Supporting Information

Theoretical investigation on the chemoselective N-heterocyclic carbene-catalyzed cross-benzoin reactions

Tao Liu[a], Shu-Min Han[b], Ling-Li Han[a,c], Lu Wang[a], Xiang-Yang Cui[a], Chong-Yang Du[a] and Siwei Bi[b,*]

[a] *Department of Chemistry and Chemical Engineering, Key Lab of Inorganic Chemistry, Shandong Provincial Education Department, Jining University, Qufu 273155, Shandong, China*

[b] *School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, China*

[c] *Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China*

Author Email Address: siweibi@126.com

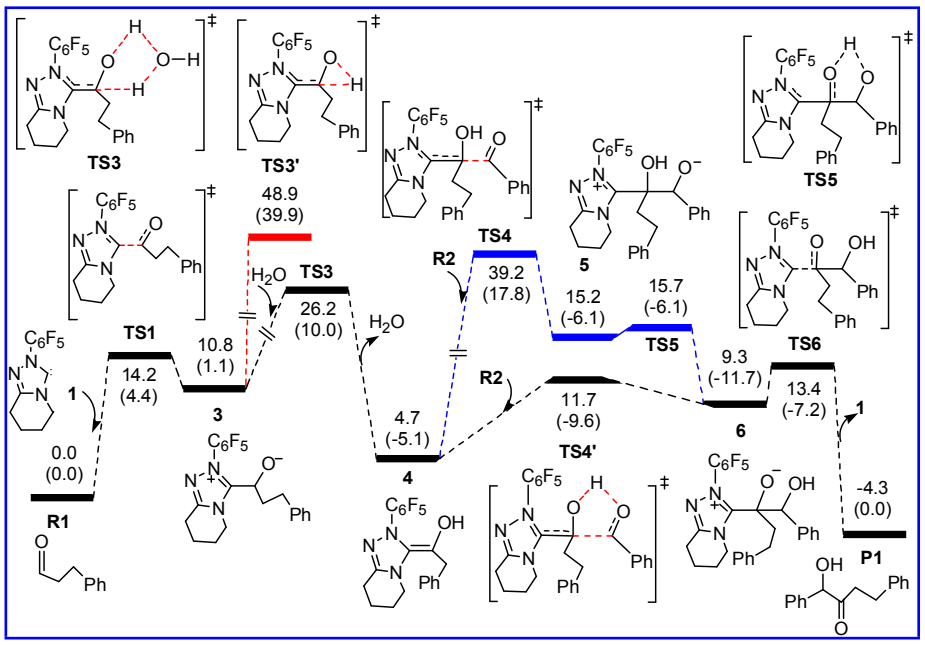

Fig. S1 Free energy diagram calculated for formation of **P1** catalyzed by **NHC-1** calculated at M06/6-31++G(d,p)//B3LYP/6-31G(d,p) level. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

Cartesian coordinates and Gibbs free energies for all of the calculated structures

R1

Sum of electronic and thermal Free Energies: -423.779994

C	-0.92344900	-0.11424600	0.82400600
H	-1.17682100	0.72970500	1.47939600
H	-1.11421100	-1.03301700	1.39694700
C	-1.84116100	-0.09570800	-0.40231700
H	-1.57984200	-0.94686600	-1.05219000
H	-1.71896100	0.82179300	-0.99099700
C	0.52514200	-0.04391800	0.43108900
C	1.23986900	-1.20791400	0.13972600
C	1.16784700	1.18839800	0.29555500
C	2.56754400	-1.14346900	-0.27040400
H	0.74631700	-2.17476800	0.24167800
C	2.49575600	1.25732000	-0.11447000
H	0.61703100	2.10232400	0.51870200
C	3.19964700	0.09058200	-0.39872200
H	3.11230200	-2.05974500	-0.48838200
H	2.98264500	2.22555400	-0.21104500
H	4.23856700	0.14211000	-0.71660200
C	-3.28036200	-0.25773000	-0.02698300
O	-4.19257900	0.40258300	-0.47015300
H	-3.47139400	-1.06763700	0.71883500

NHC-1

Sum of electronic and thermal Free Energies: -1124.758212

C	2.57576400	-0.46858100	0.49225300
N	2.64243700	0.45937000	-0.52807100
N	1.33880800	-0.74314200	0.78001000
N	0.64420700	0.06330100	-0.11676900
C	-0.76182700	0.03771700	-0.07644900
C	-1.45458800	-1.16267900	-0.22116200
C	-1.49233100	1.20539800	0.13102200
C	-2.83899500	-1.20016900	-0.15647600
C	-2.87834200	1.17945300	0.17544300
C	-3.55140200	-0.02541600	0.03750000
F	-3.48479100	-2.34983400	-0.29831100
F	-0.79575300	-2.29135400	-0.43575100
F	-4.87372500	-0.05419700	0.08864300
F	-3.56153200	2.29946300	0.36955800
F	-0.87602000	2.36487200	0.30105700
C	3.89331800	1.03251200	-1.03361600
H	3.79715000	1.14487400	-2.11715300
H	4.00644500	2.03481200	-0.60056800
C	5.07240200	0.15840500	-0.64911700
H	5.99544000	0.69519300	-0.89328400
H	5.06564800	-0.76302600	-1.24918400
C	5.01862700	-0.19704800	0.83171100
H	4.97854100	0.72578200	1.42820900
H	5.92176600	-0.73619400	1.13592700
C	3.79108700	-1.05764800	1.11830800
H	3.61733600	-1.19156700	2.19129100
H	3.94467500	-2.06206300	0.69921200
C	1.39649300	0.82721100	-0.94398500

TS1

Sum of electronic and thermal Free Energies: -1548.508652

C	0.33394800	3.06790200	0.88461100
N	-0.35619500	2.63618100	-0.23143700
N	1.27171300	2.22226900	1.19971400
N	1.13635400	1.23984700	0.23201600
C	2.02582200	0.14398900	0.23798700
C	2.94458800	-0.01841100	-0.79109800
C	1.97847800	-0.79356800	1.26204300
C	3.80868300	-1.10077900	-0.79864000
C	2.84490800	-1.87603500	1.26784900
C	3.75991900	-2.02619900	0.23522100
F	4.68394600	-1.25527400	-1.78311000
F	2.99675400	0.85725700	-1.78034100
F	4.59045500	-3.05653400	0.23716400
F	2.79820800	-2.76842200	2.24816400
F	1.08558300	-0.67167000	2.23373500
C	0.16081400	1.46242300	-0.65776100
C	-0.02624300	4.31970900	1.60064000
H	-0.60885800	4.04530800	2.49138900
H	0.88580200	4.80649700	1.96092300
C	-0.86031100	5.23227500	0.70512300
H	-0.22199200	5.68294900	-0.06825700
H	-1.26720200	6.05366800	1.30291700
C	-1.98202400	4.44039400	0.04293800
H	-2.64570900	5.09843200	-0.52742000

H	-2.59395600	3.94975300	0.81340800
C	-1.41705900	3.39831200	-0.90285200
H	-0.97596500	3.87472300	-1.78730000
H	-2.17785100	2.68898300	-1.24398900
C	-0.48513700	-0.08024500	-1.77070500
H	-0.81562400	0.56070600	-2.62709600
C	-1.65319300	-0.42280800	-0.84930300
H	-1.26019700	-0.74068500	0.12947900
H	-2.30777100	0.44770700	-0.68764600
C	-2.45758500	-1.56668200	-1.47330800
H	-1.79418000	-2.43516400	-1.57516100
H	-2.76241700	-1.27500000	-2.48996500
C	-3.66839900	-1.91735600	-0.65877500
C	-3.58441300	-2.84292600	0.38430500
C	-4.89257400	-1.28527500	-0.89184700
C	-4.69617400	-3.13875100	1.16680100
H	-2.63305300	-3.34014600	0.57538800
C	-6.00713800	-1.57736300	-0.11198000
H	-4.96870200	-0.55926600	-1.70194500
C	-5.91206000	-2.50618200	0.92076100
H	-4.61387200	-3.86861300	1.96961900
H	-6.95413100	-1.08009700	-0.31237200
H	-6.78333500	-2.73990200	1.52868100
O	0.43153800	-0.91008600	-1.92066000

3

Sum of electronic and thermal Free Energies: -1548.516983

C	1.13386700	3.03277700	0.78471700
N	0.11300400	2.75751500	-0.10060800
N	1.88266900	1.98336000	0.97018300
N	1.30966800	1.02356600	0.16632700
C	1.88393200	-0.27066500	0.13868800
C	2.73639000	-0.64720200	-0.89372000
C	1.68623000	-1.12757900	1.21135800
C	3.35443700	-1.88448100	-0.86682300
C	2.30343300	-2.37061900	1.24502000
C	3.13629200	-2.74590200	0.20299700
F	4.16464500	-2.25167000	-1.85170300
F	2.97219300	0.17470700	-1.89801500
F	3.73600700	-3.92592700	0.22857600
F	2.10570800	-3.19038000	2.26899700
F	0.88796300	-0.77146300	2.20874400
C	0.23695400	1.47496100	-0.48660300
C	1.30001700	4.37316400	1.40237800
H	0.89450800	4.33598000	2.42291200
H	2.36955200	4.58754000	1.49539600
C	0.55807300	5.43273700	0.59160500
H	1.08824300	5.62463600	-0.35183500
H	0.54685200	6.37340800	1.15036400
C	-0.86167600	4.96758900	0.29658000
H	-1.43668200	5.75127000	-0.20693200
H	-1.38083400	4.74066000	1.23815800
C	-0.86413600	3.74255800	-0.59877700
H	-0.57283100	4.00023900	-1.62438400
H	-1.84556800	3.26215700	-0.62985000
C	-0.60483700	0.62041200	-1.43880900
H	-0.99238000	1.38321400	-2.18776400
C	-1.85879100	0.21416700	-0.60084300
H	-1.50418800	-0.39953400	0.24371900
H	-2.38892800	1.08491100	-0.17857000
C	-2.80020900	-0.60994300	-1.46909700
H	-2.19449500	-1.39658100	-1.93658300
H	-3.18903900	0.02752800	-2.27815000
C	-3.93553200	-1.20066000	-0.68624800
C	-3.79701500	-2.44288900	-0.06054900
C	-5.13402500	-0.50232300	-0.51752000
C	-4.82648200	-2.97441600	0.70932800
H	-2.86491700	-2.99482200	-0.18460900
C	-6.16721000	-1.02948100	0.25132800
H	-5.25414800	0.46768800	-1.00134500
C	-6.01652600	-2.26877200	0.86781600
H	-4.70105500	-3.94518600	1.18505700
H	-7.09537900	-0.47326100	0.36733800
H	-6.82371700	-2.68443900	1.46701600
O	0.07873200	-0.38931200	-1.91845000

TS3’

Sum of electronic and thermal Free Energies: -1548.453022

C	0.78690800	3.03732900	0.06280700
N	-0.37733500	2.30658100	-0.01603100
N	1.83831800	2.28258200	0.10204900
N	1.33381300	0.99031200	0.03821100
C	2.27675800	-0.05320800	0.02898300
C	2.51233800	-0.81278200	-1.11478800
C	3.10096000	-0.24258900	1.13349000
C	3.49593100	-1.78547900	-1.13183400
C	4.10753200	-1.19774000	1.11872500
C	4.30210000	-1.97131800	-0.01508100
F	3.69729900	-2.52134900	-2.21887600
F	1.78938000	-0.60895500	-2.20799400

F	5.25657400	-2.89018600	-0.03498500
F	4.87837500	-1.37700500	2.18496700
F	2.91863000	0.48299800	2.22883700
C	-0.03715000	0.97142900	-0.05577200
C	-0.81402300	-0.18975600	-0.27228600
C	0.78766800	4.52340400	0.08517800
H	0.83912500	4.85968400	1.13020500
H	1.69883900	4.87674200	-0.40803500
C	-0.48442900	5.06400700	-0.55685100
H	-0.47649400	4.87228100	-1.63914100
H	-0.53343100	6.14906100	-0.42196200
C	-1.68585900	4.38918200	0.08543500
H	-2.62741800	4.80790200	-0.28506600
H	-1.66044600	4.56551000	1.17009800
C	-1.71123800	2.89350700	-0.18214400
H	-2.04700900	2.67763300	-1.20604700
H	-2.39805800	2.40354200	0.51239600
O	-0.09542400	-1.42364700	-0.17498300
H	-0.46091900	-0.74272000	-1.25152900
C	-2.27344500	-0.29738000	0.10108000
H	-2.35693600	-0.45206500	1.19065100
H	-2.83558200	0.61373200	-0.13465100
C	-2.94735500	-1.47496600	-0.60665200
H	-2.36109400	-2.37746500	-0.39779000
H	-2.90525900	-1.30723800	-1.69339500
C	-4.37082200	-1.65326700	-0.16601800
C	-4.67295200	-2.42316200	0.96061600
C	-5.41814600	-1.01492600	-0.83490600
C	-5.98477100	-2.55899600	1.40278800
H	-3.86277200	-2.92444400	1.49083400
C	-6.73258900	-1.14857800	-0.39776600
H	-5.19437300	-0.41099200	-1.71490600
C	-7.02009300	-1.92168100	0.72377800
H	-6.20142600	-3.16716600	2.27874100
H	-7.53597500	-0.64920200	-0.93568900
H	-8.04720100	-2.02965000	1.06533300

