

Supporting Information

Combinational Experimental and DFT Theoretical Investigation over the Formation Mechanism of Binuclear Phthalocyanine Dimer

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Table S1. The SCF energy of different spin states of intermediate **9**. Energies are given in Hartree

References for Supporting Information.

Cartesian Coordinates (Å), SCF Energies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures.

Experimental General Remarks:

CH₂Cl₂ for voltammetric studies was distilled from CaH₂ under nitrogen. Column chromatography was carried out on silica gel (Merck, Kieselgel 60, 70-230 mesh) with the indicated eluents. Nessler reagent,^{S1} and **1-OR**,^{S2} were prepared according to the published procedures. All other reagents and solvents were used as received.

¹H NMR spectra were recorded on a Bruker DPX 400 spectrometer. Spectrum was referenced internally using the resonances of SiMe₄ ($\delta = 0$ for ¹H NMR). Electronic absorption spectra were recorded on a Hitachi U-4100 spectrophotometer. IR spectra were recorded as KBr pellets using a Bruker Tensor 37 spectrometer with 2 cm⁻¹ resolution. Elemental analyses were performed on an Elementar Vavio El III. MALDI-TOF mass spectra were taken on a Bruker BIFLEX III ultrahigh-resolution Fourier transformion cyclotron resonance (FT-ICR) mass spectrometer with alpha-cyano-4-hydroxycinnamic acid as matrix. The software of Bruker Daltonics IsotopePattern was used for the simulated mass pattern.

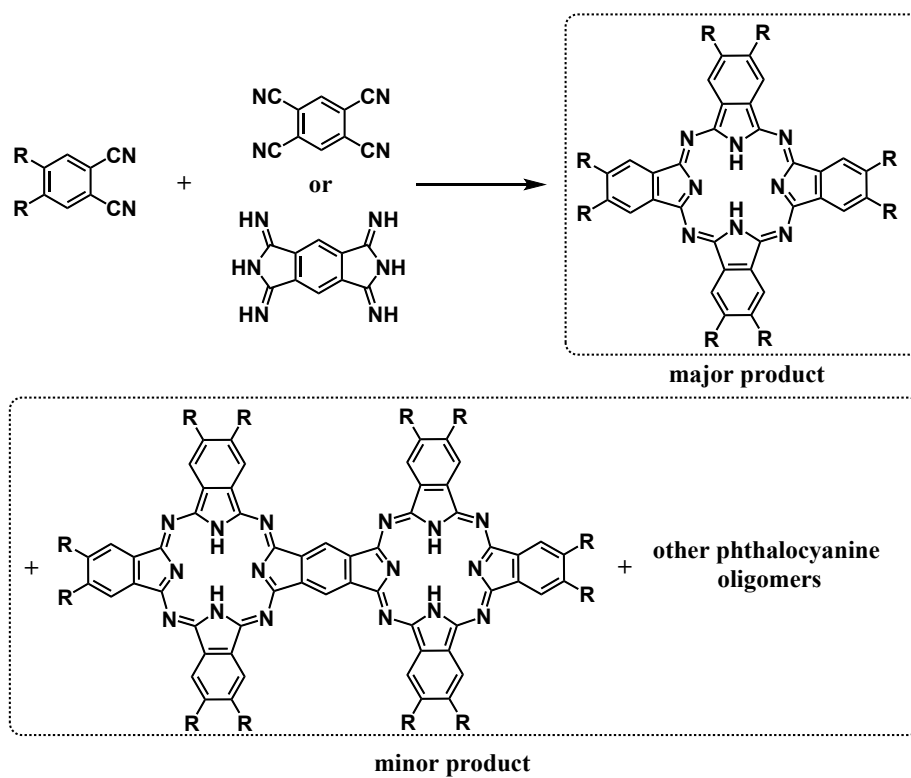
Computational Detail:

All structures are optimized at M06-2X/6-31+G(d,p)^{S3,S4} level in the gas phase. The M06-2X method is chosen due to its validity for organic mechanistic studies together with the prediction of main-group thermochemistry and energy barrier heights.^{S3,S5} Harmonic frequency analysis calculations at the same level were performed subsequently, to characterize the stationary points exhibit no imaginary frequency while the transition states exhibit one imaginary frequency. To get the improved energies, single-point calculations were carried out using the higher level of 6-311+G(2d,2p) basis set for all atoms in CH₂Cl₂ solvent, employing the SMD solvent model.^{S6} Gibbs free energies then were corrected to the refined energies at 298.15 K and 1 atm. In this study, we discuss the mechanism in terms of the corrected Gibbs free energies, which are given under corresponding compounds. All calculations were performed with Grimme-D3 dispersion corrections method.^{S7} It should be emphasized that, to the best of our knowledge, since no standard quantum mechanics-based approach is valid to accurately calculate the entropy in solution, we employed the corrections based on “the theory of free volume”^{S8} to the calculated free energies, i.e., for 2-to-1 reactions, a correction of -2.6 kcal/mol was made.

Spectroscopic characterization:

The MALDI-TOF mass spectrum of newly prepared binuclear phthalocyanine dimer **9-OR** clearly shows intense signals for the corresponding molecular ion $[M]^+$. The isotopic pattern closely resembled the simulated one as exemplified by the spectrum of **9-OR** given in Figure S1 in Supporting Information.

^1H NMR spectrum was obtained for the metal free homobinuclear phthalocyanine dimer **9-OR** in CDCl_3 , Figure S2 (Supporting Information). As can be seen, the signals appearing in the range from $\delta = 9.5$ to 8.0 ppm can be assigned to the Pc α -protons. The broad peak at $\delta = 7.37$ and the multiplet from 7.06 to 7.00 ppm are attributed to the aromatic protons of the substituents, while the multiplets $\delta 2.25$ - 2.58 ppm are due to the methyl protons. The singlet signal appearing at $\delta = -0.16$ is assigned to the inner protons of **9-OR**.



Scheme S1. Synthesis of π -conjugated phthalocyanine oligomers through cyclotetramerization pathway with 1,2,4,5-tetracyanobenzene or its bis(diiminoisoindole) counterpart as the necessary precursor.

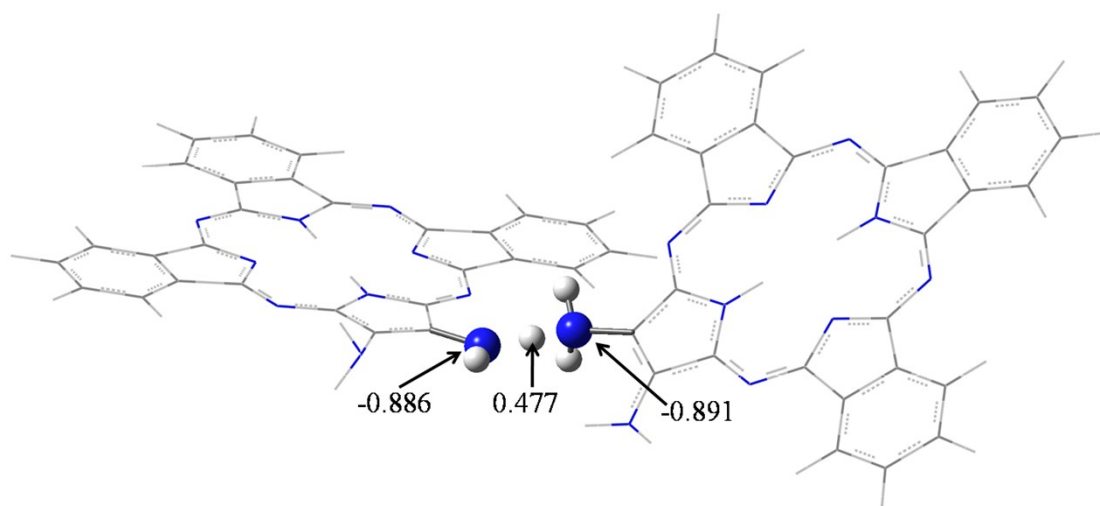


Figure S1. Optimized geometries of TS2 with NPA charge (q).

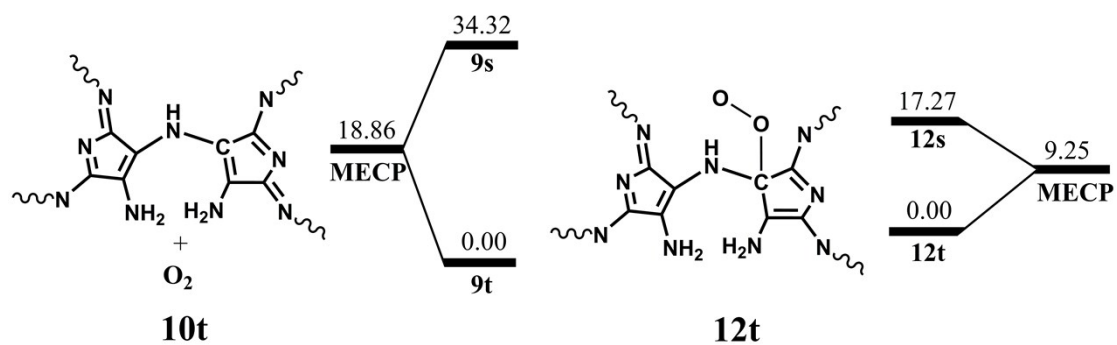


Figure S2. The minimum-energy crossing points (MECP) were identified by using the method of Harvey et al.^{S9, S10} M06-2X-D3/6-31+g(d,p) SCF energies were used to draw the energy profile. Energies are relative to **10t** and **12t**, respectively.

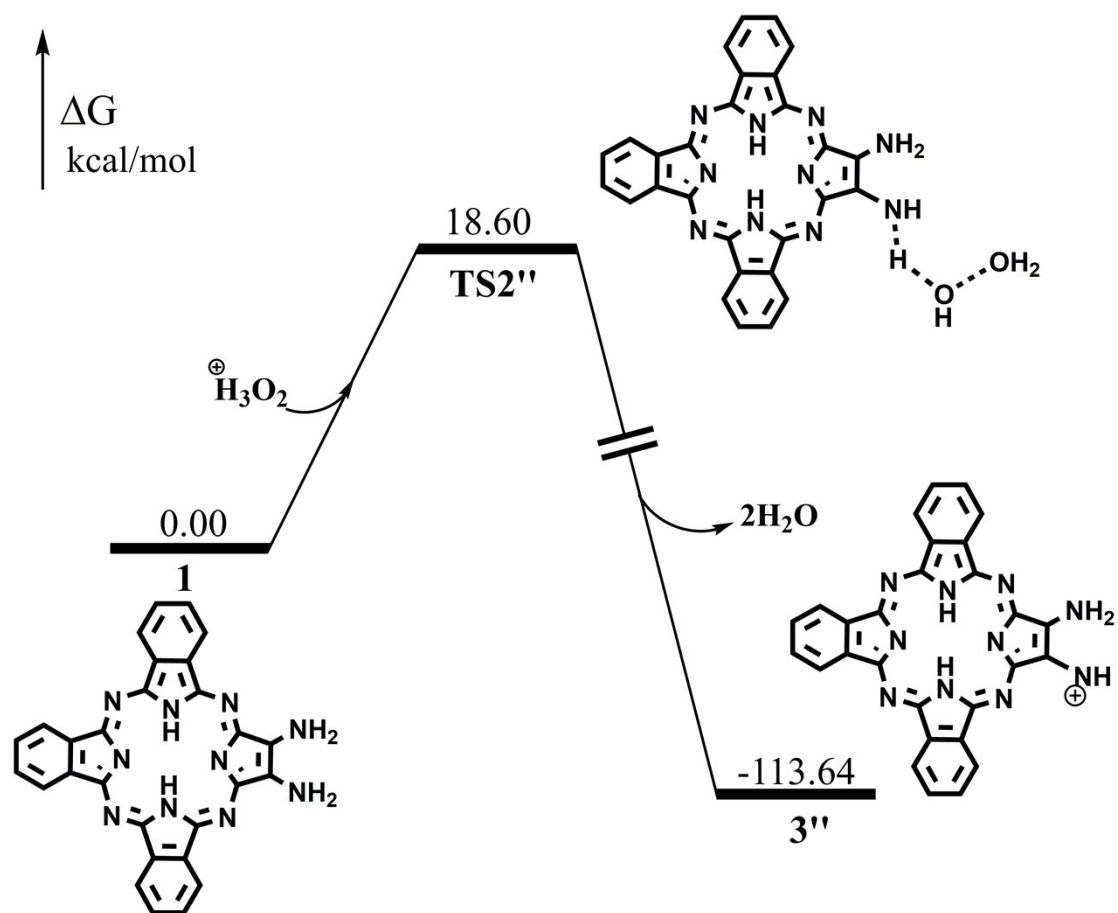


Figure S3. Free energy profile for the decomposition of the protonated H_2O_2 , along with the relative free energies.

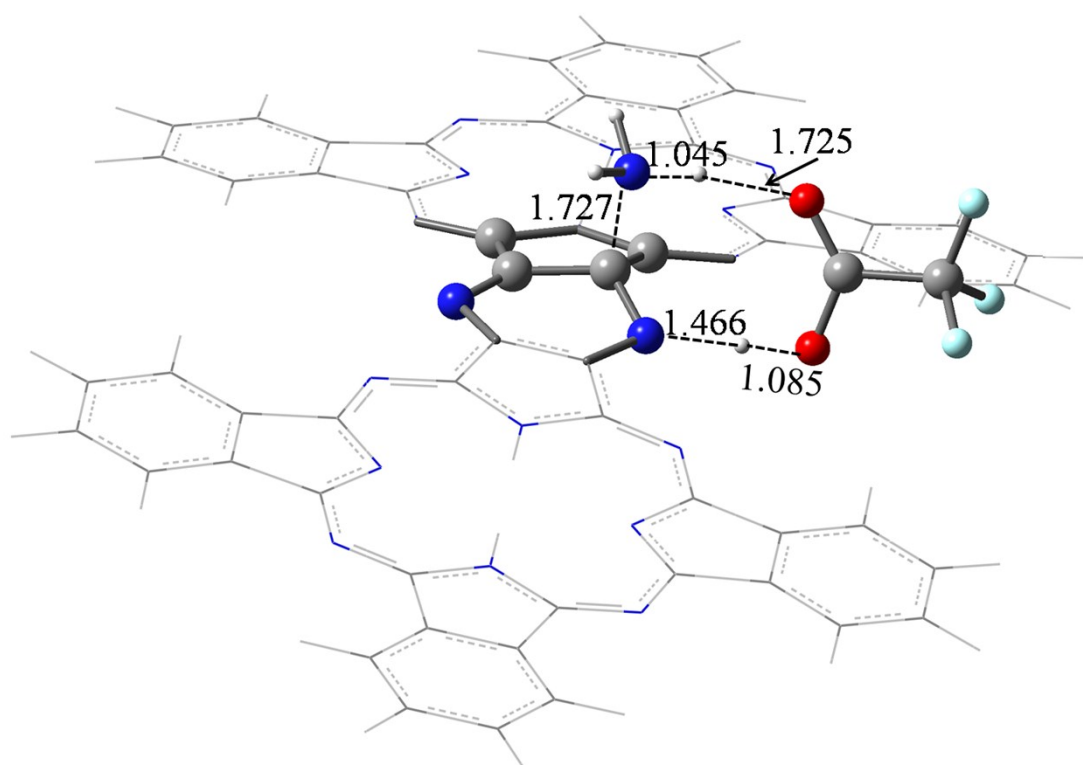


Figure S4. Optimized geometry of TS22. Key bond lengths are given in angstroms.

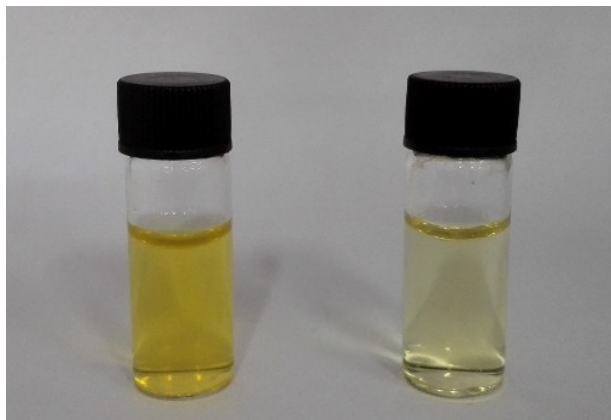


Figure S5. Photographs of Nessler's reagent with (left) and without (right) adding the 0.1 ml the aqueous solution combined during the synthesis procedure of **24-OR** from **1-OR** in mixed solvent of CH_2Cl_2 and TFA in the ratio of 20:80.

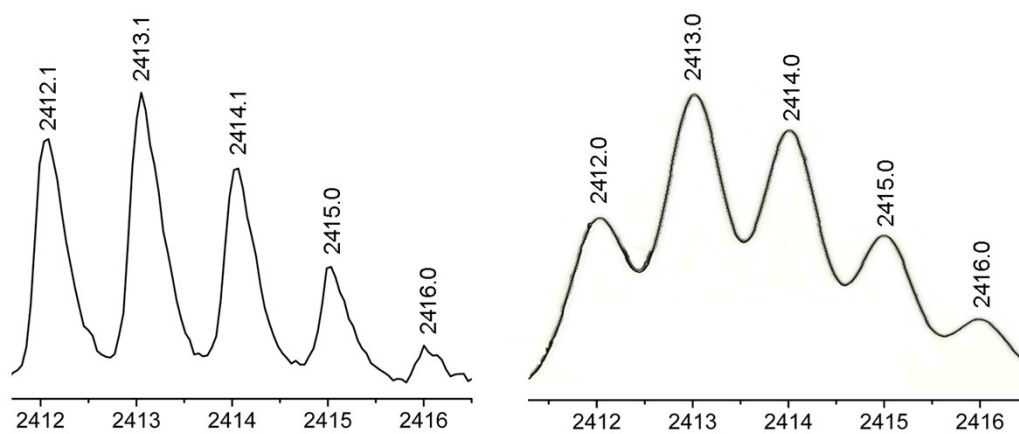


Figure S6. Experimental (left) and simulated isotopic (right) pattern for the molecular ion of **9-OR** shown in the MALDI-TOF mass spectrum.

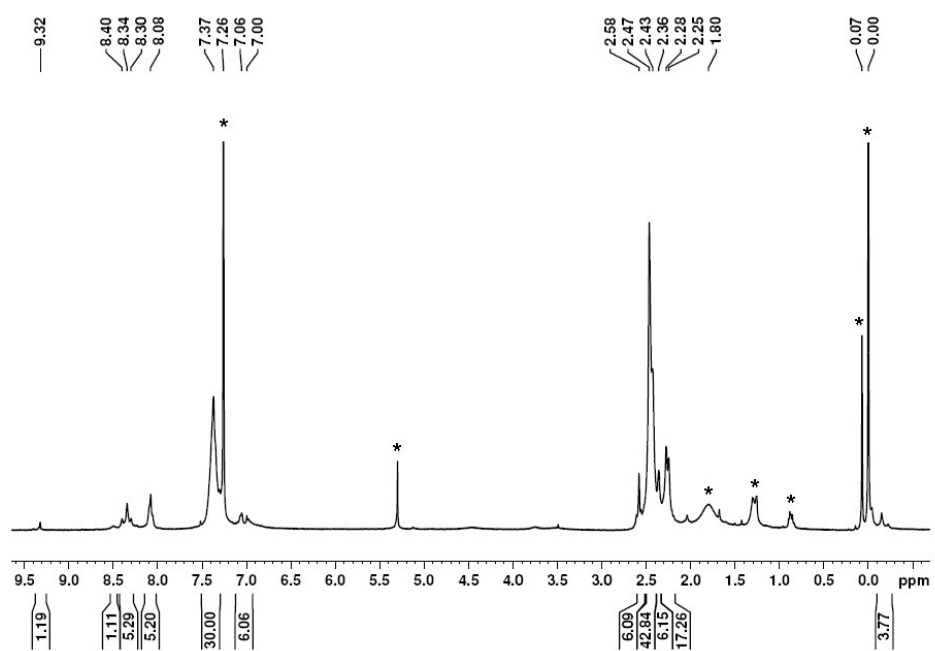


Figure S7. ^1H NMR spectrum of **9-OR** recorded in CDCl_3 . *denotes the solvent impurity and the internal SiMe_4 .

Table S1. The SCF energy on the basis of M06-2X/6-311+G(2d,2p) of different spin states of intermediate **10** and **12**. Energies are given in Hartree.

Intermediate **10**:

Spin state	Singlet	Triplet	Quintet	Septet
SCF energy	-3344.28316881	-3344.33730314	-3344.30424933	-3344.27057885

Intermediate **12**:

Spin state	Singlet	Triplet	Quintet	Septet
SCF energy	-3344.28340384	-3344.29878403	-3344.26562230	-3344.22868317

References

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Cartesian Coordinates (Å), SCF Energies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures.

All energies are given in Hartree

1

SCF energy in solution: -1625.287087

Free energy in solution: -1624.917362

C	-4.12760405	-0.46874999	0.00000000
C	-4.13280005	-2.65272399	0.00365300
C	-2.07791705	2.60466801	-0.00132700
C	-0.67517705	2.60471201	-0.00105000
C	-2.51822005	1.21494901	-0.00131100
C	-0.23480905	1.21502201	-0.00132900
H	-1.37633705	-0.56200699	-0.00185800
C	2.78964695	-0.85808699	-0.00110300
C	2.79270395	-2.25613999	-0.00279000
C	1.37460295	-0.46863599	-0.00278100
C	1.37975795	-2.65263699	-0.00623900
C	-0.68725005	-5.67568699	-0.00425800
C	-2.06569105	-5.67570699	0.00235500
C	-0.25592305	-4.30386299	-0.01065300
C	-2.49702405	-4.30379799	0.00826400
H	-1.37647405	-2.50734399	-0.00016400
N	1.01000395	-3.92506099	-0.00971300
N	-3.76298905	-3.92518599	0.00741100
N	-3.76593405	0.82187701	-0.00150400
N	1.01292495	0.82198001	-0.00116900
N	-1.37649205	0.45033601	-0.00152400
N	0.56970495	-1.54985799	-0.00592000
N	-1.37649605	-3.51530599	-0.00158400
N	-3.32271305	-1.54998599	0.00327800
N	0.16583695	-6.76668599	-0.06131900
H	1.13650495	-6.49898099	0.05676300
H	-0.09376805	-7.52412599	0.55998800
N	-2.91875605	-6.76661499	0.05937200
H	-2.65988905	-7.52384299	-0.56248700
H	-3.88961305	-6.49889799	-0.05705900
C	-5.54263905	-0.85818499	-0.00199800
C	-5.54570905	-2.25625499	-0.00017100

C	-6.73566205	-2.97672599	0.00033500
C	-7.92510505	-2.25026199	-0.00225900
C	-7.92104905	-0.84562099	-0.00488000
C	-6.72637305	-0.12790599	-0.00451200
H	-6.73123605	-4.06186199	0.00363600
H	-8.87461005	-2.77631999	-0.00181200
H	-8.86717505	-0.31366299	-0.00670600
H	-6.71115505	0.95713601	-0.00578800
C	0.04904795	3.79601001	-0.00082900
C	-0.67255205	4.98345201	-0.00074600
C	-2.08068705	4.98340701	-0.00098800
C	-2.80221505	3.79592001	-0.00124600
H	1.13379795	3.78217101	-0.00066500
H	-0.14460205	5.93162401	-0.00051600
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C	3.98260095	-2.97668199	-0.00355100
C	3.97340395	-0.12784699	0.00101200
C	5.16805295	-0.84561899	0.00115100
H	6.12157395	-2.77632299	-0.00196000
H	3.97807195	-4.06181699	-0.00676100
H	3.95825295	0.95719601	0.00216800
H	6.11419795	-0.31369099	0.00268800

1-ion

SCF energy in solution: -1625.714519

Free energy in solution: -1625.330479

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C	-1.30283664	-1.55639998	-0.00012800
C	-3.35522864	3.74139702	0.00014200
C	-4.75324164	3.75053902	0.00007600
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C	-8.29033064	-1.07372298	-0.00001800
C	-6.81765364	0.67455902	-0.00018800
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C	-4.78890064	-4.46928898	0.00030600
C	-3.39962564	-4.53190998	0.00019900
C	-5.22700464	-3.14561498	0.00023200
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C	2.48667736	-1.09298198	-0.00035300
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H	3.44320836	-1.60530898	-0.00044500
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H	1.22419136	2.09403902	-0.00019200
C	-5.47341464	4.93583502	0.00022700
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C	-10.62186464	0.40407302	-0.00050200
H	-11.62957564	-1.49368098	-0.00020000
H	-9.52812264	-2.84390698	0.00021400
H	-9.35555664	2.17237102	-0.00077000
H	-11.55126564	0.96361802	-0.00068400
H	-4.93870664	-6.45530198	0.00048000

TS2

SCF energy in solution: -3250.5558

Free energy in solution: -3249.794929

C	-6.78385398	-2.65624996	0.00000000
C	-5.89231798	-3.73158196	0.13445400
C	-8.08092198	-3.16171996	0.43188100
C	-6.69873398	-4.83801796	0.65203900
C	-11.56109898	-1.98223296	0.79538800
C	-12.61162498	-2.78829896	1.26918300
C	-10.35645198	-2.78826396	0.79964700
C	-12.05809798	-4.09493896	1.56847000
H	-10.09065098	-4.80988796	1.38848900
C	-12.99828898	-7.41257996	2.82724000
C	-12.10690798	-8.47248596	2.98742100
C	-12.19346298	-6.29641596	2.29849800
C	-10.79388998	-7.96038596	2.54781300
C	-7.34976498	-9.13467096	2.24198600
C	-6.28131998	-8.37375596	1.75362700
C	-8.51557798	-8.33693396	2.19463700
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N	-7.98628198	-4.46888996	0.81378900
N	-1.60006398	-9.33556396	0.01306700
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C	-0.86303298	-3.78786196	2.00661600
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C	5.40356302	-3.63050696	2.57224800
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C	-1.24981198	-8.11867196	0.52538200

C	-2.04029098	-7.02353196	0.81578900
C	0.11135802	-7.72164296	0.79200700
C	-1.20226498	-5.96337396	1.25675200
H	0.89505902	-5.89058496	1.49933400
N	1.16024002	-8.51156696	0.64083500
N	-1.65473598	-4.76331996	1.62070500
N	2.15107702	-2.17723896	2.75132100
N	4.96282402	-5.92134296	1.81429800
N	3.25358302	-4.25259396	2.18608900
N	2.80163102	-6.87514796	1.31833000
N	0.08093702	-6.42050196	1.22705700
N	0.51012802	-3.81758296	2.10012400
N	-7.21676198	-10.47043496	2.69815000
H	-7.53843998	-10.56240196	3.65722400
H	-7.77390298	-11.10758096	2.13621600
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H	-4.82458598	-9.63707496	1.98020500
H	-3.79321298	-6.79245196	-0.23047400
H	-3.79224498	-6.09621796	1.23742600
H	-4.13864198	-7.83478596	1.18837000
C	-13.87354598	-9.84065696	3.79898800
C	-12.52258798	-9.70437796	3.47466800
C	-14.34365498	-7.53863696	3.14756000
C	-14.77024798	-8.77408096	3.63772600
H	-14.24045398	-10.78734696	4.18318300
H	-11.81878598	-10.52156196	3.59500800
H	-15.02775098	-6.70622296	3.01867900
H	-15.81407498	-8.91563296	3.89999900
C	-11.78662098	-0.65483396	0.42017500
C	-13.07955298	-0.16614596	0.53359400
C	-14.13318198	-0.97571596	1.00979500
C	-13.91353798	-2.29308796	1.38238900
H	-10.97084598	-0.04013296	0.05454700
H	-13.29071598	0.86043904	0.25103100
H	-15.13088698	-0.55503496	1.08323400
H	-14.71300298	-2.92793996	1.74978900
C	-4.54519098	-3.58248196	-0.20454100
C	-4.12059298	-2.34199796	-0.66892500
C	-5.01802098	-1.26616196	-0.79635100
C	-6.36090798	-1.41119696	-0.46469000
H	-3.82709198	-4.38801896	-0.09406600
H	-3.07502598	-2.19784896	-0.92428600

H	-4.65135298	-0.31068196	-1.15839800
H	-7.06493098	-0.59065796	-0.55991000
C	-2.66129498	-1.93661096	2.47635000
C	-1.37959698	-2.46682696	2.39593100
C	-0.35895798	-0.38416896	3.12787300
C	-1.64326898	0.15758504	3.20479500
C	-2.77506198	-0.60624896	2.88423000
H	-3.53488398	-2.52852496	2.22247300
H	0.52316802	0.19699504	3.37568900
H	-1.77204198	1.18845204	3.51902000
H	-3.75923598	-0.15373796	2.95266600
C	6.78543502	-3.55082096	2.72007300
C	7.31301902	-2.33683996	3.14909100
C	6.48336902	-1.23492296	3.42270800
C	5.10243202	-1.31699596	3.27486200
H	7.41492902	-4.40800596	2.50630500
H	8.38586102	-2.23460896	3.27637700
H	6.93248002	-0.30485396	3.75549700
H	4.45014202	-0.47552696	3.48277200
C	5.95694302	-8.75469796	1.01516900
C	6.09588702	-10.08011096	0.60900400
C	4.97641802	-10.85426796	0.26049600
C	3.68782102	-10.32639996	0.30838900
H	6.81410402	-8.14689096	1.28586900
H	7.08410002	-10.52606096	0.55923700
H	5.12219802	-11.88338596	-0.05232400
H	2.82019402	-10.91968896	0.03887900

