Electronic Supplementary Material (ESI) for ChemComm.

An Efficient Computational Model to Predict Protonation at the Amide Nitrogen and Reactivity along the C–N Rotational Pathway

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Electronic Supplementary Information

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Computational Methods

Computational Methods. All of the calculations were performed using Gaussian 09 suite of programs. All of the geometry optimizations were performed at the MP2/6-311++G(d,p) level of theory in the gas phase. The absence of imaginary frequencies was used to characterize the structures as minima on the potential energy surface. All of the optimized geometries were verified as minima (no imaginary frequencies). Electronic and thermal energies were calculated for all structures. Energetic parameters were calculated under standard conditions (298.15 K and 1 atm). NBO calculations were performed on all of the optimized structures using MP2 electron densities. For geometry optimizations, we employed the published structure of a 4-methoxy-phenyl derivative of the [4.3.1] ring system as the starting geometry and performed full optimization. Optimized lactam conformations were used as starting geometries for isodesmic calculations for the 1-aza, 2-keto, and hydrocarbon derivatives. Optimization of all of the protonated structures started with the optimized geometries of the lactams. Structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, University of Sherbrooke). Representations of frontier molecular orbitals were generated using GaussView (GaussView, version 5, Dennington, R.; Keith, T.; Millam, J. Semichem Inc., Shawnee Mission, KS, 2009).

Additonal Discussion. Ab inito molecular orbital calculations were carried out at the MP2/6-311++G(d,p) level. This method has been shown to be accurate in predicting properties and resonance energies of amides (e.g. resonance energy, N,N-dimethyl-acetamide: experimental value of 16.8±1.3 kcal/mol; calculated value of 16.4 kcal/mol). This method was further verified by obtaining good correlations between the calculated structures and available X-ray structures

in the series: the parent [4.3.1] bridged bicyclic lactam (τ = 41.78°; χ_N = 36.01°; χ_C = 15.42°) vs. the X-ray structure of an α-4-methoxyphenyl derivative (τ = 42.8°; χ_N = 34.1°; χ_C = 16.5°), which is one of the few available twisted amide geometries determined in the solid state (Szostak, M.; Aubé, J. *Chem. Rev.* **2013**, *113*, 5701). Several X-ray structures of one-carbon bridged lactams have been reported; however, these structures are exclusively limited to derivatives of the [4.3.1] ring system, and one X-ray structure of the [4.1.1] ring system (τ = 35.3°; χ_N = 57.1°; χ_C = 6.0°) for which also very accurate calculated structure at the MP2/6-311++G(d,p) level has been found (parent lactam: τ = 38.23°; χ_N = 57.48°; χ_C = 6.33°). Due to conformational constraint of bridged systems, calculations of energy minima of unsubstituted medium-bridged bicyclic lactams typically result in a significant reduction of computational time compared to similar molecules with large degree of conformational freedom (Greenberg, A.; Venanzi, C. A. *J. Am. Chem. Soc.* **1993**, *115*, 6951). The use of lower level methods to compute properties of amides has been shown to be problematic due to inaccuracies in treatment of N-inversion barriers (Glover, S. A.; Rosser, A. A. *J. Org. Chem.* **2012**, *77*, 5492). To our knowledge, the optimization of structures of non-planar amides using a sufficiently high level of theory has not been reported to date. Cartesian coordinates and energies for all reported structures are given in the Supplementary Information.

Full Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

A[2.2.1]
Energy: -363.060509 au
Sum of electronic and thermal Energies: -362.906857 au
Geometry:

C	-0.66754900	-1.19387600	-0.82553600
C	-0.00200100	-0.00000800	1.15679300
C	-0.80600300	-1.24162600	0.74114300
H	-1.62845100	-1.10630200	-1.33816600
H	-0.15199200	-2.08106100	-1.20202800
H	-1.84596000	-1.17654100	1.07450700
H	-0.36731900	-2.15808100	1.14652400
C	-0.66749100	1.19391100	-0.82552700
H	-0.15188500	2.08107200	-1.20201000
H	-1.62839500	1.10639000	-1.33816300
C	-0.80594700	1.24165200	0.74115100
H	-0.36722200	2.15808300	1.14654200
H	-1.84590700	1.17661100	1.07451200
H	0.40364200	-0.00002100	2.16717500
C	1.03905500	-0.00002200	0.03417400
N	0.16099100	-0.00000300	-1.14961600
O	2.23952100	-0.00003900	0.04815400

A[2.2.1] N+
Energy: -363.431558 au
Sum of electronic and thermal Energies: -363.263564 au
Geometry:

C	-0.73189900	1.23566200	0.78630700
C	0.02394800	0.00000900	-1.18713500
C	-0.77836600	1.25285500	-0.77369900
H	-1.71092500	1.15389700	1.26031400
H	-0.19437900	2.09259600	1.19699400
H	-1.80125800	1.19174300	-1.14954900
H	-0.31840600	2.16475500	-1.16023700
C	-0.73188300	-1.23568400	0.78628900
H	-0.19434200	-2.09261400	1.19695700
H	-1.71090400	-1.15394300	1.26030900
C	-0.77836100	-1.25284600	-0.77371500
H	-0.31840500	-2.16473900	-1.16027400
H	-1.80125700	-1.19172700	-1.14955600
H	0.40778200	0.00001700	-2.20548800
C	1.09276200	0.00000500	-0.13499900
N	0.06342100	-0.00000500	1.09696500
O	2.26273200	0.00000700	-0.00002000
H	0.51908800	-0.00000800	2.01364600

A[2.2.1] O+
Energy: -363.370844 au
Sum of electronic and thermal Energies: -363.203781 au
Geometry:

C	0.71093800	1.21575400	-0.81903200
C	0.02053300	-0.00005100	1.16569800
C	0.83133500	1.25500600	0.74887000
H	1.66276600	1.09645800	-1.33654100
H	0.19943200	2.09591900	-1.21152400
H	1.86103400	1.16872500	1.10108100
H	0.39604900	2.16998600	1.15716600

C	0.71063000	-1.21579000	-0.81918500
H	0.19896100	-2.09576500	-1.21188600
H	1.66253000	-1.09660000	-1.33658600
C	0.83089500	-1.25534800	0.74872300
H	0.39522200	-2.17022900	1.15683300
H	1.86059800	-1.16952200	1.10103000
H	-0.40362900	-0.00004400	2.16949000
C	-0.91476300	0.00012400	0.00307700
N	-0.13598900	0.00011400	-1.14579100
O	-2.17835700	0.00023400	-0.06922300
H	-2.59160100	0.00023600	0.81634500

A[2.2.1] amine
Energy: -289.176313 au
Sum of electronic and thermal Energies: -289.003716 au
Geometry:

C	-1.19214900	-0.78951300	-0.45565800
C	0.00003600	1.12812800	0.34219000
C	-1.24131800	0.77498600	-0.49282800
H	-1.11283300	-1.24546900	-1.44607700
H	-2.07697300	-1.19944300	0.04033600
H	-1.18194300	1.17842100	-1.50848200
H	-2.15672200	1.15266600	-0.02534900
C	1.19209800	-0.78957700	-0.45566300
H	2.07690000	-1.19960000	0.04029300
H	1.11271800	-1.24549400	-1.44609400
C	1.24138500	0.77491600	-0.49279700
H	2.15680000	1.15249900	-0.02526000
H	1.18209600	1.17838500	-1.50844400
H	0.00006200	2.13613800	0.76338500
C	-0.00001800	-0.04700800	1.34064400
N	-0.00004000	-1.14744600	0.35180200
H	0.89553600	-0.09380600	1.96887900
H	-0.89557200	-0.09377000	1.96887900

A[2.2.1] ketone
Energy: -347.048555 au
Sum of electronic and thermal Energies: -346.883131 au
Geometry:

C	0.75901700	-1.24789700	0.78538500
C	-0.06605000	0.00000200	-1.15559100
C	0.75900100	-1.24790900	-0.78538200
H	1.77006800	-1.18893700	1.20021200
H	0.28670600	-2.15591800	1.17292300
H	1.77004400	-1.18898800	-1.20023400
H	0.28665100	-2.15592200	-1.17289300
C	0.75904100	1.24788900	0.78537800
H	0.28673600	2.15591900	1.17290300
H	1.77008400	1.18891800	1.20022000
C	0.75904000	1.24788400	-0.78538800
H	0.28673200	2.15591300	-1.17291400
H	1.77008500	1.18892400	-1.20023000
H	-0.50267900	0.00000400	-2.15451700
C	-1.06825200	0.00001300	0.00000300
O	-2.27953000	0.00002100	0.00000400
C	-0.06605000	0.00000300	1.15559200

H	-0.50267800	0.00001300	2.15451800

A[2.2.1] hydrocarbon
Energy: -273.168279 au
Sum of electronic and thermal Energies: -272.984292 au
Geometry:

C	-1.24881200	-0.78052100	-0.49215000
C	-0.00000100	1.13054400	0.33968700
C	-1.24881800	0.78050600	-0.49215300
H	-1.19419300	-1.20253400	-1.50115800
H	-2.15363300	-1.17198400	-0.01492000
H	-1.19424000	1.20251500	-1.50116400
H	-2.15362600	1.17195700	-0.01488900
C	1.24881900	-0.78051900	-0.49214000
H	2.15363200	-1.17198000	-0.01489500
H	1.19421200	-1.20253200	-1.50114800
C	1.24882000	0.78050700	-0.49215400
H	2.15362500	1.17196700	-0.01489500
H	1.19423300	1.20250500	-1.50117000
H	-0.00000300	2.15149900	0.73199600
C	-0.00000400	0.00001800	1.38375600
H	0.89510800	0.00002700	2.01637900
H	-0.89511300	0.00003600	2.01638300
C	-0.00000300	-1.13053400	0.33972400
H	-0.00000600	-2.15147900	0.73205900

B[3.2.1]
Energy: -402.272807 au
Sum of electronic and thermal Energies: -402.088371 au
Geometry:

C	0.06931100	1.38568900	-1.02778500
C	-0.37230100	0.40624600	1.14910300
C	0.07782100	1.71800800	0.50084800
H	1.05391000	1.50153100	-1.48922000
H	-0.62928500	2.03629200	-1.56020200
H	1.06841600	2.02835000	0.84787100
H	-0.62581000	2.52429000	0.72613900
C	0.74637700	-0.96771700	-1.13742800
H	0.31287800	-1.97344000	-1.10950400
H	1.31407800	-0.87347500	-2.06870400
C	0.82683900	-0.55509500	1.37932700
H	0.43682200	-1.52523900	1.71224700
H	1.45995500	-0.15937800	2.18231400
H	-0.96717600	0.52015100	2.05779000
C	-1.12815900	-0.28946100	0.03260200
N	-0.39365900	-0.01000500	-1.18203800
O	-2.05940900	-1.05502900	0.11759000
C	1.64727200	-0.72712800	0.08918000
H	2.34948600	-1.56193600	0.19682900
H	2.25465200	0.16987500	-0.07709300

B[3.2.1] N+
Energy: -402.645001 au
Sum of electronic and thermal Energies: -402.446200 au
Geometry:

C	0.14144600	1.25476000	1.18985100

C	0.30595300	0.49076900	-1.15661200
C	0.08250300	1.74277500	-0.28687100
H	-0.77765600	1.42799300	1.75093200
H	0.98117500	1.69351000	1.73192900
H	-0.87737000	2.21187300	-0.51234900
H	0.86960200	2.47835100	-0.46500000
C	-0.87711200	-1.05751700	1.02393200
H	-0.55093400	-2.08203000	0.81748300
H	-1.35367200	-1.02328700	2.00708000
C	-1.01476800	-0.29164500	-1.39728600
H	-0.78054100	-1.25165800	-1.87166000
H	-1.63127800	0.27909400	-2.09811000
H	0.82994100	0.68813300	-2.09311800
C	1.12465300	-0.39194500	-0.27133700
N	0.38889900	-0.22561700	1.10391400
O	2.05946600	-1.11355600	-0.37344500
C	-1.77456900	-0.50823900	-0.08145400
H	-2.59290900	-1.21910600	-0.23071500
H	-2.23826000	0.42646600	0.24885600
H	0.99525300	-0.57531800	1.85348400

B[3.2.1] O+
Energy: -402.606271 au
Sum of electronic and thermal Energies: -402.408411 au
Geometry:

C	-1.41526300	0.07723000	-1.06237500
C	-0.37251900	-0.94684900	0.85662000
C	-1.75413300	-0.67434300	0.25458300
H	-1.76365300	1.10990300	-1.07740900
H	-1.80721000	-0.43174100	-1.94346000
H	-2.36988500	-0.07427500	0.92820300
H	-2.27654600	-1.61112800	0.05248600
C	0.72973100	1.36271400	-0.75807100
H	1.81142600	1.22764200	-0.80714100
H	0.43551300	2.13949800	-1.46434700
C	0.20829500	0.36515200	1.57911700
H	1.21500000	0.14424100	1.95128900
H	-0.43775100	0.52591900	2.44860100
H	-0.28996100	-1.81417400	1.51468800
C	0.52292500	-0.86034500	-0.30646800
N	0.07411100	0.06245800	-1.16278700
O	1.76224400	-1.24001900	-0.38495300
C	0.21660800	1.62186400	0.68281100
H	0.85232300	2.38274600	1.14839300
H	-0.79101100	2.04357900	0.64027700
H	1.99115900	-1.83180800	0.35025100

B[3.2.1] amine
Energy: -328.381049 au
Sum of electronic and thermal Energies: -328.177944 au
Geometry:

C	-1.23911200	-0.77656400	-0.72870200
C	-0.35496300	1.19837100	0.39789500
C	-1.19983100	0.78443600	-0.82477600
H	-0.84832600	-1.27157000	-1.62311200
H	-2.26678400	-1.12148100	-0.57410400

H	-0.76264000	1.13486900	-1.76564100
H	-2.21096100	1.19807800	-0.75156300
C	0.98772400	-1.29310400	0.10320800
H	1.52852300	-1.45670800	1.04367300
H	1.11273200	-2.19536900	-0.50606400
C	1.14248100	1.23816200	0.05616200
H	1.71507300	1.37768900	0.98352800
H	1.36549200	2.09286000	-0.59408800
H	-0.68188800	2.15197700	0.82704700
C	-0.60405200	0.00290800	1.33126100
N	-0.43917900	-1.16536400	0.45175500
C	1.56646100	-0.07016100	-0.62805000
H	2.65935100	-0.14852700	-0.67459000
H	1.21101000	-0.06828900	-1.66560400
H	0.09095700	-0.05170300	2.17592900
H	-1.63052100	0.01143800	1.72032000

B[3.2.1] ketone
Energy: -386.259562 au
Sum of electronic and thermal Energies: -386.063382 au
Geometry:

C	-0.10046700	1.57366000	-0.78355500
C	-0.37085800	0.11613400	1.20161700
C	-0.10049200	1.57371400	0.78344700
H	0.84671700	1.94001900	-1.19276500
H	-0.89411100	2.22534100	-1.16158300
H	0.84666800	1.94013300	1.19266300
H	-0.89416600	2.22540400	1.16139700
C	0.93749900	-0.70703500	-1.27382700
H	0.68008300	-1.76627400	-1.40593800
H	1.51427900	-0.39835900	-2.15438300
C	0.93749100	-0.70693800	1.27388400
H	0.68007700	-1.76616700	1.40608000
H	1.51426500	-0.39818900	2.15442000
H	-0.94918100	0.01408800	2.12361900
C	-1.12404100	-0.43000600	0.00000900
O	-2.09131000	-1.16792100	0.00003200
C	1.77543700	-0.52434200	0.00002500
H	2.61251800	-1.23165100	0.00005200
H	2.22017400	0.47766000	-0.00001200
C	-0.37084700	0.11604900	-1.20163100
H	-0.94916800	0.01394900	-2.12362800

B[3.2.1] hydrocarbon
Energy: -312.374400 au
Sum of electronic and thermal Energies: -312.159697 au
Geometry:

C	-1.23261700	-0.77926800	-0.81195400
C	-0.39514700	1.18578900	0.42138800
C	-1.23265200	0.77923900	-0.81193700
H	-0.81999500	-1.19662400	-1.73727600
H	-2.25477000	-1.15981200	-0.71159500
H	-0.82007400	1.19664000	-1.73725800
H	-2.25482000	1.15973000	-0.71153300
C	1.10058700	-1.27187400	0.07955500
H	1.66739000	-1.41430000	1.01007900

H	1.29313300	-2.14762300	-0.55328800
C	1.10054500	1.27190600	0.07954200
H	1.66736100	1.41437600	1.01005100
H	1.29305300	2.14764600	-0.55332700
H	-0.73538300	2.13698100	0.84677800
C	-0.62487800	-0.00001200	1.36982600
C	1.58274300	0.00001700	-0.63296000
H	2.67624900	0.00003600	-0.71117300
H	1.20204600	0.00000600	-1.66180900
H	0.05689400	-0.00001300	2.22877500
H	-1.65649700	-0.00000700	1.74576600
C	-0.39512300	-1.18580100	0.42138100
H	-0.73533500	-2.13700600	0.84675900

C[3.3.1]
Energy: -441.468673 au
Sum of electronic and thermal Energies: -441.253878 au
Geometry:

C	1.24891500	-0.28535800	-1.28298400
C	-0.00002000	0.35028100	1.26632600
C	1.30387800	-0.47959300	1.24712800
H	1.21277000	-0.85941400	-2.21597500
H	2.05892900	0.44779800	-1.38753000
H	1.29072000	-1.19415300	2.07968200
H	2.13544100	0.21287400	1.43527800
C	-1.24887500	-0.28527200	-1.28303400
H	-2.05883600	0.44793900	-1.38761200
H	-1.21273000	-0.85931500	-2.21603500
C	-1.30399200	-0.47947000	1.24706100
H	-2.13551000	0.21307200	1.43513600
H	-1.29095600	-1.19401500	2.07962500
H	-0.00001100	0.98636600	2.15793400
C	0.00005000	1.24232000	0.04370200
N	0.00004500	0.49700600	-1.19579700
O	0.00010700	2.45416200	0.06898400
C	-1.55328600	-1.20264300	-0.08516800
H	-2.60452900	-1.51141900	-0.14138400
H	-0.96098300	-2.11774000	-0.14334400
C	1.55320300	-1.20275300	-0.08510600
H	2.60442900	-1.51159300	-0.14127300
H	0.96084800	-2.11781100	-0.14334300

C[3.3.1] N+
Energy: -441.846675 au
Sum of electronic and thermal Energies: -441.616994 au
Geometry:

C	-1.29455700	-0.18281000	1.30573300
C	-0.00008400	0.18622100	-1.34426000
C	-1.31306400	-0.62315900	-1.20343600
H	-1.24422500	-0.64005500	2.29781800
H	-2.07422700	0.58640100	1.31256200
H	-1.30475900	-1.42857600	-1.94450800
H	-2.14396900	0.04272400	-1.46622200
C	1.29474800	-0.18286000	1.30555500
H	2.07445600	0.58631400	1.31221000
H	1.24456200	-0.64005400	2.29767100

C	1.31282000	-0.62331200	-1.20360500
H	2.14375900	0.04246100	-1.46656000
H	1.30429600	-1.42876300	-1.94463800
H	-0.00011800	0.69912300	-2.31055900
C	0.00004300	1.24277800	-0.29308200
N	0.00009500	0.58135700	1.10337300
O	0.00007000	2.43530100	-0.33340800
C	1.54982900	-1.20214100	0.19884300
H	2.59768600	-1.50688900	0.28999200
H	0.95959200	-2.10283400	0.36324600
C	-1.54989600	-1.20202700	0.19902100
H	-2.59776300	-1.50669200	0.29032800
H	-0.95970400	-2.10277500	0.36328500
H	0.00015600	1.37157300	1.76042500

C[3.3.1] O+
Energy: -441.804906 au
Sum of electronic and thermal Energies: -441.576566 au
Geometry:

C	-1.14900700	1.45151400	0.18016200
C	0.18847700	-1.34489600	0.10147700
C	-0.52907600	-0.75679900	1.43490600
H	-0.94972600	2.52407500	0.16960500
H	-2.19596700	1.28682000	-0.07505800
H	0.10705400	-1.08825700	2.26282700
H	-1.49099600	-1.27155800	1.52969100
C	1.15581100	1.15487300	-0.87719200
H	1.49062800	0.98194800	-1.90383400
H	1.20016400	2.23140200	-0.69894000
C	1.69890000	-1.11542000	0.05666000
H	2.08579600	-1.56587600	-0.86471100
H	2.15911200	-1.64830300	0.89392300
H	-0.05632600	-2.40942300	0.02594200
C	-0.58942900	-0.50032000	-0.81229100
N	-0.29284800	0.79685900	-0.87103900
O	-1.79675300	-0.82805200	-1.19381300
C	2.03451200	0.37630000	0.10341400
H	3.07991400	0.53236800	-0.17993200
H	1.92653000	0.76026100	1.11911800
C	-0.74191000	0.77680500	1.51768400
H	-1.53057000	0.96845100	2.25433500
H	0.15956700	1.25816900	1.89837700
H	-1.97089600	-1.76601600	-1.01248200

C[3.3.1] amine
Energy: -367.579985 au
Sum of electronic and thermal Energies: -367.346373 au
Geometry:

C	-1.23715800	-1.28029400	-0.10799000
C	-0.00005900	1.25354000	0.61477200
C	-1.29899000	1.26607600	-0.21027500
H	-1.19999800	-2.18227800	-0.73046000
H	-2.05041400	-1.42050300	0.61774900
H	-1.30037900	2.11488600	-0.90598400
H	-2.12968800	1.43107300	0.49088100
C	1.23728300	-1.28019600	-0.10796700

H	2.05053800	-1.42031600	0.61778900
H	1.20021700	-2.18219500	-0.73042100
C	1.29886100	1.26618000	-0.21029500
H	2.12955100	1.43128100	0.49084500
H	1.30015400	2.11497400	-0.90602400
H	-0.00008600	2.14702100	1.25486900
C	-0.00000200	-0.00085100	1.49464000
N	0.00005200	-1.21110700	0.67337100
C	1.55605900	-0.04483700	-0.97368100
H	2.60924900	-0.09140600	-1.27914100
H	0.96955600	-0.06907700	-1.89509100
C	-1.55604600	-0.04495200	-0.97368700
H	-2.60922600	-0.09163000	-1.27916300
H	-0.96952600	-0.06910900	-1.89508900
H	-0.88773300	-0.02152200	2.14127000
H	0.88773300	-0.02144200	2.14126700

C[3.3.1] ketone
Energy: -425.459883 au
Sum of electronic and thermal Energies: -425.232923 au
Geometry:

C	-1.30452700	-0.40453200	1.27711800
C	0.00000700	0.42239500	-1.25616300
C	-1.30456500	-0.40455000	-1.27707700
H	-1.30185100	-1.06358200	2.15488700
H	-2.13432200	0.30211400	1.41520500
H	-1.30192100	-1.06360800	-2.15484100
H	-2.13436000	0.30210000	-1.41514600
C	1.30451400	-0.40468000	1.27708300
H	2.13439100	0.30187700	1.41513100
H	1.30179300	-1.06371700	2.15486100
C	1.30447300	-0.40472000	-1.27710900
H	2.13435400	0.30182100	-1.41521100
H	1.30171300	-1.06378600	-2.15486700
H	0.00004200	1.10001600	-2.11757200
C	0.00007900	1.26621200	-0.00001200
O	0.00016700	2.48886000	-0.00002400
C	1.55943000	-1.22055700	-0.00000400
H	2.60178700	-1.56169900	-0.00001500
H	0.94904800	-2.12547400	0.00002200
C	-1.55958300	-1.22036600	0.00002900
H	-2.60198200	-1.56138000	0.00004700
H	-0.94931100	-2.12535700	0.00002700
C	0.00003800	0.42242100	1.25615500
H	0.00009100	1.10005900	2.11755000

C[3.3.1] hydrocarbon
Energy: -351.573050 au
Sum of electronic and thermal Energies: -351.327572 au
Geometry:

C	1.29739500	1.27861700	-0.17926800
C	-0.00002900	-1.24726200	0.64680300
C	1.29733300	-1.27866800	-0.17927800
H	1.29661900	2.15043100	-0.84667300
H	2.12838800	1.42329400	0.52612100
H	1.29651400	-2.15047900	-0.84668700

H	2.12832200	-1.42339000	0.52610600
C	-1.29733400	1.27866700	-0.17927800
H	-2.12832500	1.42338400	0.52610500
H	-1.29651500	2.15048000	-0.84668500
C	-1.29739800	-1.27861500	-0.17926700
H	-2.12839000	-1.42328200	0.52612400
H	-1.29662700	-2.15043600	-0.84666400
H	-0.00004500	-2.14285600	1.28356800
C	0.00000000	0.00000000	1.53751200
C	-1.56306900	0.00002800	-0.99078200
H	-2.60711300	0.00005500	-1.32797700
H	-0.95711600	0.00000900	-1.89970300
C	1.56307300	-0.00002900	-0.99077700
H	2.60711900	-0.00005300	-1.32796700
H	0.95712700	-0.00000800	-1.89970300
H	0.88578700	-0.00002000	2.18782100
H	-0.88578100	0.00002000	2.18782900
C	0.00002700	1.24726100	0.64680400
H	0.00003900	2.14285600	1.28356900

D[4.1.1]
Energy: -402.255533 au
Sum of electronic and thermal Energies: -402.071557 au
Geometry:

C	0.96461100	-1.46929600	-0.04444600
C	-1.07607400	0.85073400	0.59419600
C	0.08245400	1.73825900	0.08456800
H	1.40385100	-2.25989900	0.57233200
H	0.84540900	-1.85949700	-1.06070700
H	0.52561600	2.25446800	0.94602800
H	-0.33566900	2.50734700	-0.57485400
C	-0.53009200	-0.20590300	1.57812200
H	-1.25445900	-0.58082800	2.30461700
H	0.40353500	0.05529400	2.08128600
H	-1.96707400	1.42931300	0.85220900
C	-1.16354200	-0.31117200	-0.39827300
N	-0.38578300	-1.15728900	0.43904500
O	-1.58179300	-0.47911200	-1.51785000
C	1.19403000	1.00932600	-0.71317100
C	1.86276300	-0.21842900	-0.06186100
H	1.97124700	1.75390600	-0.92115900
H	0.79074500	0.70860000	-1.68783300
H	2.19816700	0.03062700	0.95185300
H	2.76855500	-0.46653700	-0.62910300

D[4.1.1] N+
Energy: -402.617591 au
Sum of electronic and thermal Energies: -402.420047 au
Geometry:

C	0.76956100	-1.57734500	-0.26231700
C	-0.78716100	0.97658300	0.69607300
C	0.50317500	1.70283400	0.25407700
H	1.08154300	-2.48887700	0.25475200
H	0.56580400	-1.81688300	-1.31103000
H	1.04249800	1.98741100	1.16462200
H	0.21002300	2.62626000	-0.25438400

C	-0.55125700	-0.29123800	1.54988800
H	-1.40072700	-0.54898200	2.18449600
H	0.38158100	-0.35323400	2.10705100
H	-1.53836100	1.67812000	1.06574800
C	-1.26203600	0.08251500	-0.42687000
N	-0.56340500	-1.17767000	0.32214700
O	-1.86067600	0.04883800	-1.43507900
C	1.41750600	0.88996200	-0.67638000
C	1.83160800	-0.48798900	-0.14051900
H	2.32095400	1.48254000	-0.84754000
H	0.94448300	0.77515600	-1.66139700
H	2.18420100	-0.40619900	0.89337200
H	2.68596100	-0.85671900	-0.71853000
H	-1.17709200	-1.99754400	0.38473000

D[4.1.1] O+
Energy: -402.595216 au
Sum of electronic and thermal Energies: -402.397489 au
Geometry:

C	1.18624900	-1.37575100	0.09423300
C	-1.17293100	0.81767600	0.59479400
C	-0.14604000	1.73160700	-0.14710000
H	1.68629800	-2.00705300	0.82972400
H	1.04190200	-1.93791500	-0.83168700
H	0.24793300	2.43640100	0.59286800
H	-0.68659200	2.32006900	-0.89598800
C	-0.37372600	0.02233700	1.66552800
H	-0.96131800	-0.40570900	2.47678900
H	0.53740500	0.49554400	2.02749900
H	-2.11966900	1.30131000	0.83741000
C	-1.09317000	-0.47155600	-0.16400700
N	-0.15034900	-0.99715300	0.59411100
O	-1.48196900	-0.94209800	-1.31098400
C	1.02394900	1.01127400	-0.88951000
C	1.90288600	-0.03192300	-0.15271800
H	1.68629600	1.81053000	-1.23562600
H	0.63485700	0.54178700	-1.80227900
H	2.28797200	0.37459500	0.78756400
H	2.77807300	-0.24059300	-0.77704800
H	-2.18826300	-0.39409900	-1.68745700

D[4.1.1] amine
Energy: -328.342425 au
Sum of electronic and thermal Energies: -321.140294 au
Geometry:

C	-0.40367000	-1.61330200	0.13945900
C	0.95854200	1.07554100	-0.09507000
C	-0.46576300	1.63686600	-0.15205300
H	-0.42320200	-2.52758300	-0.46712400
H	-0.59084800	-1.91610600	1.17783400
H	-0.67684200	1.93532400	-1.18883100
H	-0.51081100	2.55250800	0.45173100
C	1.20662000	-0.13301300	-1.02857300
H	2.25021300	-0.20587300	-1.35325000
H	0.55266100	-0.25327300	-1.89862500
H	1.68685000	1.89084200	-0.17653700

C	1.19706800	0.05580600	1.04271800
N	0.96609200	-1.08697900	0.10153800
C	-1.57238900	0.68628400	0.32932300
C	-1.54882100	-0.69585300	-0.33048100
H	-2.53855400	1.16590700	0.12971300
H	-1.51400600	0.56614200	1.41849500
H	-1.51498500	-0.57460100	-1.42069900
H	-2.48861500	-1.22066600	-0.11390600
H	0.53731100	0.08062700	1.91640600
H	2.23866400	0.04163100	1.38208000

D[4.1.1] ketone
Energy: -386.229836 au
Sum of electronic and thermal Energies: -386.034626 au
Geometry:

C	0.79699800	-1.57603800	-0.25834900
C	-0.80004500	0.94720600	0.67659400
C	0.48003700	1.68451400	0.24710000
H	1.16231800	-2.47602500	0.25141200
H	0.66960100	-1.83845300	-1.31713000
H	1.02900900	1.98186800	1.15053600
H	0.18507200	2.60527500	-0.26991300
C	-0.56276600	-0.30744100	1.57289100
H	-1.41849100	-0.49943200	2.22606600
H	0.35416200	-0.31106600	2.16714700
H	-1.55860900	1.65739800	1.02070000
C	-1.25023700	-0.03794000	-0.41040500
O	-1.93318100	0.05643400	-1.40360500
C	1.41576500	0.89214900	-0.68054100
C	1.85724100	-0.47275000	-0.13606200
H	2.30300500	1.51010400	-0.86328600
H	0.93212200	0.75220300	-1.65708500
H	2.16997800	-0.36171700	0.90988500
H	2.74630200	-0.80668000	-0.68450200
C	-0.58593300	-1.22113800	0.31139900
H	-1.21537100	-2.11631000	0.35924400

D[4.1.1] hydrocarbon
Energy: -312.338819 au
Sum of electronic and thermal Energies: -312.124886 au
Geometry:

C	-0.47819800	-1.63266000	0.14569700
C	0.95151400	1.08339100	-0.10314200
C	-0.47812200	1.63267700	-0.14569600
H	-0.51796700	-2.54588100	-0.46308700
H	-0.69944400	-1.93535600	1.17940300
H	-0.69935500	1.93537100	-1.17940600
H	-0.51786700	2.54590100	0.46308200
C	1.22975700	-0.10298700	-1.06895100
H	2.28547300	-0.12816200	-1.35874500
H	0.61323800	-0.18472800	-1.97051800
H	1.65335800	1.92000200	-0.19515700
C	1.22976500	0.10293900	1.06895400
C	-1.58318200	0.68539800	0.34124600
C	-1.58321700	-0.68533600	-0.34124700
H	-2.54807900	1.17757600	0.16591000

H	-1.50590700	0.54576300	1.42734200
H	-1.50593100	-0.54571500	-1.42734300
H	-2.54813700	-1.17746300	-0.16590500
C	0.95145900	-1.08342500	0.10314100
H	1.65327300	-1.92006500	0.19515200
H	0.61321800	0.18471700	1.97049700
H	2.28547400	0.12806000	1.35876700

E[4.2.1]
Energy: -441.478957 au
Sum of electronic and thermal Energies: -441.263763 au
Geometry:

C	-1.45903700	-1.06841000	-0.51340500
C	1.25383100	0.55373800	0.61601300
C	0.28616300	1.72840600	0.32630700
H	-1.59057200	-1.35386400	-1.56119400
H	-2.05421300	-1.75172900	0.09830900
H	0.87969700	2.56947900	-0.05589300
H	-0.14661300	2.04423600	1.28415000
C	0.93632600	-0.93899700	-1.26173100
H	1.40688200	-1.86458900	-1.60893600
H	0.43309400	-0.48212200	-2.11855700
C	1.96877000	0.02428100	-0.62568800
H	2.87096000	-0.52157100	-0.33380500
H	2.26203700	0.81932600	-1.31816300
H	1.92763100	0.82623400	1.43224400
C	0.31001800	-0.57090700	0.98876100
N	-0.02998600	-1.23860400	-0.19464200
O	-0.24202700	-0.74189700	2.06079600
C	-0.87629900	1.47244400	-0.66624200
C	-1.91063300	0.38932900	-0.27581700
H	-0.48346800	1.28033300	-1.67089500
H	-1.41694200	2.42395400	-0.74103200
H	-2.83471500	0.55831200	-0.84212700
H	-2.16248900	0.51809700	0.78282500