TS3

Sum of electronic and thermal Free Energies: -1624.876106

C	-0.78867300	2.96437200	-0.79526000
N	0.30751200	2.31730500	-0.26604600
N	-1.82333100	2.18214400	-0.84933300
N	-1.36831200	0.98591100	-0.32368000
C	-2.26852000	-0.09846200	-0.27105300
C	-3.48576900	0.04974200	0.38682400
C	-1.99183400	-1.30002600	-0.91573200
C	-4.41012400	-0.98418200	0.40582300
C	-2.90182800	-2.34352900	-0.88414800
C	-4.11720200	-2.18041400	-0.23208100
F	-5.56644800	-0.83428700	1.03668100
F	-3.77191600	1.17651600	1.01979100
F	-4.99550500	-3.16932900	-0.21738400
F	-2.62825100	-3.48836400	-1.49388500
F	-0.84971700	-1.46034400	-1.56265100
C	-0.07324700	1.05280800	0.05278600
C	-0.72813300	4.38320600	-1.22654100
H	-0.48566000	4.40948800	-2.29831400
H	-1.72300700	4.82511400	-1.11336800
C	0.34618100	5.12987500	-0.44083500
H	0.02835500	5.25675300	0.60346000
H	0.47607700	6.13136200	-0.86211300
C	1.65479100	4.35404400	-0.49398300
H	2.46134500	4.90280300	0.00281300
H	1.95626600	4.21432200	-1.54149100
C	1.53475100	3.00094800	0.18163000
H	1.46604500	3.09934900	1.27316600
H	2.39764700	2.37083000	-0.04698700
H	0.90409300	0.50992600	1.94384100
O	0.72891300	0.11346100	3.31888100
H	0.01913300	0.69922300	3.60710700
H	0.00885800	-0.90842300	2.16685500
C	0.71260400	0.08455200	0.79088300
C	2.02354100	-0.32941100	0.12833600
H	1.80195900	-1.16010300	-0.56026200
H	2.45094000	0.46887500	-0.49413700
C	3.05893300	-0.78365100	1.15502100
H	2.60679100	-1.56609700	1.77896100
H	3.29213600	0.05629500	1.82522300
C	4.31000500	-1.28739500	0.49687400
C	4.41651900	-2.61861000	0.08567700
C	5.37092400	-0.42011100	0.22491700
C	5.55479100	-3.07272000	-0.57302300
H	3.59326400	-3.30333700	0.29052500
C	6.51194500	-0.86912700	-0.43316900
H	5.29706200	0.62162200	0.54013700
C	6.60718900	-2.19902900	-0.83408500
H	5.62215400	-4.11413400	-0.88113100
H	7.33032400	-0.17976000	-0.63063100
H	7.49908400	-2.55413800	-1.34574000

O	-0.04497300	-1.03752500	1.17104100

4

Sum of electronic and thermal Free Energies: -1548.529085

C	0.59811700	2.92575900	0.34504500
N	-0.48103600	2.07188100	0.46649100
N	1.70212100	2.33964500	0.02713100
N	1.34722000	0.98400900	-0.12312600
C	2.36397900	0.03903500	-0.00817600
C	3.49554500	0.13611000	-0.82718500
C	2.31877600	-1.02590000	0.89614300
C	4.53446000	-0.77583400	-0.74079700
C	3.33652600	-1.96683900	0.95784200
C	4.45320600	-1.83916600	0.14717700
F	5.59470800	-0.65638900	-1.53296700
F	3.58316100	1.10839100	-1.72775800
F	5.43848200	-2.72522000	0.22020600
F	3.26411900	-2.96900800	1.82720100
F	1.30562000	-1.14634000	1.74424800
C	-0.03520100	0.79433800	0.07872600
C	0.44475300	4.38776500	0.56151200
H	0.52596700	4.59833700	1.63792400
H	1.27513600	4.90112800	0.06715600
C	-0.92128800	4.84598500	0.06261700
H	-0.97539800	4.74253000	-1.03088300
H	-1.06830600	5.90578900	0.29528300
C	-1.99677100	3.99641400	0.72001600
H	-3.00026000	4.32640000	0.42970700
H	-1.92554200	4.10630700	1.81147600
C	-1.86622300	2.52776000	0.35323000
H	-2.20471900	2.34713200	-0.68130600
H	-2.49856300	1.93216100	1.01768800
H	0.43148000	-1.09809500	-1.56278300
C	-0.72300200	-0.33471800	-0.20846400
C	-2.12487000	-0.69514700	0.14018800
H	-2.09712000	-1.65435300	0.68399600
H	-2.57059100	0.02285000	0.83635200
C	-3.03594900	-0.86664000	-1.08436700
H	-2.57668400	-1.60326100	-1.75764700
H	-3.08208300	0.08588200	-1.63131900
C	-4.41633300	-1.30187600	-0.68960800
C	-4.70113600	-2.65075400	-0.46171600
C	-5.42485400	-0.36012600	-0.47157800
C	-5.96249200	-3.05016200	-0.03291800
H	-3.91903000	-3.39283700	-0.62481800
C	-6.68923900	-0.75489700	-0.04507400
H	-5.20798900	0.69562000	-0.64156700
C	-6.96154300	-2.10230100	0.17499000
H	-6.16865100	-4.10499400	0.13687500
H	-7.46510000	-0.00856300	0.11325200
H	-7.94983900	-2.41356600	0.50617000
O	-0.03680400	-1.40412100	-0.77287600

R2

Sum of electronic and thermal Free Energies: -345.267658

C	2.20595100	-0.24691400	0.00000300
C	1.72569000	1.05993700	-0.00000100
C	0.35514200	1.28873800	-0.00000900
C	-0.53172700	0.21020700	-0.00001000
C	-0.04461500	-1.10079200	-0.00000800
C	1.32258600	-1.32774200	-0.00000100
H	3.27852300	-0.42749300	0.00001000
H	2.42007200	1.89637600	0.00000300
H	-0.04001100	2.30410000	-0.00001200
H	-0.75517500	-1.92438100	-0.00001000
H	1.70849700	-2.34414400	0.00000200
C	-1.97904600	0.46731700	-0.00001500
O	-2.83543200	-0.39460800	0.00002900
H	-2.25235200	1.54789900	0.00002000

H_2O

Sum of electronic and thermal Free Energies: -76.389306

O	0.00000000	0.00000000	0.11940200
H	0.00000000	0.75616300	-0.47761000
H	0.00000000	-0.75616300	-0.47761000

TS4-3

Sum of electronic and thermal Free Energies: -1972.289834

C	-3.90359800	-0.08828800	-1.14273100
N	-3.58986100	-0.14228700	0.19826300
N	-2.88132400	-0.33426600	-1.89835200
N	-1.85043200	-0.57376600	-0.99674700
C	-0.56184000	-0.76051100	-1.52615400
C	0.17666400	0.33404900	-1.97299500
C	-0.01913500	-2.03462400	-1.66580500
C	1.45992800	0.17152400	-2.47156400
C	1.26452500	-2.21038600	-2.16097900
C	2.00215800	-1.10448900	-2.56178200
F	2.16719400	1.21692800	-2.87510700
F	-0.33561600	1.55378600	-1.88567400
F	3.22237900	-1.26640900	-3.03942700
F	1.78719000	-3.42476700	-2.25941700

F	-0.71038600	-3.09670800	-1.27780200	C	2.26654300	3.70262600	-0.67820100
C	-2.24430600	-0.40930400	0.30766500	C	2.68486600	4.39929200	1.58208100
C	-1.45015100	-0.29483800	1.46853200	C	3.60251100	3.91608400	-0.99737900
C	-1.33520100	1.88114700	1.38749900	H	1.57582300	3.33995600	-1.43942400
H	-1.88932800	2.00249000	0.42613300	C	4.02268100	4.62062600	1.26566700
O	-1.91769400	2.14613200	2.47140300	H	2.32410100	4.58572000	2.59367300
C	-5.27702100	0.20952800	-1.62556600	C	4.48566300	4.37923900	-0.02462300
H	-5.20184700	0.72895400	-2.58628600	H	3.95363900	3.72211100	-2.00927200
H	-5.79103100	-0.74290400	-1.81856000	H	4.70643700	4.98422200	2.03006200
C	-6.05315500	0.99874800	-0.57866900	H	5.53067900	4.55272900	-0.27189100
H	-7.09840300	1.09362200	-0.88949000	**6**			
H	-5.64564400	2.01611400	-0.49158300	Sum of electronic and thermal Free Energies: -1893.770558			
C	-5.94766100	0.28374800	0.75917600	C	3.35461300	2.12515100	0.11316600
H	-6.32312900	-0.74429400	0.65285000	N	2.01075700	2.43922600	0.07788500
H	-6.56387800	0.77206900	1.52169300	N	3.53768300	0.83742600	0.08582500
C	-4.52123200	0.25759500	1.27423500	N	2.27039000	0.32788700	0.02460900
H	-4.40454500	-0.44485200	2.09878800	C	2.13053900	-1.07928900	-0.04024200
H	-4.20578300	1.24703700	1.63079400	C	2.29145000	-1.83296300	1.11815200
O	-2.13747600	-0.36341000	2.66184300	C	1.93010800	-1.72469300	-1.25781900
H	-2.17444000	0.58115600	2.97312400	C	2.18671600	-3.21443200	1.08325600
C	-0.07313700	-0.89270200	1.57363500	C	1.81216700	-3.10654900	-1.29697700
H	0.53105100	-0.72605100	0.67303800	C	1.94395300	-3.84721800	-0.12839000
H	0.44595900	-0.36020900	2.38451200	F	2.32407800	-3.92765000	2.19039000
C	-0.09341500	-2.39146600	1.91503400	F	2.51402900	-1.22692200	2.27398000
H	-0.61475800	-2.51464300	2.87388600	F	1.84616000	-5.16312000	-0.17234100
H	-0.68084500	-2.92917300	1.15831300	F	1.61364200	-3.72820900	-2.44922700
C	1.29107400	-2.96946300	1.98139700	F	1.86650800	-1.04309300	-2.38292600
C	1.78520400	-3.75370800	0.93685400	C	1.32019700	1.27974800	0.03596400
C	2.13785300	-2.68626800	3.05721600	C	-0.18355600	0.92714600	0.00869400
C	3.09134100	-4.23391000	0.95505400	C	-0.99375400	2.23791100	-0.29143400
H	1.13207400	-3.99292600	0.09877600	H	-0.70146400	2.94771200	0.52669300
C	3.44173300	-3.16975600	3.08436300	O	-0.64342000	2.59892800	-1.53968900
H	1.76413500	-2.07998600	3.88271400	C	4.43520200	3.14476400	0.15001000
C	3.92476400	-3.94298300	2.03059800	H	5.19533800	2.81715100	0.86705500
H	3.45515400	-4.83691700	0.12510700	H	4.91836400	3.15325100	-0.83655300
H	4.08467300	-2.94182600	3.93212000	C	3.88011800	4.52700500	0.46642600
H	4.94587800	-4.31720900	2.05027600	H	4.65013400	5.28068100	0.27571100
C	0.14124400	2.14748500	1.22402300	H	3.61672600	4.59485900	1.53130200
H	0.67887100	1.85520100	2.13659100	C	2.64423300	4.77232100	-0.38375000
H	0.55418800	1.57298900	0.38397100	H	2.89337900	4.64632500	-1.44720200
C	0.35804800	3.64252900	0.95251200	H	2.27187300	5.79491900	-0.26217600
H	0.03816500	4.21498800	1.83333500	C	1.51464400	3.83740800	-0.00358400
H	-0.29148200	3.94674500	0.11753800	H	0.70876200	3.80936000	-0.75333600
C	1.78974000	3.94178800	0.61389600	H	1.11603800	4.09709100	0.98344800

O	-0.32835600	0.13978200	-1.14076000	F	2.27440900	-5.05350900	0.01115000
H	-0.43444600	0.88902700	-1.80052200	F	2.14078200	-3.66043400	-2.30517500
C	-2.50239500	2.06249400	-0.11319300	F	2.13290800	-0.95923800	-2.24898600
C	-3.15104800	2.43837100	1.06465700	C	1.22376600	1.34253700	0.07588300
C	-3.28041100	1.61704300	-1.18390000	C	-0.25895100	0.89919600	-0.03857900
C	-4.53791700	2.36946400	1.17920000	C	-1.17422000	2.18919200	-0.19479400
H	-2.55925400	2.82003900	1.89862200	H	-0.82456800	2.92019700	0.56739000
C	-4.66422800	1.54074900	-1.07594900	O	-0.97460500	2.56226500	-1.48722400
H	-2.78021100	1.37146700	-2.11840200	C	4.22400700	3.39389700	-0.03730500
C	-5.29935700	1.91831500	0.10610800	H	5.04195400	3.15000400	0.64857800
H	-5.02344800	2.68140200	2.10223900	H	4.64764800	3.37649400	-1.05093600
H	-5.25518500	1.19051300	-1.92085100	C	3.60793300	4.75834000	0.23574300
H	-6.38357300	1.86706800	0.18559300	H	4.32533600	5.54141000	-0.02736800
C	-0.56712900	0.17153800	1.29747800	H	3.38509600	4.86883400	1.30620800
H	0.28122500	0.15765600	1.99347700	C	2.32857400	4.89202200	-0.57382300
H	-1.34623900	0.74603800	1.81571900	H	2.54558400	4.73799100	-1.64031900
C	-1.05168200	-1.27317900	1.11417600	H	1.89742600	5.89411400	-0.47772900
H	-0.37623900	-1.80899800	0.43936800	C	1.27056700	3.91001300	-0.11274100
H	-0.96279700	-1.76092200	2.09630800	H	0.43861000	3.82232600	-0.82443900
C	-2.46430900	-1.45767100	0.62727300	H	0.89743300	4.19116300	0.87857500
C	-3.54331500	-1.21083900	1.47984000	O	-0.32002800	0.31285800	-1.29072900
C	-2.72734000	-1.94359000	-0.65527100	H	-0.59981900	1.25901000	-1.77430000
C	-4.84974800	-1.44486800	1.06362900	C	-2.64313100	1.96136400	0.13073300
H	-3.35233600	-0.84215900	2.48859600	C	-3.16659600	2.27085500	1.38817300
C	-4.03169600	-2.18628800	-1.07456000	C	-3.51782800	1.52504900	-0.86468600
H	-1.88921500	-2.12188900	-1.32835000	C	-4.52769900	2.14152000	1.65245000
C	-5.09806100	-1.93660300	-0.21551500	H	-2.49529100	2.63906700	2.16610100
H	-5.67757300	-1.24414800	1.74125800	C	-4.87843500	1.39692500	-0.60878100
H	-4.21572500	-2.56986300	-2.07623700	H	-3.11129700	1.32131000	-1.85325400
H	-6.11946400	-2.12458200	-0.53995200	C	-5.38953500	1.70480800	0.65108600