3+4

SCF energy in solution: -3250.565138

Free energy in solution: -3249.804196

C	-1.97657483	0.73643410	0.02587468
C	-2.32754083	-1.41338890	-0.16650832
C	0.46817017	3.46810710	0.55245268
C	1.84461217	3.25974410	0.66853868
C	-0.15648383	2.16564310	0.28152968
C	2.09542917	1.82882810	0.46321168
H	0.74447417	0.27383810	-0.02809532
C	4.79157717	-0.63913090	0.50074368
C	4.62105117	-2.01697190	0.37100368
C	3.43672217	-0.06596690	0.43206468
C	3.16618317	-2.22089090	0.23457868
C	0.69545417	-4.80164090	-0.36044732

C	-0.67975383	-4.63977090	-0.44573232
C	1.29863717	-3.57167790	-0.05327332
C	-0.92827483	-3.27018190	-0.20493632
H	0.40785017	-1.68208990	0.22496768
N	2.63120917	-3.39543090	0.08113068
N	-2.14612083	-2.69600390	-0.25699132
N	-1.43382283	1.97348110	0.17969668
N	3.26493217	1.27231310	0.54656768
N	0.87118417	1.24998310	0.21409368
N	2.50240517	-0.99956890	0.28480968
N	0.28355617	-2.66861090	0.03796568
N	-1.34717583	-0.42905990	-0.01687932
N	1.44513617	-5.93453690	-0.85444132
H	1.85431217	-5.65461290	-1.75226032
H	2.20060317	-6.19737390	-0.21682732
N	-1.59552683	-5.64676590	-0.82029132
H	-2.42373483	-5.22054890	-1.22884732
H	-1.90504483	-6.18630890	-0.01528032
C	-3.43880183	0.58214410	-0.07860532
C	-3.66190083	-0.79000490	-0.20446032
C	-4.94449783	-1.30404190	-0.32577732
C	-6.00345983	-0.39242090	-0.31598732
C	-5.77739983	0.98420410	-0.18887032
C	-4.48276383	1.49507710	-0.07012232
H	-5.11276783	-2.37170490	-0.42378832
H	-7.02259583	-0.75520890	-0.40845332
H	-6.62420783	1.66348110	-0.18948232
H	-4.29109883	2.55966410	0.01658268
C	2.72081417	4.30772710	0.91918868
C	2.16807717	5.58020710	1.05215768
C	0.78472917	5.78751010	0.94043668
C	-0.09028383	4.73150310	0.68893868
H	3.79000717	4.13232010	0.98183568
H	2.81912517	6.43068310	1.22645468
H	0.39339117	6.79534110	1.03682268
H	-1.15991483	4.87823910	0.58387668
C	6.97397717	-2.31286690	0.50356468
C	5.70468817	-2.88153290	0.36959968
C	6.04749817	-0.06393590	0.62558768
C	7.14445717	-0.92804490	0.62728568
H	7.85075017	-2.95317490	0.49290368
H	5.56907417	-3.95190590	0.25346068
H	6.16346017	1.01313710	0.69415668
H	8.14764517	-0.52125490	0.70328468

H	0.81513617	-6.72891190	-0.99640132
C	-0.71907383	2.08254610	-2.92951832
C	-1.04712783	-0.07661790	-3.14842032
C	1.76426617	4.75089710	-2.43916532
C	3.14894017	4.52139310	-2.30313032
C	1.12189817	3.46664410	-2.60453232
C	3.36600917	3.09778110	-2.38511432
H	1.95082917	1.53665710	-2.66928532
C	6.02708517	0.57355810	-2.55132932
C	5.80127517	-0.79940690	-2.72841032
C	4.70395317	1.18482510	-2.48792932
C	4.34898117	-0.95730790	-2.75817132
C	1.82948217	-3.66255390	-3.13350432
C	0.45349817	-3.38029790	-3.30796632
C	2.49269917	-2.32878090	-2.98928132
C	0.27577017	-1.99963890	-3.18541932
H	1.66259817	-0.38702790	-2.95840532
N	3.77825517	-2.18269990	-2.89643232
N	-0.90804883	-1.38344390	-3.25513132
N	-0.18630083	3.28353310	-2.76827032
N	4.53325617	2.49202110	-2.35517532
N	2.11135317	2.53140110	-2.55882832
N	3.72637317	0.22410810	-2.62436332
N	1.51233017	-1.38326890	-2.97606732
N	-0.09136883	0.87807610	-2.93850232
N	2.42345717	-4.83313990	-3.01896432
H	3.42861017	-4.67094290	-2.92208432
N	-0.56736383	-4.28440690	-3.61679232
H	-1.48041283	-3.86277690	-3.47898832
H	-0.50011383	-5.17200590	-3.13325432
C	-2.17146783	1.91869510	-3.12749432
C	-2.37971583	0.54713810	-3.26679232
C	-3.65054183	0.02203110	-3.46926132
C	-4.71315383	0.92309610	-3.52968532
C	-4.50191083	2.30443310	-3.39502832
C	-3.22382583	2.82393210	-3.18919932
H	-3.80047583	-1.04883990	-3.56690832
H	-5.72327483	0.55294310	-3.67667932
H	-5.35332783	2.97673010	-3.44649332
H	-3.04671683	3.88921510	-3.08025832
C	4.03638317	5.59000810	-2.12340032
C	3.50704217	6.87019310	-2.08857332
C	2.11947317	7.09936610	-2.23346632
C	1.23649117	6.04657810	-2.40901332

H	5.10121617	5.40695210	-2.02073532
H	4.16989017	7.71999410	-1.95545332
H	1.74606017	8.11840810	-2.20753132
H	0.16799217	6.20341810	-2.51947632
C	8.15129517	-1.18850690	-2.77688132
C	6.85837117	-1.69951390	-2.84545832
C	7.32147017	1.08690310	-2.48125632
C	8.37867117	0.18832210	-2.59432532
H	9.00091517	-1.85881390	-2.86654732
H	6.66930017	-2.75970190	-2.98393232
H	7.48908217	2.15127010	-2.34820732
H	9.40039117	0.55385510	-2.54891832

TS5

SCF energy in solution: -3250.502572

Free energy in solution: -3249.740674

C	-0.32299742	0.32296973	0.00422789
C	-1.59749342	-1.55827527	-0.21374011
C	0.47146158	-0.86830927	-0.28963111
C	-3.85597042	-4.45640927	-0.50311611
C	-2.69161442	-3.60265427	-0.49229311
C	-1.99119342	-5.70865827	-1.00580211
H	-0.66540642	-4.08018227	-0.87078511
C	0.88621858	-7.83328527	-1.86429611
C	2.19844458	-7.37122227	-1.97173011
C	0.08020758	-6.65750727	-1.49209411
C	2.14110858	-5.93256227	-1.65531511
C	4.38197858	-3.05616827	-1.35876511
C	3.97507158	-1.87096127	-0.73997011
C	3.25099958	-3.91209727	-1.32794011
C	2.51976158	-1.88342227	-0.65088711
H	1.20827858	-3.52088027	-0.87445111
N	3.24576258	-5.19237327	-1.67254411
N	1.82017358	-0.81561627	-0.40284311
N	-2.68625142	-2.30901127	-0.23934811
N	-1.22546342	-6.74690627	-1.32470111
N	-1.61849642	-4.41272027	-0.79865511
N	0.87170558	-5.55025227	-1.37270511
N	2.15828858	-3.17741227	-0.87554711
N	-0.29888042	-1.95897827	-0.41634011
N	4.35419358	-4.87041027	1.86345389
N	4.29165558	-1.93802227	1.26063689
C	9.82047058	0.38767673	-1.18221911

C	8.51611058	0.46762273	-0.67938211
C	10.26619058	-0.97945527	-0.90279111
C	8.23451358	-0.85760927	-0.12432411
C	13.23901558	-3.11380727	-1.38148711
C	11.90557758	-2.62469327	-1.06339411
C	11.97253458	-4.84004627	-0.52057911
H	10.24289558	-3.65842427	-0.26123611
C	10.05661258	-7.70809827	0.72489689
C	8.72593058	-7.64681627	1.14728089
C	10.41534958	-6.33257627	0.35627989
C	8.34036158	-6.23566527	1.02991689
C	5.41267358	-4.08823727	1.50700289
C	5.41082958	-2.70059927	1.33993789
C	6.74830458	-4.55727227	1.27819389
C	6.74631758	-2.34340227	0.91026389
H	8.50919958	-3.50821427	0.70277089
N	7.11993458	-5.82152227	1.33993489
N	7.05176558	-1.14995227	0.42434089
N	11.48725658	-1.39791527	-1.24934311
N	11.63020258	-6.04057627	-0.12179911
N	11.21146258	-3.69848927	-0.55543811
N	9.38193958	-5.48700327	0.55598289
N	7.52747958	-3.46445727	0.93315389
N	9.29740458	-1.68715727	-0.27362411
N	5.66777558	-3.28182327	-1.90853211
H	5.59465358	-3.84893027	-2.74779511
H	6.30355958	-3.76551227	-1.27641511
H	4.40479558	-5.84293427	1.59302289
H	3.44819758	-4.43250527	1.75312389
N	4.67427858	-0.60857827	-0.98199111
H	4.92113158	-0.52864527	-1.97449311
H	4.04038958	0.15517873	-0.71390711
H	4.50075058	-0.96224027	1.47998989
H	5.57573458	-0.58949627	-0.41691811
C	-5.20885742	-4.18633727	-0.26442411
C	-3.42285242	-5.75976827	-0.81825311
C	-4.32817742	-6.82387227	-0.90426311
C	-5.66483442	-6.55011927	-0.66789311
C	-6.09993542	-5.24292327	-0.35095011
H	-5.53380942	-3.18023327	-0.02119411
H	-3.98026442	-7.82216827	-1.14819911
H	-6.39613042	-7.34996427	-0.72549311
H	-7.15635842	-5.06890027	-0.17218111
C	-1.04168342	2.54181873	0.48881289

C	0.00199058	1.66002173	0.22255989
C	-1.65055942	-0.12173727	0.05565589
C	-2.69677842	0.75824673	0.32260589
C	-2.37445742	2.09535173	0.53769689
H	-0.82782742	3.59141273	0.66462289
H	1.03295658	1.99790473	0.18872789
H	-3.72212642	0.40488773	0.36104789
H	-3.16360142	2.81006873	0.74951589
C	14.35271958	-2.46591127	-1.91613911
C	15.50366158	-3.22073027	-2.10292011
C	15.54593758	-4.58759527	-1.76470211
C	14.43752258	-5.23300827	-1.23158211
C	13.28166258	-4.47542027	-1.04426511
H	14.30860358	-1.41259527	-2.17188211
H	16.39051158	-2.75198527	-2.51711911
H	16.46432558	-5.14302827	-1.92506211
H	14.45665458	-6.28472927	-0.96632011
C	8.39096758	2.74634873	-1.36947911
C	9.69553658	2.65955273	-1.88505811
C	10.42991658	1.47950473	-1.79385211
C	7.78612858	1.65214873	-0.75551711
H	7.85317058	3.68620973	-1.44374911
H	10.13768258	3.53277073	-2.35387511
H	11.44160958	1.40581573	-2.17927511
H	6.79038558	1.73259373	-0.32726211
C	3.24522258	-8.22059527	-2.30728111
C	2.93133858	-9.56065127	-2.53839011
C	1.61148758	-10.02534127	-2.43319511
C	0.56601858	-9.16551827	-2.09336011
H	4.26218158	-7.84903427	-2.38306811
H	3.71934258	-10.25849227	-2.80366611
H	1.40345558	-11.07430627	-2.61981411
H	-0.45777442	-9.51492527	-2.00785611
C	10.75838858	-8.90829027	0.70468189
C	10.08094058	-10.05159127	1.12636289
C	8.74386358	-9.99005527	1.55148189
C	8.04499158	-8.78383327	1.56871389
H	11.79117858	-8.94493227	0.37385789
H	10.59293958	-11.00865227	1.12793789
H	8.24839258	-10.90083327	1.87263289
H	7.01221258	-8.72656727	1.89670689

6

SCF energy in solution: -3250.54801

Free energy in solution: -3249.783845

C	-0.16795866	0.50387596	0.00000000
C	2.00783034	0.64570396	-0.09137900
C	-1.77267666	-1.05168004	-0.69546300
C	-1.65456666	-3.04739604	-1.79229000
H	0.05515434	-1.91961604	-1.35666500
C	0.08516634	-4.32842404	-2.65558500
C	2.27787034	-4.17821904	-2.74806200
C	5.20250934	-2.23318304	-1.90539000
C	5.19517934	-0.98329604	-1.09677300
C	3.92198334	-2.70520404	-1.96940600
C	3.71060634	-0.74019704	-0.84497000
H	2.03864534	-1.92738704	-1.28890200
N	3.53341334	-3.81702604	-2.63542700
N	3.34084134	0.38282196	-0.33175900
N	-1.41177166	0.07722096	-0.12733400
N	-1.19626366	-4.12947804	-2.43851700
N	-0.95142066	-2.00444004	-1.29154800
N	1.14820234	-3.55640804	-2.29296500
N	3.04633734	-1.83209004	-1.27343500
N	0.98928034	-0.14848304	-0.40410900
N	6.79124234	-3.57670304	1.48732100
N	5.89896034	-1.02025304	0.15173500
C	10.82978034	1.96407096	-3.00402800
C	11.56931734	0.81082796	-2.47030700
C	9.52434034	0.57741296	-1.74873100
C	13.56757834	-0.36608104	-2.28648300
C	14.17082434	-2.30542404	-1.24815500
H	12.19912734	-1.54515904	-1.19420600
C	13.00961934	-5.13223004	0.77308600
C	11.69764034	-5.30181204	1.22666300
C	13.00571734	-3.87217004	0.02501000
C	10.96104734	-4.13493604	0.73546800
C	7.57009134	-2.72808704	0.78692800
C	7.21104134	-1.53319204	0.18153800
C	8.98697534	-2.92160104	0.55712700
C	8.38477134	-0.99825304	-0.43690600
H	10.36908734	-1.72170304	-0.50619100
N	9.66815434	-3.96441304	0.97984200
N	8.42765334	0.12044696	-1.16549400
N	12.86927534	0.65106896	-2.73261800
N	14.12416434	-3.41074004	-0.55830100
N	13.14920634	-1.42087704	-1.52108500

N	11.78281434	-3.30500804	0.02174700
N	9.42188034	-1.84677804	-0.17927500
N	10.76741634	0.01508496	-1.73133100
N	6.33677934	-2.65952504	-2.63901900
H	6.03085334	-3.25955104	-3.40108100
H	6.99237434	-3.19673904	-2.07432600
H	7.16365134	-4.48634704	1.71515000
H	5.78964334	-3.47086004	1.40865200
N	5.70559734	0.22872496	-1.92154100
H	6.74017834	0.34593296	-1.76529800
H	5.51158434	0.08456496	-2.91490500
H	5.18941434	1.04938896	-1.57627700
H	5.68166434	-0.24173404	0.76917700
C	15.36000034	-1.76631604	-1.89828000
C	16.66902434	-2.23998204	-1.95429500
C	17.59155834	-1.48395304	-2.66875200
C	17.21863434	-0.28791904	-3.31008100
C	15.91240334	0.18413496	-3.25365700
C	14.98855934	-0.57444004	-2.53735200
H	16.94500534	-3.16319804	-1.45615300
H	18.62132334	-1.81957704	-2.73579900
H	17.96835234	0.27343196	-3.85801700
H	15.61186734	1.10427696	-3.74324800
C	9.52096734	1.81935696	-2.53779700
C	8.54274234	2.76004196	-2.83880400
C	8.91274234	3.84351096	-3.63584400
C	10.22565134	3.98036396	-4.11037300
C	11.20745434	3.04038696	-3.79681800
H	7.53018534	2.67158096	-2.45648800
H	8.17544934	4.59810196	-3.89004600
H	10.47865334	4.83667996	-4.72691700
H	12.22813934	3.13935996	-4.15120400
C	12.32352634	-7.34585604	2.26995800
C	13.64120334	-7.17501704	1.81323400
C	14.00412134	-6.06297804	1.05637800
C	11.33125934	-6.41061504	1.98346700
H	12.07756534	-8.22465004	2.85747100
H	14.38677834	-7.92501604	2.05707600
H	15.01876834	-5.92121704	0.69896200
H	10.31243334	-6.53685504	2.33470800
C	0.17030034	1.78012896	0.60520000
C	1.57203134	1.87606496	0.54355600
C	2.24626334	2.99324196	1.04393600
C	1.48587934	4.01242296	1.60256400

C	0.07990834	3.91811696	1.66232900
C	-0.59184766	2.80759696	1.16762500
H	3.32962434	3.05714196	0.99976900
H	1.97569334	4.89503196	2.00227800
H	-0.48464166	4.73239896	2.10657300
H	-1.67356566	2.73007596	1.21239200
C	0.62184034	-7.57763704	-4.59777400
C	2.01852934	-7.48181704	-4.66112500
C	2.69424234	-6.40193404	-4.08669900
C	1.92659134	-5.43327004	-3.45737400
C	0.54004534	-5.52937904	-3.39349900
C	-0.14160266	-6.59721704	-3.95902300
H	0.12790634	-8.43015604	-5.05382900
H	2.58137934	-8.26161004	-5.16499400
H	3.77551434	-6.31658304	-4.12630800
H	-1.22351866	-6.65847704	-3.90139500
C	-5.48896166	-1.76625004	-0.71808800
C	-5.41537266	-3.00578004	-1.39777500
C	-4.19825866	-3.52600504	-1.79978200
C	-3.04422666	-2.78524304	-1.51157700
C	-3.11551166	-1.54886604	-0.83416500
C	-4.35396966	-1.02927304	-0.42979500
H	-6.46185266	-1.38907104	-0.41757500
H	-6.33084366	-3.55127204	-1.60346300
H	-4.12231766	-4.47446404	-2.32166600
H	-4.40584766	-0.07905904	0.09145000

TS7

SCF energy in solution: -3250.533605

Free energy in solution: -3249.768877

C	-0.89147288	-0.78811368	0.00000000
C	-2.27856288	-0.66829468	-0.18047300
C	-0.31902488	0.45989832	-0.48484200
C	-2.47484788	0.64820732	-0.76695000
C	1.54947412	1.80610032	-0.89901000
C	1.82219112	3.89061632	-1.77697000
H	-0.06901188	3.01231032	-1.56109200
C	0.15014212	6.84076832	-3.20633000
C	-1.22847688	6.96749232	-3.35732300
C	0.36699312	5.51262332	-2.59463600
C	-1.80718588	5.71055632	-2.82966400
C	-5.06373488	4.19346132	-2.33236300
C	-5.26601788	2.78896532	-1.97177400

C	-3.69639788	4.41456432	-2.36200000
C	-3.89247088	2.28424832	-1.59213000
H	-2.01913688	3.23069232	-1.75853600
N	-3.11550088	5.53309232	-2.82597300
N	-3.72446788	1.10935332	-1.09284800
N	0.98039312	0.69946532	-0.47214400
N	1.58045512	5.08967632	-2.32100800
N	0.93158812	2.92590432	-1.43640700
N	-0.82684788	4.87762232	-2.39082800
N	-3.01460988	3.26322632	-1.93628200
N	-1.32268688	1.29761732	-0.93939900
N	-6.89251288	5.14119032	0.03580200
N	-6.28455788	2.34274032	-1.16710800
C	-12.24243188	0.43069532	-2.58574700
C	-10.10088088	0.71256132	-2.25702800
C	-15.62293088	1.88830932	-2.29418700
C	-15.87797988	3.16444232	-1.77261700
C	-14.18023288	1.67278132	-2.24610800
C	-14.59540688	3.75130432	-1.39661500
H	-12.64612288	2.94592732	-1.55480900
C	-13.11037188	6.77830532	0.03867000
C	-11.74194688	6.96790432	0.25794300
C	-13.23271088	5.43681032	-0.53902600
C	-11.09808388	5.73283332	-0.19614100
C	-7.75974688	4.24415132	-0.49315500
C	-7.51816588	2.99170832	-1.03977400
C	-9.18940188	4.45672732	-0.54900400
C	-8.77551888	2.42249132	-1.40330600
H	-10.73962088	3.18281532	-1.21616600
N	-9.78565288	5.55905232	-0.13999400
N	-8.92398288	1.21421832	-1.93759000
N	-13.57219288	0.58633132	-2.65138700
N	-14.43430688	4.93462532	-0.87456500
N	-13.63757088	2.81006132	-1.70708800
N	-12.03099688	4.84424932	-0.66477000
N	-9.74955888	3.32514432	-1.08328900
N	-11.33145688	1.30451032	-2.12060100
N	-6.00966288	4.91354132	-3.11350400
H	-5.51813888	5.64774532	-3.61921200
H	-6.73449788	5.35830032	-2.55457500
H	-7.25620988	6.05161832	0.27698700
H	-5.90728588	5.05485432	-0.17964700
N	-5.47176088	2.06077632	-3.59396700
H	-5.66802888	1.06138632	-3.60082400

H	-6.21455588	2.60965432	-4.03232200
H	-4.57495788	2.28054732	-4.02414900
H	-6.17351588	1.40939632	-0.78518900
C	-1.79800288	8.10753432	-3.90610700
C	-0.93131288	9.12749332	-4.30602900
C	0.45636612	8.99899932	-4.15519200
C	1.01992412	7.84789032	-3.59987300
H	-2.87408588	8.19629932	-4.01569000
H	-1.33560988	10.03651132	-4.74042800
H	1.10148512	9.81098232	-4.47613900
H	2.09222312	7.73624032	-3.47632200
C	4.40313112	3.95489632	-1.58161600
C	3.13065212	3.38439332	-1.44500200
C	2.96061512	2.09385932	-0.90037200
C	4.06814312	1.34475132	-0.47920700
C	5.32170212	1.91448132	-0.61714600
C	5.49067012	3.20889832	-1.16370800
H	4.51519712	4.94882332	-2.00230600
H	3.93257812	0.35302432	-0.06060500
H	6.19932012	1.35963432	-0.29986400
H	6.49205812	3.61753532	-1.25362200
C	-1.20555888	-2.96897268	0.91126900
C	-2.59781588	-2.84731368	0.73102500
C	-3.15081688	-1.69590068	0.18345800
C	-0.33737888	-1.94533868	0.55004800
H	-0.80742688	-3.88230468	1.34276400
H	-3.24429088	-3.66726468	1.02800300
H	-4.22274388	-1.59307468	0.04465700
H	0.73560512	-2.03295368	0.68775300
C	-14.04200588	7.76128332	0.35827400
C	-13.55825588	8.94652632	0.90772600
C	-12.18384888	9.13765032	1.12914500
C	-11.25507088	8.15031932	0.80731000
H	-15.10117788	7.60261432	0.18377700
H	-14.25181788	9.73851332	1.17169800
H	-11.84301788	10.07371232	1.56014300
H	-10.19284688	8.29195632	0.97786800
C	-16.65529588	1.06869632	-2.74530600
C	-17.95052788	1.56646132	-2.65804400
C	-18.20680388	2.84716632	-2.13435200
C	-17.17536488	3.66401232	-1.68428500
H	-16.44354988	0.08325432	-3.14636400
H	-18.78246288	0.95888932	-2.99905600
H	-19.23142588	3.20084132	-2.08216500

H	-17.36039788	4.65280832	-1.27834500
C	-12.11090788	-1.98238068	-3.60225500
C	-11.60584388	-0.80934468	-3.05463200
C	-10.23705788	-0.62992068	-2.84268300
C	-9.31919888	-1.62229068	-3.16532700
C	-9.81849988	-2.80309068	-3.71536000
C	-11.19372088	-2.98025568	-3.93208800
H	-13.17664788	-2.10964668	-3.76154200
H	-8.25785588	-1.48259568	-2.98654400
H	-9.13393788	-3.60314368	-3.97875800
H	-11.54605588	-3.91282668	-4.36104800

8

SCF energy in solution: -3250.580725

Free energy in solution: -3249.834828

C	0.14211887	1.95090436	0.00000000
C	1.52561787	2.07429236	0.15476100
C	-0.43428213	3.11759136	0.67942300
C	1.72714087	3.30175736	0.93578400
C	-2.31456313	4.35137836	1.28054500
C	-2.61729513	6.32330436	2.38892000
H	-0.70732313	5.49210836	2.04110400
C	-0.95795413	9.12576836	4.07020800
C	0.42491187	9.24445236	4.23776000
C	-1.15955213	7.86075436	3.35519100
C	0.99940487	8.04577936	3.61769200
C	4.26823487	6.49179336	3.05318500
C	4.46513187	5.29195136	2.38082900
C	2.85143787	6.76026636	3.04559600
C	3.16703287	4.81215436	1.97180000
H	1.23824987	5.62561136	2.27519400
N	2.30702687	7.82822636	3.59645800
N	2.94030387	3.70146836	1.28856400
N	-1.75858813	3.31199736	0.71057500
N	-2.39013713	7.43819136	3.03345300
N	-1.70908213	5.40253036	1.92319300
N	0.01551987	7.24802236	3.10247700
N	2.23443987	5.71650636	2.40781300
N	0.52805087	3.89507036	1.21844400
N	6.08173487	7.29808336	0.50446700
N	5.65707787	4.63656436	2.13478600
C	11.73737787	3.09810036	3.39954900
C	9.57197687	3.29172736	3.18800400

C	15.03636587	4.60855736	2.71357400
C	15.20864687	5.82943436	2.04318400
C	13.60577787	4.34634536	2.78850800
C	13.88598887	6.33190536	1.69786700
H	11.98426287	5.49089236	2.06718600
C	12.20058487	9.14707036	0.05991200
C	10.81506587	9.26749236	-0.08260800
C	12.41424387	7.87874736	0.76658300
C	10.24987187	8.06701736	0.54375000
C	6.99205887	6.51776136	1.18093600
C	6.81682887	5.32010736	1.86178200
C	8.40835187	6.78408036	1.14944800
C	8.12789587	4.83733036	2.22888700
H	10.04693087	5.65596736	1.87373500
N	8.94094687	7.85339036	0.58885400
N	8.35215587	3.71487636	2.88204700
N	13.05982087	3.29676836	3.35049100
N	13.64749187	7.45387436	1.06558300
N	12.98804887	5.40479636	2.16747400
N	11.24104187	7.26703236	1.03734500
N	9.04751287	5.74264036	1.76951700
N	10.76462287	3.89148936	2.90010800
N	5.16312887	7.27568736	3.73244100
H	4.82305587	8.19705436	3.97384400
H	6.13528287	7.22374436	3.46068600
H	6.43386587	8.21385836	0.25590100
H	5.12702587	7.28787636	0.83706500
N	5.12737187	1.82270736	2.56811400
H	5.72181087	1.13719836	2.11327100
H	4.89665887	1.47112236	3.49162200
H	4.26406387	1.91114236	2.03587700
H	5.69779487	3.62287436	2.33245900
C	0.98348187	10.34017036	4.88824300
C	0.11026987	11.31617536	5.36465500
C	-1.27917513	11.19664536	5.19490700
C	-1.83434513	10.09660036	4.54402700
H	2.05748387	10.42506636	5.01794900
H	0.50744187	12.18620336	5.87800900
H	-1.92825413	11.97682236	5.57979800
H	-2.90598413	9.99334736	4.40823800
C	-5.20925413	6.34179936	2.23367900
C	-3.93417413	5.82067736	2.01820700
C	-3.74803613	4.60843536	1.33702500
C	-4.83068413	3.87792036	0.84898100

C	-6.10158313	4.39688436	1.06406200
C	-6.28843313	5.61363336	1.74788800
H	-5.33974813	7.28045736	2.76162800
H	-4.67311113	2.94205136	0.32347700
H	-6.96972813	3.85732136	0.69950200
H	-7.29679013	5.98644436	1.89617700
C	0.45240387	-0.05495664	-1.23992900
C	1.84330187	0.07296436	-1.09321200
C	2.40082787	1.14288536	-0.39484500
C	-0.42007313	0.88693436	-0.69706900
H	0.05418987	-0.90044564	-1.79182700
H	2.49339787	-0.67354164	-1.53845600
H	3.47609287	1.25689136	-0.29627000
H	-1.49583713	0.80262836	-0.81156900
C	13.06883387	10.11913636	-0.42596800
C	12.50300387	11.22200136	-1.06301400
C	11.11093387	11.34312036	-1.20766800
C	10.24579087	10.36581436	-0.71908000
H	14.14265087	10.01452136	-0.30969600
H	13.14583187	12.00304436	-1.45664600
H	10.70527487	12.21515336	-1.71095500
H	9.16964587	10.45138036	-0.82929300
C	16.12957587	3.87622136	3.17631100
C	17.39500687	4.40148736	2.94771100
C	17.56788287	5.62689736	2.27463000
C	16.47946487	6.35665136	1.81396100
H	15.98297487	2.93385036	3.69335300
H	18.27036687	3.86056536	3.29262300
H	18.57279987	6.00439836	2.11505300
H	16.59887287	7.30149536	1.29442900
C	11.74042587	0.82196036	4.70340800
C	11.17111887	1.91152536	4.05207500
C	9.78544987	2.03881236	3.91949600
C	8.91566487	1.08374636	4.43540800
C	9.48060787	-0.01000064	5.08866600
C	10.87361287	-0.13950564	5.21990300
H	12.81736487	0.73210936	4.80186200
H	7.84136287	1.20100736	4.33269000
H	8.83693087	-0.77717464	5.50773900
H	11.27801387	-1.00472964	5.73571200