E[4.2.1] N+
Energy: -441.842033 au
Sum of electronic and thermal Energies: -441.612860 au
Geometry:

C	-1.24374000	-1.30042000	-0.55546300
C	1.02264500	0.87264600	0.57104700
C	-0.25050800	1.75316100	0.58525900
H	-1.45598800	-1.41522100	-1.62107900
H	-1.54115400	-2.21290900	-0.03282900
H	0.06551900	2.76201100	0.29861600
H	-0.61097900	1.80892200	1.61930100
C	0.95854500	-0.42304000	-1.52401000
H	1.64537000	-1.08518500	-2.05342800
H	0.19725900	-0.07747400	-2.22110200
C	1.68225000	0.73794400	-0.80754800
H	2.74347000	0.50214500	-0.69219500
H	1.60192900	1.66158600	-1.38502000
H	1.71734800	1.24121900	1.33024400
C	0.65377800	-0.53521100	0.92745400
N	0.27055300	-1.21747700	-0.44168400

O	0.59050800	-1.17282300	1.92574700
C	-1.40784300	1.29911000	-0.31578500
C	-1.96095200	-0.09093200	0.04566400
H	-1.13666400	1.35669000	-1.37610800
H	-2.21568800	2.02505800	-0.18111600
H	-2.99855300	-0.17532700	-0.29466500
H	-1.99274000	-0.19238800	1.13726400
H	0.63788400	-2.17374800	-0.40177200

E[4.2.1] O+
Energy: -441.829486 au
Sum of electronic and thermal Energies: -441.600638 au
Geometry:

C	-1.53012000	-1.12933500	-0.31034500
C	1.32097300	0.60763800	0.52439200
C	0.38824800	1.71776000	-0.08030900
H	-1.61857600	-1.71670500	-1.22495500
H	-2.12692600	-1.60308700	0.47044900
H	1.04782800	2.40137400	-0.62761000
H	-0.05120300	2.29580600	0.74271000
C	0.95813100	-1.25607100	-0.98466900
H	1.32271000	-2.28511800	-1.00791800
H	0.51182700	-1.02145300	-1.95083200
C	2.03350800	-0.23770800	-0.54157700
H	2.89291800	-0.74873100	-0.10246900
H	2.38323700	0.37372800	-1.37605800
H	1.98537300	1.03011700	1.28220700
C	0.28054500	-0.32986600	1.01245200
N	-0.08808300	-1.15165100	0.06372900
O	-0.48754800	-0.18028500	2.06154200
C	-0.74902900	1.27202500	-1.04706200
C	-1.89487900	0.36108800	-0.51633600
H	-0.31826400	0.85001000	-1.96067400
H	-1.22558100	2.20570400	-1.36386500
H	-2.72408400	0.40728500	-1.22890900
H	-2.27275400	0.77473900	0.42402700
H	-0.13379900	0.50698800	2.64617500

E[4.2.1] amine
Energy: -367.572433 au
Sum of electronic and thermal Energies: -367.339209 au
Geometry:

C	-1.12694900	-1.44536300	0.01271800
C	0.98214800	0.95253600	0.56110300
C	-0.26113600	1.76527200	0.18178600
H	-1.22449300	-1.92250700	-0.96903400
H	-1.56476200	-2.14203200	0.73999100
H	0.07368100	2.66766800	-0.34766400
H	-0.75900400	2.10595600	1.10124400
C	1.16092700	-1.02291600	-0.87805400
H	1.98279800	-1.74662400	-0.93688600
H	0.57968300	-1.11122800	-1.80171500
C	1.72518100	0.41185200	-0.67494500
H	2.80163200	0.36854500	-0.48014200
H	1.57188000	1.04673200	-1.55422500
H	1.63972400	1.59374700	1.16162900

C	0.66511400	-0.35462800	1.31212800
N	0.30876500	-1.33675800	0.28540200
C	-1.30045500	1.04089900	-0.68424300
C	-1.95608900	-0.14739400	0.02797900
H	-0.85063400	0.71326800	-1.63080400
H	-2.07661500	1.76857800	-0.95157500
H	-2.92579400	-0.37689100	-0.43320400
H	-2.17440400	0.14521200	1.06346100
H	1.56788300	-0.69665900	1.83752300
H	-0.13537100	-0.25799700	2.05275100

E[4.2.1] ketone
Energy: -425.453447 au
Sum of electronic and thermal Energies: -425.226851 au
Geometry:

C	-1.27629900	-1.30534900	-0.54390300
C	1.03930900	0.83400400	0.55355700
C	-0.22288600	1.71756400	0.60672800
H	-1.54791800	-1.41107600	-1.60181900
H	-1.65064900	-2.19511900	-0.02491500
H	0.08106100	2.74093700	0.35088400
H	-0.58310500	1.73728200	1.64405800
C	0.95332600	-0.45244700	-1.55392200
H	1.67887700	-1.05631700	-2.10687400
H	0.21780100	-0.09856600	-2.28174100
C	1.65774500	0.74145600	-0.84786400
H	2.73033200	0.53817200	-0.75826600
H	1.54764900	1.67601100	-1.40812700
H	1.74584700	1.19276900	1.30872400
C	0.66387400	-0.60992200	0.85985200
O	0.65403500	-1.13209300	1.95971000
C	-1.39143800	1.29765100	-0.29829000
C	-1.98690700	-0.07739100	0.05377100
H	-1.09850700	1.33529700	-1.35437800
H	-2.17609200	2.05429000	-0.17623800
H	-3.03394500	-0.11175500	-0.26990700
H	-2.00239100	-0.17136100	1.14788200
C	0.26767100	-1.28788500	-0.44875600
H	0.63239100	-2.31990500	-0.43401100

E[4.2.1] hydrocarbon
Energy: -351.564403 au
Sum of electronic and thermal Energies: -351.319262 au
Geometry:

C	-1.24839500	-1.41477800	-0.01092000
C	1.02341600	0.91810900	0.57252800
C	-0.19133300	1.77425400	0.19225100
H	-1.40732600	-1.87430800	-0.99586000
H	-1.73120000	-2.07875400	0.71840700
H	0.17939700	2.66390500	-0.33546700
H	-0.66844200	2.13317900	1.11579500
C	1.11326200	-0.99211900	-0.97865800
H	1.87547600	-1.74987800	-1.18804500
H	0.47989400	-0.93106400	-1.86938000
C	1.77163600	0.37137600	-0.65701500
H	2.82713700	0.22280100	-0.40151000