TS6

Sum of electronic and thermal Free Energies: -1893.770239

C	3.20631200	2.31389500	0.04144000	H	-4.91716600	2.39840100	2.63588700
N	1.84377100	2.54272900	0.00937200	H	-5.54771500	1.05698600	-1.39741200
N	3.46831200	1.04320800	0.11309300	H	-6.45587900	1.61206800	0.84737000
N	2.23288900	0.45497500	0.12948100	C	-0.62472800	-0.03443700	1.13552100
C	2.19532700	-0.95929200	0.10204700	H	0.20530600	-0.08084500	1.85153600
C	2.30667400	-1.68555800	1.28234400	H	-1.45305600	0.41372900	1.69858200
C	2.16238700	-1.63120200	-1.11703600	C	-1.00311300	-1.47070000	0.75003700
C	2.31754400	-3.07089600	1.25878700	H	-0.27875400	-1.86202700	0.02763900
C	2.17441600	-3.01791400	-1.14825700	H	-0.89869500	-2.07828500	1.66128300
C	2.25325900	-3.73388600	0.03989900	C	-2.39208500	-1.68612400	0.21009500
F	2.40208400	-3.76002500	2.38587100	C	-3.49365400	-1.63937200	1.06879700
F	2.36776500	-1.05538700	2.44503200	C	-2.61144400	-2.00086900	-1.13261100
				C	-4.77703100	-1.90639500	0.60508800
				H	-3.33689500	-1.39541700	2.12042100

C	-3.89375800	-2.27095100	-1.60239900
H	-1.76129000	-2.02999600	-1.81180900
C	-4.98138600	-2.22807500	-0.73455100
H	-5.61993700	-1.86662900	1.29251100
H	-4.04296300	-2.51974600	-2.65133400
H	-5.98335000	-2.44382400	-1.09956900

TS4-2

Sum of electronic and thermal Free Energies: -1893.780438

C	3.60654500	-1.39907000	-0.43332100
N	3.18938900	-0.15755400	-0.86203900
N	2.62660600	-2.10529700	0.03826100
N	1.52268300	-1.28418200	-0.11193000
C	0.30842000	-1.72899400	0.44426000
C	0.08847800	-1.58902300	1.81074600
C	-0.66077700	-2.36132000	-0.32907700
C	-1.12197300	-1.95202000	2.37901500
C	-1.86910500	-2.74773800	0.23101100
C	-2.09951900	-2.53715200	1.58431500
F	-1.34586400	-1.74672500	3.66752600
F	1.03097500	-1.06010100	2.57804500
F	-3.25124700	-2.89833500	2.11845500
F	-2.80130200	-3.32005200	-0.51612700
F	-0.45996000	-2.55852800	-1.62327100
C	1.84468500	-0.05936100	-0.62413400
C	1.04278400	1.12805300	-0.69397000
C	1.61946900	1.99603500	1.11511000
H	1.92572800	1.06967000	1.64696100
O	2.50890800	2.80228100	0.68813000
C	5.02075100	-1.84896100	-0.52214500
H	5.24101900	-2.46895900	0.35302700
H	5.12073400	-2.49847300	-1.40300900
C	5.96247100	-0.65912400	-0.65817100
H	6.97155000	-1.01519500	-0.88811100
H	6.02055000	-0.10994100	0.29222000
C	5.44553900	0.25961000	-1.75319100
H	5.34268700	-0.30739000	-2.68963900
H	6.14552100	1.07875500	-1.94938500
C	4.11536100	0.88067500	-1.37679200
H	3.63433600	1.36087900	-2.22826900
H	4.22699300	1.62811600	-0.58247800
C	0.31858600	2.53424600	1.60914500
C	-0.50141000	1.79162300	2.46134400
C	-0.10775500	3.79907700	1.19374700
C	-1.73960100	2.28140600	2.86159000
H	-0.15644500	0.82766600	2.82866200
C	-1.34423400	4.29196000	1.59368900
H	0.54833300	4.38109100	0.54933200
C	-2.16868500	3.53070000	2.42093300
H	-2.36698500	1.68663500	3.52321800
H	-1.67075000	5.27492600	1.25981800
H	-3.13801800	3.91531800	2.73047200
C	-0.45402700	1.02827600	-0.84608100
H	-0.90892100	0.34018000	-0.12049500
H	-0.86436500	2.01885300	-0.60464600
C	-0.89474700	0.65659700	-2.26928400
H	-0.46569600	1.39502700	-2.95990800
H	-0.47854900	-0.32134000	-2.54692300
C	-2.39143600	0.63030000	-2.39462000
C	-3.09087900	-0.57772600	-2.42825800
C	-3.12232200	1.82229300	-2.41734900
C	-4.48195200	-0.59925900	-2.47781900
H	-2.53198400	-1.51266700	-2.42345000
C	-4.51145900	1.80644900	-2.47115200
H	-2.58886500	2.77299800	-2.39354700
C	-5.19742600	0.59385700	-2.49773700
H	-5.00620800	-1.55279300	-2.50123100
H	-5.06285900	2.74431300	-2.49193600
H	-6.28432400	0.58071100	-2.53731800
O	1.57302800	2.10692700	-1.50606000
H	2.07218800	2.69242400	-0.86243500

5

Sum of electronic and thermal Free Energies: -1893.787302

C	3.48200600	-1.65038800	-0.00382800
N	3.16158600	-0.42041400	-0.53794400
N	2.46315000	-2.17208300	0.61434300
N	1.47171000	-1.23171800	0.46197900
C	0.20296100	-1.53446000	1.01132400
C	-0.21757100	-0.98073300	2.21592300
C	-0.62747400	-2.44376600	0.36232300
C	-1.49051800	-1.23345500	2.70320800
C	-1.89777900	-2.71243200	0.84669300
C	-2.32904500	-2.10202100	2.01730900
F	-1.89785700	-0.66235700	3.82502100
F	0.57310900	-0.16394000	2.89493700
F	-3.53924500	-2.34988000	2.47962800
F	-2.69880500	-3.54328000	0.19867500
F	-0.22482900	-3.02524100	-0.75759600
C	1.87312300	-0.15606300	-0.24641200

C	1.11023900	1.15401900	-0.64580000
C	1.33294500	2.10633200	0.64888900
H	1.43221200	1.49513200	1.55792600
O	2.54391400	2.75214900	0.38113500
C	4.81615600	-2.28188300	-0.17364400
H	5.06865100	-2.82107500	0.74510700
H	4.72770400	-3.03739100	-0.96691500
C	5.86967800	-1.25117800	-0.56352600
H	6.78405200	-1.76807400	-0.87034200
H	6.12590600	-0.62675400	0.30381400
C	5.33391700	-0.37326300	-1.68464500
H	5.04323500	-0.99755400	-2.54190000
H	6.09982700	0.32371000	-2.04119800
C	4.15255000	0.45014100	-1.22011300
H	3.60716400	0.95607100	-2.01681800
H	4.45560000	1.20466800	-0.48498900
C	0.19958500	3.07385200	0.85995200
C	-0.79428300	2.80852800	1.80448200
C	0.10291300	4.23525400	0.09004400
C	-1.86704600	3.67859300	1.97289800
H	-0.71922600	1.91073300	2.42004900
C	-0.96999100	5.10478000	0.25371000
H	0.88083300	4.44970400	-0.63923000
C	-1.95887600	4.82994900	1.19582100
H	-2.62983600	3.46227300	2.71814300
H	-1.03323800	6.00517600	-0.35421000
H	-2.79405900	5.51437900	1.32726600
C	-0.37727300	0.85246600	-0.90360300
H	-0.89330300	0.40926500	-0.03898200
H	-0.84205300	1.83488600	-1.05586800
C	-0.59627600	0.02002200	-2.16586300
H	-0.06920100	0.53657400	-2.97864400
H	-0.12982600	-0.97102300	-2.06948800
C	-2.05430900	-0.14341700	-2.49314200
C	-2.69575500	-1.37766300	-2.36757800
C	-2.81508000	0.95861500	-2.89847700
C	-4.05849800	-1.50866900	-2.62353400
H	-2.11731400	-2.25027500	-2.06585800
C	-4.17436400	0.83262700	-3.15989600
H	-2.32902300	1.92800100	-3.01165600
C	-4.80356800	-0.40283900	-3.01883700
H	-4.53657700	-2.48024800	-2.51248800
H	-4.74726400	1.70227900	-3.47538500
H	-5.86802200	-0.50168700	-3.22004600
O	1.68776200	1.72464000	-1.69728700
H	2.55366600	2.66105900	-0.61577700

TS5

Sum of electronic and thermal Free Energies: -1893.776885

C	3.89893200	-0.44003300	-1.05175000
N	2.85637700	-1.33301100	-0.89650700
N	3.52872700	0.76175700	-0.71911800
N	2.20612800	0.59037600	-0.35623300
C	1.51471700	1.71035500	0.16263400
C	0.75037500	2.52934400	-0.65812400
C	1.62388300	2.02029100	1.51447800
C	0.07285400	3.62250300	-0.13713000
C	0.95427100	3.11114200	2.04411000
C	0.17655700	3.91091900	1.21597900
F	-0.67571500	4.38356700	-0.92561100
F	0.62383800	2.25282300	-1.94894700
F	-0.46271100	4.95337200	1.71869200
F	1.05331100	3.39829900	3.33468100
F	2.36663400	1.27095700	2.30574500
C	1.75933900	-0.67360700	-0.45379100
C	0.03035700	-1.03501300	0.48798100
C	0.09580800	-2.58072700	0.56383200
H	0.35766500	-2.98727900	-0.42495800
O	1.09993200	-2.89736300	1.49250600
C	5.24053300	-0.85138600	-1.54291800
H	5.63170800	-0.06769300	-2.19999800
H	5.92339000	-0.91151500	-0.68403900
C	5.16358900	-2.20891100	-2.23411400
H	6.17545000	-2.57345600	-2.43701300
H	4.65564400	-2.10911000	-3.20406100
C	4.40207900	-3.18853100	-1.35248500
H	4.88454900	-3.24541400	-0.36639000
H	4.41761400	-4.19878400	-1.77449000
C	2.95090500	-2.77360300	-1.18869100
H	2.47499500	-3.30256100	-0.35774300
H	2.38579200	-2.96619600	-2.10884200
O	0.19217400	-0.46000900	1.59727100
H	1.15390300	-2.07689900	2.02720800
C	-1.25758700	-3.12377700	0.96268200
C	-2.13080400	-3.62492800	-0.00355200
C	-1.68002400	-3.07382600	2.29346200
C	-3.41015800	-4.04892100	0.34507800
H	-1.80193500	-3.68492800	-1.04135200
C	-2.95677900	-3.49687600	2.64471700

H	-1.00045300	-2.69644700	3.05415300
C	-3.82918700	-3.97856500	1.67077500
H	-4.07946100	-4.43925200	-0.41889900
H	-3.27422000	-3.45022200	3.68436400
H	-4.82813200	-4.30856500	1.94719800
C	-0.97300900	-0.48488700	-0.52713100
H	-0.53296700	0.31732800	-1.12893000
H	-1.24507100	-1.27774300	-1.23979500
C	-2.22312100	0.06535400	0.16245600
H	-2.64382500	-0.68829500	0.84226400
H	-1.91488900	0.91645100	0.78627300
C	-3.26161300	0.48477400	-0.83702200
C	-4.37323400	-0.32059100	-1.09308600
C	-3.11250300	1.66669900	-1.56845200
C	-5.31706100	0.04699200	-2.04821100
H	-4.49683500	-1.24557800	-0.52844900
C	-4.05261300	2.03857800	-2.52293400
H	-2.24553500	2.30223100	-1.38416400
C	-5.16000300	1.22920500	-2.76550700
H	-6.17962600	-0.59061200	-2.23106200
H	-3.92269600	2.96566900	-3.07753600
H	-5.89776000	1.52098500	-3.50972300