9s

SCF energy in solution: -3194.017272

Free energy in solution: -3193.294444

C	0.24486268	1.79456514	-0.07050403
C	1.63326968	1.74949314	-0.21746503
C	-0.26415032	0.61615214	-0.78550603
C	1.90751168	0.54720414	-1.01670203
C	-3.61175632	-2.18570186	-2.29926703
C	-2.07293132	-0.68241786	-1.46349303
C	-2.26870232	-2.60436586	-2.67920203
H	-0.40420632	-1.70350786	-2.25473103
C	-0.46078432	-5.21454586	-4.51077603
C	0.92926968	-5.26391986	-4.65785703
C	-0.72845532	-4.01457386	-3.71253103
C	1.44079568	-4.09267286	-3.94114803
C	4.63126768	-2.45711786	-3.17109003
C	4.74732368	-1.28313986	-2.44221603
C	3.22274068	-2.78216386	-3.22851103
C	3.42490168	-0.87824186	-2.05296503
H	1.54178968	-1.75198586	-2.46133703
N	2.73977568	-3.82493086	-3.87054003
N	3.14223568	0.20492814	-1.34580803
N	-1.57583832	0.35750514	-0.83935303
N	-1.98076432	-3.66573486	-3.38523303
N	-1.41056832	-1.66776686	-2.14931903
N	0.41616168	-3.37462786	-3.39225103
N	2.54546768	-1.80221186	-2.55221103
N	0.74216968	-0.09797486	-1.33128503
N	6.28444968	-3.23203186	-0.49279803
N	5.90971168	-0.60179486	-2.08814303
C	11.98843868	0.65700614	-3.70676803
C	9.83004968	0.56969914	-3.38368503
C	15.26179168	-0.93375686	-3.07672703
C	15.42451568	-2.11096786	-2.33146403
C	13.83768368	-0.62340686	-3.10417403
C	14.10247768	-2.53984486	-1.89144803
H	12.21410968	-1.65641586	-2.23550303
C	12.40418968	-5.16081186	0.02889497
C	11.02285868	-5.22397886	0.23649097
C	12.62400968	-3.96148586	-0.78684003
C	10.46683668	-4.06127886	-0.46338403
C	7.23572368	-2.45799786	-1.10371903
C	7.08165968	-1.28960886	-1.83286203
C	8.64253568	-2.77125486	-1.10308603
C	8.38372468	-0.87461086	-2.27591003
H	10.28779668	-1.73974386	-1.94600503

N	9.16543768	-3.80870586	-0.47756303
N	8.61549468	0.20942914	-2.99791303
N	13.30496668	0.40855014	-3.70797203
N	13.85783568	-3.60196486	-1.16953303
N	13.21432068	-1.61361986	-2.38567603
N	11.46154568	-3.33567286	-1.06030903
N	9.28962568	-1.79238286	-1.81314303
N	11.01331868	-0.06478086	-3.11843703
N	5.58769668	-3.23516786	-3.74655703
H	5.25176168	-3.95642386	-4.36886703
H	6.47996268	-2.81993686	-3.96531203
H	6.65697568	-3.92509086	0.14270997
H	5.45778068	-2.75238186	-0.16467303
H	5.99675268	0.37325514	-2.34297503
C	11.43946968	1.82903914	-4.40004203
C	10.05814168	1.77242214	-4.19417003
C	9.20761368	2.73954214	-4.71922403
C	9.78776768	3.76906714	-5.45876403
C	11.17587868	3.82561314	-5.66480403
C	12.02395068	2.85336314	-5.13686403
H	8.13591968	2.68843614	-4.55660403
H	9.15777568	4.54332714	-5.88521603
H	11.59164268	4.64248414	-6.24617903
H	13.09773968	2.88687314	-5.28974103
C	17.77501968	-2.01102386	-2.68281203
C	16.68562468	-2.66763286	-2.12329703
C	16.35453968	-0.27463486	-3.63809303
C	17.61164668	-0.82928986	-3.43086803
H	18.77314068	-2.41338786	-2.54266603
H	16.79801368	-3.57847586	-1.54487003
H	16.21485068	0.63521914	-4.21211703
H	18.48710868	-0.34558686	-3.85199603
C	12.69339868	-7.14933786	1.30149197
C	11.30546168	-7.21417886	1.50944097
C	10.44908568	-6.25138986	0.97880097
C	13.26364968	-6.11935986	0.55601997
H	13.32914168	-7.91753086	1.73025797
H	10.89611168	-8.03163886	2.09466097
H	9.37600268	-6.29630786	1.13372397
H	14.33409268	-6.05980186	0.38826197
C	-0.37870432	2.81403814	0.63982797
C	0.43919368	3.79346614	1.20220297
C	1.83486968	3.74784114	1.05523297
C	2.45423268	2.72214114	0.34173397

H	-1.45817632	2.83897614	0.74766997
H	-0.00724732	4.60729814	1.76481197
H	2.44000368	4.52716514	1.50769297
H	3.53206068	2.67658314	0.22408297
C	-3.49136632	-1.00445186	-1.55179203
C	-4.85860032	-2.75310586	-2.55958603
C	-5.97616532	-2.10345686	-2.05021403
C	-5.85512132	-0.91766186	-1.30007703
C	-4.61283632	-0.35221986	-1.04074103
H	-4.93891132	-3.66680886	-3.13884803
H	-6.96403232	-2.51455586	-2.23179903
H	-6.75195032	-0.43980286	-0.91921603
H	-4.50523832	0.56067814	-0.46461503
C	0.72339368	-7.26370286	-5.93118703
C	-0.67328732	-7.21282486	-5.78382503
C	-1.28612132	-6.18561486	-5.06979203
C	1.54535868	-6.28933986	-5.36935303
H	1.16630768	-8.07971886	-6.49353203
H	-1.28154432	-7.99014186	-6.23545103
H	-2.36343832	-6.13704386	-4.94895503
H	2.62455268	-6.32377686	-5.47760303

9t

SCF energy in solution: -3194.01032097

Free energy in solution: -3193.26129709

C	0.70769229	1.26153844	0.00000000
C	2.09536729	1.07907644	-0.12154500
C	0.10860829	0.08206344	-0.59994800
C	2.26123229	-0.20037156	-0.79035300
C	-3.47311571	-2.56089956	-1.89586600
C	-1.80342871	-1.11584256	-1.18047600
C	-2.15510371	-3.13528056	-2.22441100
H	-0.21970171	-2.35388656	-1.85825500
C	-0.56541071	-6.03724756	-3.77469700
C	0.82304529	-6.20838356	-3.90613400
C	-0.73713971	-4.75774356	-3.10738200
C	1.41508129	-5.02314656	-3.31058900
C	4.76274629	-3.57631956	-2.67178600
C	4.96961329	-2.39771756	-2.01739700
C	3.29791129	-3.79783156	-2.72278600
C	3.66314229	-1.83068756	-1.67324100
H	1.70648429	-2.57083656	-2.04822600
N	2.76940929	-4.84650756	-3.25828900

N	3.50113729	-0.69793556	-1.07204600
N	-1.24461671	-0.07906656	-0.65416200
N	-1.97635471	-4.26744256	-2.81905600
N	-1.21788171	-2.22514956	-1.77019400
N	0.46208629	-4.17858856	-2.84399400
N	2.70144329	-2.71341056	-2.13073600
N	1.06020629	-0.76991156	-1.06177000
N	6.72071229	-4.49123756	-0.32483200
N	6.14297729	-1.73768756	-1.68225700
C	12.06543029	0.12543844	-3.19690600
C	9.92451329	-0.16429556	-2.88095500
C	15.46160429	-1.25694256	-2.74062800
C	15.72390929	-2.48431056	-2.11516500
C	14.01671429	-1.05661756	-2.72953800
C	14.44374629	-3.05533756	-1.71094200
H	12.48910029	-2.29114856	-1.95323700
C	12.98011029	-5.97234256	-0.04154800
C	11.61118129	-6.16548956	0.16571500
C	13.09391529	-4.68826156	-0.74350400
C	10.95531129	-4.99157256	-0.42212300
C	7.60652229	-3.59156356	-0.88965900
C	7.34843329	-2.38152456	-1.51585700
C	9.02877429	-3.79526856	-0.93471800
C	8.61160629	-1.82540656	-1.92500800
H	10.57636129	-2.57689056	-1.70872900
N	9.64064229	-4.84325256	-0.40812700
N	8.74784529	-0.65862756	-2.53101500
N	13.39912329	-0.01701756	-3.22599900
N	14.29266529	-4.19791456	-1.09447800
N	13.48082629	-2.15814156	-2.10649800
N	11.88429529	-4.13568456	-0.95372600
N	9.58797129	-2.71117256	-1.55943600
N	11.15767329	-0.72789056	-2.68494400
N	5.60003929	-4.44158456	-3.31280500
H	5.17039029	-5.33581856	-3.51897600
H	6.54813529	-4.50151656	-2.96538500
H	7.18579029	-5.18647456	0.24705300
H	5.92231229	-4.07083056	0.13392400
H	6.17216329	-0.73613756	-1.82980600
C	11.42002829	1.31571244	-3.76400600
C	10.04945029	1.12959244	-3.56198000
C	9.12014829	2.07493844	-3.98276500
C	9.61057429	3.21769244	-4.61279400
C	10.98783229	3.40472044	-4.81469900

C	11.91502029	2.45338444	-4.39218400
H	8.05734129	1.92221844	-3.82572100
H	8.91745629	3.97915544	-4.95621000
H	11.33220829	4.30721044	-5.30967500
H	12.98115629	2.58705044	-4.54379400
C	18.05470529	-2.16926556	-2.46839900
C	17.02582129	-2.95969756	-1.96954300
C	16.49256629	-0.46384656	-3.24112900
C	17.79141629	-0.93711956	-3.09602900
H	19.08238629	-2.50498956	-2.37412700
H	17.21509929	-3.91106956	-1.48386700
H	16.27602529	0.48375944	-3.72274600
H	18.62152029	-0.34823756	-3.47270300
C	13.44361229	-8.03841756	1.04115500
C	12.06833629	-8.23377056	1.24922600
C	11.13080629	-7.29885756	0.81345800
C	13.92025929	-6.90162156	0.39073700
H	14.14409429	-8.78855256	1.39425900
H	11.73302729	-9.13136456	1.75926800
H	10.06689529	-7.44427656	0.96996600
H	14.98028129	-6.74026656	0.22397800
C	0.17867929	2.40075444	0.60240800
C	1.07795029	3.35220844	1.07993500
C	2.46685329	3.16869044	0.95935400
C	2.99519229	2.02843644	0.35692100
H	-0.89445271	2.53487144	0.69266300
H	0.70299329	4.25319044	1.55517400
H	3.13662829	3.93106644	1.34447000
H	4.06581229	1.87797244	0.26199000
C	-3.25922571	-1.33423356	-1.26197800
C	-4.75174171	-3.04695756	-2.12114900
C	-5.82295571	-2.26092456	-1.68802600
C	-5.60875871	-1.03201956	-1.05286000
C	-4.31666271	-0.54866256	-0.82981000
H	-4.90175671	-4.00120056	-2.61506000
H	-6.83923871	-2.60717156	-1.84595200
H	-6.46268271	-0.44592156	-0.72881300
H	-4.13529671	0.40187044	-0.33930400
C	0.46252929	-8.30320856	-4.98194600
C	-0.92660371	-8.13203856	-4.84949900
C	-1.46008271	-6.99565856	-4.24403700
C	1.35695729	-7.34321456	-4.51223200
H	0.84180329	-9.20067856	-5.46027400
H	-1.59265471	-8.90102756	-5.22783400

H	-2.53101871	-6.85516756	-4.13880500
H	2.43010229	-7.46904956	-4.61343000

10s

SCF energy in solution: -3344.283169

Free energy in solution: -3343.554448

C	1.53733598	-0.19379845	0.02012475
C	3.25386398	-1.11972445	-1.16793325
C	1.29345498	-1.60000445	-0.33665925
C	6.28437498	-3.64999145	-3.56518025
C	4.88927998	-2.24480645	-2.38004525
C	5.06642098	-4.36528445	-3.20504825
H	3.37847898	-3.69368445	-2.12173825
C	3.66417398	-6.22741145	-3.16495025
C	1.69375298	-6.71054245	-2.36330425
C	-1.18259902	-5.47096345	-0.44801225
C	-1.25340702	-4.19013345	0.09729075
C	0.08363198	-5.56314045	-1.14645225
C	-0.08275502	-3.48285445	-0.30089925
H	1.62620598	-4.13251745	-1.37039025
N	0.51198798	-6.64277445	-1.75870325
N	0.17636298	-2.21494045	0.01010575
N	4.43962398	-1.16600845	-1.78347125
N	4.80254598	-5.60610745	-3.51046025
N	4.28893098	-3.46894545	-2.50346225
N	2.62764698	-5.71828145	-2.46736025
N	0.71566298	-4.35291845	-0.99317325
N	2.34632998	-2.10950945	-1.04425325
N	-2.65777102	-0.82211545	-0.18488925
N	-2.30887802	-3.69604345	0.88520875
C	-7.89031802	-6.27142645	-1.09490125
C	-5.93657102	-5.76864745	-0.25845025
C	-10.85066502	-5.05967945	-2.93533525
C	-10.99275702	-3.74484545	-3.40287025
C	-9.55818302	-5.15156245	-2.26722925
C	-9.78894502	-3.01253845	-3.02883325
H	-8.07715402	-3.67645845	-1.97966325
C	-8.21456602	0.28730855	-3.27759725
C	-6.95690902	0.60968855	-2.75694425
C	-8.43052602	-1.12098945	-2.93579225
C	-6.47042302	-0.61663545	-2.12108625
C	-3.53358802	-1.85499645	-0.29853725
C	-3.40574902	-3.14665145	0.18137675

C	-4.83258002	-1.76035645	-0.93288025
C	-4.59621802	-3.85984445	-0.16327925
H	-6.32944402	-3.23083345	-1.20093725
N	-5.28907602	-0.67372945	-1.51689825
N	-4.82813402	-5.14464645	0.09648175
N	-9.08022002	-6.23565745	-1.70471625
N	-9.55553702	-1.75720145	-3.29815825
N	-8.98668002	-3.91033745	-2.35851925
N	-7.38339502	-1.62595445	-2.25159125
N	-5.42536102	-2.99193145	-0.82142325
N	-7.00777902	-5.26343945	-0.94405425
N	-2.07970402	-6.46246145	-0.34801225
H	-3.01055002	-6.23980945	-0.00378925
H	-1.92236902	-7.30691745	-0.87682125
H	-1.67678802	-1.07012545	-0.07320625
H	-2.86126502	-0.01236945	-0.75485925
H	-1.97183402	-3.08003345	1.61912175
O	1.52340098	-5.14728645	1.45411675
O	0.39357698	-5.31666045	1.85436975
C	2.33212998	-10.13171045	-3.91493625
C	3.60242898	-9.82087445	-4.43009325
C	4.16390598	-8.55872245	-4.25167425
C	3.41745698	-7.62074045	-3.54430825
C	2.15306098	-7.92949045	-3.03140625
C	1.58888498	-9.18990945	-3.20745525
H	1.92637698	-11.12599945	-4.07318525
H	4.15243598	-10.58101845	-4.97586225
H	5.14385698	-8.30845345	-4.64486725
H	0.60816998	-9.42336745	-2.80597125
C	7.41406498	-4.05874245	-4.27223625
C	8.42684298	-3.12485545	-4.45517725
C	8.31688298	-1.81626345	-3.94705825
C	7.19060198	-1.40890745	-3.24256325
C	6.17506498	-2.34631445	-3.05904525
H	7.48729898	-5.06965145	-4.65885125
H	9.32234398	-3.40585545	-5.00009625
H	9.12953798	-1.11596445	-4.11082125
H	7.09263098	-0.40413845	-2.84549725
C	1.35884498	2.01868155	0.87603275
C	0.80058798	0.74849655	0.72885975
C	2.79028998	0.11410855	-0.51471325
C	3.35310398	1.37614355	-0.36997925
C	2.61548498	2.32843255	0.33374175
H	0.81524898	2.78204355	1.42362475

H	-0.16553702	0.50341655	1.16035675
H	4.32804798	1.60268955	-0.78898125
H	3.01895198	3.32675955	0.46982375
C	-6.42092802	1.88654155	-2.89883625
C	-7.18530802	2.83043155	-3.58072925
C	-8.44864602	2.50563955	-4.10412225
C	-8.98201002	1.22704055	-3.95960025
H	-5.44526202	2.13084655	-2.49151325
H	-6.80156402	3.83724355	-3.71241325
H	-9.01542102	3.26777055	-4.62955025
H	-9.95632002	0.96566955	-4.35951525
C	-12.98600202	-5.61226445	-3.82508025
C	-11.84605102	-6.01411345	-3.13946125
C	-12.13612602	-3.34149045	-4.09067825
C	-13.12882502	-4.29253845	-4.29449825
H	-13.78377102	-6.32582345	-4.00404625
H	-11.72284802	-7.02740045	-2.77216125
H	-12.23476702	-2.32180345	-4.44747225
H	-14.03399802	-4.01642045	-4.82574725
C	-7.16491602	-9.74470945	0.30490775
C	-5.91571302	-9.41945845	0.85548175
C	-5.38829302	-8.13268645	0.74300475
C	-6.14769802	-7.18979645	0.05923875
C	-7.39443802	-7.51247045	-0.48104825
C	-7.92665802	-8.79134445	-0.37088025
H	-7.54403202	-10.75582945	0.41381575
H	-5.35409202	-10.18367945	1.38331375
H	-4.43071102	-7.87444445	1.18564875
H	-8.89690102	-9.02954745	-0.79430925

10t

SCF energy in solution: -3344.337303

Free energy in solution: -3343.608762

C	-1.66666669	-0.94315244	0.00000000
C	0.04029631	-1.87669044	-1.19589600
C	-1.91201369	-2.35276344	-0.34181500
C	3.03933231	-4.42594144	-3.61206800
C	1.66265931	-3.01316244	-2.41605200
C	1.82883231	-5.13860844	-3.22896200
H	0.15828731	-4.46207344	-2.12265700
C	0.42858731	-7.00142244	-3.15856600
C	-1.52795269	-7.47788144	-2.31804600
C	-4.36640569	-6.23380244	-0.34221600

C	-4.44330969	-4.95075444	0.16806300
C	-3.12024069	-6.32219844	-1.08524200
C	-3.28422869	-4.23842644	-0.26727400
H	-1.60896169	-4.87540244	-1.39688500
N	-2.69758869	-7.41059044	-1.68483300
N	-3.02458269	-2.96751944	0.02804900
N	1.21781631	-1.92907544	-1.82207100
N	1.55937031	-6.38303544	-3.52330100
N	1.06215031	-4.23902844	-2.52080000
N	-0.59958269	-6.48703044	-2.44700900
N	-2.51237869	-5.09529644	-1.00532600
N	-0.86688369	-2.86771144	-1.05232800
N	-5.84798769	-1.55948544	-0.10518600
N	-5.49311569	-4.43812144	0.96041200
C	-11.04448069	-7.03534044	-1.06939300
C	-9.10107469	-6.52369544	-0.21401200
C	-13.99372169	-5.83655844	-2.93615200
C	-14.13846369	-4.52168344	-3.40292500
C	-12.70720269	-5.92264244	-2.25611400
C	-12.94235469	-3.78359944	-3.01629200
H	-11.23671869	-4.44001744	-1.95277700
C	-11.38368369	-0.47468544	-3.24361200
C	-10.13310569	-0.14670544	-2.70965000
C	-11.59578669	-1.88473244	-2.90636000
C	-9.64664669	-1.37164344	-2.07088200
C	-6.71907769	-2.59790244	-0.22567600
C	-6.58665669	-3.88945644	0.25153200
C	-8.01365869	-2.50872244	-0.86942000
C	-7.77096469	-4.60874044	-0.10444100
H	-9.50029369	-3.98670044	-1.15329300
N	-8.47084669	-1.42329244	-1.45528400
N	-7.99880169	-5.89451344	0.15188900
N	-12.22876069	-7.00478544	-1.69037700
N	-12.71341069	-2.52619344	-3.28108900
N	-12.14157369	-4.67804944	-2.34019100
N	-10.55280769	-2.38528644	-2.21226100
N	-8.60040769	-3.74368744	-0.76661600
N	-10.16798069	-6.02336344	-0.90977500
N	-5.23512769	-7.25565644	-0.18217600
H	-6.17805569	-7.01288344	0.11233100
H	-5.11024369	-8.06137144	-0.77769200
H	-4.86534269	-1.80986544	-0.01349200
H	-6.05584469	-0.75307144	-0.67876600
H	-5.14881069	-3.80230944	1.67344600

O	-1.27531069	-5.16661444	1.76458700
O	-1.68204869	-6.28976744	1.66203900
C	-0.91538369	-10.91300544	-3.84923000
C	0.34491831	-10.60598944	-4.39069300
C	0.90896531	-9.34209044	-4.23415100
C	0.17532931	-8.39786044	-3.52161300
C	-1.07912369	-8.70296144	-2.98250100
C	-1.64595669	-9.96507844	-3.13671500
H	-1.32339769	-11.90881944	-3.99115500
H	0.88505831	-11.37061144	-4.94008300
H	1.88110731	-9.09498544	-4.64818500
H	-2.61916169	-10.19481744	-2.71526500
C	4.15877331	-4.83818844	-4.33461400
C	5.16733331	-3.90523844	-4.53958500
C	5.06427531	-2.59270644	-4.03834900
C	3.94940831	-2.18141144	-3.31932400
C	2.93692531	-3.11834344	-3.11261400
H	4.22663731	-5.85144444	-4.71606500
H	6.05436331	-4.18902144	-5.09679600
H	5.87370931	-1.89303544	-4.21988800
H	3.85691631	-1.17384344	-2.92804900
C	-1.84068069	1.27691956	0.83778600
C	-2.39784569	0.00457756	0.70779900
C	-0.41962769	-0.63785444	-0.55053700
C	0.14181031	0.62688356	-0.42309200
C	-0.59026869	1.58406956	0.27943000
H	-2.38015569	2.04425156	1.38391000
H	-3.35919769	-0.23769444	1.15147700
H	1.11174131	0.85162656	-0.85454400
H	-0.18759369	2.58450456	0.40177500
C	-9.60229369	1.13310556	-2.84397500
C	-10.36451569	2.07423256	-3.53211400
C	-11.62072969	1.74380356	-4.06892700
C	-12.14893969	0.46223056	-3.93190000
H	-8.63209069	1.38164256	-2.42628700
H	-9.98461169	3.08321256	-3.65827800
H	-12.18603769	2.50387856	-4.59891700
H	-13.11771769	0.19647256	-4.34223600
C	-16.11771569	-6.39899044	-3.84682900
C	-14.98218669	-6.79587244	-3.15118400
C	-15.27757969	-4.12330544	-4.10079500
C	-16.26319069	-5.07919844	-4.31547700
H	-16.90996169	-7.11648244	-4.03443800
H	-14.85704569	-7.80909344	-2.78434300

H	-15.37828469	-3.10354444	-4.45681600
H	-17.16480269	-4.80702144	-4.85476600
C	-10.31704869	-10.50576844	0.33579600
C	-9.07450169	-10.17518644	0.89823300
C	-8.55171469	-8.88607944	0.79161400
C	-9.30879369	-7.94590344	0.10124200
C	-10.54886869	-8.27408344	-0.45114100
C	-11.07643669	-9.55543444	-0.34670700
H	-10.69262769	-11.51867344	0.44045100
H	-8.51425569	-10.93730944	1.43057200
H	-7.59894869	-8.62470344	1.24267500
H	-12.04147469	-9.79763444	-0.77967200

10-quintet

SCF energy in solution: -3344.30424933

C	0.18461538	1.47692305	0.00000000
C	1.88395938	0.58239105	-1.21770600
C	-0.04226862	0.07864505	-0.33091100
C	4.90460238	-1.93974595	-3.66851500
C	3.51006638	-0.53323095	-2.45975200
C	3.68766438	-2.67581195	-3.27692800
H	2.01380738	-2.01150295	-2.16471200
C	2.30737138	-4.54851695	-3.19887900
C	0.36169738	-5.03569495	-2.35276000
C	-2.49688962	-3.80516995	-0.33705800
C	-2.56988162	-2.55445695	0.20675300
C	-1.22060362	-3.89309295	-1.09979900
C	-1.40517362	-1.81443195	-0.22461400
H	0.28302938	-2.42630595	-1.36933600
N	-0.83348162	-4.96911995	-1.69583100
N	-1.17072062	-0.56773895	0.07482400
N	3.07739538	0.53106905	-1.87476100
N	3.45212438	-3.91057495	-3.57652700
N	2.91295738	-1.78262195	-2.56469500
N	1.27922738	-4.04142095	-2.47727400
N	-0.62102762	-2.66667095	-0.99142000
N	0.98784138	-0.42557995	-1.05415200
N	-3.98033362	0.84375305	-0.04123100
N	-3.62353562	-2.04704095	0.99482600
C	-9.12199562	-4.65672095	-1.14788100
C	-7.19820562	-4.13939295	-0.25207300
C	-12.04941462	-3.45891895	-3.04845400
C	-12.19885962	-2.13863195	-3.49883500

C	-10.77399562	-3.54270895	-2.34856900
C	-11.01672762	-1.39552095	-3.08185800
H	-9.32216562	-2.05121495	-2.00096100
C	-9.48560262	1.93076605	-3.23533500
C	-8.24669062	2.26157405	-2.67659400
C	-9.69079962	0.51421605	-2.92186000
C	-7.76011162	1.03166005	-2.04747600
C	-4.84592562	-0.19510295	-0.17949100
C	-4.71113062	-1.49162395	0.28328700
C	-6.13527162	-0.10705895	-0.83656500
C	-5.88539062	-2.21521095	-0.09634300
H	-7.60767262	-1.59171895	-1.15727700
N	-6.59248962	0.98160205	-1.41485600
N	-6.10518262	-3.50659495	0.13831800
N	-10.29460562	-4.62828295	-1.78907500
N	-10.79514862	-0.13174995	-3.32430500
N	-10.21866862	-2.29207895	-2.40571400
N	-8.65414162	0.01282805	-2.21730600
N	-6.71465162	-1.34725795	-0.75586800
N	-8.25609762	-3.63943995	-0.95970700
N	-3.35087162	-4.83356895	-0.25844500
H	-4.29210062	-4.64556295	0.08049200
H	-3.17056062	-5.64250395	-0.83568600
H	-2.99697362	0.59413405	0.05564100
H	-4.18725162	1.65904105	-0.60228100
H	-3.28312662	-1.42061095	1.71812800
O	1.09941438	-4.42956995	0.82466600
O	0.25062638	-4.06910795	1.59058000
C	0.97373138	-8.45539395	-3.89764100
C	2.23005138	-8.14131995	-4.44415800
C	2.79091938	-6.87504095	-4.28459700
C	2.05967138	-5.93474995	-3.56422600
C	0.80360438	-6.24786295	-3.01826100
C	0.24250838	-7.51292095	-3.17678600
H	0.56836338	-9.45188395	-4.04186900
H	2.77035138	-8.90123495	-4.99972100
H	3.76018538	-6.62373295	-4.70295400
H	-0.72768362	-7.75050595	-2.75258700
C	6.01350438	-2.35058995	-4.39164300
C	7.02390638	-1.40958095	-4.60696300
C	6.91497638	-0.10506995	-4.11082900
C	5.79339238	0.30151905	-3.38326200
C	4.79534238	-0.63785395	-3.17317700
H	6.08245838	-3.36517595	-4.76964700

H	7.90866038	-1.69242495	-5.16803100
H	7.71751438	0.60169405	-4.29567600
H	5.69601938	1.30914905	-2.99319800
C	-0.00751662	3.69991005	0.83857200
C	-0.54575862	2.42015205	0.72103000
C	1.42412838	1.80145305	-0.57705000
C	1.96376538	3.08062005	-0.45815200
C	1.22986338	4.02579405	0.25497100
H	-0.54810362	4.45979405	1.39389400
H	-1.49407662	2.16486605	1.18536900
H	2.92196338	3.32301905	-0.90627500
H	1.61876238	5.03278105	0.36837100
C	-7.72441762	3.54736905	-2.78427500
C	-8.48342062	4.49182305	-3.47148600
C	-9.72794362	4.15863105	-4.03317500
C	-10.24752762	2.87093705	-3.92280900
H	-6.76318162	3.79786105	-2.34748400
H	-8.11001662	5.50553405	-3.57738800
H	-10.29103062	4.92144405	-4.56159600
H	-11.20720862	2.60309105	-4.35268700
C	-14.15280062	-4.02756395	-4.00232500
C	-13.02540862	-4.42401795	-3.29368000
C	-13.33024862	-1.74074895	-4.20979400
C	-14.30295162	-2.70234995	-4.45450700
H	-14.93505762	-4.74946895	-4.21343000
H	-12.89700462	-5.44124095	-2.93924600
H	-13.43470862	-0.71691795	-4.55282600
H	-15.19807462	-2.43077195	-5.00479000
C	-8.39380162	-8.13687095	0.23257800
C	-7.16572162	-7.80265295	0.82398000
C	-6.65138962	-6.50853095	0.74105500
C	-7.40045362	-5.56660195	0.04402600
C	-8.62722262	-5.89845895	-0.53543000
C	-9.14670262	-7.18491095	-0.45462700
H	-8.76368562	-9.15354595	0.31930100
H	-6.61108962	-8.56559795	1.36100700
H	-5.71202962	-6.24457595	1.21803000
H	-10.10146762	-7.42943195	-0.90855200