H	1.73604300	1.06693600	-1.50337600
H	1.68876700	1.55259500	1.17225100
C	0.67617500	-0.36661700	1.34487400
C	-1.27205700	1.10547700	-0.66777100
C	-1.97620700	-0.06209500	0.03706300
H	-0.85623300	0.78056900	-1.62968000
H	-2.02031100	1.87226100	-0.90553400
H	-2.97236400	-0.20538300	-0.40001700
H	-2.14568700	0.22699500	1.08288800
H	1.58007100	-0.72170400	1.85676900
H	-0.09572100	-0.21738800	2.10898600
C	0.26686100	-1.39035600	0.26579500
H	0.55035000	-2.40025900	0.58488200

F[4.3.1]
Energy: -480.672387 au
Sum of electronic and thermal Energies: -480.427077 au
Geometry:

C	-1.38330500	-1.47398500	-0.13767600
C	0.70928700	1.18559800	0.51879200
C	-0.44830300	1.82675100	-0.29766400
H	-1.27939200	-2.15970700	-0.98508700
H	-1.94113800	-1.99138100	0.64826900
H	-0.02676600	2.64465600	-0.89678800
H	-1.16004300	2.27032800	0.40906300
C	1.07329500	-1.44451000	-0.61365600
H	1.28414400	-2.52090800	-0.56885200
H	0.79248500	-1.21011900	-1.65197200
C	1.94321200	0.85275500	-0.34570000
H	2.78781500	1.48042800	-0.04320800
H	1.73696200	1.08475100	-1.39892400
H	0.97035900	1.86573300	1.33531700
C	0.00601300	-0.01857000	1.11350700
N	-0.02070200	-1.15616100	0.31403100
O	-0.73228700	0.09302300	2.08434700
C	2.30006600	-0.62871300	-0.23683800
H	2.60542300	-0.87447700	0.78798600
H	3.12957600	-0.88739600	-0.90336800
C	-2.12651500	-0.18903400	-0.56840500
H	-2.60774900	0.25968900	0.30732000
H	-2.92957400	-0.47367700	-1.25887900
C	-1.22948300	0.87945100	-1.24170600
H	-1.88135000	1.52152300	-1.84658100
H	-0.54314700	0.40104200	-1.95121300

F[4.3.1] N+
Energy: -481.038282 au
Sum of electronic and thermal Energies: -480.778649 au
Geometry:

C	-1.32042100	-1.50119500	-0.38667400
C	0.53816100	1.19559900	0.61653900
C	-0.72247600	1.86735600	0.01648900
H	-1.21929800	-1.93843000	-1.38282200
H	-1.78279300	-2.23625900	0.27619600
H	-0.39075500	2.80914700	-0.43410600
H	-1.40435500	2.12522800	0.83531900

C	1.14211100	-1.20323100	-0.98525300
H	1.45634100	-2.22557400	-1.21117900
H	0.64327900	-0.78915500	-1.86299900
C	1.72749200	1.12283100	-0.37916300
H	2.51482900	1.79889700	-0.03694000
H	1.40104900	1.48354300	-1.36124200
H	0.82612900	1.76776400	1.50406400
C	0.15678200	-0.14568700	1.16449500
N	0.10710900	-1.29851600	0.11774400
O	-0.14168400	-0.46398600	2.27632400
C	2.27491700	-0.29602300	-0.53978000
H	2.71939700	-0.66379000	0.39463700
H	3.06198500	-0.32275500	-1.29905000
C	-2.15130100	-0.21889600	-0.40745800
H	-2.48880300	0.00879100	0.61086000
H	-3.05368800	-0.47636600	-0.97249200
C	-1.49312500	1.03438000	-1.01540300
H	-2.28794800	1.67078800	-1.41631500
H	-0.86252100	0.77524300	-1.87460500
H	0.33802100	-2.11637200	0.69312700

F[4.3.1] O+
Energy: -481.030904 au
Sum of electronic and thermal Energies: -480.771877 au
Geometry:

C	-1.42208000	-1.48990000	-0.03009800
C	0.77513200	1.21199100	0.45113900
C	-0.38877700	1.78496300	-0.45431400
H	-1.28798900	-2.30507400	-0.74356500
H	-1.96040100	-1.87065500	0.83911000
H	0.08093900	2.53011600	-1.10588400
H	-1.11198500	2.32030900	0.17283200
C	1.10307400	-1.52281800	-0.45498100
H	1.23850000	-2.58038000	-0.20648400
H	0.84540300	-1.44786500	-1.51635600
C	2.01191900	0.78360000	-0.36496000
H	2.86098200	1.41454800	-0.09169400
H	1.82035300	0.94568800	-1.43140900
H	1.02939900	1.94447600	1.22448900
C	0.01932700	0.06511100	1.01200500
N	-0.04759400	-1.05733800	0.34799600
O	-0.92597500	0.25937000	1.91173000
C	2.33189800	-0.69279800	-0.12809600
H	2.62884100	-0.86020400	0.91423300
H	3.15869100	-1.02184700	-0.76317000
C	-2.11120200	-0.25856900	-0.67240000
H	-2.71994900	0.25704300	0.07612800
H	-2.80477500	-0.62713700	-1.43403800
C	-1.14850100	0.76270400	-1.34610600
H	-1.76164500	1.37012500	-2.01993400
H	-0.43783200	0.23763100	-1.99536600
H	-0.86231400	1.15393100	2.27815500

F[4.3.1] amine
Energy: -406.764514 au
Sum of electronic and thermal Energies: -406.500931 au

Geometry:

C	-1.30011700	-1.53036400	0.10032300
C	0.54350900	1.20759800	0.66730000
C	-0.72513200	1.79886500	0.03794500
H	-1.26743700	-2.14540400	-0.80691400
H	-1.78081200	-2.14693500	0.87367100
H	-0.44354400	2.70482000	-0.51663500
H	-1.40226300	2.12312900	0.84159100
C	1.04963200	-1.36240700	-0.62427400
H	1.40764300	-2.39808900	-0.70995900
H	0.57780900	-1.10816500	-1.58861000
C	1.68361100	1.03367000	-0.37399500
H	2.49741800	1.73747700	-0.16621300
H	1.30488600	1.28228100	-1.37471500
H	0.87685100	1.91538000	1.43978200
C	0.28179500	-0.13292600	1.37742000
N	0.08419700	-1.26533900	0.47937100
C	2.21695500	-0.40240000	-0.41817300
H	2.75248500	-0.65066700	0.50536000
H	2.92981100	-0.51967300	-1.24201100
C	-2.19376600	-0.29878100	-0.15495100
H	-2.58173500	0.07918900	0.80001200
H	-3.07009300	-0.64262300	-0.71999000
C	-1.51514900	0.86592900	-0.89194500
H	-2.29101500	1.46747700	-1.38185200
H	-0.87304000	0.48582500	-1.69585700
H	1.12625300	-0.34761700	2.04538000
H	-0.60061900	-0.05413700	2.02346800