P1

Sum of electronic and thermal Free Energies: -769.050857

C	0.84128600	-1.62664100	-0.09809600
C	2.08560800	-1.32987400	0.74263600
H	1.76800700	-1.36126800	1.80097000
O	3.05649500	-2.29840200	0.48678300
O	0.88493600	-2.55375300	-0.88813100
H	2.66339400	-2.88329900	-0.18616700
C	2.57887700	0.06624900	0.42833500
C	2.27545400	1.14221300	1.26041800
C	3.30408800	0.28707300	-0.74318100
C	2.69029000	2.42773400	0.92499500
H	1.71585000	0.96774400	2.17932600
C	3.72287700	1.56990700	-1.07617500
H	3.54606800	-0.55929300	-1.38397400
C	3.41345000	2.64377000	-0.24430700
H	2.45365100	3.26157700	1.58212400
H	4.29000600	1.73450300	-1.98975400
H	3.74049500	3.64770200	-0.50522100
C	-0.36873600	-0.76778900	0.09870200
H	-0.11542700	0.25382100	-0.22457400
H	-0.55447700	-0.68164100	1.18084600
C	-1.60687900	-1.26859400	-0.63556000
H	-1.81043800	-2.30462700	-0.33467700
H	-1.40011900	-1.28870500	-1.71295900
C	-2.79995300	-0.40238900	-0.34491600
C	-3.08644300	0.71237700	-1.13579700
C	-3.61722600	-0.66944500	0.75586900
C	-4.16647200	1.53780200	-0.83773900
H	-2.45490800	0.93062100	-1.99721700
C	-4.69779300	0.15292100	1.05788200
H	-3.39952700	-1.53784000	1.37813000
C	-4.97596200	1.25969400	0.26035100
H	-4.37976300	2.39987700	-1.46631000
H	-5.32628200	-0.07345200	1.91669000
H	-5.82278600	1.90147300	0.49303900

TS1'

Sum of electronic and thermal Free Energies: -1469.995307

C	-1.43193000	-2.56584000	-0.54893200
N	-1.99936500	-1.40472900	-0.06419500
N	-0.14251200	-2.43561700	-0.66023100
N	0.08107100	-1.14556000	-0.21383900
C	1.40389100	-0.65892900	-0.20325000
C	2.40641800	-1.35277300	0.46633000
C	1.72611300	0.52853700	-0.84911800
C	3.70684300	-0.87266600	0.48590500
C	3.01753800	1.02723500	-0.81508400
C	4.01076200	0.32224300	-0.15115900
F	4.65643000	-1.54226500	1.12518000
F	2.13125400	-2.47529500	1.11337900
F	5.24948400	0.78712500	-0.12759200
F	3.30876500	2.16799200	-1.42635800
F	0.79694700	1.20651200	-1.50384700
C	-1.02890200	-0.48924700	0.16016500
C	-0.86973700	0.97425800	1.42096000
C	-2.24132200	-3.76016700	-0.90561900
H	-2.35609000	-3.78355400	-1.99831400
H	-1.68555500	-4.66212400	-0.62901000
C	-3.61734700	-3.69563100	-0.24818100
H	-3.52980200	-3.89247100	0.82987000
H	-4.25749500	-4.47889500	-0.66593700
C	-4.23480600	-2.32093400	-0.46813300
H	-5.26017400	-2.28164600	-0.08612800
H	-4.28217300	-2.10506700	-1.54501700
C	-3.42908700	-1.24313000	0.23314900
H	-3.55283400	-1.31321700	1.32208700

H	-3.72499300	-0.23785400	-0.08022900
O	0.34703800	1.14371600	1.66029900
C	-1.67942700	2.08913000	0.79494900
C	-1.02509200	3.12256100	0.12699700
C	-3.06346600	2.14934900	0.95075300
C	-1.74903700	4.17626100	-0.41932500
H	0.05981800	3.08463300	0.05798700
C	-3.79258900	3.20312900	0.40749300
H	-3.57089700	1.36966300	1.52059200
C	-3.13584100	4.21573000	-0.28681800
H	-1.23139600	4.97704700	-0.94388500
H	-4.87229300	3.24185100	0.53670400
H	-3.70151100	5.04227100	-0.71154900
H	-1.50907100	0.39966700	2.14493900

7

Sum of electronic and thermal Free Energies: -1469.999842

C	1.46711200	-2.23228900	0.69231500
N	1.97835500	-1.28488800	-0.16739800
N	0.19237400	-2.04293400	0.88473200
N	-0.09737700	-0.93701300	0.11745500
C	-1.43987000	-0.48436100	0.07285400
C	-2.24953300	-0.76689700	-1.02167300
C	-1.99312200	0.11820300	1.19251900
C	-3.58534600	-0.40922200	-1.01070800
C	-3.33396200	0.47605700	1.21368200
C	-4.12977500	0.20573600	0.11199200
F	-4.35517300	-0.66364400	-2.06168000
F	-1.75037700	-1.37914100	-2.08009600
F	-5.41148700	0.53833700	0.12475000
F	-3.85334500	1.06403800	2.28341900
F	-1.23139500	0.39298400	2.24460900
C	0.97384800	-0.46485900	-0.52167200
C	0.94383700	0.78054200	-1.43140900
C	2.31943100	-3.28683800	1.29723300
H	2.54943600	-2.98758200	2.32923300
H	1.74399100	-4.21601900	1.35949700
C	3.61495600	-3.45180400	0.50634500
H	3.41124800	-3.95511100	-0.44925400
H	4.30018700	-4.09432900	1.06733600
C	4.24815500	-2.09113800	0.24609100
H	5.22353800	-2.19540700	-0.23957400
H	4.41494800	-1.57240400	1.20055700
C	3.36927400	-1.23727200	-0.64872000
H	3.36941500	-1.60710700	-1.68137100

TS7

Sum of electronic and thermal Free Energies: -1546.358528

C	0.99356500	2.55165400	-0.66160900
N	1.70113000	1.48319200	-0.15653200
N	-0.28037800	2.30009600	-0.70237500
N	-0.38683300	1.01798300	-0.19511600
C	-1.66087000	0.41263400	-0.18538700
C	-2.72668000	1.04937600	0.44284400
C	-1.88980400	-0.78429900	-0.85727800
C	-3.99867600	0.49681100	0.40732200
C	-3.15282100	-1.35158200	-0.87933900
C	-4.20953800	-0.70559900	-0.25158700
F	-5.00807700	1.10895100	1.00980400
F	-2.53917000	2.18678200	1.09348500
F	-5.41992000	-1.23781700	-0.28293300
F	-3.36120700	-2.49535600	-1.51571200
F	-0.89880700	-1.39570800	-1.48353000
C	0.81106900	0.51235100	0.16485200
C	1.10508700	-0.70571800	0.89519500
C	1.66789500	3.80811900	-1.07322700
H	1.85957700	3.76348800	-2.15441300
H	0.98187500	4.64387100	-0.90495600
C	2.98920700	3.96583900	-0.32687700
H	2.79798300	4.17553400	0.73498500
H	3.53591800	4.82265700	-0.73203500
C	3.81153600	2.69193000	-0.46411800
H	4.79944400	2.80676400	-0.00681500
H	3.97297500	2.47215400	-1.52866200
C	3.12973400	1.51066800	0.20092800
H	3.18619800	1.57657400	1.29529900
H	3.68259300	-0.18884800	-0.65701800
O	-0.28709200	1.16619200	-1.65384000
C	1.82326800	1.82856000	-0.71657300
C	1.35896900	2.38688000	0.47660100
C	3.01229500	2.30095900	-1.26645700
C	2.08167100	3.38334100	1.11888700
H	0.41663300	2.02633100	0.89042800
C	3.73596700	3.31059200	-0.63195400
H	3.36850100	1.88168000	-2.20888800
C	3.27361400	3.85047900	0.56330800
H	1.71541200	3.80413300	2.05345000
H	4.65878900	3.67969700	-1.07543900
H	3.83505800	4.63788000	1.06162700
H	1.56479400	0.43823600	-2.31837700

H	3.57882600	0.56173500	-0.10497800
O	-0.05314700	-1.42616700	1.23923200
C	2.17951400	-1.58168500	0.30515400
C	2.38469600	-1.71774800	-1.06986300
C	2.95371400	-2.34378100	1.18616200
C	3.35809100	-2.58704900	-1.55603600
H	1.77418700	-1.14350300	-1.76695300
C	3.91801400	-3.21842400	0.70053600
H	2.78066200	-2.22855100	2.25631600
C	4.12514800	-3.33977700	-0.67227300
H	3.51036300	-2.68282600	-2.62910400
H	4.51601600	-3.80528200	1.39464700
H	4.88238400	-4.02198900	-1.05241900
H	1.43212000	-0.42151400	2.04686100
O	1.13170100	-0.84693400	3.41621900
H	0.78265200	-0.04664000	3.82384900
H	0.05428500	-1.38054600	2.24050300

TS7'

Sum of electronic and thermal Free Energies: -1469.941179

C	1.10072800	2.58389200	-0.46079500
N	1.79410000	1.44950900	-0.09794300
N	-0.18369500	2.40374700	-0.45051500
N	-0.33349900	1.08664200	-0.03493400
C	-1.59077400	0.47631000	-0.09843200
C	-2.71581000	1.09970000	0.44015900
C	-1.74288700	-0.77665100	-0.68895600
C	-3.96080000	0.49423700	0.37595300
C	-2.98204200	-1.39613400	-0.73710600
C	-4.09320100	-0.75957900	-0.20552300
F	-5.02325000	1.09836400	0.89461100
F	-2.60940400	2.27663000	1.04230100
F	-5.28201200	-1.34311000	-0.26010700
F	-3.11179700	-2.58672200	-1.30926400
F	-0.71212100	-1.36438700	-1.27994100
C	0.86559200	0.48621100	0.21708900
C	1.04233100	-0.75387700	0.89279700
C	1.80682700	3.84390600	-0.80340700
H	2.02164500	3.84444300	-1.88152300
H	1.13418100	4.68488600	-0.60971500
C	3.11631000	3.94022700	-0.02562400
H	2.90764200	4.08796200	1.04345600
H	3.68343900	4.81227400	-0.36632300
C	3.92289000	2.66525400	-0.22602000
H	4.89518100	2.72820900	0.27388700
H	4.12123300	2.52517600	-1.29806800
C	3.20116300	1.44454100	0.31651700
H	3.21514700	1.41934800	1.41626600
H	3.67046500	0.52421900	-0.04160400
O	-0.12376400	-1.32815200	1.47739400
C	2.11657200	-1.69946700	0.50173900
C	2.74711200	-1.66752000	-0.74722300
C	2.45717400	-2.72677600	1.39144300
C	3.72522300	-2.60310000	-1.07573800
H	2.45166700	-0.91795500	-1.48137900
C	3.42711100	-3.66241600	1.06250700
H	1.94150400	-2.78218800	2.34815800
C	4.07329700	-3.60084100	-0.17193100
H	4.20247800	-2.56078900	-2.05264800
H	3.68148800	-4.44734000	1.77180200
H	4.83398400	-4.33408500	-0.42989800
H	0.83808800	-0.59269900	2.03907000

8

Sum of electronic and thermal Free Energies: -1470.017728

C	1.06423000	2.53510000	-0.12890600
N	1.76183700	1.34664300	-0.18383300
N	-0.20716600	2.38789100	-0.30120200
N	-0.37572000	1.01166000	-0.54801500
C	-1.63485600	0.47657600	-0.22016600
C	-2.50929900	0.04686600	-1.21587500
C	-2.05718000	0.40204000	1.10596300
C	-3.76544600	-0.44653500	-0.89809100
C	-3.31450500	-0.08115400	1.43629200
C	-4.16846600	-0.50638000	0.42901800
F	-4.59028200	-0.85262600	-1.85610900
F	-2.15260500	0.09964200	-2.48815300
F	-5.37087100	-0.97060100	0.73326800
F	-3.70235200	-0.14128600	2.70438000
F	-1.24791300	0.79630000	2.08057300
C	0.83539700	0.32578200	-0.38498100
C	1.02463800	-1.01939100	-0.51467100
O	-0.00422700	-1.70142100	-1.15565600
H	-0.24547200	-2.46542500	-0.61137500
C	2.17515000	-1.80660100	-0.09345800
C	2.52812000	-2.96197900	-0.81612500
C	2.90084100	-1.52161100	1.07843900
C	3.59024300	-3.76004900	-0.41543100
H	1.96210400	-3.21627500	-1.70995500
C	3.97280800	-2.31577800	1.46644100

H	2.59291000	-0.68997100	1.71037600
C	4.32923000	-3.43707000	0.72117000
H	3.84883700	-4.64060400	-1.00061500
H	4.51857600	-2.07115800	2.37572100
H	5.16331900	-4.06206800	1.03157400
C	3.80040100	2.61057600	-0.65619400
H	4.89046500	2.53341900	-0.58449000
H	3.56250500	2.91039000	-1.68716700
C	3.20773600	1.24471400	-0.36105500
H	3.66060000	0.82976400	0.54992100
H	3.39527000	0.52629300	-1.16945800
C	3.24981400	3.64375900	0.31601200
H	3.76800800	4.60228100	0.20903500
H	3.41644500	3.30172200	1.34775500
C	1.76025700	3.84054100	0.05818700
H	1.61819700	4.43334400	-0.85510300
H	1.27092000	4.39698400	0.86532100