10-septet

SCF energy in solution: -3344.27057885

C	0.04615385	0.49226550	-0.00644408
C	1.72789285	-0.39306050	-1.25485708

C	-0.18524515	-0.90420950	-0.34322608
C	4.72128585	-2.89753250	-3.75672408
C	3.33897485	-1.49918550	-2.52492008
C	3.51036585	-3.63751150	-3.35411608
H	1.84842785	-2.98139650	-2.21970308
C	2.13415085	-5.51254850	-3.26733408
C	0.19926085	-6.00640650	-2.40104108
C	-2.64175215	-4.78768650	-0.35251008
C	-2.70622615	-3.54093050	0.20497492
C	-1.36850115	-4.87327050	-1.12120208
C	-1.54505015	-2.80027950	-0.22774308
H	0.13307285	-3.40347150	-1.39197708
N	-0.98913915	-5.94329550	-1.73263808
N	-1.30934115	-1.55192950	0.07132092
N	2.91211885	-0.43883150	-1.92847308
N	3.27356585	-4.87146150	-3.65603108
N	2.74243485	-2.74889350	-2.62905708
N	1.11448485	-5.01014850	-2.53133008
N	-0.76310915	-3.65038350	-0.99976908
N	0.83480785	-1.40266350	-1.08465808
N	-4.09539615	-0.16554050	-0.14170208
N	-3.75874815	-3.04403550	0.99923592
C	-9.27506915	-5.61673750	-1.19947408
C	-7.37346215	-5.10228750	-0.26636708
C	-12.18438115	-4.39473850	-3.15617308
C	-12.31839015	-3.07773550	-3.60307008
C	-10.90298115	-4.49788650	-2.43527208
C	-11.12179815	-2.33076350	-3.17219408
H	-9.43376515	-3.00465050	-2.08582908
C	-9.58027515	0.97975150	-3.28227108
C	-8.34221715	1.30056450	-2.70093808
C	-9.79526615	-0.42780750	-2.98635508
C	-7.87843515	0.07064350	-2.08402408
C	-4.95516415	-1.19720450	-0.18947708
C	-4.84168215	-2.46680850	0.30019992
C	-6.28682515	-1.07979650	-0.84601408
C	-6.04169115	-3.19423050	-0.06582808
H	-7.77108415	-2.55981250	-1.13274208
N	-6.68088415	-0.00032850	-1.43091008
N	-6.24634915	-4.46066550	0.14981692
N	-10.45811915	-5.57095450	-1.87572208
N	-10.91583415	-1.07793950	-3.41163008
N	-10.32915715	-3.23549350	-2.49389608
N	-8.76517115	-0.94021050	-2.26904008

N	-6.89127715	-2.30066950	-0.71102208
N	-8.39911515	-4.59845850	-0.99722408
N	-3.50591915	-5.80541250	-0.28329608
H	-4.44405315	-5.61190850	0.06551192
H	-3.33238515	-6.61747650	-0.85813508
H	-3.11278215	-0.37745750	0.02885192
H	-4.33422615	0.65182650	-0.68671708
H	-3.42559215	-2.45666050	1.75673492
O	0.97152685	-5.44923950	0.77371192
O	0.12358985	-5.10705550	1.54891292
C	0.79741485	-9.41782350	-3.96926608
C	2.04697485	-9.09962650	-4.52857108
C	2.60819985	-7.83339250	-4.36936308
C	1.88410285	-6.89765350	-3.63610908
C	0.63488585	-7.21492250	-3.07727208
C	0.07331785	-8.47978150	-3.23546508
H	0.39153085	-10.41405850	-4.11372908
H	2.58172485	-9.85621850	-5.09393708
H	3.57224185	-7.57880850	-4.79768108
H	-0.89172615	-8.72056350	-2.80146908
C	5.82227785	-3.30329850	-4.49466008
C	6.82850385	-2.35963050	-4.71761408
C	6.72324885	-1.05753750	-4.21431608
C	5.60970985	-0.65612150	-3.47173708
C	4.61564985	-1.59807650	-3.25424408
H	5.88845285	-4.31608150	-4.87795208
H	7.70708085	-2.63840750	-5.29028408
H	7.52242485	-0.34862550	-4.40538208
H	5.51538785	0.34954450	-3.07590308
C	-0.13293515	2.70980450	0.85112092
C	-0.67196315	1.43055750	0.73329692
C	1.27649085	0.82156450	-0.60019508
C	1.81743185	2.10024150	-0.48097108
C	1.09472285	3.04040450	0.24970992
H	-0.66443415	3.46528150	1.42103092
H	-1.61117315	1.17147550	1.21377792
H	2.76863085	2.34576550	-0.94211208
H	1.48506485	4.04673050	0.36385292
C	-7.81296915	2.58581850	-2.79222308
C	-8.55796815	3.54093950	-3.48161708
C	-9.79682215	3.21945550	-4.06274408
C	-10.32550015	1.93290950	-3.97105608
H	-6.85626315	2.82928450	-2.34154908
H	-8.17737515	4.55325450	-3.57354708

H	-10.34868815	3.98977350	-4.59198908
H	-11.28075715	1.67567450	-4.41710608
C	-14.28635915	-4.93677250	-4.12744208
C	-13.16107915	-5.34629950	-3.40723008
C	-13.43199915	-2.66333950	-4.31692608
C	-14.42013115	-3.61711550	-4.57509508
H	-15.07235115	-5.65293350	-4.34433708
H	-13.04498315	-6.36522250	-3.05325208
H	-13.52121915	-1.63664850	-4.65602708
H	-15.30727215	-3.33225150	-5.13135908
C	-8.59564515	-9.07937050	0.21607492
C	-7.37631915	-8.74573150	0.83235792
C	-6.85644115	-7.45551350	0.75125192
C	-7.58593015	-6.51024350	0.03213292
C	-8.80806515	-6.84223650	-0.57601608
C	-9.33003315	-8.13147950	-0.49314308
H	-8.97093815	-10.09421150	0.30194292
H	-6.83644615	-9.50744850	1.38588092
H	-5.92565015	-7.19192150	1.24534692
H	-10.27533815	-8.37949150	-0.96495608

TS11s

SCF energy in solution: -3344.27422

Free energy in solution: -3343.5437

C	-0.68475453	3.03617567	0.00000000
C	0.92038247	2.15563267	-1.36315400
C	-0.93934153	1.63676367	-0.35377400
C	3.72828147	-0.33474133	-4.05098300
C	2.43799847	1.05313467	-2.74397500
C	2.54393947	-1.04729533	-3.61346300
H	0.93772347	-0.39338233	-2.40938800
C	1.15604047	-2.91600933	-3.49569400
C	-0.74059053	-3.40995533	-2.54090100
C	-3.47967253	-2.22168133	-0.41271400
C	-3.41580553	-1.01998133	0.37772500
C	-2.22938153	-2.31153533	-1.13975500
C	-2.28720353	-0.24788333	-0.19104100
H	-0.64215553	-0.93394033	-1.30657800
N	-1.88179153	-3.35461733	-1.84388600
N	-2.03020853	0.99551467	0.09913100
N	2.03047347	2.11999867	-2.08513500
N	2.24819547	-2.29220433	-3.92078100
N	1.82422547	-0.16791733	-2.84447600

N	0.17898147	-2.42771733	-2.67940500
N	-1.56004253	-1.13235733	-0.92183500
N	0.02235947	1.14508367	-1.15790600
N	-4.71877853	2.44516967	-0.08725500
N	-4.55308853	-0.47000533	0.99332500
C	-10.08837553	-2.78681333	-1.37204400
C	-8.17076353	-2.37263233	-0.41392400
C	-12.85337453	-1.45154833	-3.41832800
C	-12.90197653	-0.13415733	-3.89761900
C	-11.61807353	-1.59745233	-2.65836800
C	-11.69661453	0.54530467	-3.43860000
H	-10.09784453	-0.18764033	-2.26492500
C	-9.96503053	3.77192167	-3.57162100
C	-8.73284653	4.03977967	-2.96629700
C	-10.26272753	2.37331267	-3.25236500
C	-8.34215953	2.79190867	-2.30664400
C	-5.59165953	1.43035767	-0.29201900
C	-5.53880753	0.12449067	0.17376700
C	-6.83597653	1.57424767	-1.02218300
C	-6.73728553	-0.53404133	-0.25157300
H	-8.36330153	0.16298967	-1.40891800
N	-7.20802753	2.68238967	-1.62430300
N	-7.05417753	-1.80215933	0.00261900
N	-11.23083553	-2.69924133	-2.06056700
N	-11.38773453	1.78747767	-3.69146000
N	-10.98598953	-0.38397733	-2.71005100
N	-9.28562053	1.82201167	-2.50309900
N	-7.47996553	0.36592267	-0.96395900
N	-9.16722253	-1.82177233	-1.17085100
N	-4.44077153	-3.12193833	-0.42802700
H	-5.34877753	-2.89676033	-0.01551300
H	-4.29274153	-3.98298933	-0.93669200
H	-3.75489753	2.18527367	0.11027300
H	-4.87279653	3.27848467	-0.63851700
H	-4.29772753	0.07689967	1.81070800
O	-2.65808653	-1.87048833	1.61310200
O	-1.36361553	-1.71294933	1.68193900
C	-0.28890753	-6.77875833	-4.26421000
C	0.93537447	-6.46146633	-4.87578600
C	1.52779347	-5.21210033	-4.70194400
C	0.85882447	-4.29452233	-3.89871900
C	-0.35983553	-4.60967833	-3.29078900
C	-0.95519653	-5.85561533	-3.46079900
H	-0.71981853	-7.76241533	-4.42169700

H	1.42635747	-7.20649433	-5.49383000
H	2.47326047	-4.95755833	-5.16957300
H	-1.89963253	-6.09443733	-2.98290300
C	4.80438347	-0.73492433	-4.84722300
C	5.80284147	0.19669267	-5.08866000
C	5.73656247	1.49971167	-4.55051800
C	4.67046347	1.89966467	-3.75914200
C	3.66185947	0.96356767	-3.51509900
H	4.84507447	-1.73972933	-5.25406300
H	6.65495647	-0.07722333	-5.70237200
H	6.53916847	2.19880367	-4.76230700
H	4.60963447	2.89780967	-3.33866900
C	-0.80572153	5.23065167	0.91192200
C	-1.35848553	3.95588267	0.79826500
C	0.50773347	3.36940167	-0.64975600
C	1.06441247	4.63853267	-0.53700500
C	0.38730147	5.56729867	0.25204300
H	-1.30018153	5.97607467	1.52650100
H	-2.26957353	3.68861967	1.32570300
H	1.99139847	4.88679167	-1.04344300
H	0.79008747	6.56862967	0.36652200
C	-8.13540053	5.29306767	-3.06570900
C	-8.81258353	6.26973467	-3.79242300
C	-10.05059153	5.99965867	-4.40040800
C	-10.64554353	4.74436567	-4.29835500
H	-7.17958453	5.49559067	-2.59361900
H	-8.37899853	7.25969267	-3.89316600
H	-10.54865153	6.78617767	-4.95842900
H	-11.60099653	4.52509167	-4.76365700
C	-14.94102453	-1.91286533	-4.45977200
C	-13.87293153	-2.36181233	-3.69239900
C	-13.97295453	0.31634567	-4.66754500
C	-14.98997253	-0.59065533	-4.94096000
H	-15.75495753	-2.59097933	-4.69478000
H	-13.82253953	-3.37768833	-3.31525200
H	-13.99967153	1.33737467	-5.03293700
H	-15.84098053	-0.27721433	-5.53699400
C	-9.63228953	-6.27477133	0.10368200
C	-8.40819853	-6.00502433	0.73454400
C	-7.81065453	-4.74731833	0.64597100
C	-8.47379053	-3.77717033	-0.09714600
C	-9.69664853	-4.04399133	-0.71674200
C	-10.29865153	-5.29331733	-0.63049100
H	-10.06842453	-7.26422133	0.19639500

H	-7.92296353	-6.78876633	1.30742300
H	-6.87531453	-4.53085633	1.15399000
H	-11.24965553	-5.48850633	-1.11509300

TS11t

SCF energy in solution: -3344.289664

Free energy in solution: -3343.563084

C	0.58139536	1.07235141	0.00000000
C	2.05553336	0.22517841	-1.51994200
C	0.25725736	-0.29502559	-0.40448500
C	4.55102336	-2.17276359	-4.58140400
C	3.42462036	-0.83335559	-3.07914100
C	3.36735636	-2.87343959	-4.10112400
H	1.89362736	-2.24948659	-2.72618200
C	1.89842836	-4.67859059	-4.01238500
C	0.05192936	-5.17317959	-2.95582600
C	-2.43973764	-4.05092459	-0.54376900
C	-2.31173564	-2.87886859	0.28845300
C	-1.27987464	-4.13403359	-1.35417100
C	-1.14213364	-2.14529759	-0.27455800
H	0.33708636	-2.77691159	-1.62838400
N	-1.01647164	-5.13501859	-2.17155000
N	-0.81955764	-0.93407259	0.09118000
N	3.11646236	0.19543141	-2.32916000
N	2.99807536	-4.07227559	-4.47810400
N	2.75118736	-2.02585159	-3.21531900
N	1.01999536	-4.21639159	-3.09636000
N	-0.52968064	-2.97833259	-1.14675900
N	1.14585436	-0.76747959	-1.30483700
N	-3.43048764	0.64219441	-0.28704000
N	-3.43361464	-2.24473759	0.86514700
C	-9.01054864	-4.34910959	-1.62428900
C	-7.10585464	-4.00755859	-0.61271500
C	-11.62911764	-2.93559059	-3.80665500
C	-11.59048764	-1.63339259	-4.32644300
C	-10.43044864	-3.12214859	-2.99817700
C	-10.36712964	-1.00360059	-3.84390700
H	-8.85184564	-1.78241259	-2.59142100
C	-8.46433264	2.12370041	-4.00545200
C	-7.24178964	2.34576241	-3.36323400
C	-8.84537864	0.75194841	-3.65895700
C	-6.93931064	1.09908941	-2.65673400
C	-4.33551264	-0.34176259	-0.50885000

C	-4.36359764	-1.63614659	-0.01095200
C	-5.54230864	-0.15814859	-1.28981000
C	-5.57892064	-2.24620259	-0.45916800
H	-7.12345664	-1.50281259	-1.69597300
N	-5.83708464	0.95143641	-1.93150500
N	-5.97565464	-3.48421759	-0.17354600
N	-10.12385664	-4.22299559	-2.35449900
N	-9.98435464	0.21229441	-4.12149700
N	-9.73301064	-1.94548259	-3.06291400
N	-7.92474164	0.17318541	-2.86107100
N	-6.24643764	-1.33167559	-1.22600600
N	-8.04546464	-3.42922659	-1.42178100
N	-3.40849364	-4.97787859	-0.44646600
H	-4.30908664	-4.68175859	-0.07057500
H	-3.39652364	-5.72262959	-1.13035700
H	-2.48809164	0.35691541	-0.03473600
H	-3.52791464	1.47005941	-0.85888500
H	-3.14796964	-1.62749159	1.62173200
O	-1.64391764	-3.48911359	1.81520700
O	-0.53025764	-4.05691259	1.69503300
C	0.22676936	-8.40350459	-4.97394600
C	1.41641636	-8.08625659	-5.64984100
C	2.07569536	-6.87943759	-5.42231800
C	1.50817436	-6.00647459	-4.50054200
C	0.32419636	-6.32082859	-3.82834100
C	-0.33725364	-7.52389159	-4.05124500
H	-0.25926064	-9.35285059	-5.17578200
H	1.82667036	-8.79648259	-6.36077000
H	2.99539636	-6.62356759	-5.93820400
H	-1.25486564	-7.76309759	-3.52375600
C	5.53830236	-2.55728959	-5.48771900
C	6.55809036	-1.65001259	-5.74664100
C	6.59241536	-0.39037859	-5.11737600
C	5.60881436	-0.00707159	-4.21429300
C	4.58443336	-0.91752659	-3.95441200
H	5.49966136	-3.53078359	-5.96488900
H	7.34521436	-1.91275059	-6.44601100
H	7.40559836	0.29134541	-5.34503200
H	5.62520336	0.96008741	-3.72320400
C	0.58774736	3.22324341	1.02041900
C	-0.00924464	1.97177941	0.88471100
C	1.73620736	1.40652841	-0.71811400
C	2.33651836	2.65497241	-0.58214500
C	1.74415336	3.56000441	0.29602500

H	0.15763036	3.95145041	1.70063700
H	-0.89406064	1.70397741	1.45501000
H	3.23205736	2.90512141	-1.14159000
H	2.18331436	4.54359541	0.42939000
C	-6.57697664	3.56368741	-3.47439800
C	-7.17682964	4.55240841	-4.25090400
C	-8.40515264	4.32838441	-4.89609400
C	-9.06763464	3.10834241	-4.78217400
H	-5.62882964	3.73051341	-2.97373900
H	-6.68911064	5.51569341	-4.36233700
H	-8.84172264	5.12292441	-5.49291100
H	-10.01635364	2.92472341	-5.27585800
C	-13.70062364	-3.32025759	-4.90952500
C	-12.68544764	-3.79963159	-4.09038100
C	-12.60830264	-1.15240159	-5.14827000
C	-13.66207864	-2.01334459	-5.43157300
H	-14.54082164	-3.96212359	-5.15378700
H	-12.70221164	-4.80425259	-3.68138900
H	-12.56772464	-0.14349859	-5.54479000
H	-14.47362164	-1.67498959	-6.06769600
C	-8.79224564	-7.80936559	-0.03463500
C	-7.57504664	-7.58684259	0.62723000
C	-6.90770364	-6.36581359	0.52375900
C	-7.49539764	-5.38324159	-0.26500500
C	-8.71019564	-5.60347959	-0.91779900
C	-9.38118964	-6.81609959	-0.81733700
H	-9.28352364	-8.77138459	0.07056700
H	-7.14954364	-8.37919159	1.23472900
H	-5.97470464	-6.18660159	1.04999000
H	-10.32494364	-6.97499359	-1.32865000

12s

SCF energy in solution: -3344.283404

Free energy in solution: -3343.551219

C	-2.58397932	0.73643410	0.00000000
C	-1.10287732	-0.10078890	-1.52314300
C	-2.84750032	-0.66537790	-0.34352000
C	1.44400568	-2.52213290	-4.51359200
C	0.28061368	-1.16956490	-3.06503600
C	0.31122568	-3.24562590	-3.98747200
H	-1.17752832	-2.62888190	-2.62481300
C	-1.06525132	-5.11908890	-3.79921500
C	-2.87493632	-5.62971690	-2.69496100

C	-5.42832632	-4.50747390	-0.31873700
C	-5.27188332	-3.36508390	0.61872400
C	-4.21592032	-4.58441390	-1.11378700
C	-4.13368932	-2.57180490	-0.02974300
H	-2.64975932	-3.20224490	-1.37006900
N	-3.95696832	-5.59258190	-1.89428500
N	-3.88693532	-1.32634390	0.21857200
N	-0.07730832	-0.11388790	-2.34526500
N	-0.02035132	-4.48730490	-4.29860100
N	-0.33560232	-2.38887590	-3.13412600
N	-1.97138532	-4.65225490	-2.87692800
N	-3.52365332	-3.41869190	-0.89815100
N	-1.97090432	-1.13544990	-1.23521100
N	-6.44736332	0.22379610	0.07831400
N	-6.43334332	-2.72471290	1.12694200
C	-11.87649632	-4.82673290	-1.60954300
C	-10.01418632	-4.48230590	-0.52400400
C	-14.44260432	-3.39325090	-3.83920500
C	-14.41239032	-2.07379790	-4.31488600
C	-13.27033332	-3.58269090	-2.99470900
C	-13.22062632	-1.43709690	-3.76810600
H	-11.73515732	-2.22632890	-2.48781300
C	-11.38093032	1.73236510	-3.75332600
C	-10.18624432	1.95571310	-3.06129000
C	-11.74369332	0.34116710	-3.46979900
C	-9.88104132	0.69023010	-2.39021500
C	-7.31443632	-0.77311590	-0.21120400
C	-7.32170832	-2.08953990	0.23239200
C	-8.50194332	-0.58637190	-1.02328900
C	-8.51643932	-2.70280790	-0.27263800
H	-10.03960432	-1.94707390	-1.52855700
N	-8.79985132	0.53920410	-1.63325800
N	-8.90241332	-3.95519190	-0.03845700
N	-12.96400732	-4.69804390	-2.37459500
N	-12.85315632	-0.20453390	-3.99039000
N	-12.59518332	-2.39163790	-2.99606300
N	-10.83733132	-0.24759790	-2.66105800
N	-9.18137332	-1.77543890	-1.02492900
N	-10.93351432	-3.89668990	-1.34685600
N	-6.40461832	-5.37113190	-0.34317300
H	-7.30914832	-5.11820390	0.07230800
H	-6.29421532	-6.21307390	-0.89666100
H	-5.50180132	-0.06186390	0.32272900
H	-6.55365032	1.07231510	-0.46145000

H	-6.20472332	-2.18276090	1.95616100
O	-4.66264332	-4.16827690	1.62926800
O	-3.34496632	-3.79455090	1.84339300
C	-2.61198432	-8.94674890	-4.55212500
C	-1.44263732	-8.61904290	-5.25871300
C	-0.82486932	-7.38007790	-5.10051800
C	-1.41120732	-6.48213490	-4.21446900
C	-2.57516032	-6.80775590	-3.51219300
C	-3.19579832	-8.04364690	-3.66621600
H	-3.06452332	-9.92203990	-4.70043200
H	-1.01472032	-9.34830490	-5.93935200
H	0.07855568	-7.11829090	-5.64151600
H	-4.09680532	-8.29073490	-3.11429500
C	2.44506468	-2.89617890	-5.41780600
C	3.41118168	-1.95467090	-5.72938100
C	3.39089868	-0.66189290	-5.15681800
C	2.40410068	-0.28605290	-4.26168600
C	1.42321068	-1.23356690	-3.94333400
H	2.45194268	-3.89100190	-5.85041400
H	4.20320368	-2.20909590	-6.42641100
H	4.16770668	0.04597010	-5.42760800
H	2.37983568	0.70245610	-3.81543600
C	-2.65108432	2.91667010	0.95082200
C	-3.18958832	1.63240610	0.87566900
C	-1.46675632	1.09758010	-0.75835100
C	-0.92375432	2.37496510	-0.68391400
C	-1.53630432	3.28242210	0.18005400
H	-3.09381132	3.64483110	1.62278800
H	-4.03503732	1.34094510	1.49218400
H	-0.05470432	2.64556910	-1.27459400
H	-1.14096032	4.28946010	0.26742500
C	-9.54411832	3.18977010	-3.10506200
C	-10.13824832	4.19395410	-3.86614300
C	-11.33847832	3.96877310	-4.56154200
C	-11.97828632	2.73217610	-4.51488200
H	-8.61743832	3.35723210	-2.56594700
H	-9.66793232	5.17035110	-3.92574000
H	-11.77130232	4.77558410	-5.14440800
H	-12.90527532	2.54778410	-5.04792400
C	-16.46547132	-3.78117790	-5.02772400
C	-15.47041132	-4.26776890	-4.18868400
C	-15.41036232	-1.58566490	-5.15680800
C	-16.43534932	-2.45705690	-5.50546800
H	-17.28314332	-4.43066090	-5.32286800

H	-15.48130632	-5.28549590	-3.81334000
H	-15.37671332	-0.56361790	-5.51875600
H	-17.23073532	-2.11373090	-6.15904700
C	-11.66008832	-8.32228990	-0.09908400
C	-10.47479732	-8.09664990	0.61731100
C	-9.82405832	-6.86336690	0.56842700
C	-10.39318132	-5.87188690	-0.22341500
C	-11.57913632	-6.09466290	-0.92694800
C	-12.23386532	-7.31936490	-0.88062500
H	-12.13997732	-9.29356490	-0.03523500
H	-10.06322332	-8.89499090	1.22649300
H	-8.92193932	-6.68143390	1.14558800
H	-13.15525632	-7.47961590	-1.43078400

12t

SCF energy in solution: -3344.298784

Free energy in solution: -3343.570056

C	0.28423772	0.91731265	0.00000000
C	-0.68982428	0.35372165	1.98103400
C	0.89328072	-0.26155435	0.61500300
C	-2.07211628	-1.38685835	6.03360500
C	-1.51718628	-0.39199235	4.02680500
C	-0.92846628	-2.08523435	5.44538500
H	0.08750872	-1.72211635	3.63460500
C	0.74355972	-3.70215735	5.40385700
C	2.37752272	-4.30227235	4.07507900
C	4.08968172	-3.64565335	0.96416300
C	3.68861572	-2.64408035	-0.08692600
C	3.18434572	-3.58921735	1.99999000
C	2.50112572	-1.93029935	0.58265500
H	1.51274972	-2.29568235	2.37854900
N	3.21647072	-4.37955935	3.08122600
N	1.93812772	-0.89361735	0.02878900
N	-1.53625628	0.42989165	3.01152800
N	-0.31702028	-3.10228035	5.98890700
N	-0.65803328	-1.44924535	4.26230200
N	1.31649572	-3.41324835	4.23441900
N	2.25173872	-2.55330635	1.73559200
N	0.30301972	-0.57169435	1.78243500
N	4.24466572	1.08464865	0.38368000
N	4.74650272	-1.83825135	-0.62238900
C	10.36268372	-2.97321435	2.34693400
C	8.53172772	-2.94497435	1.15639600

C	12.50715172	-1.15202835	4.73500300
C	12.22117772	0.13492865	5.21409300
C	11.43605872	-1.52919735	3.82095300
C	10.97040372	0.56434165	4.60011400
H	9.71855772	-0.45283835	3.23354000
C	8.61701172	3.37045865	4.48117600
C	7.44352972	3.39271265	3.72045200
C	9.22907472	2.06511565	4.21894300
C	7.39864772	2.10022965	3.03318600
C	5.24133672	0.23323565	0.72581800
C	5.49615772	-1.06034235	0.29169600
C	6.33584372	0.61443465	1.59680700
C	6.75591172	-1.46157135	0.84651200
H	8.06038472	-0.46325635	2.17554300
N	6.40346072	1.77153065	2.21813700
N	7.37446572	-2.61543935	0.61208200
N	11.36693572	-2.66905535	3.17610500
N	10.38460172	1.71243165	4.80375500
N	10.56499072	-0.47306235	3.78901200
N	8.48607072	1.33827965	3.35887500
N	7.20818772	-0.43966635	1.63444600
N	9.28482872	-2.22257235	2.04172000
N	5.10424172	-4.51593835	0.77645900
H	5.90909472	-4.14108935	0.27686100
H	5.32510072	-5.09629835	1.57672300
H	3.37443872	0.68559765	0.04853100
H	4.18815472	1.93952965	0.92017300
H	4.39068972	-1.28340835	-1.39895000
O	3.19905972	-3.33974435	-1.28689400
O	2.11790072	-4.02071135	-1.05023800
C	3.08954872	-6.89871035	6.77931000
C	2.04065772	-6.51574335	7.62909000
C	1.18467672	-5.46771435	7.29002900
C	1.41559272	-4.82408535	6.08053800
C	2.45826972	-5.20347535	5.23542200
C	3.31413172	-6.24663435	5.56655700
H	3.73680072	-7.71873435	7.07423100
H	1.89622172	-7.04631035	8.56488400
H	0.36970472	-5.16079135	7.93733900
H	4.12280072	-6.53787635	4.90423000
C	-2.76212528	-1.60762935	7.22198100
C	-3.82400428	-0.75698035	7.51395800
C	-4.18303128	0.28512565	6.64041200
C	-3.49189328	0.50484765	5.45353100

C	-2.42928128	-0.34813435	5.16237800
H	-2.47278828	-2.41547135	7.88579900
H	-4.38740428	-0.89691935	8.43077500
H	-5.01708928	0.92888665	6.90090700
H	-3.76024428	1.30536765	4.77240100
C	-0.26224928	2.72406165	-1.45053700
C	0.53413072	1.61265365	-1.18018900
C	-0.73158528	1.31151565	0.88069400
C	-1.53036728	2.41971265	0.61140400
C	-1.27972128	3.12124865	-0.56604000
H	-0.09958928	3.29215565	-2.36085600
H	1.31329572	1.29288565	-1.86566200
H	-2.31639228	2.71859965	1.29724700
H	-1.88203728	3.99061465	-0.81025300
C	6.59758972	4.49809865	3.72709400
C	6.96584672	5.58176265	4.52108300
C	8.14492472	5.55864265	5.28546300
C	8.98888972	4.45035965	5.27631700
H	5.68834472	4.50963865	3.13497800
H	6.33228872	6.46255065	4.55297000
H	8.39872172	6.42185965	5.89251200
H	9.90136372	4.42188665	5.86290300
C	14.49442472	-1.20252835	6.04029500
C	13.64895472	-1.84088735	5.14091200
C	13.06910272	0.77548865	6.11610200
C	14.20773772	0.08913265	6.52148200
H	15.39369072	-1.70554235	6.38072800
H	13.85744072	-2.83579235	4.76208100
H	12.83780572	1.77086765	6.48008000
H	14.89225472	0.55491065	7.22309200
C	10.86187272	-6.42100635	0.79536600
C	9.69444072	-6.39878235	0.01712200
C	8.83131572	-5.30266535	0.03851400
C	9.17233972	-4.23735935	0.86436500
C	10.33805172	-4.25850635	1.63331900
C	11.20323972	-5.34568535	1.61565200
H	11.51003172	-7.29045335	0.75237000
H	9.46307972	-7.24942835	-0.61595100
H	7.93717372	-5.27876535	-0.57722000
H	12.10583472	-5.34927435	2.21788400