TS8-2

Sum of electronic and thermal Free Energies: -1893.771297

C	2.19994900	2.94767500	0.84140600
N	1.20335700	2.83269600	-0.10112000
N	2.64742600	1.78868600	1.21578100
N	1.90328200	0.88769400	0.47487500
C	2.40779500	-0.42800800	0.41879300
C	2.49274900	-1.17837200	1.58805500
C	2.89917900	-0.96973500	-0.76576300
C	3.03050300	-2.45492000	1.57438600
C	3.41748700	-2.25568600	-0.79336700
C	3.49013400	-2.99389000	0.38009900
F	3.09765200	-3.16450700	2.69071200
F	2.01646700	-0.68858200	2.72145800
F	3.99866100	-4.21379500	0.36184600
F	3.87155200	-2.76841900	-1.92682400
F	2.85746600	-0.27148800	-1.88955500
C	0.97546800	1.50122500	-0.31079400
C	-0.09747600	0.93807200	-1.09943000
C	-0.23269100	-0.53916400	-1.16923400
C	-0.34921900	-1.17472900	-2.40996300
C	-0.30568400	-1.33030000	-0.01325200
C	-0.51117700	-2.55519200	-2.49149300
H	-0.30532400	-0.56820900	-3.31084800
C	-0.45921400	-2.70786700	-0.09408500
H	-0.25372500	-0.85397500	0.96651000
C	-0.55853900	-3.33035700	-1.33722600
H	-0.59540800	-3.02794900	-3.46807700
H	-0.51078000	-3.29739400	0.81934400
H	-0.68213500	-4.40884700	-1.40311700
C	-1.81061200	1.70920200	-0.21182500
H	-1.35090500	2.02265200	0.75521500
C	-2.78932200	0.56286100	-0.05160000
H	-2.93084800	0.06481000	-1.02312500
H	-2.43525700	-0.19230000	0.66101700
C	-4.13202600	1.12537900	0.43138200
H	-4.46224200	1.88317800	-0.29079300
H	-3.98126500	1.64088400	1.39185400
C	-5.17582000	0.05670800	0.58042400
C	-5.95083500	-0.33149700	-0.51584200
C	-5.36774500	-0.60163900	1.79726700
C	-6.89721900	-1.34411500	-0.39820300
H	-5.80804500	0.17401100	-1.47132300
C	-6.31401300	-1.61495600	1.92049100
H	-4.76769300	-0.30867300	2.65933200
C	-7.08322300	-1.98851600	0.82213800
H	-7.49571200	-1.62837500	-1.26142500
H	-6.45366900	-2.11175600	2.87855900
H	-7.82674300	-2.77683000	0.91724600
O	-2.11357200	2.60353000	-1.06590400
C	2.68466900	4.25876900	1.34884100
H	2.87127000	4.16447900	2.42371300
H	3.65521600	4.46960500	0.87910900
C	1.70093100	5.37256300	1.01457200
H	2.16205100	6.34229500	1.22569200
H	0.80656100	5.29351600	1.64823500
C	1.30485900	5.26380100	-0.44936800
H	2.20756700	5.28837600	-1.07674900
H	0.67747600	6.10723200	-0.75615100
C	0.52142200	3.99402300	-0.71600700
H	0.42999700	3.78244200	-1.78227400
H	-0.49371800	4.04650500	-0.30997200
O	-0.23222000	1.59569600	-2.30511300
H	-1.08694200	2.11008700	-2.19171400

TS8-1

Sum of electronic and thermal Free Energies: -1815.260967

C	2.01851500	-2.78744200	0.51540000
N	2.35969000	-1.64617500	-0.17326800
N	0.74750800	-2.81787300	0.78471400
N	0.26258800	-1.64798100	0.24233100
C	-1.14301900	-1.51168800	0.19905500

C	-1.85989400	-1.44504500	1.38926700
C	-1.83156600	-1.52688700	-1.00993100
C	-3.24246600	-1.36771200	1.37722700
C	-3.21424200	-1.42748100	-1.03158600
C	-3.91861700	-1.36296700	0.16356800
F	-3.91905100	-1.28915800	2.51274800
F	-1.21597900	-1.40288000	2.54430800
F	-5.23710500	-1.28547700	0.14686100
F	-3.86577100	-1.42561700	-2.18401500
F	-1.17050100	-1.61403000	-2.15214600
C	1.23546600	-0.89723400	-0.32182800
C	1.19338000	0.44588200	-0.92269500
C	-0.12732000	1.14606900	-0.93115300
C	-0.63359900	1.64733400	-2.13145900
C	-0.84292100	1.39187600	0.24730200
C	-1.82113700	2.37415400	-2.15605400
H	-0.07619000	1.45999800	-3.04537300
C	-2.02628200	2.11809200	0.22609600
H	-0.45683800	1.02879300	1.19987400
C	-2.52134000	2.61539600	-0.97854500
H	-2.19910500	2.75508200	-3.10271300
H	-2.55861000	2.30479800	1.15711700
H	-3.44465900	3.19011300	-0.99542400
C	2.47964700	1.48996800	0.04372500
H	2.72061700	0.80139800	0.88882800
O	3.38947000	1.66866800	-0.86701000
C	3.01011200	-3.82900500	0.88927900
H	2.77062500	-4.18885900	1.89520300
H	2.88353500	-4.68282500	0.20961100
C	4.43017900	-3.28865400	0.77516500
H	5.14349500	-4.11159300	0.88013200
H	4.63237600	-2.57720700	1.58824800
C	4.59286900	-2.59467100	-0.56821700
H	4.33203500	-3.29181200	-1.37692600
H	5.62975600	-2.28488000	-0.73458100
C	3.72989800	-1.35186600	-0.65591700
H	3.63228600	-0.97776100	-1.67609800
H	4.13448600	-0.53742400	-0.04732500
O	1.82571700	0.40949900	-2.14165900
H	2.65050400	1.00440200	-1.93463000
C	1.80418200	2.71635500	0.58058400
C	1.44487600	2.80879600	1.92387400
C	1.53463000	3.79218200	-0.26783300
C	0.79993600	3.94287800	2.41132300
H	1.66625500	1.97418400	2.59121500
C	0.88095700	4.92029400	0.20960500
H	1.83986800	3.71728400	-1.31055200
C	0.50768500	4.99742400	1.55201800
H	0.52593100	4.00343400	3.46279400
H	0.66082900	5.74694900	-0.46308900
H	-0.00110400	5.88295700	1.92717100

9

Sum of electronic and thermal Free Energies: -1815.270429

C	0.04521200	3.52626600	0.21337300
N	-0.98227400	2.61259300	0.05406300
N	1.20363300	2.93898600	0.16102200
N	0.89482600	1.62046500	-0.03800000
C	1.94581000	0.68547800	-0.18874700
C	2.53000300	0.11518600	0.93534000
C	2.41048700	0.34542800	-1.45562400
C	3.53567700	-0.83016600	0.80341900
C	3.41662900	-0.59819500	-1.59335700
C	3.97365500	-1.18553300	-0.46358500
F	4.07000800	-1.39828600	1.87525900
F	2.11110100	0.44950700	2.14463600
F	4.93783400	-2.08008900	-0.59664700
F	3.86597900	-0.92878800	-2.79663200
F	1.93218200	0.93759200	-2.53003400
C	-0.42759000	1.39107600	-0.09409000
C	-0.96062200	-0.04192300	-0.42864000
C	-0.58531600	-0.93005000	0.76277100
C	0.14090900	-2.09296400	0.52547300
C	-0.97064800	-0.61750000	2.06776200
C	0.48045600	-2.93794900	1.57797200
H	0.43655800	-2.29951200	-0.50240200
C	-0.63075100	-1.45850300	3.12252200
H	-1.53714000	0.29471700	2.26796900
C	0.09655800	-2.62148900	2.87874400
H	1.05239900	-3.84353400	1.38421100
H	-0.93036900	-1.20587400	4.13753600
H	0.36593400	-3.27800600	3.70328600
C	-2.52594200	-0.03562200	-0.61347100
H	-3.02530500	0.52645100	0.19024100
O	-2.73532000	0.61525300	-1.84323900
C	-0.19039500	4.97879900	0.41834800
H	0.56671000	5.35845700	1.11202500
H	-0.02941900	5.49370200	-0.53905000
C	-1.61327900	5.22953800	0.90150900

H	-1.81835000	6.30421700	0.89511700
H	-1.72755400	4.88285100	1.93830800
C	-2.58341900	4.48594400	-0.00262900
H	-2.42823800	4.79803000	-1.04484400
H	-3.62359400	4.71752300	0.24920600
C	-2.41571400	2.98287800	0.11216800
H	-2.91441300	2.45914000	-0.70753300
H	-2.80402400	2.62082900	1.07211500
O	-0.39977700	-0.34682400	-1.59816200
H	-1.87417600	0.40694900	-2.29009700
C	-3.08789300	-1.43708800	-0.61618300
C	-3.87934700	-1.88950300	0.43944700
C	-2.81955200	-2.30620300	-1.67718700
C	-4.39382600	-3.18329500	0.44207900
H	-4.09709200	-1.21717900	1.26982100
C	-3.33040800	-3.59900700	-1.67689200
H	-2.18579200	-1.95823400	-2.48924800
C	-4.12115800	-4.04148600	-0.61811600
H	-5.01355800	-3.51818000	1.27139800
H	-3.11138900	-4.26647200	-2.50806000
H	-4.52486900	-5.05172400	-0.62206800

TS9

Sum of electronic and thermal Free Energies: -1815.264829

C	0.79898500	3.58546100	0.17309500
N	-0.38266000	2.87019400	0.19890100
N	1.81846100	2.78816600	0.04147700
N	1.22818400	1.53930100	-0.00748100
C	2.04898500	0.40505700	-0.19899900
C	2.53752100	-0.30662800	0.88960200
C	2.35677400	-0.02086800	-1.48694600
C	3.30729600	-1.44455900	0.70129900
C	3.12849000	-1.15528100	-1.68424300
C	3.60074300	-1.86569000	-0.58768400
F	3.74090100	-2.14073900	1.74364500
F	2.24788000	0.07810700	2.12204200
F	4.33696800	-2.94864600	-0.77445400
F	3.42174500	-1.56459600	-2.91134000
F	1.92746900	0.65772100	-2.53373300
C	-0.11024400	1.54828300	0.08818300
C	-1.04040700	-0.17888400	-0.44811600
C	-0.66109200	-1.05029300	0.72513100
C	-0.04641700	-2.27262800	0.46252000
C	-0.94467100	-0.69906400	2.04674100
C	0.30756800	-3.12338700	1.50606200
H	0.16490000	-2.53227500	-0.57309700
C	-0.59583400	-1.54733800	3.08999900
H	-1.41821400	0.26007000	2.25990400
C	0.03759600	-2.76011600	2.82168400
H	0.80359700	-4.06801300	1.29146200
H	-0.80998800	-1.26061400	4.11725400
H	0.31882600	-3.41955300	3.63973200
C	-2.51068700	0.30457900	-0.47096000
H	-2.74292800	0.88943900	0.43111500
O	-2.64642100	1.12329700	-1.60536400
C	0.83591500	5.06933100	0.25872300
H	1.71170400	5.37140600	0.84241100
H	0.98170800	5.46622500	-0.75575800
C	-0.46900500	5.61077600	0.83453200
H	-0.49148900	6.69948300	0.72383700
H	-0.52555400	5.39579500	1.91112200
C	-1.65090900	4.97105800	0.11933000
H	-1.56938600	5.15618000	-0.96139200
H	-2.59863600	5.40950900	0.44894000
C	-1.71260900	3.47633400	0.37658900
H	-2.39111900	2.97376300	-0.31946700
H	-2.03467000	3.27106000	1.40577000
O	-0.55644600	-0.41565200	-1.58395300
H	-1.90253800	0.82799200	-2.17096700
C	-3.43672600	-0.89113100	-0.51493900
C	-4.21501900	-1.22624100	0.59241900
C	-3.50605600	-1.69150500	-1.65784100
C	-5.05224100	-2.33815200	0.56318200
H	-4.17291900	-0.60180600	1.48487000
C	-4.34252000	-2.80105700	-1.69054800
H	-2.89781000	-1.43675400	-2.52325000
C	-5.11652000	-3.12910200	-0.57924800
H	-5.65778200	-2.58398900	1.43297700
H	-4.38951400	-3.41572400	-2.58712900
H	-5.77131900	-3.99734800	-0.60689600

P4

Sum of electronic and thermal Free Energies: -690.532286

C	-0.52531400	1.44925700	0.07167000
O	-0.58685900	2.45568000	-0.62218100
C	-1.57278400	0.40869400	0.03108300
C	-2.48842100	0.42953500	-1.02762700
C	-1.68559700	-0.57410800	1.02042300
C	-3.48937400	-0.52664300	-1.10535400
H	-2.39250500	1.20283300	-1.78594400

C	-2.69574200	-1.52428100	0.94643600
H	-0.99305600	-0.59204500	1.85836600
C	-3.59335900	-1.50437200	-0.11744000
H	-4.19188400	-0.51185100	-1.93486800
H	-2.78456000	-2.28259000	1.72024400
H	-4.37958700	-2.25341800	-0.17743600
C	0.71768800	1.27349200	0.94901200
H	0.40857000	0.97568200	1.96350000
O	1.40410700	2.48906000	1.00487500
H	0.98665600	3.04636100	0.32346700
C	1.57586800	0.16964400	0.35583100
C	1.78990300	-1.02866900	1.03315200
C	2.16958900	0.36492900	-0.89262100
C	2.58385500	-2.02402400	0.47048500
H	1.33800600	-1.17845800	2.01363100
C	2.96088500	-0.62822400	-1.45652100
H	2.01691500	1.30723700	-1.41765400
C	3.16849600	-1.82647700	-0.77640100
H	2.75068100	-2.95355000	1.01027000
H	3.41919200	-0.46798900	-2.43007800
H	3.78942800	-2.60266400	-1.21781000

NHC-2

Sum of electronic and thermal Free Energies: -1085.490558

C	-2.85428500	-0.50737100	-0.48082500
N	-2.92695100	0.40611700	0.54412300
N	-1.62516300	-0.77909500	-0.78145300
N	-0.93868100	0.02599000	0.13984100
C	0.46708900	0.02249400	0.08860000
C	1.17809500	-1.17329100	0.17571600
C	1.18189000	1.20725800	-0.07442900
C	2.56222000	-1.18941100	0.09732300
C	2.56782000	1.20168700	-0.12925100
C	3.25837100	0.00152000	-0.04984900
F	3.22360700	-2.33568800	0.18573300
F	0.53831500	-2.32012200	0.34942800
F	4.58060500	-0.00783500	-0.11221800
F	3.23408700	2.33837700	-0.28184100
F	0.55069400	2.36525800	-0.19395600
C	-1.69918900	0.77750000	0.98377600
C	-4.21543300	-0.90968900	-0.92321700
C	-5.08495900	0.20575800	-0.30488900
C	-4.30572500	0.71473400	0.91793300
H	-4.46392400	-1.89357000	-0.50556400
H	-4.31028400	-0.97982700	-2.00960200
H	-5.19585700	1.02100300	-1.02834000
H	-6.08523200	-0.14207400	-0.03698800
H	-4.42617300	1.78510900	1.09919100
H	-4.56409400	0.17125100	1.83409200

TS2

Sum of electronic and thermal Free Energies: -1509.241632

C	0.74337100	0.14492600	1.30336600
H	0.82476800	0.97311100	2.05910100
C	2.04110600	-0.02678700	0.53418400
H	1.83894800	-0.55556700	-0.40733600
H	2.47631700	0.95492000	0.29061600
C	3.02357900	-0.84213400	1.37891700
H	2.56321700	-1.81564300	1.59407300
H	3.17465800	-0.33834700	2.34581000
C	4.34193500	-1.02884800	0.68575300
C	5.38040500	-0.11021000	0.85742700
C	4.53441100	-2.09422500	-0.19746300
C	6.58361200	-0.25635700	0.17379500
H	5.23998200	0.72599300	1.54302800
C	5.73508800	-2.24452700	-0.88357600
H	3.72923400	-2.81521200	-0.34073400
C	6.76431400	-1.32449500	-0.70063900
H	7.38291000	0.46644200	0.32493100
H	5.86916300	-3.08338600	-1.56345000
H	7.70545200	-1.44210500	-1.23334200
O	0.00647500	-0.82889900	1.53129800
C	-1.31402400	3.30086100	-0.52838000
N	-0.11753000	2.77022500	-0.11138700
N	-2.22588800	2.38446500	-0.63274700
N	-1.52543200	1.24204900	-0.24130400
C	-2.18854200	-0.00021200	-0.23269800
C	-3.38509200	-0.16105600	0.45979700
C	-1.63875500	-1.09869400	-0.88575200
C	-4.03104400	-1.38759400	0.48346000
C	-2.26925900	-2.33251200	-0.85131300
C	-3.46803400	-2.47544700	-0.16850600
F	-5.17170400	-1.52989900	1.14536400
F	-3.92068900	0.85440300	1.12089600
F	-4.07846800	-3.64964400	-0.14113300
F	-1.73864500	-3.37243200	-1.48127500
F	-0.51103900	-0.97669700	-1.56857700
C	-0.23126900	1.44459500	0.08305800
C	-1.19679800	4.77327800	-0.69403900
C	0.33535400	4.96677600	-0.71411100

C	0.92441900	3.78040900	0.06621600
H	-1.65799800	5.27266600	0.16732400
H	-1.69041500	5.14601000	-1.59465300
H	0.69163800	4.92876500	-1.74889100
H	0.64077700	5.92519100	-0.28918800
H	1.87822000	3.42394200	-0.33040300
H	1.03952300	3.98917800	1.13633100

10

Sum of electronic and thermal Free Energies: -1509.247030

H	-1.00932200	0.59810400	-2.03229100
C	-0.73655200	0.11141700	-1.03392400
C	-2.10784500	-0.06872700	-0.32365100
H	-1.92723400	-0.34963600	0.72538800
H	-2.70610900	0.85682700	-0.32304000
C	-2.88051700	-1.18131700	-1.02230000
H	-2.24203500	-2.07362000	-1.00993500
H	-3.02349400	-0.90542200	-2.07859600
C	-4.21128200	-1.45555700	-0.38607900
C	-4.30452600	-2.23923600	0.76838600
C	-5.38339500	-0.90389200	-0.90910800
C	-5.53229900	-2.46514400	1.38124100
H	-3.39736500	-2.67870700	1.18443200
C	-6.61497800	-1.12807300	-0.30074400
H	-5.32403300	-0.29382900	-1.81080200
C	-6.69346600	-1.91052100	0.84760300
H	-5.58463300	-3.08176000	2.27637500
H	-7.51720500	-0.69419600	-0.72752000
H	-7.65489400	-2.08989500	1.32398900
O	0.00297000	-0.96674400	-1.07627200
C	0.66903100	3.21463300	0.45246900
N	-0.37695100	2.55607300	-0.13993600
N	1.68545000	2.42841500	0.63791900
N	1.23841900	1.22169400	0.12641000
C	2.14349000	0.13245200	0.09941900
C	2.69549000	-0.29251800	-1.10507200
C	2.58261600	-0.43153600	1.28814900
C	3.63763700	-1.30414800	-1.12177200
C	3.53506800	-1.44213400	1.27930000
C	4.06130600	-1.87617100	0.07332900
F	4.15523800	-1.72188500	-2.27075800
F	2.33525500	0.27859200	-2.24065800
F	4.97443200	-2.83535300	0.05714300
F	3.94184600	-1.98795500	2.41846400
F	2.07721500	-0.02942300	2.44656200
C	-0.01387400	1.28379300	-0.35445400
C	0.33655400	4.64843900	0.65041000
C	-1.19321900	4.64763500	0.45390000
C	-1.51016000	3.43978600	-0.44112800
H	0.84665800	5.24257000	-0.11797300
H	0.64990400	5.02756800	1.62571600
H	-1.68491600	4.51356400	1.42305100
H	-1.55904000	5.57861100	0.01654200
H	-2.45721400	2.95517500	-0.19737600
H	-1.49161400	3.67443600	-1.51115600

TS10

Sum of electronic and thermal Free Energies: -1585.608003

H	-0.45324700	-0.54544900	-1.30468500
O	0.05409400	-1.75312800	-1.93167400
H	0.79282900	-1.42931300	-2.45743500
H	0.22900900	-1.68632200	-0.22941800
C	-0.70476400	-0.09187000	-0.17937600
C	-2.20628900	-0.08886300	0.05266800
H	-2.44406800	0.15296300	1.10247600
H	-2.68502900	0.68018400	-0.57189700
C	-2.81191800	-1.44958200	-0.29362200
H	-2.31060600	-2.20996800	0.31914400
H	-2.57974900	-1.68831100	-1.34052100
C	-4.29355900	-1.48207600	-0.05526000
C	-4.80158400	-1.69005600	1.23058100
C	-5.19597200	-1.26441500	-1.09876000
C	-6.17185900	-1.68474000	1.46756600
H	-4.10607800	-1.86440900	2.05211300
C	-6.56861100	-1.26010300	-0.86755100
H	-4.81067200	-1.10345000	-2.10575800
C	-7.06123000	-1.47081600	0.41712400
H	-6.54845400	-1.85345500	2.47449600
H	-7.25684900	-1.09589500	-1.69422300
H	-8.13361400	-1.47149900	0.59954500
O	-0.04436700	-1.11018300	0.54297100
C	0.59959800	3.29216500	-0.01193600
N	-0.47881400	2.44342700	-0.07696400
N	1.71901400	2.65296400	0.10811000
N	1.31889900	1.32575500	0.11407100
C	2.30670200	0.31753800	0.12557800
C	2.79662600	-0.18930600	-1.07072600
C	2.79764900	-0.17706300	1.32778200
C	3.75910600	-1.18710400	-1.07357800
C	3.76713200	-1.16590300	1.33663000

C	4.24669200	-1.66883800	0.13306800
F	4.21544200	-1.67517700	-2.21751800
F	2.33286400	0.27046000	-2.22406900
F	5.17098700	-2.61413500	0.13879900
F	4.23302800	-1.64091500	2.48277500
F	2.31608700	0.27694200	2.47162700
C	-0.02548000	1.17420700	-0.01503800
C	0.15892700	4.70653700	-0.10897500
C	-1.34778000	4.58626600	0.19217200
C	-1.75493100	3.16095800	-0.20946000
H	0.34288400	5.07637400	-1.12509200
H	0.69001200	5.36225900	0.58453000
H	-1.51693200	4.71800800	1.26587500
H	-1.94056400	5.33532500	-0.33651300
H	-2.50977200	2.73046100	0.45019900
H	-2.09699900	3.08775400	-1.24758900

11

Sum of electronic and thermal Free Energies: -1509.265879

H	0.17713600	-1.35827800	-1.32389400
C	-0.77113100	-0.30369700	-0.00562800
C	-2.21411800	-0.53056800	0.28360500
H	-2.31473900	-1.37447000	0.98613400
H	-2.66056400	0.33559400	0.78728600
C	-3.02728000	-0.85380000	-0.98014700
H	-2.57193300	-1.72259800	-1.47459900
H	-2.94478800	-0.00576900	-1.67569700
C	-4.46880000	-1.12854900	-0.66712900
C	-4.91251300	-2.42665700	-0.40464600
C	-5.38578000	-0.07841100	-0.56858900
C	-6.23868400	-2.67137500	-0.06091800
H	-4.20491700	-3.25296900	-0.47531700
C	-6.71234100	-0.31754200	-0.22510900
H	-5.04968400	0.93954000	-0.77089100
C	-7.14326300	-1.61707300	0.02911800
H	-6.56751000	-3.68986400	0.13529600
H	-7.41384000	0.51164500	-0.15925800
H	-8.18098200	-1.80767400	0.29382300
O	-0.07261800	-1.44241500	-0.39251000
C	0.47421900	3.02329200	0.18229800
N	-0.54509300	2.14317800	0.42088900
N	1.59276100	2.47275800	-0.14357800
N	1.27157200	1.08943200	-0.16668800
C	2.32354600	0.18430400	-0.05561200
C	3.38044800	0.22931400	-0.97113100
C	2.39855000	-0.76969800	0.96269000
C	4.45289200	-0.64349800	-0.88442200
C	3.44659700	-1.67541000	1.03048100
C	4.48477600	-1.60626600	0.11451500
F	5.43759000	-0.58278000	-1.77490900
F	3.36151700	1.10937600	-1.96533800
F	5.50066400	-2.45706100	0.18881500
F	3.48244300	-2.58035200	2.00314300
F	1.46458800	-0.81843600	1.90305100
C	-0.09736200	0.86023900	0.11237900
C	-0.02123200	4.42216100	0.29509400
C	-1.38437700	4.22657100	0.98239300
C	-1.82727900	2.79638300	0.63188900
H	-0.13301600	4.84439000	-0.71154200
H	0.65888800	5.07285700	0.85065200
H	-1.26290800	4.30645700	2.06801500
H	-2.12295400	4.96922800	0.67218900
H	-2.38688100	2.32764700	1.44678900
H	-2.43747100	2.75096600	-0.28292000

TS11

Sum of electronic and thermal Free Energies: -1854.514366

C	3.61983100	-1.74794300	-0.52486200
N	3.26262000	-0.50618900	-0.97691400
N	2.63771700	-2.37369000	0.04104500
N	1.58206100	-1.47196500	-0.09075300
C	0.37525500	-1.75262800	0.57596500
C	0.22281200	-1.38432600	1.90868000
C	-0.67416300	-2.40187900	-0.06625600
C	-0.99231000	-1.54405100	2.55545700
C	-1.88862700	-2.59083300	0.57718100
C	-2.04692100	-2.15286200	1.88612400
F	-1.14649400	-1.12545700	3.80199200
F	1.23523100	-0.82536300	2.55527000
F	-3.20445200	-2.31935800	2.49814800
F	-2.89471000	-3.18277400	-0.04863400
F	-0.54078200	-2.79426700	-1.32395400
C	1.94963200	-0.30292200	-0.70811700
C	1.24765700	0.92442200	-0.90291500
C	2.01535200	1.97549300	0.73662700
H	2.27024000	1.10539300	1.37824800
O	2.94586900	2.62232100	0.15558200
C	5.04411100	-2.02397100	-0.84111200
H	5.56610300	-2.53968700	-0.03197900
H	5.09789600	-2.66030700	-1.73337000

C	5.57961200	-0.60546700	-1.11842500
H	6.39024000	-0.60092900	-1.85019800
H	5.96313900	-0.17474800	-0.18709400
C	4.37741400	0.22217500	-1.59960000
H	4.25304400	0.20865500	-2.68719000
H	4.38895400	1.25141900	-1.23964600
C	0.79756900	2.69773900	1.20361800
C	-0.04620600	2.14998100	2.17246000
C	0.47429800	3.93796300	0.64656600
C	-1.20725000	2.81187600	2.55581200
H	0.21897300	1.20322300	2.63950800
C	-0.68518900	4.60192000	1.02887200
H	1.15044800	4.36402000	-0.09215700
C	-1.53415000	4.03701700	1.97951900
H	-1.85618500	2.37165500	3.31067300
H	-0.93008500	5.56512800	0.58568200
H	-2.44298200	4.55590400	2.27606200
C	-0.25618800	0.94463500	-0.97433100
H	-0.71776300	0.41211900	-0.13130100
H	-0.57208100	1.99151000	-0.86698800
C	-0.81763600	0.40021100	-2.29534800
H	-0.40311900	1.00279600	-3.11511200
H	-0.47271100	-0.63134200	-2.45187300
C	-2.31994600	0.43352100	-2.31793000
C	-3.06176400	-0.74794600	-2.26361700
C	-3.01048200	1.65012900	-2.34196900
C	-4.45316600	-0.72234000	-2.22891200
H	-2.53708100	-1.70256400	-2.24879100
C	-4.40005800	1.68094200	-2.31015200
H	-2.44789800	2.58287900	-2.38911500
C	-5.12770500	0.49401100	-2.25228100
H	-5.00918500	-1.65681600	-2.18380600
H	-4.91956500	2.63684700	-2.33301400
H	-6.21479400	0.51957500	-2.22655900
O	1.84344200	1.70620500	-1.87141300
H	2.40330900	2.34574600	-1.34068700