12-quintet

SCF energy in solution: -3344.26562230

C	0.55384614	0.01538462	0.00000000
C	-0.46315886	-0.49086438	1.97465500
C	1.13306914	-1.15915838	0.64939800
C	-1.94635686	-2.13261638	6.03252700
C	-1.33848086	-1.18258238	4.01938800
C	-0.79863386	-2.85439738	5.48231500
H	0.25921514	-2.53724538	3.68681500
C	0.85601614	-4.48984038	5.50867300
C	2.51022114	-5.13456138	4.22730900
C	4.29352014	-4.55980238	1.13783600
C	3.91110014	-3.58911038	0.05137700
C	3.36177314	-4.48006438	2.15118600
C	2.71733214	-2.85146638	0.68035200
H	1.68744114	-3.17402438	2.46240000
N	3.36891114	-5.24138338	3.25185800
N	2.18018014	-1.81768038	0.09608200
N	-1.32726686	-0.38139238	2.98797500
N	-0.20967586	-3.86652038	6.05844100
N	-0.49640186	-2.24438138	4.29306800
N	1.45435014	-4.23407138	4.34357500
N	2.43761214	-3.44975638	1.84003500
N	0.51769714	-1.43563238	1.81230200
N	4.47382414	0.12240262	0.58043900
N	4.97998114	-2.80392138	-0.48717800
C	10.65888314	-3.86019838	2.43838100
C	8.81367914	-3.85843638	1.27849500
C	12.83446814	-1.97640838	4.78510900
C	12.54368414	-0.69045538	5.24780500
C	11.74529014	-2.38798638	3.88175700
C	11.26491114	-0.27210938	4.64306600
H	9.99892214	-1.32175538	3.31139400
C	8.88973514	2.50116262	4.52022200
C	7.69896814	2.49715062	3.77484100
C	9.50769814	1.20775562	4.27272900
C	7.66297014	1.20284262	3.11862800
C	5.46558114	-0.73528538	0.85065500
C	5.71941014	-2.01147938	0.42106100
C	6.60055114	-0.31351038	1.71989200
C	7.01269814	-2.40797038	0.95682400
H	8.34004014	-1.38713038	2.26695300
N	6.63083314	0.83547962	2.30353800
N	7.60825014	-3.53889838	0.72930800
N	11.68608914	-3.51982738	3.26758600
N	10.69412614	0.86798662	4.85263600

N	10.85362214	-1.32451938	3.85027400
N	8.75345314	0.45742862	3.43293100
N	7.48052714	-1.35766638	1.73780800
N	9.55801214	-3.12186938	2.14045900
N	5.32133514	-5.42037838	1.00047600
H	6.13410014	-5.05834738	0.50134000
H	5.52660314	-5.98398838	1.81651300
H	3.61648114	-0.21732138	0.15822200
H	4.47590014	1.00383662	1.07586500
H	4.64864014	-2.27598838	-1.29203200
O	3.43844314	-4.31899738	-1.13534200
O	2.34855414	-4.98574938	-0.89824000
C	3.14552314	-7.67121738	7.00656500
C	2.08298014	-7.25919238	7.82550300
C	1.24350914	-6.21266338	7.44408300
C	1.50461814	-5.60041438	6.22443200
C	2.56095014	-6.00829438	5.40981700
C	3.40059114	-7.05056538	5.78345400
H	3.77941614	-8.48927138	7.33414900
H	1.91502014	-7.76600738	8.77048300
H	0.41823914	-5.88341638	8.06691000
H	4.21998514	-7.36467838	5.14519300
C	-2.66375886	-2.32449038	7.20962500
C	-3.72246586	-1.45786338	7.46323600
C	-4.05149686	-0.42836338	6.56336600
C	-3.33291486	-0.23761538	5.38774100
C	-2.27346386	-1.10665338	5.13486700
H	-2.39733286	-3.12311338	7.89386000
H	-4.30687786	-1.57520338	8.37001700
H	-4.88402486	0.22863562	6.79400200
H	-3.57849786	0.55286162	4.68659000
C	0.06158514	1.79828262	-1.49909700
C	0.83394414	0.68008262	-1.19137100
C	-0.47011786	0.44482362	0.85489500
C	-1.24521586	1.56039962	0.54769100
C	-0.96311686	2.23187462	-0.63994100
H	0.24760714	2.34274062	-2.41934200
H	1.61622914	0.33032562	-1.85855400
H	-2.03779986	1.88699562	1.21306200
H	-1.54664186	3.10545162	-0.91299300
C	6.84116114	3.59472562	3.77834800
C	7.20950414	4.69660362	4.54816000
C	8.40104414	4.70009362	5.29350200
C	9.25854014	3.60084862	5.28993400

H	5.92152414	3.58790862	3.20230000
H	6.56584614	5.57010262	4.57531100
H	8.65460414	5.57626362	5.88168200
H	10.18005014	3.59446462	5.86297100
C	14.84052814	-1.98145538	6.06197900
C	13.98289114	-2.64498638	5.18042900
C	13.38921914	-0.02559038	6.12202900
C	14.54895814	-0.69318138	6.52533900
H	15.74960414	-2.47202838	6.39454300
H	14.19652914	-3.64324138	4.81327600
H	13.14928614	0.97280862	6.47220800
H	15.23653814	-0.20644238	7.20936900
C	11.16737014	-7.30248038	0.90807800
C	9.98393014	-7.29853938	0.14869800
C	9.11156614	-6.21216838	0.17765900
C	9.45341814	-5.13261138	0.99000600
C	10.63913614	-5.13484738	1.74356700
C	11.51285314	-6.21969738	1.71381200
H	11.82332714	-8.16587638	0.85985600
H	9.75062114	-8.15650638	-0.47364500
H	8.20597514	-6.20221538	-0.42177200
H	12.42676114	-6.21351838	2.29894400

12-septet

SCF energy in solution: -3344.22868317

C	0.68492308	0.61969230	0.00000000
C	-0.43685292	0.04320030	1.89888900
C	1.15557008	-0.62611770	0.57471300
C	-2.19836392	-1.78168070	5.77147500
C	-1.43370192	-0.72130870	3.85386000
C	-1.06234892	-2.52617570	5.22383600
H	0.11699308	-2.11397070	3.50262000
C	0.46890708	-4.28069270	5.19645100
C	2.12988708	-4.88781170	3.91601800
C	4.17013808	-4.13189770	0.96607900
C	3.84819008	-3.14177070	-0.09131600
C	3.13214308	-4.13931370	1.94867200
C	2.64869808	-2.41147270	0.52824500
H	1.47492808	-2.84188070	2.22761700
N	3.09841708	-4.96753270	2.95136000
N	2.19477208	-1.31676270	0.02246400
N	-1.35699192	0.14978930	2.89567900
N	-0.57072892	-3.61657770	5.72794100

N	-0.65766392	-1.83152570	4.08773600
N	1.19039308	-3.94843470	4.06159400
N	2.25116808	-3.10692970	1.63270300
N	0.46877808	-0.94413270	1.70514300
N	4.53498908	0.56119830	0.51123700
N	4.93560008	-2.36053570	-0.59719900
C	10.56382108	-3.67478570	2.32842100
C	8.72043108	-3.58925770	1.16890100
C	12.80427808	-1.90544970	4.70251800
C	12.56183908	-0.61497470	5.18022200
C	11.70289908	-2.26318970	3.79117600
C	11.30259508	-0.13980570	4.57706500
H	10.00088508	-1.12375770	3.22917700
C	9.03777408	2.72502330	4.48024200
C	7.84878808	2.77589530	3.73392800
C	9.60457808	1.41082030	4.22014000
C	7.76280708	1.49064030	3.06424000
C	5.49423608	-0.33559270	0.77371600
C	5.69843408	-1.61536570	0.32894900
C	6.64419008	0.03301630	1.64689700
C	6.97492308	-2.06712670	0.86162300
H	8.33924808	-1.11467570	2.18505100
N	6.71787608	1.17256430	2.24487800
N	7.52600008	-3.21969570	0.62563400
N	11.60176508	-3.38479070	3.16308200
N	10.77540208	1.01877830	4.79862900
N	10.85347508	-1.16591370	3.76977500
N	8.82263808	0.69946830	3.37186700
N	7.48453108	-1.04421770	1.65179700
N	9.49044008	-2.89250570	2.04089200
N	5.20014808	-4.99054670	0.93946400
H	6.05422908	-4.68244070	0.47125500
H	5.30153408	-5.58148670	1.75704000
H	3.66341208	0.25148830	0.09552000
H	4.56514808	1.43472430	1.01965200
H	4.62663708	-1.80536770	-1.39201500
O	3.37939608	-3.81760870	-1.33494200
O	2.29781708	-4.50605670	-1.13950900
C	2.43552008	-7.78597370	6.36756100
C	1.36697708	-7.39084170	7.18922900
C	0.62656508	-6.24185570	6.91397400
C	0.98640208	-5.49936570	5.79180500
C	2.05428008	-5.89488770	4.97296700
C	2.79434808	-7.03946470	5.24437000

H	2.98847008	-8.68696970	6.61313400
H	1.11506008	-7.99482570	8.05533100
H	-0.19993292	-5.93173570	7.54510200
H	3.61776308	-7.33584070	4.60262300
C	-2.98760892	-2.01615670	6.89026600
C	-4.01675992	-1.11047170	7.15227000
C	-4.24598392	-0.00792770	6.31821000
C	-3.44996592	0.22240730	5.19405200
C	-2.42798592	-0.67996470	4.93964000
H	-2.80193992	-2.87383870	7.52808200
H	-4.65381992	-1.26157070	8.01786100
H	-5.05586692	0.67559530	6.55129800
H	-3.61469392	1.06994730	4.53699200
C	0.36157708	2.54485130	-1.36754800
C	1.04735908	1.35582030	-1.12786800
C	-0.33973892	1.05648930	0.85580300
C	-1.02772592	2.24182230	0.61462700
C	-0.66112192	2.98283130	-0.50806400
H	0.61517908	3.14324930	-2.23683900
H	1.82532108	1.00746730	-1.80112300
H	-1.81926792	2.56910430	1.28099300
H	-1.17505492	3.91290330	-0.72869500
C	7.03517308	3.90645330	3.74827900
C	7.44624608	4.98475630	4.52997300
C	8.63622208	4.93322630	5.27604300
C	9.44937208	3.80091030	5.26163100
H	6.11662208	3.94213030	3.17155300
H	6.83769408	5.88273630	4.56604300
H	8.92364008	5.79258130	5.87338300
H	10.36932108	3.75169130	5.83511700
C	14.80351708	-2.00396470	5.98628100
C	13.92436308	-2.62286370	5.09348500
C	13.42897908	0.00581330	6.06572300
C	14.56024208	-0.71114570	6.46476100
H	15.69151108	-2.53350470	6.31601300
H	14.10049808	-3.62414070	4.71485000
H	13.22654308	1.00832330	6.42765000
H	15.26338808	-0.25996170	7.15727400
C	10.94698408	-7.11067170	0.74721600
C	9.76537508	-7.05177970	-0.01285200
C	8.93352308	-5.93476870	0.03224700
C	9.31345308	-4.88137870	0.86195300
C	10.49778008	-4.93807570	1.61558000
C	11.33118808	-6.05361470	1.56946800

H	11.57098008	-7.99661470	0.68598100
H	9.50197108	-7.89072170	-0.64894800
H	8.03070708	-5.88185970	-0.56928800
H	12.24433908	-6.08965970	2.15471000

TS13s

SCF energy in solution: -3344.28721

Free energy in solution: -3343.560843

C	2.32558138	0.14211886	0.00000000
C	0.46482038	-0.33104414	1.03401700
C	3.52179538	-0.76102714	-1.77797400
C	3.18444038	-2.51779714	-3.18348300
H	1.81872338	-1.99119014	-1.65334000
C	1.47459238	-4.09042014	-3.40449300
C	-0.41384462	-4.52996214	-2.41464400
C	-2.76483862	-3.57834414	0.23717200
C	-2.52092162	-2.55647514	1.33347600
C	-1.59858762	-3.64697414	-0.61570700
C	-1.21224962	-1.92627114	0.86544400
H	0.11535638	-2.41704814	-0.67145600
N	-1.46989862	-4.49678614	-1.59224300
N	-0.68789362	-0.87599614	1.43403800
N	3.36399138	0.13553886	-0.81689300
N	2.64187738	-3.55360814	-3.76717100
N	2.69405038	-1.78701914	-2.12036800
N	0.65647338	-3.69693214	-2.39107300
N	-0.75793262	-2.63000214	-0.19450100
N	1.26880838	-0.72915714	0.02575900
N	-3.23165762	0.79408086	0.22182800
N	-3.58074262	-1.76817314	1.79682800
C	-9.16136562	-4.86181414	0.47868500
C	-7.89735762	-4.69111914	1.04990500
C	-9.40469662	-3.64313714	-0.30746900
C	-7.42856362	-3.38104214	0.58001200
C	-12.00713462	-2.16682014	-2.46558700
C	-11.87869862	-0.92144514	-3.09972400
C	-10.78429562	-2.40429914	-1.71143800
C	-10.57441662	-0.37932214	-2.74401100
H	-9.06388262	-1.20069914	-1.51212800
C	-8.88763462	1.23012686	-2.80956600
C	-6.89429162	1.47239286	-1.95219900
C	-4.32593262	-0.02103214	0.20967700
C	-4.46885862	-1.22583014	0.87794100

C	-5.53662962	0.21828886	-0.54423100
C	-5.76332462	-1.74251614	0.52276000
H	-7.29345862	-0.94892014	-0.71314000
N	-5.76076962	1.28447286	-1.28158200
N	-6.23868762	-2.91467214	0.92697200
N	-10.54002662	-3.47449814	-0.99156300
N	-10.09677762	0.76676186	-3.15330700
N	-9.98459962	-1.31044314	-1.91897500
N	-7.97325662	0.63760586	-2.01110200
N	-6.37431462	-0.84502214	-0.31162400
N	-8.35977962	-2.79078814	-0.22320300
N	-3.79939962	-4.34436214	0.17569600
H	-4.60114262	-4.15789514	0.79367200
H	-3.81528662	-5.11486414	-0.48596800
H	-2.61644962	0.66411686	1.01929900
H	-3.38436762	1.74655486	-0.07943600
H	-3.90497062	-2.67990614	2.60650700
O	-2.18347262	-3.45102514	2.42425700
O	-3.43884462	-3.78307914	2.99722800
C	-13.15793562	-2.94086814	-2.61351800
C	-12.89799062	-0.41106214	-3.90338300
C	-14.04407862	-1.18216014	-4.05071800
C	-14.17289362	-2.43186614	-3.41357900
H	-13.24407962	-3.90135214	-2.11658600
H	-12.78731662	0.55284086	-4.38865500
H	-14.85916362	-0.81789414	-4.66782400
H	-15.08429862	-3.00428214	-3.55288200
C	-8.40069562	2.52010186	-3.30678300
C	-7.12286762	2.67396186	-2.75902800
C	-6.35174862	3.80149386	-3.02680300
C	-6.90298162	4.77199286	-3.86035000
C	-8.18757862	4.61740786	-4.40920000
C	-8.95566062	3.48686586	-4.13996200
H	-5.36019062	3.91309186	-2.60030000
H	-6.33264862	5.66580286	-4.09309300
H	-8.58434662	5.39506586	-5.05423200
H	-9.94819562	3.35698686	-4.55900100
C	-8.08750062	-6.80271714	2.12418700
C	-7.33811762	-5.65006014	1.88823000
C	-9.91247662	-6.00786014	0.71344300
C	-9.35374962	-6.97961414	1.54368200
H	-7.69018162	-7.57526214	2.77481300
H	-6.36825262	-5.49627914	2.35446900
H	-10.89415562	-6.13244814	0.26815300

H	-9.90875262	-7.88852414	1.75343500
C	-1.11774462	-6.56271114	-3.91233100
C	-0.67631062	-7.31636914	-4.99564200
C	0.54565438	-7.03324614	-5.63229200
C	1.35821138	-5.98834114	-5.20265600
C	0.91347438	-5.23600814	-4.11814500
C	-0.30203462	-5.51698514	-3.48437600
H	-2.05937662	-6.77764014	-3.41784200
H	-1.28351362	-8.13926014	-5.35911300
H	0.85648438	-7.64377214	-6.47407400
H	2.30223038	-5.76194214	-5.68731400
C	5.37263538	-2.21697214	-4.54641100
C	6.50331738	-1.41773214	-4.64416800
C	6.71131938	-0.32813614	-3.77356500
C	5.79218938	-0.01204314	-2.78330300
C	4.65398838	-0.81510814	-2.68348900
C	4.44679538	-1.90115514	-3.55102200
H	5.20376838	-3.05721314	-5.21133200
H	7.24611138	-1.63246914	-5.40567100
H	7.60896438	0.27142886	-3.88377800
H	5.94000338	0.82288486	-2.10671000
C	1.32780238	2.69706886	3.17754500
C	2.52111338	3.00863686	2.51039400
C	2.97371938	2.24182986	1.43390900
C	2.18916638	1.16211686	1.05238300
C	0.99993038	0.85670186	1.71471700
C	0.54414138	1.60813786	2.78893200
H	1.01203138	3.31298486	4.01336100
H	3.10462138	3.86162686	2.84174000
H	3.89811238	2.47386886	0.91539000
H	-0.37560062	1.34837286	3.30355700

TS13t

SCF energy in solution: -3344.248697

Free energy in solution: -3343.527196

C	2.19619421	0.19379845	0.02874965
C	0.33541821	-0.27940555	1.06272265
C	3.39238221	-0.70919955	-1.74931435
C	3.05500421	-2.46585255	-3.15496935
H	1.68927921	-1.93933355	-1.62480135
C	1.34513521	-4.03843655	-3.37609135
C	-0.54331779	-4.47802855	-2.38629535
C	-2.89429579	-3.52658655	0.26558965

C	-2.65038979	-2.50477255	1.36195165
C	-1.72805979	-3.59515655	-0.58729635
C	-1.34169379	-1.87456855	0.89397765
H	-0.01410379	-2.36523655	-0.64296235
N	-1.59936279	-4.44490055	-1.56389735
N	-0.81730979	-0.82435455	1.46267465
N	3.23460721	0.18727745	-0.78815235
N	2.51243521	-3.50160555	-3.73873735
N	2.56461121	-1.73513555	-2.09181035
N	0.52703921	-3.64503155	-2.36263835
N	-0.88740679	-2.57820055	-0.16603435
N	1.13941121	-0.67745255	0.05442865
N	-3.36102679	0.84577645	0.25030765
N	-3.71020179	-1.71649055	1.82532265
C	-9.29096379	-4.80990855	0.50731165
C	-8.02695279	-4.63925055	1.07852965
C	-9.53424879	-3.59123455	-0.27885935
C	-7.55810379	-3.32920455	0.60861165
C	-12.13664779	-2.11485855	-2.43699635
C	-12.00817979	-0.86948655	-3.07113135
C	-10.91382079	-2.35236055	-1.68283335
C	-10.70389079	-0.32738855	-2.71540635
H	-9.19340279	-1.14878255	-1.48347035
C	-9.01706979	1.28201045	-2.78096935
C	-7.02371179	1.52420745	-1.92361735
C	-4.45536179	0.03069345	0.23820765
C	-4.59830479	-1.17410155	0.90645465
C	-5.66605479	0.27004645	-0.51568535
C	-5.89279879	-1.69076155	0.55129165
H	-7.42291779	-0.89710455	-0.68459035
N	-5.89019079	1.33625145	-1.25301435
N	-6.36819879	-2.86288355	0.95554065
N	-10.66957679	-3.42255955	-0.96295535
N	-10.22622679	0.81868345	-3.12470435
N	-10.11410279	-1.25851455	-1.89036135
N	-8.10270179	0.68945245	-1.98252435
N	-6.50376779	-0.79324455	-0.28307535
N	-8.48929779	-2.73892555	-0.19461035
N	-3.92884779	-4.29262555	0.20412265
H	-4.73052579	-4.10624055	0.82219565
H	-3.94473979	-5.06313355	-0.45753135
H	-2.74592379	0.71584145	1.04787065
H	-3.51384679	1.79830845	-0.05074135
H	-4.03441879	-2.62821655	2.63500565

O	-2.31295779	-3.39939555	2.45269865
O	-3.56832379	-3.73142855	3.02564865
C	-13.28746079	-2.88888455	-2.58494535
C	-13.02744879	-0.35908255	-3.87480635
C	-14.17354879	-1.13015855	-4.02215835
C	-14.30239679	-2.37986155	-3.38502135
H	-13.37363079	-3.84936755	-2.08801535
H	-12.91674679	0.60481745	-4.36007835
H	-14.98861779	-0.76587755	-4.63927735
H	-15.21381079	-2.95226155	-3.52433935
C	-8.53009679	2.57197745	-3.27817735
C	-7.25225879	2.72579345	-2.73043335
C	-6.48110779	3.85330345	-2.99820735
C	-7.03232079	4.82382445	-3.83174235
C	-8.31692679	4.66928245	-4.38058235
C	-9.08504179	3.53876045	-4.11134635
H	-5.48954179	3.96486745	-2.57171435
H	-6.46196379	5.71761945	-4.06448535
H	-8.71367579	5.44695745	-5.02560635
H	-10.07758379	3.40891345	-4.53037535
C	-8.21718179	-6.75080955	2.15288365
C	-7.46775079	-5.59819155	1.91689965
C	-10.04212079	-5.95592055	0.74210365
C	-9.48343479	-6.92767155	1.57237165
H	-7.81990379	-7.52335355	2.80353565
H	-6.49788679	-5.44442255	2.38314265
H	-11.02380479	-6.08048455	0.29681665
H	-10.03847279	-7.83655655	1.78214365
C	-1.24725579	-6.51061455	-3.88418935
C	-0.80583079	-7.26417355	-4.96757235
C	0.41614821	-6.98102055	-5.60418335
C	1.22872921	-5.93618255	-5.17443435
C	0.78400221	-5.18394955	-4.08984935
C	-0.43151979	-5.46495655	-3.45611535
H	-2.18890079	-6.72556655	-3.38973435
H	-1.41305379	-8.08700955	-5.33113435
H	0.72696621	-7.59146855	-6.44602735
H	2.17275621	-5.70975355	-5.65906035
C	5.24321821	-2.16496255	-4.51785335
C	6.37391821	-1.36573555	-4.61553935
C	6.58193121	-0.27621155	-3.74485235
C	5.66279721	0.03982245	-2.75457235
C	4.52458321	-0.76322855	-2.65483035
C	4.31737821	-1.84920255	-3.52244835

H	5.07433821	-3.00514855	-5.18283935
H	7.11671421	-1.58042655	-5.37705235
H	7.47958621	0.32334745	-3.85501135
H	5.81062121	0.87469845	-2.07791735
C	1.19849821	2.74846745	3.20654765
C	2.39181721	3.06006545	2.53942465
C	2.84440121	2.29334945	1.46286465
C	2.05981821	1.21369545	1.08123665
C	0.87057321	0.90825345	1.74354165
C	0.41480421	1.65959645	2.81782765
H	0.88275021	3.36430845	4.04242565
H	2.97535021	3.91300745	2.87085065
H	3.76879921	2.52541645	0.94436665
H	-0.50494179	1.39980245	3.33242965

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SCF energy in solution: -3344.289103

Free energy in solution: -3343.560262

C	-1.43410857	1.43410851	0.00000000
C	-3.16873057	0.74471551	1.12744900
C	-0.47603657	0.96690151	-2.06006300
C	-1.01622157	-0.43193949	-3.77824300
H	-2.16962857	-0.28243449	-2.00233100
C	-2.76841657	-1.93555349	-4.11036600
C	-4.51302457	-2.63858049	-3.01120400
C	-6.43913057	-2.40272949	0.07582100
C	-6.15534457	-1.52494649	1.29290900
C	-5.44155257	-2.21931549	-0.90963600
C	-4.88904857	-0.78109349	0.79853900
H	-3.75642457	-0.92741449	-0.93637000
N	-5.42661457	-2.82110949	-2.07942100
N	-4.26615257	0.13669551	1.52304700
N	-0.48765657	1.62478851	-0.92196600
N	-1.63387557	-1.30647049	-4.50339500
N	-1.35655857	0.03534351	-2.51728600
N	-3.42007257	-1.79802449	-2.94798600
N	-4.56001657	-1.25116349	-0.40272600
N	-2.47720057	0.57792951	-0.04287800
N	-6.55310557	1.92396851	0.52967500
N	-7.26682057	-0.84138649	1.76354200
C	-13.04738557	-3.05568849	-0.15070600
C	-11.80727257	-3.10150449	0.49373000

C	-13.11932557	-1.72707149	-0.76928300
C	-11.17908357	-1.80064349	0.23230500
C	-15.44436157	0.29492251	-2.79960100
C	-15.16139757	1.59683251	-3.24311900
C	-14.29307357	-0.17083549	-2.04233000
C	-13.83196057	1.94385351	-2.76508500
H	-12.47208057	0.81039451	-1.61417500
C	-11.99613957	3.35814751	-2.53179600
C	-10.03584457	3.25411551	-1.57416400
C	-7.72450457	1.21144751	0.40843100
C	-8.00329557	-0.04792749	0.92525400
C	-8.87801357	1.67494451	-0.31734300
C	-9.35277657	-0.36664349	0.47515500
H	-10.74651257	0.74164251	-0.67608400
N	-8.95929957	2.85125151	-0.90575400
N	-9.96495157	-1.51802149	0.69472100
N	-14.19111457	-1.34670949	-1.46957200
N	-13.22241857	3.08332551	-2.98637000
N	-13.37911557	0.85349451	-2.06291000
N	-11.18960357	2.56173151	-1.79311600
N	-9.83755457	0.69528751	-0.24220200
N	-11.99655057	-1.01338049	-0.52151000
N	-7.53847657	-3.08958849	0.00569400
H	-8.25367257	-2.90472149	0.72074600
H	-7.78208557	-3.58772749	-0.84227900
H	-6.03989257	1.71961151	1.38202000
H	-6.65189057	2.91085251	0.32599100
H	-6.52876457	-1.30373449	3.49156000
O	-5.71417457	-2.46600249	2.28626400
O	-5.67705657	-1.79825549	3.53990100
C	-16.65800857	-0.32474249	-3.10107600
C	-16.08344757	2.31860751	-4.00251400
C	-17.29025957	1.70097551	-4.30214500
C	-17.57431857	0.39426851	-3.85655800
H	-16.86459657	-1.33068249	-2.75124000
H	-15.85298157	3.32392351	-4.33895500
H	-18.03257557	2.23117051	-4.89018800
H	-18.52931557	-0.05427849	-4.11092000
C	-11.35204357	4.64545851	-2.81512600
C	-10.09647057	4.57781851	-2.20378500
C	-9.19943057	5.63933151	-2.27281900
C	-9.60169057	6.77440251	-2.97386600
C	-10.86400557	6.84217751	-3.58729000
C	-11.75847357	5.77599851	-3.51693300

H	-8.22595857	5.57795351	-1.79717200
H	-8.93029457	7.62404251	-3.05001600
H	-11.14348457	7.74289551	-4.12486800
H	-12.73539257	5.81714051	-3.98766300
C	-12.27950157	-5.30987049	1.24796400
C	-11.40474157	-4.22549649	1.20964900
C	-13.92520557	-4.13453249	-0.11378900
C	-13.52176757	-5.26575349	0.59308300
H	-12.00213657	-6.20337849	1.79842100
H	-10.45332957	-4.24742249	1.73296200
H	-14.88578957	-4.08703549	-0.61647500
H	-14.17865557	-6.12825749	0.64641200
C	-5.42016557	-4.28101249	-4.84104300
C	-5.13159657	-4.74970849	-6.11933300
C	-4.00412157	-4.29658249	-6.82765500
C	-3.13488957	-3.36110749	-6.27476300
C	-3.42743757	-2.89477749	-4.99507700
C	-4.54832357	-3.34464949	-4.28992500
H	-6.28913457	-4.62797149	-4.29169900
H	-5.78806957	-5.47939249	-6.58271000
H	-3.81316657	-4.68566149	-7.82263300
H	-2.26244757	-3.00397749	-6.81203700
C	0.99236543	0.20646351	-5.30048400
C	2.11735743	1.02530151	-5.35470400
C	2.44847743	1.88696051	-4.29480700
C	1.66245643	1.95426351	-3.14833300
C	0.53917243	1.13410851	-3.09751700
C	0.20862343	0.27520851	-4.15342500
H	0.72810543	-0.46157249	-6.11316800
H	2.75423343	1.00031351	-6.23300100
H	3.33359643	2.50923551	-4.37566000
H	1.90426443	2.61423951	-2.32212200
C	-1.98619657	3.25946051	3.73837700
C	-0.87538957	3.70869051	3.01340800
C	-0.57140757	3.18630551	1.75209400
C	-1.42020957	2.20960551	1.25480600
C	-2.52715357	1.76623851	1.97561600
C	-2.83589357	2.27228751	3.22827800
H	-2.18742257	3.68487751	4.71622900
H	-0.23825657	4.47528651	3.44245300
H	0.28865743	3.52534651	1.18428400
H	-3.69397757	1.90679751	3.78334900

SCF energy in solution: -3871.138633

Free energy in solution: -3870.380522

C	-2.72609825	0.68475451	0.00000000
C	-4.83892725	1.19075151	0.19137500
C	-1.21474625	-0.61925249	1.20900100
C	-1.34604825	-1.79824949	3.14297500
H	-2.97374125	-0.70477749	2.37171800
C	-3.03435425	-2.14805449	4.71500700
C	-5.12230325	-1.54246349	4.91160800
C	-8.09032525	0.11324251	3.40274800
C	-8.04281225	0.74396851	2.05202900
C	-6.70103725	-0.41543349	3.62792800
C	-6.61132825	0.64244251	1.60378800
H	-4.97057225	-0.36528649	2.42967600
N	-6.36482725	-1.02463149	4.71344600
N	-6.14422825	1.27641451	0.57627000
N	-1.53572725	0.17527951	0.19026700
N	-1.81167825	-2.31431849	4.27945000
N	-2.01165125	-0.99865549	2.25524500
N	-4.07372725	-1.46338049	4.09582200
N	-5.95684325	-0.13396049	2.51231700
N	-3.87418725	0.47087951	0.75546100
N	-9.58735225	-3.11753549	1.28370800
N	-8.64106225	-0.58773349	2.20594200
C	-13.99821525	3.35622251	3.72087200
C	-12.63307125	3.09907551	3.57432500
C	-14.68569225	2.14225251	3.26523000
C	-12.55631725	1.72633951	3.03248300
C	-18.14645825	0.92563051	2.85646300
C	-18.47575725	-0.34269549	2.35791800
C	-16.69124825	1.02696851	2.87379300
C	-17.22649725	-1.03606949	2.06433000
H	-15.22994625	-0.38810249	2.29683900
C	-15.94497325	-2.83308949	1.33203800
C	-13.82232825	-3.28289149	1.13441700
C	-10.39505625	-2.08718249	1.60458900
C	-10.02294125	-0.83081349	2.06591000
C	-11.83284825	-2.14901449	1.56689900
C	-11.24167725	-0.10378749	2.32402900
H	-13.25813425	-0.66705149	2.09334800
N	-12.50018425	-3.20687149	1.15939200
N	-11.39588425	1.14669651	2.77323400
N	-16.02139725	2.07935651	3.27433000