12

Sum of electronic and thermal Free Energies: -1854.521029

C	3.28377300	-2.26611500	-0.22623700
N	3.14470500	-0.99076400	-0.70474400
N	2.22506000	-2.65765900	0.41555300
N	1.39287600	-1.55529400	0.32767700
C	0.11137600	-1.64563300	0.91691700
C	-0.17405400	-1.02349100	2.12748900
C	-0.88097200	-2.39382700	0.29062600
C	-1.45686200	-1.05798500	2.65155600
C	-2.16152400	-2.45224800	0.81674900
C	-2.44804200	-1.77714100	1.99721600
F	-1.72955500	-0.42321000	3.77980700
F	0.76409300	-0.35437000	2.77772600
F	-3.66668100	-1.82368400	2.49995400
F	-3.10975000	-3.14090700	0.20184000
F	-0.61698500	-3.01815000	-0.84730000
C	1.93450700	-0.53240400	-0.37311600
C	1.44118600	0.88841300	-0.74704900
C	1.93251500	1.79440500	0.52654900
H	1.99668000	1.17089500	1.43202500
O	3.20433800	2.21984500	0.14719400
C	4.60058000	-2.83365400	-0.60763700
H	5.07127400	-3.38730800	0.20793500
H	4.46753500	-3.52678400	-1.44737700
C	5.37724700	-1.56651100	-1.01947300
H	6.09740200	-1.76111900	-1.81663600
H	5.92852400	-1.18313400	-0.15456900
C	4.32807000	-0.52947100	-1.44918400
H	4.09347300	-0.55144000	-2.51633900
H	4.57218200	0.48971600	-1.15414200
C	1.00046400	2.94171100	0.81051000
C	-0.00968500	2.82513100	1.76888700
C	1.10208900	4.12892000	0.08254600
C	-0.91016900	3.86392500	1.98209600
H	-0.08616300	1.90838900	2.35607400
C	0.20239300	5.16859300	0.29311400
H	1.89840200	4.22868100	-0.65162200
C	-0.80924900	5.03888200	1.24168500
H	-1.68914700	3.75857800	2.73466100
H	0.29193800	6.08726600	-0.28353700
H	-1.51236700	5.85205000	1.40830600
C	-0.08402700	0.90903400	-0.93830100
H	-0.63959100	0.55015800	-0.05749100
H	-0.35453400	1.96680100	-1.05128500
C	-0.52755200	0.15768800	-2.19269400
H	0.00222600	0.60616000	-3.04284000
H	-0.21014800	-0.89497000	-2.14447700
C	-2.01706100	0.21785200	-2.38616200
C	-2.81314200	-0.91489000	-2.20458400
C	-2.64982300	1.42448600	-2.70470100
C	-4.19937100	-0.84897500	-2.31924900

H	-2.33574900	-1.86773200	-1.98071100
C	-4.03316200	1.49494700	-2.82775400
H	-2.04564000	2.31820600	-2.86154300
C	-4.81538000	0.35892400	-2.62858400
H	-4.79589200	-1.74612100	-2.16450200
H	-4.50522100	2.44286700	-3.07838700
H	-5.89777900	0.41655500	-2.71924100
O	2.10608300	1.29076800	-1.82602400
H	3.11589900	2.08288800	-0.84859800

TS12

Sum of electronic and thermal Free Energies: -1854.512587

C	-0.23222800	-1.04862900	0.34051800
C	-0.63414800	-2.54806700	0.37894400
H	-0.59363900	-2.96752500	-0.63813700
O	0.29903900	-3.19679500	1.20141700
O	0.24864300	-0.61537300	1.41965100
H	0.65772700	-2.45577000	1.73484400
C	-2.05050900	-2.67600300	0.89172300
C	-3.11350200	-2.83541500	0.00183800
C	-2.32180800	-2.56700000	2.25732800
C	-4.42692200	-2.86410700	0.46220000
H	-2.90687700	-2.93847300	-1.06376000
C	-3.63242300	-2.59661300	2.72022800
H	-1.49588900	-2.45497300	2.95656000
C	-4.68982400	-2.73793600	1.82354800
H	-5.24518200	-2.99069500	-0.24376600
H	-3.83187700	-2.50780400	3.78612200
H	-5.71497200	-2.76016800	2.18642600
C	-1.11408400	-0.15024900	-0.51927700
H	-0.50047900	0.54457900	-1.10069000
H	-1.66054400	-0.75847300	-1.25612800
C	-2.08827800	0.66884800	0.33106100
H	-2.69593200	0.00439400	0.96097700
H	-1.49811700	1.29674800	1.01310600
C	-2.98330800	1.51364700	-0.52834600
C	-4.28225900	1.09668700	-0.82669200
C	-2.51958500	2.70627500	-1.09114900
C	-5.10242300	1.85440800	-1.65760700
H	-4.64959800	0.16465500	-0.39452400
C	-3.33557400	3.46695600	-1.92154800
H	-1.50337800	3.03992200	-0.87448200
C	-4.63166700	3.04361300	-2.20626900
H	-6.11395400	1.51721400	-1.87490100
H	-2.95991700	4.39625100	-2.34509800
H	-5.27180300	3.64039900	-2.85232700
C	3.45486900	-1.97525400	-1.30127000
N	2.11911300	-2.29301400	-1.25070800
N	3.66498900	-0.75301900	-0.92276000
N	2.37558000	-0.31959000	-0.62710500
C	2.21931900	0.96333000	-0.05916400
C	2.64712400	1.18658000	1.24639500
C	1.63857300	2.00932200	-0.76573500
C	2.49408400	2.42947500	1.83814400
C	1.46226400	3.25217200	-0.17467000
C	1.89278200	3.46051300	1.12730900
F	2.90099800	2.63663800	3.08251700
F	3.20094600	0.20583200	1.93587600
F	1.73650600	4.64567200	1.69168700
F	0.88473200	4.23852300	-0.84904500
F	1.21613800	1.82836100	-2.01036200
C	1.40605700	-1.24527300	-0.79887100
C	4.25906200	-3.15142600	-1.72117400
C	3.17404300	-4.08760000	-2.29367900
C	1.86043500	-3.69221100	-1.60193600
H	4.74674100	-3.58754800	-0.84033200
H	5.04099300	-2.90258500	-2.44236100
H	3.07958100	-3.91818100	-3.37169300
H	3.41040400	-5.14257600	-2.13964200
H	0.98944600	-3.77034900	-2.25667400
H	1.66371400	-4.24382800	-0.67520100

TS2'

Sum of electronic and thermal Free Energies: -1430.728122

C	-0.86636800	-1.32393200	0.54471200
O	-0.38156500	-1.03191000	1.65982800
C	-2.33001300	-1.67323500	0.40855600
C	-3.18151500	-1.48906200	1.49416500
C	-2.83690900	-2.17716200	-0.78837000
C	-4.53620500	-1.79065800	1.38016000
H	-2.75689800	-1.10856300	2.42139900
C	-4.18862600	-2.47868200	-0.90639100
H	-2.16119300	-2.32136700	-1.63281200
C	-5.04217600	-2.28097500	0.17853700
H	-5.20004700	-1.64615000	2.23012300
H	-4.58041300	-2.87011500	-1.84303300
H	-6.10014500	-2.51785700	0.08852600
H	-0.25592600	-1.87361300	-0.21413800
C	-1.10798600	2.57830300	-0.46137200
N	-1.74552800	1.35964200	-0.45706500

N	0.18121400	2.44075200	-0.42265300
N	0.31852400	1.05563900	-0.41043400
C	1.59892400	0.48787700	-0.25514200
C	2.17025200	-0.27203000	-1.26985100
C	2.29042300	0.65382600	0.94156700
C	3.42262800	-0.84522800	-1.10326200
C	3.54804700	0.09675400	1.11062000
C	4.10965000	-0.65605700	0.08735200
F	3.96771100	-1.56336400	-2.07562500
F	1.52271700	-0.46092500	-2.40983100
F	5.30606500	-1.19550300	0.24942500
F	4.21011500	0.26273000	2.24730800
F	1.75393700	1.35392600	1.92383500
C	-0.84009900	0.36554600	-0.42512100
C	-2.09531000	3.68425000	-0.54622200
C	-3.40797500	2.96137600	-0.17622600
C	-3.20360100	1.48595800	-0.55288600
H	-2.12175500	4.07366700	-1.57158600
H	-1.85751200	4.51808200	0.11874300
H	-3.57126500	3.03668600	0.90403400
H	-4.27743100	3.39170000	-0.67767600
H	-3.69660000	0.78710700	0.12789200
H	-3.51151800	1.26048400	-1.58000300

13

Sum of electronic and thermal Free Energies: -1430.732188

C	1.11584900	0.41398400	-1.54088600
O	-0.09025300	0.83376200	-1.82067900
C	2.05610500	1.45706000	-0.89222900
C	1.51747100	2.32051000	0.06166600
C	3.39645000	1.58852900	-1.24782300
C	2.31011500	3.28868200	0.66532200
H	0.45962400	2.22343600	0.30410700
C	4.19460200	2.56359700	-0.65055300
H	3.81223900	0.93279700	-2.01475700
C	3.65345400	3.41245600	0.30958000
H	1.88271000	3.95630400	1.41109100
H	5.23768400	2.66643400	-0.94365500
H	4.27313700	4.17604900	0.77484400
H	1.73098000	-0.04832600	-2.37647600
C	1.45729400	-2.38838800	0.88612000
N	2.01654700	-1.57064400	-0.06065900
N	0.20127600	-2.11220100	1.07210000
N	-0.01995400	-1.07534900	0.18119100
C	-1.31775600	-0.50913300	0.11953200
C	-2.20918500	-0.88589200	-0.87784100
C	-1.74695600	0.32788000	1.13821900
C	-3.50376300	-0.39884300	-0.87537400
C	-3.04382800	0.82081700	1.14930700
C	-3.92294500	0.45002400	0.14364900
F	-4.35307700	-0.74552300	-1.83428900
F	-1.82303300	-1.70467300	-1.84027400
F	-5.16678600	0.90466800	0.15056100
F	-3.44108400	1.63508500	2.11830600
F	-0.90233400	0.69660500	2.09272700
C	1.07612900	-0.73344100	-0.51042100
C	2.45795100	-3.37094200	1.37469100
C	3.78163600	-2.74493100	0.88632700
C	3.42713700	-1.86825900	-0.32659200
H	2.26637400	-4.34251000	0.90235600
H	2.42148500	-3.51560400	2.45656700
H	4.19700000	-2.11124000	1.67652400
H	4.52874100	-3.49891900	0.63157900
H	4.00526700	-0.94251300	-0.38120000
H	3.49998000	-2.39635000	-1.28340500

TS13

Sum of electronic and thermal Free Energies: -1507.091661

C	-1.03073100	-0.93847500	-0.15980900
O	-0.04535500	-1.58450400	0.61651200
H	0.41826500	-2.07595200	-0.12705500
C	-2.42590600	-1.43807500	0.09330400
C	-2.90707700	-1.56925600	1.39899500
C	-3.25878600	-1.76970900	-0.97469900
C	-4.21019700	-1.99370700	1.62925200
H	-2.24701500	-1.33195500	2.23228500
C	-4.56646600	-2.19369500	-0.74695400
H	-2.87203700	-1.69241800	-1.99034900
C	-5.04473200	-2.29975300	0.55491500
H	-4.58025800	-2.08525100	2.64826800
H	-5.20820000	-2.44834500	-1.58758200
H	-6.06566100	-2.62904800	0.73561000
C	-1.16746900	2.68989900	-0.04253300
N	-1.81432200	1.48270100	-0.13837800
N	0.11507300	2.54960800	0.07948100
N	0.27757200	1.17367200	0.06839100
C	1.57982600	0.62903700	0.08169000
C	2.20713800	0.27994900	-1.10654000
C	2.23622400	0.41290800	1.28761900
C	3.47087100	-0.29087400	-1.09653600

C	3.50407400	-0.14268300	1.30875300
C	4.11880800	-0.49620600	0.11333900
F	4.05525400	-0.63999500	-2.23297300
F	1.59329100	0.47156500	-2.26492600
F	5.32672100	-1.03213900	0.13107700
F	4.12769600	-0.34814200	2.45953000
F	1.63761000	0.71614400	2.42550300
C	-0.89465500	0.50258300	-0.05568000
C	-2.14248900	3.80856500	-0.06629800
C	-3.40929500	3.11030500	-0.60009900
C	-3.27562900	1.62676400	-0.22427800
H	-1.81111000	4.64296500	-0.68856800
H	-2.28256500	4.18865300	0.95316800
H	-4.32677600	3.54302900	-0.19632400
H	-3.44393400	3.20261600	-1.69047700
H	-3.71321700	1.38457200	0.75043800
H	-3.68602000	0.94775900	-0.97431400
O	0.31189000	-2.30184300	-1.81407700
H	0.90189700	-1.74145500	-2.32909800
H	-0.63011400	-1.32862100	-1.25247600