N	-17.12636125	-2.24231149	1.58259800
N	-16.21286525	-0.16233649	2.39704600
N	-14.71354125	-2.31918549	1.51973100
N	-12.28652025	-0.93536249	2.01437000
N	-13.80791725	1.19761051	2.87102000
N	-8.90854225	0.50183851	4.47640100
H	-8.70506725	1.46206651	4.74152700
H	-8.72856225	-0.11126849	5.26760200
H	-8.59961825	-2.93284749	1.19470000
H	-9.99165425	-3.91400549	0.81579200
H	-10.12299525	2.13814351	2.78880800
O	-8.76351525	1.79566951	1.55712500
O	-9.24905425	2.62569451	2.61086800
C	-19.13147325	1.83711251	3.23151100
C	-19.80302425	-0.74277049	2.21801000
C	-20.78689525	0.16544451	2.59253200
C	-20.45604725	1.43871951	3.09272700
H	-18.86198725	2.81547551	3.61484000
H	-20.04598925	-1.72654049	1.83087900
H	-21.83259525	-0.10918149	2.49856800
H	-21.25299025	2.11941751	3.37386000
C	-15.88259825	-4.19453849	0.79561500
C	-14.52022825	-4.48351749	0.66962300
C	-14.08401125	-5.71338449	0.18485500
C	-15.05757925	-6.64382249	-0.17094400
C	-16.42669125	-6.35205149	-0.04457400
C	-16.85947125	-5.12088349	0.44207000
H	-13.02567825	-5.93356049	0.09052800
H	-14.75707125	-7.61428149	-0.55319100
H	-17.15621225	-7.10250649	-0.33211000
H	-17.91371625	-4.88522349	0.54455600
C	-12.15673425	5.26828151	4.43961100
C	-11.68707525	4.05382451	3.93798500
C	-14.47364325	4.56164351	4.22034800
C	-13.52814825	5.52181351	4.57884500
H	-11.44076425	6.03217151	4.72564500
H	-10.62013825	3.89020151	3.83876300
H	-15.53926125	4.73721451	4.32456100
H	-13.85452125	6.47894251	4.97269400
C	-5.57666725	-2.63775749	7.24729800
C	-4.94870125	-3.38996649	8.23891300
C	-3.60764925	-3.78589749	8.10928900
C	-2.85478725	-3.44186249	6.98704000
C	-3.48587425	-2.69232949	6.00072500

C	-4.81995325	-2.29769549	6.13117000
H	-6.61240825	-2.32685249	7.33669800
H	-5.50221025	-3.67623749	9.12747300
H	-3.15097125	-4.37128649	8.90114700
H	-1.81787925	-3.74315449	6.88010800
C	1.09168075	-2.67609949	3.11855400
C	2.25957175	-2.63153549	2.38103700
C	2.34244975	-1.89352649	1.17444000
C	1.25882775	-1.18851049	0.68571200
C	0.06852175	-1.22772949	1.42746800
C	-0.01401525	-1.96370549	2.63030000
H	1.01820775	-3.23749349	4.04398500
H	3.13510875	-3.17063349	2.72853400
H	3.27960275	-1.88485649	0.62706000
H	1.31288175	-0.62011249	-0.23676700
C	-4.21870825	3.33206851	-2.89698400
C	-2.85868325	3.00451051	-3.02172700
C	-2.23629625	2.13426651	-2.12763400
C	-3.01555725	1.60436551	-1.10510200
C	-4.36828325	1.93371251	-0.98018800
C	-4.99708925	2.79752251	-1.87180300
H	-4.66851025	4.01204751	-3.61316400
H	-2.28355125	3.43896451	-3.83332700
H	-1.18643825	1.87572251	-2.21883000
H	-6.05114825	3.03928051	-1.77466000
C	-7.54181725	4.94228151	3.51156600
C	-6.91673025	3.76201251	2.73919300
O	-6.46352525	2.81412051	3.32943100
O	-6.92874525	3.97268851	1.44217300
H	-6.67007625	3.14591551	0.97135200
F	-8.47425225	5.58347251	2.81093500
F	-8.09659325	4.50324651	4.64492600
F	-6.58296825	5.82283651	3.83484500

TS16

SCF energy in solution: -3871.124066

Free energy in solution: -3870.362553

C	-3.21705433	-2.05426354	0.00000000
C	-5.37942133	-1.94278354	0.26867200
C	-1.56202533	-0.69413654	-0.89286500
C	-1.56263633	1.36732646	-1.86930000
H	-3.32652733	0.42192746	-1.16507500
C	-3.25511233	2.89973946	-2.34577900

C	-5.41585333	3.03264146	-2.09944900
C	-8.43351533	1.36338546	-0.91716700
C	-8.49486333	0.00394846	-0.25892000
C	-7.06852133	1.64777646	-1.21116300
C	-7.04888233	-0.42288954	-0.24015400
H	-5.31579733	0.49240546	-0.93209500
N	-6.66871933	2.75807846	-1.79176300
N	-6.64094633	-1.56729754	0.27435900
N	-1.94045033	-1.80688154	-0.30619700
N	-1.96083033	2.50288646	-2.34691600
N	-2.32190733	0.36703146	-1.28381000
N	-4.31750333	2.23033446	-1.87546300
N	-6.32219933	0.54707246	-0.80109900
N	-4.29189633	-1.26748154	-0.22167800
N	-10.27556533	2.30383446	1.97372800
N	-9.23960333	-0.36173254	0.75410500
C	-13.77844533	-3.73404854	-2.32774700
C	-12.54231133	-3.55241554	-1.70466600
C	-14.57299233	-2.54788854	-1.98364000
C	-12.64205033	-2.25919054	-1.01286100
C	-17.95773533	-1.19970754	-2.56549100
C	-18.42824633	-0.00350954	-2.00892400
C	-16.57260933	-1.37272054	-2.13492800
C	-17.33833133	0.57780446	-1.22877000
H	-15.35609433	-0.11106554	-0.95633500
C	-16.39704533	2.17033346	0.18610600
C	-14.46166033	2.49651246	1.13900000
C	-11.01301633	1.30017446	1.37871400
C	-10.54055433	0.13682546	0.79256200
C	-12.43000733	1.36585946	1.14488300
C	-11.68196733	-0.55014654	0.25433700
H	-13.71521733	0.01867546	0.13529700
N	-13.19273733	2.38734746	1.49527000
N	-11.62158333	-1.72401654	-0.37378600
N	-15.82819833	-2.40473854	-2.43432700
N	-17.41836133	1.68309346	-0.54408800
N	-16.26898133	-0.28129754	-1.36239400
N	-15.17716333	1.63465446	0.34660700
N	-12.78765433	0.21763746	0.48038400
N	-13.88195233	-1.70066454	-1.20065300
N	-9.42001333	2.15947646	-1.21101000
H	-10.38601633	1.87063446	-1.08721000
H	-9.21093133	3.04159646	-1.66693100
H	-9.44605533	1.97291546	2.45133800

H	-10.83544633	2.93777846	2.53100100
H	-9.84745933	-2.16509454	-0.96972700
O	-8.93604133	-0.77010654	-1.84180000
O	-9.06644233	-2.14550754	-1.56888500
C	-18.77202233	-1.99979454	-3.36321800
C	-19.73158533	0.43427346	-2.23068500
C	-20.54575433	-0.36109554	-3.03022900
C	-20.07250533	-1.56215854	-3.58949600
H	-18.39279333	-2.92386454	-3.78638300
H	-20.08513733	1.36137646	-1.79215600
H	-21.56713333	-0.05242254	-3.22871500
H	-20.73794033	-2.15553554	-4.20822900
C	-16.52863033	3.43454746	0.91769100
C	-15.28669233	3.64425546	1.52653300
C	-15.04655833	4.77122546	2.30721100
C	-16.09084233	5.68064346	2.46059300
C	-17.33796633	5.46906946	1.84844100
C	-17.57380333	4.34140046	1.06512000
H	-14.08080133	4.92950846	2.77623000
H	-15.94210833	6.57115046	3.06341500
H	-18.12819033	6.19954946	1.99044600
H	-18.53184333	4.16864846	0.58558300
C	-11.78552833	-5.61307254	-2.61468900
C	-11.52151533	-4.48507054	-1.83748200
C	-14.04812333	-4.85355954	-3.10377800
C	-13.02897833	-5.79625354	-3.23735900
H	-11.01091133	-6.36150254	-2.74819100
H	-10.55278333	-4.34009654	-1.37060000
H	-15.01096833	-4.97734654	-3.58829500
H	-13.19476233	-6.68494654	-3.83813600
C	-5.72934833	5.40159246	-3.17746900
C	-5.00241633	6.43053746	-3.76929600
C	-3.60774333	6.34365746	-3.92757000
C	-2.90289733	5.22346546	-3.49731300
C	-3.63422733	4.19650946	-2.90531100
C	-5.02143933	4.28169646	-2.74743000
H	-6.80564533	5.46530546	-3.05561500
H	-5.51918533	7.31906646	-4.11789100
H	-3.07631633	7.16653546	-4.39472000
H	-1.82710333	5.14490146	-3.61504300
C	0.99866567	1.47445246	-2.29916500
C	2.17553867	0.74986446	-2.13063100
C	2.17413567	-0.52048654	-1.52886100
C	0.99371567	-1.10317754	-1.07780600

C	-0.18096433	-0.37609054	-1.24778900
C	-0.18017033	0.88997846	-1.84751000
H	0.98899567	2.45507346	-2.76270400
H	3.11588167	1.17163346	-2.47044400
H	3.11250267	-1.05344954	-1.41633400
H	0.97629067	-2.08269354	-0.61206100
C	-4.97123133	-5.37743554	1.86602700
C	-3.58292133	-5.45331454	1.69462100
C	-2.86796133	-4.41621954	1.08747300
C	-3.59588633	-3.31379254	0.66609000
C	-4.97672833	-3.23993654	0.83887000
C	-5.69695833	-4.26178754	1.43667500
H	-5.49138133	-6.20343254	2.34025600
H	-3.05468833	-6.33634454	2.03958500
H	-1.79317133	-4.46692154	0.94830900
H	-6.77267433	-4.18765054	1.55832800
C	-11.96883833	-0.30808854	-3.28047900
O	-11.92905433	-1.39223854	-3.80059900
O	-11.05463233	0.29067346	-2.56135900
H	-10.17702933	-0.28134254	-2.35167600
C	-13.20363033	0.60863846	-3.45125100
F	-14.26905833	-0.07793254	-3.85868400
F	-13.52536033	1.23901746	-2.31153700
F	-12.94171233	1.55414846	-4.37061300

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SCF energy in solution: -3871.162312

Free energy in solution: -3870.402566

C	-6.13695103	2.88089002	0.03771277
C	-4.03712503	3.47157202	0.08288877
C	-8.16523303	3.89113902	0.57440477
C	-8.74644903	5.91769402	1.42753777
H	-6.73764403	5.34947802	1.08606377
C	-7.52877303	7.78340902	2.12310477
C	-5.42371303	8.34001302	2.22267777
C	-1.92438203	7.35402602	1.55415777
C	-1.55553203	6.07353102	0.92446977
C	-3.40611103	7.34544802	1.64067977
C	-2.82199403	5.33663402	0.71972677
H	-4.81540703	5.88296302	1.08426677
N	-4.07753903	8.34031902	2.12844277
N	-2.88481503	4.14188502	0.21202577
N	-7.45221503	2.86628802	0.12751077

N	-8.66618103	7.13338502	1.92388377
N	-7.71614503	5.09467802	1.03347977
N	-6.25618503	7.35097102	1.84952777
N	-3.83580303	6.14819802	1.13447477
N	-5.28285103	3.91244002	0.34208077
N	0.55355397	8.36316502	-0.26537523
N	-0.42264403	5.48224902	0.74995777
C	4.26827197	1.67603702	2.71166177
C	2.94431597	2.07495402	2.52081777
C	5.08970597	2.77513902	2.17827477
C	3.02079497	3.39237002	1.87269277
C	8.65656197	3.65632702	1.79405177
C	9.10317397	4.87662002	1.27158077
C	7.19415097	3.68013702	1.78457077
C	7.92196497	5.67112102	0.93344177
H	5.86983897	5.18603602	1.13516777
C	6.82764997	7.56831102	0.13596277
C	4.76527497	8.22600602	-0.14030623
C	1.24614997	7.31683102	0.23679577
C	0.79361897	6.06289202	0.71579877
C	2.68062597	7.26585602	0.23010377
C	1.97524197	5.27441102	1.00093477
H	4.01382597	5.75702302	0.87334677
N	3.44798497	8.26831502	-0.16370323
N	1.93909797	4.06347302	1.54604377
N	6.43207997	2.70814202	2.21112277
N	7.94506997	6.86843102	0.42942577
N	6.83075097	4.89381802	1.26275777
N	5.55442897	7.18003502	0.28700177
N	3.05539397	6.03293802	0.70513477
N	4.33190097	3.77215902	1.69468077
N	-1.15231203	8.24717602	2.06503077
H	0.31580597	7.87905602	2.83157777
H	-1.72835503	8.95897702	2.52716677
H	-0.28674503	8.64212602	0.22917777
H	1.14366597	9.12483602	-0.58166023
H	-0.68355303	3.49232502	1.55092877
O	-1.90610503	3.72357202	2.97776477
O	-0.98325503	2.90203602	2.26945177
C	9.54930797	2.67492702	2.21438877
C	10.46043697	5.15897702	1.15152077
C	11.35603797	4.17928002	1.57059077
C	10.90730997	2.95447702	2.09463977
H	9.18809097	1.73480602	2.61742777

H	10.79461997	6.10800302	0.74609877
H	12.42303397	4.36129202	1.49290477
H	11.63654097	2.21576202	2.41088777
C	6.91819797	8.92387602	-0.41481623
C	5.59652197	9.34622902	-0.58868623
C	5.30336497	10.60646902	-1.10085823
C	6.37733597	11.42992202	-1.43212123
C	7.70483997	11.00451102	-1.25640123
C	7.99455997	9.74204002	-0.74366823
H	4.27663197	10.93103402	-1.23474323
H	6.18864397	12.42040102	-1.83410023
H	8.51533197	11.67412602	-1.52587823
H	9.01551197	9.40229402	-0.60344123
C	2.18460197	0.07550702	3.54242577
C	1.87291897	1.29513202	2.93536777
C	4.58215297	0.46579402	3.31470777
C	3.51309997	-0.33383598	3.72592277
H	1.38065197	-0.56839198	3.88469777
H	0.84800997	1.63280302	2.80337977
H	5.61359597	0.16250502	3.46121077
H	3.71185197	-1.28844298	4.20284277
C	-5.74888203	10.71745002	3.27524877
C	-6.74527003	11.58422902	3.71484577
C	-8.10362303	11.22582802	3.64763977
C	-8.50148703	9.99212802	3.13990777
C	-7.50240503	9.12726902	2.70024277
C	-6.15067403	9.48395902	2.76716877
H	-4.69880503	10.98684602	3.32489777
H	-6.47338203	12.55454702	4.11809077
H	-8.85298703	11.92760702	4.00002977
H	-9.54707903	9.70713402	3.08511077
C	-11.30926803	5.51278902	1.40847277
C	-12.26562203	4.56500502	1.08045577
C	-11.90387903	3.30604002	0.55164977
C	-10.57673103	2.96937302	0.33988277
C	-9.60795203	3.92303902	0.66959077
C	-9.96805303	5.17788302	1.19647877
H	-11.57737103	6.48193802	1.81548677
H	-13.31657403	4.78995902	1.23163377
H	-12.68444303	2.59239802	0.30853477
H	-10.28525603	2.00609102	-0.06507923
C	-3.40609203	-0.06154898	-1.18749023
C	-4.75624103	-0.44116398	-1.22930323
C	-5.77070203	0.44037102	-0.85180423

C	-5.38591903	1.70924002	-0.43833223
C	-4.04292403	2.08657102	-0.40418623
C	-3.02618303	1.21486702	-0.77019123
H	-2.64553803	-0.77799498	-1.48106323
H	-5.01357303	-1.44319798	-1.55792323
H	-6.81661103	0.15248102	-0.87466823
H	-1.98612503	1.51954602	-0.71903923
C	0.90283397	6.38311002	3.85129177
O	-0.13926403	5.77510602	3.83890877
O	1.13600297	7.56562102	3.33899377
H	-1.31957403	4.19584402	3.59125777
C	2.16380897	5.80981002	4.53466477
F	1.99081797	4.53168402	4.84742177
F	3.23170897	5.91037902	3.73361677
F	2.42344097	6.49304102	5.65724477

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SCF energy in solution: -3192.767616

Free energy in solution: -3192.064452

C	-3.52682961	-0.09043928	0.04616855
C	-4.81999061	0.43310372	0.00374555
C	-2.63576161	1.03098172	-0.28346345
C	-4.66029861	1.84820672	-0.35210245
C	1.45787039	3.02331372	-1.03029345
C	-0.48971261	1.87112072	-0.62724645
C	0.33327039	3.91144672	-1.19464145
H	-1.73434561	3.53179772	-0.98484345
C	-0.51473261	7.38272672	-2.04798345
C	-1.81832061	7.88646572	-2.10342645
C	-0.64936461	5.97482272	-1.66849445
C	-2.68271961	6.75957472	-1.75298745
C	-6.31028961	6.09915572	-1.36154745
C	-6.85634761	4.77727372	-0.96854945
C	-4.82571261	5.92885872	-1.39939245
C	-5.67548561	3.88995972	-0.80538445
H	-3.61162961	4.25803372	-0.99750145
N	-4.02870661	6.89937672	-1.71008745
N	-5.74314861	2.63592272	-0.47754045
N	-1.33004561	0.88590672	-0.32974845
N	0.39952739	5.18933372	-1.52757345
N	-0.79114461	3.16579472	-0.94075745
N	-1.97932361	5.64806272	-1.50049045
N	-4.55337061	4.63686672	-1.05463745

N	-3.36921661	2.17640272	-0.51563045
N	-9.24598261	7.16775472	-0.12517945
N	-8.03174961	4.26365372	-0.90727245
C	-13.33393161	1.01402072	-1.88489945
C	-11.31777061	1.83219472	-1.69174645
C	-16.95451461	1.70359372	-1.71791345
C	-17.49340261	2.95819872	-1.39736145
C	-15.50203061	1.82539772	-1.67685245
C	-16.37842861	3.86647872	-1.15409045
H	-14.29584561	3.49526872	-1.23092845
C	-15.61352961	7.32846672	-0.23513045
C	-14.32355261	7.85120372	-0.09373345
C	-15.42943461	5.92629072	-0.61422445
C	-13.41819961	6.74168372	-0.39485745
C	-9.82339261	6.04881972	-0.58148745
C	-9.26575361	4.79594772	-0.94145245
C	-11.26303261	5.89980372	-0.62818145
C	-10.39109361	3.89766372	-1.17157445
H	-12.46716461	4.23567072	-1.12753845
N	-12.09821261	6.87701872	-0.35523045
N	-10.27887661	2.62217072	-1.50275445
N	-14.66035361	0.84943172	-1.92378745
N	-16.48586861	5.12353272	-0.82741645
N	-15.23150961	3.12312372	-1.33868445
N	-14.12182961	5.60911072	-0.70278045
N	-11.53495661	4.60707772	-0.99774945
N	-12.64915161	2.14447872	-1.61219545
N	-6.93878661	7.15728772	-1.69635545
H	-6.26055161	7.86962172	-1.98701745
H	-9.89602161	7.92244372	0.06294755
H	-8.34302361	7.41171172	-0.54931145
C	-12.42493561	-0.11061128	-2.15966345
C	-11.13769961	0.41372672	-2.03623545
C	-10.00750061	-0.36939528	-2.23116145
C	-10.21338761	-1.71153528	-2.55466045
C	-11.50722561	-2.24099328	-2.67691945
C	-12.63731661	-1.44533428	-2.48123745
H	-9.01324461	0.05539772	-2.13614645
H	-9.35830461	-2.36028828	-2.71707645
H	-11.62784761	-3.28952528	-2.93021745
H	-13.64161561	-1.84523728	-2.57522345
C	-19.68886461	2.07637272	-1.64082245
C	-18.87110361	3.16340172	-1.35418745
C	-17.77354461	0.61319472	-2.00572345

C	-19.14765361	0.81729172	-1.96233145
H	-20.76716261	2.19683272	-1.61725845
H	-19.27690561	4.13815072	-1.10531345
H	-17.34245261	-0.35129128	-2.25215645
H	-19.81944261	-0.00671828	-2.17978845
C	-16.54184561	9.44225172	0.33874755
C	-15.24597561	9.96855872	0.48111955
C	-14.11812861	9.18049372	0.26686055
C	-16.74398161	8.11257072	-0.02161845
H	-17.39692461	10.08738472	0.51407055
H	-15.12656861	11.00981072	0.76360055
H	-13.11576961	9.58179672	0.37528255
H	-17.73954361	7.69579972	-0.13408945
C	-3.29897261	-1.42671128	0.35377155
C	-4.41577761	-2.22009528	0.61849655
C	-5.71547761	-1.69015628	0.57781655
C	-5.93841761	-0.34833028	0.26854255
H	-2.29168761	-1.82899528	0.38501155
H	-4.28054761	-3.26900328	0.86318855
H	-6.55905361	-2.33846028	0.79327955
H	-6.93560261	0.07918172	0.23638355
C	0.94701339	1.75715972	-0.67870445
C	2.83641839	3.23387772	-1.16049145
C	3.67393539	2.15582372	-0.93175045
C	3.16111439	0.88568272	-0.57899745
C	1.80024839	0.67045572	-0.44846545
H	3.22039739	4.21167872	-1.43130345
H	4.74797539	2.28237872	-1.02352245
H	3.85316939	0.06729372	-0.40837045
H	1.39514639	-0.29897628	-0.17823745
C	-0.97524461	10.02436572	-2.71803045
C	0.33504439	9.51837272	-2.66288345
C	0.58449139	8.18966572	-2.32720645
C	-2.07266661	9.21368372	-2.43866445
H	-1.13012961	11.06527572	-2.98355145
H	1.16630839	10.17951072	-2.88694345
H	1.59275839	7.79112072	-2.28248545
H	-3.08752961	9.59579772	-2.47903945

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SCF energy in solution: -3192.73431

Free energy in solution: -3192.030535

C	-7.42894072	0.47803617	0.00000000
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C	-9.43481272	0.31162617	0.84868900
C	-3.91523872	-2.51147183	-0.13688500
C	-5.55952472	-0.90159883	-0.15800300
C	-5.08726572	-3.01178383	0.54898100
H	-6.94793672	-2.07258483	0.90690500
C	-7.65359972	-6.05357883	2.87257400
C	-6.29921672	-4.62701583	1.71726900
C	-8.29977472	-4.77938383	2.56831800
C	-11.54423872	-3.11619483	3.15778900
C	-11.87715172	-1.80652883	2.63118400
C	-10.17038672	-3.40839983	2.68643600
C	-10.66979672	-1.28782083	1.99539000
H	-8.81926872	-2.21577983	1.59415900
N	-9.56743572	-4.52379083	2.95415800
N	-10.55293972	-0.10568283	1.45000000
N	-6.18926172	0.24079617	-0.38794200
N	-5.20524272	-4.19878683	1.10257500
N	-6.02383572	-2.00434783	0.49847800
N	-7.48260472	-3.95599583	1.88610100
N	-9.73483572	-2.29368983	2.02460600
N	-8.27701172	-0.36169583	0.67300400
N	-12.95748672	-4.17987283	2.08524600
N	-13.06443672	-1.23892583	2.53957400
C	-19.32765972	-0.02061983	1.81897800
C	-17.21724872	-0.08205083	2.37755400
C	-22.15387072	-1.87255583	0.35895900
C	-22.05939572	-3.18770983	-0.13278600
C	-20.84351072	-1.49547783	0.84457900
C	-20.69054372	-3.62192583	0.05005500
H	-19.04156972	-2.58707483	0.87369900
C	-18.45734572	-6.47769283	-0.51663500
C	-17.10656372	-6.50996083	-0.15436400
C	-18.94730972	-5.16398983	-0.09560400
C	-16.84307072	-5.21544883	0.47344700
C	-14.02317572	-3.43742683	2.06925300
C	-14.10589272	-2.06533283	2.51205500
C	-15.35090872	-3.76656383	1.51215700
C	-15.48417172	-1.62920283	2.30504600
H	-17.15030172	-2.66402883	1.52847600
N	-15.62528172	-4.90944683	0.95724500
N	-15.95057172	-0.44532783	2.60515300
N	-20.53537072	-0.32368283	1.37572200
N	-20.20643772	-4.79673383	-0.29137100
N	-20.02598672	-2.57012883	0.63571100

N	-17.94570572	-4.44026983	0.49392600
N	-16.16007172	-2.68500883	1.74727500
N	-18.21477072	-0.81796283	1.84088500
N	-11.89107972	-3.58494283	4.37042400
H	-11.48425372	-4.48013683	4.61629900
H	-12.83156272	-3.41451383	4.69903200
H	-13.00866872	-4.98210783	1.45124300
C	-19.02842972	1.30580117	2.37671500
C	-17.67845472	1.26752117	2.72955900
C	-17.03804672	2.36533517	3.29157700
C	-17.80382072	3.51411817	3.49138200
C	-19.16177972	3.55392017	3.13753700
C	-19.79639572	2.44745417	2.57238000
H	-15.98689872	2.32017617	3.55748200
H	-17.34465872	4.39567917	3.92744000
H	-19.72592272	4.46554117	3.30772600
H	-20.84509372	2.46953417	2.29458800
C	-9.36247972	1.66086517	0.27081800
C	-8.08158072	1.76742817	-0.27234300
C	-7.65981472	2.92701917	-0.91085400
C	-8.57185772	3.98059817	-0.98659400
C	-9.86009472	3.87120017	-0.44050800
C	-10.27743772	2.70373617	0.19977700
H	-6.66218272	3.00244517	-1.33083300
H	-8.28264472	4.90444217	-1.47764600
H	-10.54177072	4.71200917	-0.52012600
H	-11.27038872	2.60315917	0.62592600
C	-7.16577372	-8.25330483	3.63881700
C	-5.87436572	-8.15394283	3.09069300
C	-5.45773272	-7.00379583	2.42600400
C	-6.36905872	-5.95547883	2.32540000
C	-8.07434172	-7.20369083	3.53694400
H	-7.45520572	-9.16659483	4.14896000
H	-5.19274872	-8.99290883	3.18943300
H	-4.46366672	-6.91905283	1.99923800
H	-9.07331972	-7.27405883	3.95511100
C	-2.67055472	-3.09581883	-0.39152100
C	-1.73951772	-2.34179083	-1.08836800
C	-2.03297072	-1.03187083	-1.52718400
C	-3.26506972	-0.44875183	-1.27758000
C	-4.20739472	-1.20599483	-0.57432800
H	-2.45468372	-4.10280083	-0.05063100
H	-0.76259472	-2.76260883	-1.30402600
H	-1.27558172	-0.47560683	-2.06999800

H	-3.50332172	0.55627317	-1.60934300
C	-18.27313972	-8.67790083	-1.40348600
C	-16.91556172	-8.71030183	-1.03908800
C	-16.31226572	-7.62531283	-0.40840600
C	-19.06388572	-7.56040483	-1.14762900
H	-18.70935472	-9.54258083	-1.89372300
H	-16.33063472	-9.59861683	-1.25561700
H	-15.26509472	-7.64182383	-0.12417700
H	-20.11226172	-7.52630783	-1.42558900
C	-24.36893972	-3.13718883	-0.70860300
C	-23.17300072	-3.83708083	-0.67456200
C	-23.36241872	-1.17001183	0.32295700
C	-24.46328172	-1.81738983	-0.21512500
H	-25.25436272	-3.60906983	-1.12251200
H	-23.09014872	-4.85115383	-1.05092200
H	-23.42153172	-0.15649083	0.70533000
H	-25.41864572	-1.30461683	-0.26070200

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SCF energy in solution: -3192.785421

Free energy in solution: -3192.078052

C	-6.29198980	1.51162788	0.00000000
C	-8.43479580	1.53757288	0.42049100
C	-4.65429980	-0.13482712	-0.22818400
C	-4.66483680	-2.40066012	-0.09166600
H	-6.40017280	-1.23567912	0.19915400
C	-6.72111880	-5.38556612	0.53001000
C	-8.08309680	-5.34893512	0.84312500
C	-6.31400080	-3.98742212	0.36266100
C	-8.43935580	-3.92851512	0.85162900
C	-11.47474080	-1.88506112	1.53630200
C	-11.50615280	-0.41748812	1.11781300
C	-10.07126480	-2.29481512	1.13670800
C	-10.11345180	-0.00186212	0.88731000
H	-8.36871280	-1.16440212	0.66379200
N	-9.70944580	-3.53441612	1.13754400
N	-9.71940680	1.21378388	0.68752500
N	-5.05662680	1.13245588	-0.22621900
N	-5.08066480	-3.65214212	0.06939700
N	-5.40832580	-1.25353312	-0.00441500
N	-7.39900380	-3.14663312	0.56685200
N	-9.36381980	-1.16247512	0.87375200
N	-7.38943580	0.71446288	0.27854600

N	-12.50947480	-2.57665112	0.79568800
N	-12.56535380	0.26801588	0.88728000
C	-17.21601580	2.90202888	0.64385200
C	-18.94128080	1.44426888	0.32420600
C	-16.77588780	1.49862688	0.60859800
C	-21.93915980	-0.65170512	-0.20121900
C	-21.90240380	-2.04809212	-0.30096800
C	-20.56702980	-0.18635112	-0.00049600
C	-20.50652280	-2.46393312	-0.16382600
H	-18.77112880	-1.28874012	0.13045300
C	-18.78353080	-4.02845912	-0.07078000
C	-16.61859580	-4.00447312	0.20243600
C	-13.68477680	-1.89275712	0.75535800
C	-13.71119680	-0.49956712	0.87287900
C	-15.01991680	-2.34719212	0.54193700
C	-15.07306280	-0.08232612	0.72108100
H	-16.81698880	-1.23134812	0.42873100
N	-15.37516680	-3.61411912	0.39213500
N	-15.51413580	1.17288888	0.75600700
N	-20.21856480	1.06423888	0.13525200
N	-20.08467080	-3.69260012	-0.20529900
N	-19.77678880	-1.30710012	0.01090700
N	-17.74201980	-3.20921012	0.12696100
N	-15.81257680	-1.21833012	0.53823400
N	-17.85627080	0.66232688	0.41204800
N	-11.53550480	-1.96215512	2.98133000
H	-11.41520880	-2.92130512	3.29755800
H	-12.41244880	-1.59080312	3.33701100
H	-12.50273680	-3.58926312	0.75550100
C	-18.32377880	-7.80223412	-0.32589000
C	-16.92964280	-7.78747712	-0.15158800
C	-16.23575580	-6.59354512	0.03451900
C	-16.97790380	-5.41653112	0.04113800
C	-18.36481480	-5.43230712	-0.13350700
C	-19.06298480	-6.62139612	-0.31968900
H	-18.82937780	-8.75200312	-0.46829300
H	-16.38577380	-8.72680312	-0.16368500
H	-15.15897780	-6.57558412	0.16778500
H	-20.13971280	-6.61997412	-0.45440400
C	-8.12608580	-7.72321812	0.97911300
C	-6.75752580	-7.76065012	0.66383500
C	-6.03421680	-6.59148912	0.43483500
C	-8.81003180	-6.51275512	1.07381900
H	-8.65576380	-8.65478812	1.15105600

H	-6.25672480	-8.72149212	0.59844200
H	-4.97697580	-6.61195312	0.19142400
H	-9.86683580	-6.47321812	1.31737500
C	-8.05443380	2.94229688	0.24055300
C	-6.68397280	2.92628888	-0.02568600
C	-5.97876080	4.10296488	-0.25160500
C	-6.69693580	5.29743388	-0.20079100
C	-8.07574880	5.31094888	0.06598800
C	-8.77856280	4.12806188	0.29120300
H	-4.91374080	4.08440188	-0.45845500
H	-6.18282280	6.23821388	-0.37115400
H	-8.59974680	6.26095888	0.09588200
H	-9.84409480	4.12071688	0.49670600
C	-3.31840280	-1.99569012	-0.39634200
C	-2.14470380	-2.73634312	-0.59659500
C	-0.98551880	-2.03706712	-0.87831900
C	-0.97866180	-0.62365012	-0.96243300
C	-2.13142480	0.11441188	-0.76608000
C	-3.31131980	-0.58674812	-0.47972000
H	-2.15993380	-3.81905812	-0.52996100
H	-0.05827980	-2.57776412	-1.03919400
H	-0.04655480	-0.11460812	-1.18595700
H	-2.13738880	1.19750088	-0.82812900
C	-18.59932880	2.86843688	0.46350900
C	-16.53242780	4.09942588	0.80979900
C	-17.28950980	5.27176288	0.78919600
C	-18.68056780	5.23872988	0.60827500
C	-19.35960180	4.03092288	0.44173700
H	-15.45608680	4.11136988	0.94735800
H	-16.79550080	6.23007588	0.91464100
H	-19.23529980	6.17155388	0.59767100
H	-20.43479080	3.99363988	0.30051600
C	-23.06318880	-2.79070812	-0.49603500
C	-23.13638880	0.05217788	-0.29306900
C	-24.29849680	-0.68788112	-0.48830900
C	-24.26201480	-2.08972712	-0.58828400
H	-23.02205380	-3.87204912	-0.57165200
H	-23.14916480	1.13400588	-0.21400700
H	-25.25272080	-0.17695812	-0.56547300
H	-25.18917980	-2.63277812	-0.74036100

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SCF energy in solution: -3719.617496

Free energy in solution: -3718.879745

C	-6.42118876	-1.45982319	-0.01911006
C	-8.58121376	-1.50422419	0.29897194
C	-4.73850376	-3.04459819	-0.35354006
C	-4.71079576	-5.30932819	-0.51584506
H	-6.48014376	-4.22090219	-0.16073106
C	-6.76408376	-8.36264419	-0.49141306
C	-8.14230776	-8.37117219	-0.25931406
C	-6.35447976	-6.95712119	-0.38915806
C	-8.49894376	-6.97669919	-0.00186306
C	-11.56572976	-5.08809519	0.94614494
C	-11.62804376	-3.58099019	0.70565894
C	-10.15514876	-5.42388819	0.49999594
C	-10.24575376	-3.11131919	0.52945194
H	-8.47587676	-4.20292619	0.17895694
N	-9.77295276	-6.64209619	0.32707194
N	-9.86761276	-1.87499219	0.48554994
N	-5.16697476	-1.79585419	-0.22105706
N	-5.11118376	-6.57549619	-0.56209606
N	-5.47986676	-4.19488319	-0.31550806
N	-7.45067076	-6.15889619	-0.09561906
N	-9.46976776	-4.25033119	0.39350794
N	-7.51548676	-2.29515319	0.11377094
N	-12.60282876	-5.73211119	0.20430494
N	-12.70623576	-2.89397819	0.58257894
C	-17.41587776	-0.34606219	0.67538094
C	-19.11429976	-1.81408519	0.26804294
C	-16.94377176	-1.72946419	0.50709494
C	-22.08485576	-3.92377219	-0.36260706
C	-22.02466576	-5.30605419	-0.57507906
C	-20.71579976	-3.44732519	-0.15570006
C	-20.61703476	-5.70379019	-0.50356906
H	-18.89658676	-4.52262419	-0.15847806
C	-18.86254876	-7.23267919	-0.56992506
C	-16.69250776	-7.17911319	-0.35348306
C	-13.78842676	-5.05801519	0.26982194
C	-13.83615776	-3.67882419	0.51253494
C	-15.11732876	-5.51584619	0.05689394
C	-15.20860676	-3.27628819	0.43511794
H	-16.93665376	-4.43062319	0.09266294
N	-15.45672076	-6.77646119	-0.17784606
N	-15.67380576	-2.03705919	0.59414894
N	-20.38979676	-2.20635719	0.07567894
N	-20.17606076	-6.91623519	-0.64924906

N	-19.90456076	-4.54927119	-0.25418006
N	-17.83777476	-6.40426519	-0.34478006
N	-15.92947276	-4.40636919	0.17357694
N	-18.01249376	-2.57314519	0.26273894
N	-11.67407976	-5.43919319	2.39112394
H	-12.58067176	-5.11866819	2.73579694
H	-10.96298376	-4.94632419	2.93422694
H	-12.59240776	-6.75360919	0.16987194
C	-18.32711676	-10.97313619	-1.06984606
C	-16.93035276	-10.93675919	-0.92439306
C	-16.25660576	-9.74032519	-0.68317906
C	-17.02738476	-8.58600919	-0.59396206
C	-18.41708176	-8.62148519	-0.73538906
C	-19.09365176	-9.81266819	-0.97637706
H	-18.81475176	-11.92461119	-1.25675406
H	-16.36692076	-11.86137319	-1.00069606
H	-15.17800476	-9.70281819	-0.56563606
H	-20.17318976	-9.83002419	-1.08485606
C	-8.20254176	-10.72395319	-0.57944906
C	-6.81532376	-10.72112219	-0.79867906
C	-6.07498376	-9.53917919	-0.76427506
C	-8.89053176	-9.54198319	-0.31074606
H	-8.74721676	-11.66169819	-0.62309106
H	-6.31209076	-11.66046619	-1.00503506
H	-5.00481876	-9.53085019	-0.94329206
H	-9.96699476	-9.52728419	-0.16879306
C	-8.21726776	-0.08531619	0.29151094
C	-6.83521976	-0.05686419	0.09162194
C	-6.13903576	1.14558881	0.02959294
C	-6.87751976	2.31912181	0.17453394
C	-8.26786476	2.28845781	0.37414694
C	-8.96139876	1.08105681	0.43592394
H	-5.06533776	1.16111181	-0.12636706
H	-6.37135376	3.27844381	0.13159594
H	-8.80789576	3.22389081	0.48054694
H	-10.03526476	1.04106881	0.58723294
C	-3.35751376	-4.85000019	-0.69065706
C	-2.16232576	-5.54348319	-0.92545606
C	-1.00370876	-4.79844219	-1.05163106
C	-1.02031576	-3.38696719	-0.94877506
C	-2.19592076	-2.69532419	-0.71804806
C	-3.37404276	-3.44296519	-0.58783506
H	-2.16058376	-6.62553519	-1.00325406
H	-0.05938876	-5.30137819	-1.23375306

H	-0.08827476	-2.84101319	-1.05434406
H	-2.21953576	-1.61365619	-0.63848206
C	-18.80196976	-0.39904019	0.52343394
C	-16.75746376	0.84975481	0.92993294
C	-17.54251776	1.99960281	1.02902594
C	-18.93630776	1.94672781	0.87695594
C	-19.59007876	0.74076581	0.62036394
H	-15.67865576	0.87803281	1.04362594
H	-17.06851776	2.95582381	1.22680994
H	-19.51312476	2.86230681	0.96049994
H	-20.66715676	0.68791381	0.50015294
C	-23.17471476	-6.05489819	-0.80216906
C	-23.29610976	-3.23958819	-0.36960006
C	-24.44909576	-3.98584519	-0.59711306
C	-24.38891376	-5.37352919	-0.81020506
H	-23.11472076	-7.12565219	-0.96520006
H	-23.32734276	-2.16808019	-0.20335706
H	-25.41427176	-3.49012419	-0.61087106
H	-25.30908176	-5.92184919	-0.98409206
C	-11.31531776	-10.31919319	2.32249194
F	-11.45840776	-11.12749119	1.27227194
F	-12.14647676	-10.73660419	3.28806994
F	-10.06468676	-10.43248619	2.77307194
C	-11.65344876	-8.86001619	1.93968194
O	-12.23710076	-8.61323519	0.90987894
O	-11.26022776	-8.03526019	2.86813694
H	-11.45905276	-7.05901319	2.63000494

TS22

SCF energy in solution: -3719.59916

Free energy in solution: -3718.862216

C	-4.32816546	1.87338499	0.00000000
C	-2.16207046	1.87079499	0.27429600
C	-5.99123446	3.49520599	-0.21504900
C	-5.98422046	5.76644699	-0.26447300
H	-4.22466046	4.62981499	-0.01391600
C	-4.30766646	7.37885399	-0.10599700
C	-2.15255046	7.35724099	0.21414300
C	0.89781654	5.35618699	0.93302300
C	0.91523154	3.87669499	0.73198200
C	-0.50951446	5.75580499	0.57953500
C	-0.46786146	3.44309499	0.53930300
H	-2.22432046	4.58011999	0.26165300

N	-0.87466546	6.98922399	0.47545100
N	-0.87227146	2.21242899	0.45354500
N	-5.58445146	2.23530699	-0.15546900
N	-5.56563846	7.02246099	-0.25963800
N	-5.22935646	4.62896599	-0.14004200
N	-3.21859746	6.55586699	0.11210200
N	-1.22662846	4.59868999	0.45879800
N	-3.22377846	2.68497099	0.14870200
N	1.95940254	6.07024399	0.40693100
N	2.00105754	3.17138499	0.65416100
C	8.38869754	1.99946499	0.31583300
C	6.21894554	1.95161099	0.56258600
C	10.01171354	3.62014199	-0.07879600
C	9.94680354	5.88054099	-0.38365100
H	8.21000154	4.72107599	-0.05582000
C	8.21726254	7.43889999	-0.42494100
C	6.04902454	7.40299099	-0.20091100
C	3.08471954	5.33595299	0.43296300
C	3.12337454	3.93850699	0.64177300
C	4.43962354	5.77176399	0.20156800
C	4.49870854	3.51587599	0.54020200
H	6.23690154	4.65639099	0.20382600
N	4.79680054	7.01894999	-0.01543500
N	4.94399154	2.27651899	0.66738600
N	9.65999154	2.37543599	0.12920200
N	9.51614754	7.10517299	-0.50899300
N	9.21812654	4.73414999	-0.15395800
N	7.17149554	6.61761999	-0.20284100
N	5.22860254	4.64632199	0.29413400
N	7.28791654	2.77873799	0.33351000
N	0.95193754	5.61495499	2.61391200
H	0.13367454	5.26537999	3.11436300
H	1.78947854	5.15525499	2.97520900
C	1.62651554	9.00869599	1.62337300
O	1.91233754	8.61711299	0.43801800
O	1.33471954	8.34370599	2.60836700
H	1.04870854	6.65240799	2.71884700
C	1.73698254	10.54382499	1.78410100
F	3.01076154	10.87332999	2.04275600
F	0.98152554	10.97790199	2.78968000
F	1.36495954	11.18852099	0.67195000
H	1.92796354	7.53434799	0.36310300
C	7.78356354	8.83150899	-0.57772800
C	6.39329054	8.80614799	-0.43516100

C	8.46594454	10.02124099	-0.81303200
C	5.62768654	9.96458599	-0.52271200
C	7.70568254	11.18601799	-0.89976000
H	9.54542554	10.03386599	-0.92308700
C	6.30772754	11.15797199	-0.75682200
H	4.54827054	9.92871799	-0.41306800
H	8.19912254	12.13562899	-1.08135400
H	5.74963054	12.08603899	-0.83046500
C	11.38275354	4.07674599	-0.27714300
C	11.34320654	5.46596799	-0.46354500
C	12.58664554	3.37521999	-0.29910500
C	12.50767354	6.20064599	-0.67788500
C	13.74866554	4.10723699	-0.51341200
H	12.60220254	2.30031699	-0.15362400
C	13.70927554	5.50180999	-0.70015700
H	12.46452754	7.27513299	-0.82063800
H	14.70654154	3.59785699	-0.53803000
H	14.63793954	6.03873199	-0.86456900
C	6.66278954	0.55689799	0.69747700
C	8.04958854	0.58676199	0.54102800
C	5.98140554	-0.63191001	0.92741300
C	8.81451954	-0.57145801	0.60958800
C	6.74319154	-1.79862201	0.99761200
H	4.90255254	-0.64128601	1.04414300
C	8.13789354	-1.76919901	0.84144700
H	9.89205654	-0.53748001	0.48639800
H	6.25129154	-2.74976701	1.17524700
H	8.69680454	-2.69766901	0.90217300
C	-3.93459646	0.45975399	0.03303100
C	-2.54895646	0.45846499	0.20551100
C	-4.65105846	-0.72728601	-0.07267000
C	-1.82042846	-0.72378701	0.27825600
C	-3.92810646	-1.91748201	-0.00011700
H	-5.72770246	-0.71939301	-0.20739500
C	-2.53414446	-1.91671301	0.17227900
H	-0.74326446	-0.70700001	0.40914900
H	-4.44988746	-2.86604501	-0.07929900
H	-2.00670946	-2.86394601	0.22230200
C	-7.35191546	5.33642699	-0.42390800
C	-7.35660246	3.92726499	-0.39194600
C	-8.53980546	6.05922399	-0.59019000
C	-8.54840846	3.20451899	-0.52627400
C	-9.71463046	5.33876999	-0.72077700
H	-8.52554446	7.14369599	-0.61394800

C	-9.71915346	3.92499599	-0.68918800
H	-8.54003346	2.11998999	-0.50160300
H	-10.65482146	5.86505299	-0.85091000
H	-10.66254046	3.39921499	-0.79588000
C	-2.50192646	8.76531999	0.04316900
C	-3.88614446	8.78225499	-0.14985100
C	-1.74372046	9.93100499	0.03137500
C	-4.56971146	9.97830199	-0.34462600
C	-2.42444646	11.13080799	-0.16209300
H	-0.66557346	9.89782199	0.14362400
C	-3.81774546	11.15251599	-0.34322100
H	-5.64439446	9.98927799	-0.49409500
H	-1.87015446	12.06375299	-0.17814100
H	-4.31546046	12.10567599	-0.49148500

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SCF energy in solution: -3719.627963

Free energy in solution: -3718.899452

C	-7.17054278	1.38242892	0.00000000
C	-9.34844978	1.41834792	-0.13338800
C	-5.50074878	-0.24149608	0.00367500
C	-5.51283278	-2.51556508	-0.14894800
H	-7.28177778	-1.36426708	-0.18547300
C	-7.20203178	-4.09620108	-0.39392200
C	-9.37289278	-4.06451708	-0.57987700
C	-12.41221978	-2.01292808	-0.53376700
C	-12.43012178	-0.58783908	-0.41519900
C	-11.03112478	-2.43845908	-0.56041300
C	-11.04128478	-0.15601508	-0.36243000
H	-9.27377278	-1.28899308	-0.42989900
N	-10.64324378	-3.69040208	-0.63619200
N	-10.62788478	1.08315292	-0.22976100
N	-5.88919478	1.00824492	0.06149300
N	-5.91612778	-3.75684208	-0.26416900
N	-6.27045278	-1.37085008	-0.12312500
N	-8.27514178	-3.27013208	-0.43046300
N	-10.28744878	-1.29524208	-0.47105200
N	-8.26156278	0.59193592	-0.13562400
N	-13.49639178	-2.76952008	-0.55058100
N	-13.53110578	0.13984892	-0.32752500
C	-19.91929678	1.24105692	0.02882400
C	-17.74098578	1.32708792	-0.07473000
C	-21.55830178	-0.41273508	0.02316600

C	-21.49727078	-2.69058708	-0.09192200
H	-19.75207778	-1.50228908	-0.12420200
C	-19.76845378	-4.23837508	-0.25454100
C	-17.59325078	-4.17742008	-0.37956400
C	-14.61284978	-2.04441508	-0.44801700
C	-14.62752478	-0.62227608	-0.34896000
C	-15.97408078	-2.50808908	-0.40212300
C	-16.01576578	-0.22124108	-0.25709400
H	-17.75914278	-1.39950508	-0.23903900
N	-16.33973778	-3.77609408	-0.44054500
N	-16.46227478	1.01712192	-0.15733300
N	-21.20111278	0.84173892	0.07099800
N	-21.07136378	-3.92198408	-0.17021100
N	-20.76344478	-1.52900508	-0.07342600
N	-18.71814978	-3.39655208	-0.28440100
N	-16.74641678	-1.38220308	-0.29341900
N	-18.81796978	0.47354492	-0.07163700
N	-11.62717878	-1.83872208	2.36074800
H	-10.70527178	-1.79429908	2.78542800
H	-12.26179978	-1.35535908	2.98937500
C	-12.85260178	-5.64463708	1.00641000
O	-13.35065978	-5.46946808	-0.18839400
O	-12.47310178	-4.81234708	1.79210700
H	-11.90280478	-2.81960708	2.34370900
C	-12.85331178	-7.14335308	1.38602800
F	-14.08766378	-7.50245408	1.77335400
F	-12.01454878	-7.38345908	2.38784400
F	-12.51086578	-7.92454608	0.35318600
H	-13.40648478	-4.48376708	-0.39560800
C	-19.33927378	-5.64145308	-0.32829700
C	-17.94561778	-5.60073008	-0.40745200
C	-20.03098178	-6.84719608	-0.32519100
C	-17.18243978	-6.75976208	-0.48443100
C	-19.27305578	-8.01568708	-0.40289900
H	-21.11399778	-6.87098008	-0.26303600
C	-17.87177378	-7.97240708	-0.48030600
H	-16.09937478	-6.71364208	-0.54141500
H	-19.77273978	-8.97919508	-0.40195100
H	-17.31579678	-8.90287308	-0.53599200
C	-22.93665078	-0.89296108	0.06889600
C	-22.89931078	-2.29218208	-0.00134100
C	-24.14272678	-0.20335308	0.16474800
C	-24.06696378	-3.05074308	0.02151400
C	-25.31002578	-0.95925108	0.18752800

H	-24.15751278	0.87996092	0.21880500
C	-25.27265878	-2.36369808	0.11686000
H	-24.02450478	-4.13327308	-0.03335100
H	-26.27041178	-0.45947608	0.26136900
H	-26.20497678	-2.91857808	0.13769700
C	-18.18530078	2.72182592	0.03045300
C	-19.57896178	2.66801192	0.09574700
C	-17.50040378	3.93065292	0.06910600
C	-20.34747578	3.82161192	0.20276400
C	-18.26573578	5.09159692	0.17643500
H	-16.41683478	3.95844492	0.01764900
C	-19.66738878	5.03844392	0.24215500
H	-21.43009978	3.76947492	0.25312300
H	-17.77160178	6.05741292	0.21020000
H	-20.22848478	5.96380092	0.32535700
C	-7.54637678	2.79853392	0.08916100
C	-8.94037878	2.82020692	0.00679300
C	-6.80892278	3.96895292	0.23104700
C	-9.65572378	4.01114592	0.06241600
C	-7.51943478	5.16736092	0.28638100
H	-5.72604878	3.94264992	0.29505000
C	-8.92141278	5.18796292	0.20359400
H	-10.73900378	4.01278392	-0.00160800
H	-6.98238178	6.10427192	0.39575100
H	-9.43959878	6.14051592	0.25138200
C	-4.12533478	-2.09259408	-0.02509500
C	-4.11781578	-0.69227808	0.06752800
C	-2.94036078	-2.82722908	0.00624100
C	-2.92505078	0.01904392	0.19499800
C	-1.75235578	-2.11845708	0.13379300
H	-2.95945878	-3.90938408	-0.06679600
C	-1.74482178	-0.71296008	0.22694900
H	-2.93255178	1.10151792	0.26548700
H	-0.80911878	-2.65429608	0.16264300
H	-0.79591078	-0.19568808	0.32542500
C	-8.99675878	-5.47778908	-0.65325200
C	-7.60633078	-5.50214508	-0.52486700
C	-9.73970478	-6.64157908	-0.80986900
C	-6.90111978	-6.70050308	-0.53622000
C	-9.03808478	-7.84642908	-0.81589400
H	-10.81783478	-6.60605008	-0.93235200
C	-7.64044578	-7.87470908	-0.68015400
H	-5.82085478	-6.71481508	-0.43481600
H	-9.58059178	-8.77989808	-0.92774500

H	-7.12822178	-8.83158408	-0.68963000
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SCF energy in solution: -3136.238359

Free energy in solution: -3135.569237

C	-3.13953495	0.58134552	-0.00761020
C	-1.74314095	0.58545652	-0.00760820
C	-3.52680195	-0.83450148	-0.00762220
C	-1.34544595	-0.82664748	-0.00762020
C	-6.60380395	-2.87589248	-0.00765020
C	-6.60364095	-4.27872848	-0.00764720
C	-5.21375495	-2.43742548	-0.00763820
C	-5.21352695	-4.71677448	-0.00763320
H	-3.43493295	-3.57726848	-0.00763120
C	-3.13880695	-7.73531248	-0.00756420
C	-1.74244095	-7.73905748	-0.00762320
C	-3.52648595	-6.31945248	-0.00758220
C	-1.34513495	-6.32668048	-0.00764620
C	1.72746005	-4.29156948	-0.00765920
C	1.72761205	-2.86155548	-0.00765320
C	0.34238905	-4.72466748	-0.00765620
C	0.34254205	-2.42836548	-0.00764020
H	-1.42293295	-3.57613048	-0.00767720
N	-0.07019295	-5.97412748	-0.00766620
N	-0.07059695	-1.17928748	-0.00762820
N	-4.81749295	-1.19091948	-0.00763520
N	-4.81704895	-5.96340248	-0.00762320
N	-4.44830995	-3.57718248	-0.00763420
N	-2.44340895	-5.51122548	-0.00752320
N	-0.40802395	-3.57666848	-0.00765820
N	-2.44370895	-1.64249848	-0.00760120
N	2.82431605	-5.04120748	-0.00766420
N	2.82468605	-2.11202348	-0.00765120
C	8.78847805	0.58133552	-0.00763420
C	7.39210405	0.58548552	-0.00763920
C	9.17568705	-0.83460048	-0.00762520
C	6.99429805	-0.82672348	-0.00763320
C	12.25305305	-2.87572948	-0.00761920
C	12.25299805	-4.27841248	-0.00762620
C	10.86273505	-2.43726648	-0.00762620
C	10.86263005	-4.71678048	-0.00763920
H	9.08396805	-3.57687048	-0.00764920
C	8.78814105	-7.73519348	-0.00764020

C	7.39178005	-7.73928348	-0.00764720
C	9.17539605	-6.31927648	-0.00765820
C	6.99400005	-6.32710248	-0.00766820
C	3.92179405	-4.29177548	-0.00765920
C	3.92197305	-2.86171248	-0.00765320
C	5.30640005	-4.72489948	-0.00766120
C	5.30663005	-2.42880648	-0.00764820
H	7.07197105	-3.57719448	-0.00765820
N	5.71964205	-5.97439848	-0.00766920
N	5.71986205	-1.17923748	-0.00763920
N	10.46671005	-1.19086948	-0.00762120
N	10.46650705	-5.96311048	-0.00764920
N	10.09735305	-3.57695948	-0.00763920
N	8.09286205	-5.51126748	-0.00762720
N	6.05707905	-3.57687848	-0.00765620
N	8.09304905	-1.64257748	-0.00764520
C	9.51903105	1.76446252	-0.00763520
C	6.66671305	1.77144352	-0.00764520
C	-1.01764995	1.77141152	-0.00760120
C	-3.86995695	1.76459952	-0.00760520
C	-7.79449295	-2.15132748	-0.00766120
C	-7.79415295	-5.00359348	-0.00765520
C	-3.86899295	-8.91865948	-0.00753220
C	-1.01665595	-8.92479348	-0.00763820
C	6.66633305	-8.92522648	-0.00764020
C	9.51864705	-8.91835748	-0.00762520
C	13.44341305	-5.00322948	-0.00762220
C	13.44352005	-2.15099548	-0.00760620
C	8.79836505	2.95809052	-0.00761520
H	9.32908705	3.90488952	-0.00760220
C	7.39391505	2.96118452	-0.00762020
H	6.86791705	3.91063652	-0.00761120
C	-1.74472395	2.96116852	-0.00763020
H	-1.21869495	3.91060352	-0.00764320
C	-3.14922395	2.95813352	-0.00763220
H	-3.67987495	3.90497552	-0.00764620
C	-8.98183595	-2.87367648	-0.00767320
H	-9.93011995	-2.34606248	-0.00768420
C	-8.98167495	-4.28154848	-0.00767020
H	-9.92983395	-4.80938248	-0.00767820
C	-3.14794695	-10.11205848	-0.00755420
H	-3.67836695	-11.05903048	-0.00753220
C	-1.74349295	-10.11475148	-0.00760520
H	-1.21722595	-11.06405448	-0.00761920

C	7.39347705	-10.11498648	-0.00767920
H	6.86744805	-11.06442148	-0.00770020
C	8.79794005	-10.11194748	-0.00767120
H	9.32861805	-11.05877148	-0.00768820
C	14.63096805	-4.28103448	-0.00760220
H	15.57914905	-4.80882948	-0.00759520
C	14.63102205	-2.87327448	-0.00759520
H	15.57924305	-2.34555148	-0.00758120
H	-4.95496795	1.75140652	-0.00760620
H	0.06746905	1.75979552	-0.00760020
H	5.58159305	1.75992952	-0.00764920
H	10.60404005	1.75119252	-0.00763220
H	13.42998505	-1.06627648	-0.00760120
H	13.42980505	-6.08794748	-0.00762720
H	10.60365605	-8.90511748	-0.00761820
H	5.58121405	-8.91366948	-0.00764420
H	0.06846005	-8.91293848	-0.00767320
H	-4.95400595	-8.90572048	-0.00749120
H	-7.78045995	-6.08831348	-0.00765220
H	-7.78110195	-1.06660448	-0.00766520

TS2'

SCF energy in solution: -3250.959923

Free energy in solution: -3250.173967

C	-4.54907155	-0.54376657	0.00000000
C	-2.27932355	-0.43658957	0.20006500
C	-4.06758355	0.80058343	0.25732200
C	1.40904945	-0.52136757	0.51046700
C	0.01431745	-0.10530957	0.48747700
C	1.26956245	1.72375843	1.02063400
H	-0.82665055	1.80497243	0.86350100
C	1.26320245	5.29049743	1.89977700
C	0.11883945	6.08234443	1.98680100
C	0.79030345	3.95022543	1.50450100
C	-1.00529055	5.19480643	1.63019700
C	-4.63532755	5.26868443	1.32244800
C	-5.43425855	4.17017243	0.86517500
C	-3.28192955	4.87087143	1.27338500
C	-4.46314755	3.05929143	0.64223700
H	-2.35485355	3.02382143	0.80719600
N	-2.24951355	5.64255743	1.61761200
N	-4.89231255	1.86112043	0.38152300
N	-1.00809355	-0.86739157	0.23180100