14

Sum of electronic and thermal Free Energies: -1430.752962

C	-1.31804000	-0.83690200	-0.15619700
O	-0.30830000	-1.78759800	-0.06956400
H	-0.36065300	-2.34945700	-0.85654600
C	-2.67974800	-1.33369900	-0.31216700
C	-3.02350300	-2.59071600	0.21882200
C	-3.65539700	-0.65252500	-1.06243300
C	-4.29826500	-3.11380300	0.05196800
H	-2.27304300	-3.14693900	0.77650900
C	-4.93358200	-1.17445200	-1.21565400
H	-3.39234700	0.27560700	-1.56575100
C	-5.26761800	-2.40510500	-0.65519400
H	-4.53978800	-4.08332300	0.48344800
H	-5.66825800	-0.62619000	-1.80218600
H	-6.26617500	-2.81630700	-0.78333700
C	-0.88566100	2.68966900	0.20897100
N	-1.71487900	1.59976500	0.15374700
N	0.36283000	2.40713200	0.06833200
N	0.35980400	1.00797700	-0.10435600
C	1.59908500	0.36324800	-0.05971000
C	2.53548500	0.58693600	-1.06886200
C	1.97934700	-0.43624800	1.01971300
C	3.79787200	0.01377000	-1.01964500
C	3.22399600	-1.04281600	1.06048000
C	4.14093900	-0.80568400	0.04502300
F	4.67335700	0.23501000	-1.99315200
F	2.22548400	1.35261400	-2.10658400
F	5.34209700	-1.36403600	0.09294100
F	3.56148800	-1.81577100	2.08661200
F	1.14389200	-0.62770300	2.02898400
C	-0.93783800	0.46640600	-0.03950400
C	-1.67315200	3.90719700	0.53441000
C	-2.87870400	3.28861800	1.26745200
C	-3.04966500	1.87843100	0.67573700
H	-1.98189300	4.41354300	-0.38889400
H	-1.11287500	4.62338700	1.13923800
H	-2.65061600	3.20740600	2.33585200
H	-3.78743500	3.88604500	1.16316100
H	-3.33135200	1.12880200	1.42247000
H	-3.79362400	1.84911900	-0.12999200

TS14

Sum of electronic and thermal Free Energies: -1854.508431

C	-2.07992100	3.23108700	-0.86215500
N	-1.06779800	3.03114300	0.03396200
N	-2.62799100	2.12229800	-1.24644200
N	-1.91339900	1.15895200	-0.53181500
C	-2.46983800	-0.13550500	-0.48984900
C	-2.51456000	-0.90592000	-1.64792500
C	-3.03260800	-0.64236500	0.67860600
C	-3.09139600	-2.16573200	-1.63970900
C	-3.59318100	-1.91037500	0.70224500
C	-3.62964300	-2.66669000	-0.46153000
F	-3.12232300	-2.89561300	-2.74459800
F	-1.95981700	-0.45442200	-2.76143700
F	-4.17858000	-3.86868200	-0.44847100
F	-4.11672800	-2.38994100	1.82009100
F	-3.01812500	0.07413200	1.79082400
C	-0.93657700	1.70233600	0.25783700
C	0.13542000	-0.35085900	1.26789200
C	0.19228100	-0.88713300	2.55868800
C	0.18141400	-1.23776500	0.18128000
C	0.26839600	-2.26197300	2.75889600
H	0.17022200	-0.20407800	3.40335300
C	0.25164000	-2.61033200	0.38123200
H	0.18081900	-0.84507900	-0.83617100
C	0.29147400	-3.13183100	1.67318300
H	0.30529300	-2.65550300	3.77268900

H	0.28294100	-3.27660000	-0.47888000
H	0.34920900	-4.20652400	1.82927900
C	2.75829200	0.58968700	0.04556400
H	2.87604800	0.12867000	1.03817100
H	2.35585900	-0.17445300	-0.63106600
C	4.12958300	1.05034600	-0.46470600
H	4.51582200	1.80658500	0.23097100
H	4.00438000	1.54420800	-1.43994500
C	5.09654500	-0.09100200	-0.58854700
C	5.85099000	-0.50375700	0.51303900
C	5.23001100	-0.79362300	-1.78830100
C	6.71873500	-1.58689600	0.41875800
H	5.75229600	0.03658600	1.45490700
C	6.09739500	-1.87751500	-1.88795300
H	4.64537300	-0.48150200	-2.65415400
C	6.84574600	-2.27668000	-0.78415900
H	7.30186800	-1.89046500	1.28585000
H	6.19305800	-2.40948700	-2.83241200
H	7.52702300	-3.12120100	-0.86109000
C	-2.27155000	4.68328300	-1.11220900
H	-2.45162200	4.91320500	-2.16474600
H	-3.14126300	5.03261900	-0.54156200
C	-0.95572600	5.27127200	-0.56580000
H	-1.08546800	6.27556500	-0.15677000
H	-0.21911000	5.33012300	-1.37453000
C	-0.45907200	4.28633200	0.50157600
H	-0.84986000	4.50409800	1.50179500
H	0.62780500	4.18020800	0.55578300
C	0.08285900	1.11955600	1.08694400
C	1.84420600	1.79029200	0.15022800
H	1.38396200	2.08011400	-0.82200000
O	2.18077500	2.70801100	0.96409300
O	0.23677100	1.86671400	2.23812800
H	1.11394700	2.32966600	2.10641500

15

Sum of electronic and thermal Free Energies: -1854.523063

C	2.13517700	3.39467000	0.26758400
N	0.82521200	2.97360600	0.23776800
N	2.96406800	2.40621700	0.14688600
N	2.12377400	1.31739400	0.03212700
C	2.68562600	0.03925300	-0.18275300
C	3.06957700	-0.74293800	0.90198900
C	2.88868300	-0.42922400	-1.47804000
C	3.60001400	-2.00783500	0.70539700
C	3.41982800	-1.69505500	-1.67988100
C	3.76927900	-2.48041300	-0.58947800
F	3.94173900	-2.76419500	1.73818600
F	2.91291600	-0.28831300	2.13444200
F	4.27892600	-3.68390500	-0.78588700
F	3.61542700	-2.15312200	-2.90817500
F	2.60686500	0.32538300	-2.51977700
C	0.81277000	1.64198200	0.06846700
C	-0.18243400	-0.61513100	0.52260400
C	-0.17856200	-1.84552100	-0.13052200
C	-0.13978500	-0.58293800	1.91683500
C	-0.12734400	-3.02978800	0.59696800
H	-0.21705500	-1.83733400	-1.21843300
C	-0.08211300	-1.76617800	2.64786500
H	-0.14417200	0.37524400	2.43961000
C	-0.07339100	-2.99322100	1.98865700
H	-0.12585300	-3.98678100	0.07849800
H	-0.04090400	-1.73037500	3.73458700
H	-0.02838200	-3.91823600	2.55947000
C	-2.84800400	0.30986700	-0.14115000
H	-2.76180800	-0.23771600	-1.09310800
H	-2.75352300	-0.43258700	0.66403200
C	-4.21997500	0.97418100	-0.04996900
H	-4.30951700	1.71657500	-0.85269200
H	-4.28845700	1.52195900	0.90286900
C	-5.33387400	-0.02961800	-0.14065400
C	-5.97593700	-0.28296900	-1.35458700
C	-5.71164600	-0.77547600	0.97955300
C	-6.97117400	-1.25176700	-1.44938000
H	-5.68750200	0.29155900	-2.23502400
C	-6.70476000	-1.74512200	0.89045400
H	-5.21681500	-0.58819300	1.93321700
C	-7.33850100	-1.98674900	-0.32609000
H	-7.46205400	-1.43188800	-2.40371000
H	-6.98683700	-2.31431900	1.77406400
H	-8.11631500	-2.74391100	-0.39731200
C	2.21507700	4.86916700	0.41340400
H	3.00286200	5.18403000	1.10121200
H	2.42623800	5.31870100	-0.56490000
C	0.79470900	5.21005700	0.90188500
H	0.46287200	6.19432500	0.56450100
H	0.77243600	5.20328500	1.99675000
C	-0.11774000	4.10082400	0.36351000
H	-0.53337700	4.30966300	-0.62476000

H	-0.93786500	3.84309100	1.03588500
C	-0.31244000	0.65401800	-0.32216900
C	-1.71177500	1.32121700	-0.07119500
H	-1.74198400	1.82757800	0.91123900
O	-1.84670000	2.27864000	-1.09446100
O	-0.12665600	0.50357900	-1.63788700
H	-1.28707200	1.84268600	-1.78958000

TS15

Sum of electronic and thermal Free Energies: -1854.515596

C	0.46426600	0.23008200	0.31524300
C	0.18466300	-0.87234000	-0.68091900
C	-0.23354200	-2.10951900	-0.19520100
C	0.35353400	-0.70393000	-2.05739600
C	-0.51219400	-3.15633800	-1.06974600
H	-0.35838900	-2.22162900	0.88008300
C	0.07973600	-1.74734600	-2.93268200
H	0.67273000	0.26181000	-2.44928700
C	-0.36461500	-2.97435300	-2.44146900
H	-0.85536400	-4.11301300	-0.67988000
H	0.20149700	-1.60221400	-4.00395700
H	-0.59008300	-3.78710600	-3.12826000
C	1.76599200	1.02723200	0.10539700
H	1.78967600	1.51341200	-0.88278000
C	2.96915000	0.09882700	0.23890900
H	2.92202300	-0.39116000	1.22406000
H	2.91365700	-0.69880500	-0.51691100
C	4.29083300	0.84897700	0.09435300
H	4.32395900	1.64993800	0.84380600
H	4.31909000	1.33249500	-0.89413100
C	5.47709700	-0.05865400	0.25241700
C	5.94224600	-0.81770900	-0.82496300
C	6.10701900	-0.20457800	1.49014600
C	7.01218600	-1.69335100	-0.67296800
H	5.45685100	-0.71270300	-1.79587100
C	7.17835400	-1.07896000	1.64765600
H	5.75098500	0.38046600	2.33822300
C	7.63466600	-1.82631400	0.56566500
H	7.36272300	-2.27303000	-1.52449700
H	7.65949600	-1.17640500	2.61882900
H	8.47269500	-2.50916700	0.68627200
O	1.79625000	2.02987200	1.09476100
O	0.15531900	0.05895000	1.52419600
H	1.27616700	1.61922300	1.81583900
C	-2.05125100	3.50285900	-0.24538300
N	-0.80498600	2.95867200	-0.44837700
N	-2.93017500	2.58804000	0.02434700
N	-2.15887800	1.43060100	-0.02556800
C	-2.77149000	0.18684900	0.23597200
C	-3.04270400	-0.19375400	1.54657800
C	-3.07834300	-0.68341800	-0.80328500
C	-3.60617100	-1.43145200	1.81557000
C	-3.62229700	-1.93207000	-0.54197400
C	-3.88620000	-2.30164100	0.76895200
F	-3.86720200	-1.79603400	3.06310100
F	-2.76933700	0.62633700	2.54525100
F	-4.40473700	-3.49100200	1.02634800
F	-3.86164600	-2.78054000	-1.53233300
F	-2.82300000	-0.34101300	-2.05561300
C	-0.85135700	1.62285600	-0.29775300
C	-2.00057700	4.98272100	-0.36639700
C	-0.65150600	5.19026500	-1.08646100
C	0.21446900	3.97630100	-0.72037900
H	-1.99850400	5.42924700	0.63597000
H	-2.85181700	5.39697500	-0.91183800
H	-0.81756700	5.20565900	-2.16913100
H	-0.16955200	6.12979200	-0.80781000
H	0.87426400	3.65056300	-1.52845000
H	0.81269600	4.11669500	0.18518100

P2

Sum of electronic and thermal Free Energies: -769.051977

C	1.92792500	1.35035000	0.15807200
O	2.25404300	2.25059800	0.92183200
C	2.67533500	0.07523700	0.09608400
C	3.66876000	-0.15865100	1.05451900
C	2.43201500	-0.88835400	-0.88976600
C	4.40077300	-1.33581600	1.03265200
H	3.84837100	0.59822300	1.81391000
C	3.16997700	-2.06487100	-0.91307000
H	1.67206800	-0.72099100	-1.65009700
C	4.15222700	-2.28985200	0.04748600
H	5.16761000	-1.51208400	1.78284700
H	2.98107000	-2.80798300	-1.68350900
H	4.72793200	-3.21225600	0.02868500
C	0.68699000	1.56747700	-0.69642400
H	0.88928700	1.25487200	-1.73414400
C	-0.46456500	0.72836100	-0.13333500
H	-0.65357800	1.06102400	0.89941400
H	-0.17599100	-0.33110100	-0.07961500

C	-1.73513700	0.87389900	-0.96676900
H	-1.99974000	1.93709400	-1.02556000
H	-1.52743700	0.53525200	-1.99300400
C	-2.87421300	0.08579800	-0.38589400
C	-3.02043200	-1.27291800	-0.67725400
C	-3.77752000	0.67921800	0.49877200
C	-4.04579800	-2.01870600	-0.10550400
H	-2.31960900	-1.74601200	-1.36576900
C	-4.80490700	-0.06267900	1.07366000
H	-3.67045100	1.73833500	0.73399700
C	-4.94238200	-1.41480100	0.77247400
H	-4.14748700	-3.07466400	-0.34756000
H	-5.50217000	0.41690900	1.75750300
H	-5.74627600	-1.99552000	1.21928800
O	0.36150400	2.92899500	-0.69882100
H	0.83775500	3.30000000	0.06531500