N	1.64562045	2.94879843	1.34958500
N	0.01551945	1.24861943	0.79826500
N	-0.55781455	3.93586343	1.35079600
N	-3.20833155	3.56617943	0.83147200
N	-2.71869055	0.83652043	0.37303500
N	-8.06549155	6.29760843	0.78839300
N	-6.57651955	3.65885343	1.81427300
C	-10.30808955	-1.45158957	2.33710500
C	-9.10242455	-0.74771657	2.36060500
C	-11.34647855	-0.44815157	2.03941100
C	-9.46225655	0.65206343	2.07417400
C	-15.01862855	-0.32387457	1.58085400
C	-13.59376955	0.02159743	1.66587100
C	-14.73560855	1.92780043	1.12302500
H	-12.63127455	1.87743743	1.36656500
C	-14.47848855	5.49725643	0.35376700
C	-13.29713455	6.24068243	0.34147300
C	-14.08133055	4.13031543	0.72558200
C	-12.23076055	5.29386143	0.70832900
C	-8.63485055	5.09938243	1.21202700
C	-7.97668655	3.91752343	1.56210200
C	-10.00695555	4.76752343	1.13978900
C	-8.92043455	2.88277143	1.70562000
H	-11.01280355	2.93782743	1.47028600
N	-10.97918555	5.63301943	0.79723300
N	-8.58469355	1.60990743	2.00381400
N	-12.64635155	-0.81976657	1.95409500
N	-15.02336455	3.15300543	0.82338000
N	-13.50189155	1.36358743	1.38241300
N	-12.77506255	4.02387243	0.93056500
N	-10.13221555	3.43256943	1.44813600
N	-10.83605955	0.77118743	1.88641400
N	-5.17492355	6.50988043	1.77353300
H	-4.87625655	7.28003643	1.17754700
H	-4.83150955	6.73746643	2.70395300
H	-7.30148055	6.63962943	1.37724300
H	-8.77408955	7.00310943	0.60878300
N	-6.27333755	4.42346743	-0.50617200
H	-5.56460355	4.69667843	-1.18883800
H	-6.72499055	3.56071243	-0.83084600
H	-6.48026355	2.62200843	1.82651900
H	-6.96334855	5.19966843	-0.40070200
C	2.00607145	-1.75892457	0.27413200
C	2.18111245	0.60532243	0.83626900

C	3.57042945	0.53311943	0.93777900
C	4.16383445	-0.70038557	0.70272100
C	3.39022445	-1.83084957	0.37527600
H	1.40388845	-2.62516957	0.02213800
H	4.15278345	1.41267443	1.19059600
H	5.24200245	-0.79976557	0.77125900
H	3.89020345	-2.77766757	0.19869500
C	-5.90059955	-2.46482657	-0.40305100
C	-5.81932055	-1.09506057	-0.18336500
C	-3.39444955	-1.34322557	-0.04051000
C	-3.47791855	-2.71835957	-0.26436400
C	-4.74264255	-3.26683857	-0.44440800
H	-6.87233155	-2.92855757	-0.54374500
H	-6.71144055	-0.47545757	-0.14716600
H	-2.58248855	-3.33062557	-0.29420500
H	-4.84490855	-4.33266657	-0.62194600
C	-15.67101755	-1.53371257	1.77249100
C	-17.05832055	-1.53864857	1.61987400
C	-17.75843655	-0.37052557	1.28764300
C	-17.09605255	0.84327843	1.09654700
C	-15.71714055	0.84152443	1.24962200
H	-15.11818555	-2.43062057	2.03009800
H	-17.60827855	-2.46310357	1.76064000
H	-18.83686855	-0.41356057	1.17766900
H	-17.62736555	1.75334143	0.83980800
C	-7.93644555	-2.76567757	2.82080300
C	-9.14576755	-3.47013957	2.80021200
C	-10.35964855	-2.81946457	2.55650900
C	-7.89537455	-1.38453057	2.60253000
H	-7.01089155	-3.30224257	3.00247800
H	-9.13804255	-4.54097157	2.97473000
H	-11.30218755	-3.35616257	2.53610500
H	-6.95583755	-0.84108957	2.60844500
C	0.18724645	7.42061143	2.34521000
C	1.45403245	7.94425243	2.61725900
C	2.60335845	7.14764643	2.53017800
C	2.52491245	5.80025643	2.16837400
H	-0.70777455	8.03054843	2.40979100
H	1.55315745	8.98682943	2.90169500
H	3.57064845	7.58826743	2.74865500
H	3.40795945	5.17387043	2.09849500
C	-15.70768855	6.06820143	0.05383400
C	-15.71647755	7.42791943	-0.26317400
C	-14.53167155	8.17629743	-0.27526900

C	-13.29933555	7.59246843	0.02810200
H	-16.61793055	5.47818743	0.06774200
H	-16.65455655	7.91689343	-0.50388400
H	-14.57585255	9.23132243	-0.52533900
H	-12.38139855	8.17068343	0.02076600
H	-6.28996955	4.00149243	2.73812400

3'

SCF energy in solution: -3194.44236022

Free energy in solution: -3193.577416

C	-2.93103444	1.63129971	0.00000000
C	-5.04199944	1.81444771	0.85389000
C	-3.56571244	2.92045171	-0.31052200
C	-8.41563744	1.81465571	2.37321300
C	-7.19502644	2.18316471	1.64720800
C	-8.64917444	3.94214671	1.49139000
H	-6.72366044	3.95496971	0.60369100
C	-9.20786144	7.31206271	0.17039000
C	-8.29346144	8.04737671	-0.58698700
C	-8.53885044	6.03740471	0.46782000
C	-7.10725344	7.18823071	-0.71772300
C	-3.77824244	7.11503871	-2.21126200
C	-2.93067544	6.02090671	-2.06714200
C	-4.95542944	6.76661171	-1.48673600
C	-3.54664844	5.02551771	-1.28971000
H	-5.46243244	5.02570671	-0.40660200
N	-6.03763844	7.54821171	-1.37171000
N	-2.97054644	3.84370371	-1.01089300
N	-6.14675244	1.42076671	1.52703600
N	-9.17808844	5.08723971	1.20014300
N	-7.40414244	3.44812171	1.15389300
N	-7.31783544	5.97879971	-0.05350500
N	-4.76900444	5.51065771	-0.95826100
N	-4.83922444	2.97782971	0.23564000
N	-1.03533144	8.56566471	-1.19078000
N	-1.61952144	5.80325371	-2.65065900
C	2.72316756	1.25008571	-1.67053400
C	1.56200156	1.80348971	-2.21265900
C	3.37585056	2.34535771	-0.92963700
C	1.55208756	3.20833571	-1.76492200
C	6.45092356	2.88217571	1.06171700
C	5.16057256	3.05502171	0.38241600
C	5.68634656	5.04342971	1.38300100

H	3.90788656	4.75293871	0.27001000
C	4.62437456	8.48934871	2.01475200
C	3.44993956	9.07367971	1.53799000
C	4.62003856	7.11340371	1.49324300
C	2.78190356	8.02865371	0.74370700
C	-0.23030344	7.41748871	-1.20724500
C	-0.47716444	6.20838571	-1.84554700
C	1.03056756	7.25875371	-0.58017600
C	0.57439456	5.31145071	-1.60197600
H	2.35667756	5.61693371	-0.51612900
N	1.64352756	8.21325471	0.14472700
N	0.59328456	4.03935471	-2.05177400
N	4.55333756	2.12778071	-0.29537000
N	5.64584256	6.27068871	1.79140600
N	4.76931756	4.35205071	0.61641800
N	3.54833256	6.85841071	0.75429100
N	1.47746856	5.98844971	-0.84560700
N	2.68030156	3.47580371	-0.99432000
N	-3.58110844	8.25507071	-2.96302400
H	-2.70262644	8.73499571	-2.78033400
H	-4.37920344	8.88013571	-2.93631900
H	-0.50872744	9.34426371	-0.80108500
H	-1.86741744	8.42736671	-0.61880100
H	-1.49803344	4.77858371	-2.77643500
C	-8.74633844	0.65514971	3.06216700
C	-9.30497644	2.89034971	2.27908000
C	-10.56016144	2.84806671	2.87074200
C	-10.89808344	1.68564471	3.56405800
C	-10.00632444	0.60707071	3.65821500
H	-8.04760544	-0.17184929	3.12762500
H	-11.24160944	3.68814971	2.79122900
H	-11.86969444	1.61142071	4.04105300
H	-10.30551644	-0.28035029	4.20589700
C	-1.41181444	-0.18612529	0.16455400
C	-1.68377744	1.10415671	-0.29677500
C	-3.87483344	0.91819471	0.73974600
C	-3.61225944	-0.36247829	1.20574700
C	-2.36092844	-0.90728329	0.90229900
H	-0.44764044	-0.63699629	-0.05196000
H	-0.95272844	1.67646271	-0.85929500
H	-4.34946844	-0.91286129	1.78074100
H	-2.11599344	-1.90675629	1.24639500
C	7.28857656	1.77901771	1.14917500
C	8.46981856	1.93384071	1.87577300

C	8.79320156	3.15272371	2.48844400
C	7.94691056	4.25860471	2.39581300
C	6.77364256	4.09811671	1.67232700
H	7.02783156	0.84185671	0.66942200
H	9.15369056	1.09690471	1.96939200
H	9.72106356	3.23531671	3.04454700
H	8.18724356	5.20674671	2.86451800
C	1.02271256	-0.29862129	-3.18621200
C	2.18818856	-0.85209529	-2.63997900
C	3.06222056	-0.08046729	-1.86973200
C	0.69137656	1.04372671	-2.98147800
H	0.36630156	-0.92577829	-3.78067400
H	2.41424956	-1.89744829	-2.82262200
H	3.96857256	-0.49705229	-1.44320700
H	-0.21242844	1.47233271	-3.40328600
C	-8.59914844	9.32015871	-1.05028500
C	-9.85663644	9.83325571	-0.72719200
C	-10.77346244	9.09369271	0.03376600
C	-10.46103444	7.81478071	0.49615000
H	-7.88837344	9.88957871	-1.63988700
H	-10.13388244	10.82446771	-1.07112700
H	-11.74143644	9.52627571	0.26412700
H	-11.16216144	7.23244871	1.08460400
C	5.52003156	9.18843471	2.81210700
C	5.19776056	10.51163171	3.12013600
C	4.01930456	11.10022071	2.64179100
C	3.12373056	10.38794271	1.84045200
H	6.42927956	8.72172871	3.17588100
H	5.86889056	11.09725371	3.73959000
H	3.80082656	12.13115771	2.90067700
H	2.21087056	10.84116671	1.46865700
H	-1.58588544	6.24244171	-3.58059000

TS21'

SCF energy in solution: -3192.719185

Free energy in solution: -3192.017246

C	-2.13178299	0.16795865	0.00000000
C	-4.26049799	0.13772065	0.48666100
C	0.90097701	-1.84247835	-0.53278600
C	0.94017301	-3.24866435	-0.42980800
C	-0.45120399	-1.42848335	-0.25606300
C	-0.38774299	-3.69224135	-0.09043400
H	-2.15173799	-2.57507335	0.22580000

C	-1.98375899	-5.32146835	0.40063100
C	-4.11075299	-5.32754535	0.88108200
C	-7.22558699	-3.37356535	1.50986300
C	-7.25850799	-1.88913935	1.26201500
C	-5.80819499	-3.75228635	1.11723800
C	-5.89258099	-1.44777935	0.97488300
H	-4.14407299	-2.57425535	0.61408300
N	-5.39413399	-4.97372135	1.15074800
N	-5.52103299	-0.21691535	0.80361300
N	-0.88938999	-0.17424735	-0.25477700
N	-0.76004799	-4.95008635	0.09588900
N	-1.16496299	-2.56564835	-0.00196000
N	-3.09449999	-4.51457835	0.58229000
N	-5.12898599	-2.59483835	0.86818800
N	-3.19668799	-0.65839935	0.30437300
N	-8.33122999	-4.14936735	0.96807700
N	-8.33799399	-1.20111735	1.07773900
C	-14.65873899	0.07988365	0.38632000
C	-12.49798499	0.07826165	0.70400600
C	-16.30827999	-1.51605735	0.01500700
C	-16.28831199	-3.78852435	-0.17862600
H	-14.53702299	-2.65150535	0.16391700
C	-14.19612199	-6.79453835	-0.15795400
C	-12.81196799	-6.79912635	0.03926200
C	-14.59702099	-5.38779735	-0.08115600
C	-12.43738799	-5.39668335	0.22917800
C	-9.43075299	-3.37269035	0.87954500
C	-9.46162499	-1.96870535	1.01506800
C	-10.79136699	-3.79744135	0.61635900
C	-10.81818399	-1.52717635	0.82312100
H	-12.56615199	-2.65372035	0.47445400
N	-11.17848199	-5.04091535	0.45010700
N	-11.23605999	-0.27261935	0.86934600
N	-15.93112399	-0.26935935	0.17414300
N	-15.88097799	-5.02694135	-0.23045900
N	-15.54075199	-2.64891135	0.02531500
N	-13.53547899	-4.58528135	0.14817000
N	-11.56309099	-2.65326935	0.60946400
N	-13.58099699	-0.72860035	0.48198500
N	-7.42616399	-3.84497435	2.95274500
H	-6.59854099	-4.20997435	3.42760100
H	-7.92875699	-3.17355935	3.53565900
C	-14.17547699	-9.16195135	-0.38675300
C	-12.78315299	-9.16583535	-0.19066600

C	-12.07994699	-7.98319535	0.02517000
C	-14.90294099	-7.97438735	-0.37401300
H	-14.68868699	-10.10396335	-0.55261800
H	-12.24967699	-10.11103435	-0.21071200
H	-11.00487899	-7.97345835	0.17325600
H	-15.97724599	-7.96047135	-0.52658300
C	-20.02420599	-3.33837735	-0.66412000
C	-18.84290399	-4.06295635	-0.56051500
C	-17.66845299	-3.34677335	-0.33380600
C	-17.68050099	-1.94899235	-0.21495500
C	-18.86542899	-1.22155235	-0.31902000
C	-20.03587199	-1.93526535	-0.54494700
H	-20.95900899	-3.86068635	-0.84066100
H	-18.82166299	-5.14377535	-0.65102900
H	-18.85941099	-0.14077035	-0.22545500
H	-20.97896599	-1.40551635	-0.63227400
C	-3.67073999	-9.10277835	1.08474100
C	-2.29874999	-9.09977935	0.77941100
C	-1.61348799	-7.91229135	0.53069600
C	-2.34113099	-6.72804435	0.59911200
C	-3.70513999	-6.73230435	0.90695700
C	-4.39630399	-7.91549035	1.15198300
H	-4.17040499	-10.04883935	1.26698600
H	-1.76617699	-10.04455935	0.73396100
H	-0.55542699	-7.90272535	0.29018900
H	-5.45782599	-7.90534335	1.37762900
C	2.13066501	-3.95516235	-0.64722900
C	3.26107801	-3.22351435	-0.96503700
C	3.22160201	-1.81274035	-1.06820700
C	2.05010001	-1.10829935	-0.85523700
H	2.15085901	-5.03681635	-0.56658100
H	4.20082901	-3.73738435	-1.14043300
H	4.13166001	-1.27790635	-1.32036900
H	2.00801601	-0.02700135	-0.93231400
C	-3.92092799	1.55308765	0.30234800
C	-2.56057199	1.57260165	-0.00957700
C	-1.89209899	2.76670865	-0.25362800
C	-2.63771699	3.94285065	-0.17458900
C	-4.00657699	3.92089465	0.13805400
C	-4.67217899	2.72004065	0.38191000
H	-0.83450099	2.77508065	-0.49612500
H	-2.15342599	4.89665065	-0.35911800
H	-4.55295499	4.85732365	0.18847400
H	-5.73000699	2.68565465	0.62170900

C	-14.28458199	1.49278365	0.54973700
C	-12.90368199	1.49112465	0.75127200
C	-12.19377799	2.66999865	0.94183300
C	-12.92125399	3.86053565	0.92471900
C	-14.31031099	3.86295065	0.72308700
C	-15.01549699	2.67440365	0.53148900
H	-11.11946899	2.65369765	1.09434800
H	-12.40639299	4.80524965	1.06854700
H	-14.84223299	4.80909165	0.71562500
H	-16.08899399	2.66489065	0.37351500
H	-8.18237799	-4.60226535	2.27827100

22'

SCF energy in solution: -3192.795879

Free energy in solution: -3192.098636

C	-5.33591742	0.58139534	0.00000000
C	-3.93961042	0.58233034	-0.03183000
C	-5.72890742	1.99519034	-0.00361200
C	-3.54760742	1.99545834	-0.05568400
C	-8.80023042	4.03719734	0.05587400
C	-8.80026242	5.44163334	0.05405800
C	-7.41402042	3.60061334	0.02982700
C	-7.41406342	5.87823834	0.02706500
H	-5.63570242	4.73956334	-0.00576700
C	-5.33627842	8.89769534	-0.00614800
C	-3.93996542	8.89683734	-0.03472100
C	-5.72908742	7.48374934	-0.00814600
C	-3.54768842	7.48365634	-0.05566800
C	-0.46860542	5.45385234	-0.11599300
C	-0.46875942	4.02532034	-0.11992000
C	-1.85894942	5.88566334	-0.11194000
C	-1.85916742	3.59379334	-0.11678200
H	-3.62265242	4.73987534	-0.11471300
N	-2.26657642	7.13124234	-0.08481900
N	-2.26641342	2.34818734	-0.08859000
N	-7.01327542	2.35096234	0.02518900
N	-7.01347242	7.12797934	0.01982300
N	-6.64902942	4.73947734	0.01380300
N	-4.64046842	6.67233834	-0.03886300
N	-2.60851442	4.73975434	-0.13748800
N	-4.64031642	2.80664734	-0.03752000
N	0.62163058	6.20321934	-0.09308800
N	0.62094458	3.27528234	-0.09919200

C	6.58566458	0.57970534	0.01999900
C	5.18964958	0.57601234	-0.01025200
C	6.97310258	1.99560334	0.03194300
C	4.79190658	1.98836434	-0.01506300
C	10.05060458	4.03588534	0.10221500
C	10.05086258	5.43833034	0.10430400
C	8.66033758	3.59750234	0.07125300
C	8.66076158	5.87732234	0.07466400
H	6.88221658	4.73784934	0.03369900
C	6.58723658	8.89608834	0.03297600
C	5.19123058	8.90035434	0.00291600
C	6.97418358	7.47999834	0.04032300
C	4.79299858	7.48814834	-0.00647000
C	1.72342958	5.45156534	-0.07435600
C	1.72319558	4.02637134	-0.07689500
C	3.10603158	5.88537634	-0.04479500
C	3.10553058	3.59192534	-0.04849900
H	4.87267258	4.73825434	-0.00986000
N	3.51952058	7.13580534	-0.03371300
N	3.51854858	2.34130434	-0.04127800
N	8.26458558	2.35141234	0.06068700
N	8.26551558	7.12362934	0.06788500
N	7.89533358	4.73760134	0.05632800
N	5.89257858	6.67234734	0.01657400
N	3.85842358	4.73850834	-0.03088300
N	5.89178858	2.80368734	0.01063100
C	7.31581158	-0.60363266	0.03227000
C	4.46437058	-0.60987966	-0.03007800
C	-3.20919642	-0.60106166	-0.03839800
C	-6.06041142	-0.60552766	0.02785100
C	-9.99311442	3.31308434	0.07929200
C	-9.99314642	6.16579134	0.07565800
C	-6.06098142	10.08450134	0.01837500
C	-3.20957542	10.08016134	-0.04088000
C	4.46628358	10.08648734	-0.01276800
C	7.31776658	10.07912934	0.04910700
C	11.24104058	6.16289734	0.13139000
C	11.24052758	3.31082234	0.12713000
C	6.59523958	-1.79712466	0.01290700
H	7.12583058	-2.74396866	0.02132800
C	5.19108858	-1.79983066	-0.01790400
H	4.66488858	-2.74906766	-0.03307000
C	-3.93041342	-1.79373166	-0.01045900
H	-3.40047542	-2.74100766	-0.01480000

C	-5.33486942	-1.79589766	0.02221700
H	-5.86166942	-2.74473866	0.04272300
C	-11.17891142	4.03464334	0.10088000
H	-12.12717542	3.50720434	0.11934800
C	-11.17893642	5.44427734	0.09908600
H	-12.12721142	5.97173634	0.11620800
C	-5.33548142	11.27494734	0.01277400
H	-5.86240042	12.22377534	0.03072100
C	-3.93099442	11.27283334	-0.01640700
H	-3.40111142	12.22013934	-0.02051100
C	5.19340058	11.27616734	0.00329800
H	4.66749258	12.22561234	-0.00847900
C	6.59754258	11.27290934	0.03385000
H	7.12843458	12.21955134	0.04541400
C	12.42825058	5.44046834	0.15628200
H	13.37624558	5.96817534	0.17784100
C	12.42799558	4.03275634	0.15418000
H	13.37580258	3.50464734	0.17415400
H	-7.14522742	-0.59705966	0.05202600
H	-2.12442242	-0.58471766	-0.06532300
H	3.37952658	-0.59818366	-0.05475100
H	8.40057458	-0.59065166	0.05556600
H	11.22675858	2.22611534	0.12511500
H	11.22764658	7.24761034	0.13261300
H	8.40252658	10.06574434	0.07224600
H	3.38142858	10.07518034	-0.03713100
H	-2.12473742	10.06374134	-0.06455700
H	-7.14584742	10.07597734	0.04014300
H	-9.98008942	7.25053834	0.07358800
H	-9.98006342	2.22833534	0.07996900
N	-1.39680442	4.63347134	2.78797100
H	-2.33607342	4.69673334	3.16938000
H	-0.84438542	5.36265134	3.22915000
H	-1.01232842	3.74032634	3.08223800

TS2''

SCF energy in solution: -1777.188462

Free energy in solution: -1776.787721

N	-2.28682175	2.08010333	0.00000000
N	0.36389525	0.66505233	-0.01946300
C	4.35305425	5.71699833	0.08948900
C	3.36592225	3.77135833	0.07059700
C	3.98038425	9.40430233	0.13792100

C	2.73732125	10.04857833	0.13939200
C	3.72851625	7.95913633	0.11664500
C	1.70375125	9.01177033	0.11907900
H	1.89404725	6.90557333	0.09539700
C	-1.93088275	8.59303233	0.03845100
C	-2.59741275	7.36334933	0.04084000
C	-0.50087275	8.27120233	0.09388200
C	-1.52641675	6.35695533	0.11698800
C	-1.07774475	2.67752433	0.04641400
C	0.16680225	2.04322333	0.07227100
C	-0.83193875	4.11162133	0.10029000
C	1.14856925	3.05293333	0.08287900
H	0.98692425	5.17548533	0.11588700
N	-1.77559475	5.04530733	0.15028200
N	2.46637625	2.82502733	0.06942700
N	4.64376525	7.04240533	0.10738100
N	0.41897925	9.24724033	0.10730500
N	2.35532725	7.80594233	0.10791700
N	-0.29348075	6.93673233	0.12395900
N	0.51256925	4.28539033	0.08232700
N	3.14966425	5.14685233	0.08914200
H	-3.11200175	2.58088733	-0.33605100
H	-2.27008575	1.08468133	-0.19228200
H	1.33153625	0.44043333	-0.22716400
C	5.44058025	4.72654933	0.06956500
C	4.80911625	3.48217433	0.05804700
C	5.53513225	2.30158733	0.03803100
C	6.92980925	2.41214133	0.02951600
C	7.56176125	3.66105933	0.04094900
C	6.82150925	4.84769233	0.06135500
H	5.04163725	1.33561133	0.02937200
H	7.53645425	1.51277533	0.01362200
H	8.64564125	3.70626533	0.03369000
H	7.30149925	5.82044533	0.07020700
C	3.82782625	12.15761833	0.17343000
C	2.63473825	11.43288533	0.15696900
C	5.16879025	10.11900833	0.15383000
C	5.07194625	11.51240833	0.17187200
H	3.79426525	13.24175133	0.18756200
H	1.66646625	11.92152833	0.15783100
H	6.12685325	9.61065533	0.15214600
H	5.97720925	12.11000733	0.18482400
C	-4.00462675	9.73487633	-0.15755600
C	-4.67173375	8.50626533	-0.18375200

C	-3.97779175	7.29381633	-0.09092700
C	-2.61074275	9.79703333	-0.05410600
H	-4.57830775	10.65242133	-0.23262400
H	-5.75181075	8.49247933	-0.28450400
H	-4.50306975	6.34577633	-0.13479300
H	-2.07840975	10.74218733	-0.05657600
O	-4.53547675	3.68218833	-0.37030500
H	-5.49396675	3.69559533	-0.20476300
O	-4.02058775	4.46597333	1.26176000
H	-3.11504675	4.69965433	0.79146600
H	0.07307025	0.15696833	0.81042400
H	-3.89056975	3.63906933	1.75624200

3''

SCF energy in solution: -416.69521062

Free energy in solution: -416.62953762

N	-4.97347473	1.15384614	0.00000000
N	-2.09794173	-0.05403186	0.31484200
C	1.15673327	5.39995614	0.75178500
C	0.44555127	3.33817414	0.62995500
C	0.33839827	9.02821314	0.84042400
C	-0.97487673	9.51035314	0.81689600
C	0.27145627	7.55978714	0.79257400
C	-1.86901073	8.35110214	0.75232200
H	-1.43401273	6.29207914	0.69345900
C	-5.42539973	7.48765114	0.63419000
C	-5.92246373	6.18944714	0.52671300
C	-3.95645073	7.34824114	0.63553500
C	-4.73060173	5.32153114	0.46214200
C	-3.86762473	1.72622914	0.21360700
C	-2.47356473	1.23164014	0.34348600
C	-3.76063173	3.22815714	0.32579700
C	-1.65815773	2.33797014	0.42523300
H	-2.08776573	4.43738514	0.48407700
N	-4.83237573	4.01514914	0.34028900
N	-0.32104673	2.30023414	0.53374300
N	1.28048527	6.76429514	0.80254200
N	-3.17799273	8.43305114	0.71993600
N	-1.08281173	7.24007314	0.74097400
N	-3.57581973	6.05815614	0.53721200
N	-2.47781473	3.50431314	0.39364600
N	0.04650927	4.69012214	0.64505600
H	-6.34545673	2.84990014	1.30616900

H	-4.88095273	0.13729214	-0.07863000
H	-1.11790173	-0.26106686	0.45648100
C	2.36253827	4.56494514	0.81464700
C	1.90924027	3.24747714	0.73984300
C	2.79298927	2.17804514	0.77060400
C	4.15291627	2.47732614	0.88126900
C	4.60614527	3.80156214	0.95692300
C	3.71215127	4.87302814	0.92429500
H	2.44164427	1.15351614	0.71061700
H	4.87650727	1.66925214	0.90890400
H	5.67055627	3.99307714	1.04150800
H	4.05078927	5.90201614	0.98074700
C	-0.16558973	11.73970714	0.91109100
C	-1.25578373	10.86873014	0.85157900
C	1.42408227	9.88673314	0.89962900
C	1.14901627	11.25709814	0.93452600
H	-0.33730373	12.81030714	0.93969700
H	-2.27858473	11.22909614	0.83277200
H	2.43917527	9.50519614	0.91732700
H	1.97055227	11.96410414	0.98070700
C	-7.63981673	8.33686014	0.69261500
C	-8.13840073	7.03691514	0.58776100
C	-7.28022173	5.93013114	0.50229100
C	-6.25976973	8.58692114	0.71848100
H	-8.33448673	9.16760614	0.75615000
H	-9.21177873	6.88064114	0.57334900
H	-7.66594773	4.91938414	0.42629900
H	-5.86252273	9.59291014	0.80086700
O	-6.57913773	2.68000914	2.23281900
H	-7.23949473	1.97934114	2.23094700
O	-3.91000873	2.18892414	2.85665300
H	-4.87525673	2.33427814	2.89162600
H	-2.75670573	-0.78894586	0.52299300
H	-3.56580673	2.36044414	3.73862300

CF₃COOH

SCF energy in solution: -526.8101468

Free energy in solution: -526.8013738

C	-4.23076917	1.97612729	0.00000000
C	-5.76548317	2.13654429	0.00001600
O	-6.31815017	3.19733529	-0.00000500
O	-6.34350517	0.93818129	-0.00001300

H	-7.30641617	1.05903129	0.00004200
F	-3.83647017	1.29898729	-1.08307700
F	-3.83645817	1.29976929	1.08357800
F	-3.64140117	3.16364029	-0.00043100

H₂O

SCF energy in solution: -76.43140526

Free energy in solution: -76.42807826

O	-2.74535805	0.99469495	0.00000000
H	-3.51401205	0.41675995	0.00002400
H	-1.97670405	0.41675995	-0.00000100

H₂O₂

SCF energy in solution: -151.5479624

Free energy in solution: -151.5430234

O	-4.36339516	0.80901856	0.00000000
H	-4.01676816	-0.09333544	0.00000900
O	-5.77132316	0.52528256	0.00000000
H	-6.11795016	1.42763656	0.00002600

H₃O₂⁺

SCF energy in solution: -151.9175769

Free energy in solution: -151.9000009

O	-3.21997481	0.40861523	-0.14263973
H	-3.58132881	0.40623323	0.77207827
O	-1.81615981	0.40802023	0.11851027
H	-1.45212481	-0.40719377	-0.30510973
H	-1.45223381	1.22491423	-0.30197073

NH₃

SCF energy in solution: -56.55423829

Free energy in solution: -56.53752429

N	-1.52519892	0.78249336	0.00000000
H	-1.52519892	1.73025836	-0.35972000
H	-2.34598692	0.30861136	-0.35972000
H	-0.70441092	0.30861136	-0.35972000

O₂

SCF energy in solution: -150.3140069

Free energy in solution: -150.3299209

○	-3.03713523	1.04774534	0.00000000
○	-3.03713523	1.04774534	-1.19799800