F[4.3.1] ketone
Energy: -464.648659 au
Sum of electronic and thermal Energies: -464.391561 au
Geometry:

C	-1.36312300	-1.51220200	-0.33553800
C	0.56722900	1.17127100	0.58508200
C	-0.66943800	1.84902900	-0.04493400
H	-1.30683400	-1.99811300	-1.31807800
H	-1.92107400	-2.18804400	0.32184800
H	-0.33168700	2.78130400	-0.51629100
H	-1.36137700	2.12796900	0.76038200
C	1.13729000	-1.27929000	-0.92195100
H	1.48615500	-2.29119800	-1.15839300
H	0.68439700	-0.88477400	-1.83963600
C	1.75418800	1.06452900	-0.40700100
H	2.54621500	1.75412000	-0.09515900
H	1.43063700	1.38749600	-1.40537700
H	0.86118400	1.77014700	1.45398500
C	0.14123200	-0.17431700	1.15198200
O	-0.20034500	-0.28853600	2.32187300
C	2.29339500	-0.36338200	-0.52512000
H	2.72182800	-0.69131600	0.43241400
H	3.09639600	-0.40317300	-1.26964600
C	-2.16941000	-0.20513300	-0.45004300
H	-2.51999100	0.08184500	0.55017400
H	-3.06980300	-0.42626500	-1.03548400
C	-1.44627600	1.00737500	-1.06895700

H	-2.20002800	1.66401200	-1.52006800
H	-0.79215400	0.69049500	-1.89043900
C	0.08351200	-1.36318100	0.20389000
H	0.30730700	-2.23440600	0.83032300

F[4.3.1] hydrocarbon
Energy: -390.756416 au
Sum of electronic and thermal Energies: -390.480708 au
Geometry:

C	-1.40378400	-1.52110500	0.03803800
C	0.57201600	1.18524100	0.68879600
C	-0.68111800	1.81753900	0.06495900
H	-1.40477200	-2.10184400	-0.89462900
H	-1.94445100	-2.13032800	0.77433300
H	-0.37171800	2.72727600	-0.46843100
H	-1.34857400	2.14400200	0.87577700
C	1.03575600	-1.33450700	-0.71055400
H	1.35607400	-2.35933500	-0.93427200
H	0.51594900	-0.97412600	-1.60688900
C	1.72274900	1.02417200	-0.34585900
H	2.54806300	1.70029000	-0.09365300
H	1.36297300	1.33146900	-1.33756500
H	0.91045700	1.89238900	1.45803600
C	0.28491700	-0.13908800	1.41859900
C	2.23134200	-0.41690000	-0.46432000
H	2.76285900	-0.71774900	0.44764800
H	2.95008800	-0.49073500	-1.28881700
C	-2.21395200	-0.22897400	-0.16954400
H	-2.56184000	0.13940600	0.80476500
H	-3.12053700	-0.49642600	-0.72685500
C	-1.50420800	0.93426600	-0.88211600
H	-2.26950100	1.57355800	-1.34052100
H	-0.88662500	0.56532100	-1.70963800
H	1.14287400	-0.35567500	2.06738500
H	-0.57493200	-0.01351600	2.09017800
C	0.06027600	-1.35270000	0.49432500
H	0.30965100	-2.24164300	1.08920500

G[4.4.1]
Energy: -519.867339 au
Sum of electronic and thermal Energies: -519.591945 au
Geometry:

C	0.51028600	1.61325300	-0.45818900
C	0.48199700	-1.28778400	0.33546800
C	2.00287500	-1.17825300	0.16168400
H	0.29003300	1.26478400	-1.47923900
H	0.32341700	2.69462600	-0.45201300
H	2.35636400	-2.10719500	-0.30543700
H	2.45152700	-1.14118500	1.16347700
C	-1.82174300	1.23557600	0.22718200
H	-2.39351500	0.98778100	1.12477000
H	-2.00343400	2.29112000	-0.00770500
C	-0.32065500	-1.42677300	-0.98012800
H	-0.18598400	-2.45685700	-1.33350300
H	0.09116800	-0.78098700	-1.76275300
H	0.29834100	-2.18735700	0.93464200

C	-0.18305600	-0.18918300	1.15101400
N	-0.39764700	1.06591300	0.54768000
O	-0.71174900	-0.44678700	2.22374200
C	-2.25336200	0.34293000	-0.95110200
H	-3.34726000	0.39775100	-1.02924100
H	-1.85882900	0.74633900	-1.89249500
C	1.98965200	1.36673100	-0.15800600
H	2.16066300	1.47671100	0.92123800
H	2.56070000	2.16112000	-0.65285000
C	2.50655000	0.01395600	-0.65243300
H	3.60293700	0.01060300	-0.61792600
H	2.23368500	-0.10339700	-1.70895400
C	-1.83647000	-1.14023700	-0.84030800
H	-2.20486400	-1.56146500	0.10500100
H	-2.35387900	-1.68077300	-1.64180300

G[4.4.1] N+
Energy: -520.241147 au
Sum of electronic and thermal Energies: -519.951249 au
Geometry:

C	0.45911900	1.51475400	-0.86156200
C	0.40555900	-1.26029200	0.52819800
C	1.92164500	-1.22310700	0.21285900
H	0.07116900	0.92630900	-1.69210800
H	0.28293700	2.57235600	-1.08054900
H	2.20542100	-2.23499100	-0.09771300
H	2.46021000	-1.01665600	1.14591600
C	-1.88448400	1.20124800	0.09968600
H	-2.33910200	1.08462000	1.08865300
H	-2.13562800	2.19440900	-0.28533000
C	-0.48372400	-1.64708500	-0.66335700
H	-0.35559400	-2.72689100	-0.79418400
H	-0.12809600	-1.19301400	-1.59388800
H	0.26268300	-2.00745400	1.31845500
C	0.03034100	0.01272500	1.22420700
N	-0.38651900	1.22485900	0.35156000
O	0.02601200	0.23757900	2.39966400
C	-2.35094000	0.11040800	-0.85429700
H	-3.44304200	0.20580400	-0.87338400
H	-2.01544400	0.32295000	-1.87542600
C	1.94326900	1.23162700	-0.62303600
H	2.23549900	1.56434400	0.38344000
H	2.49363700	1.87099900	-1.32133600
C	2.35692700	-0.22655800	-0.86530400
H	3.44948100	-0.26662300	-0.92677300
H	1.98900700	-0.53819900	-1.84989300
C	-1.97500100	-1.32790600	-0.47472400
H	-2.28293500	-1.54431400	0.55782000
H	-2.55907000	-1.99696800	-1.11396100
H	-0.22986500	1.99379600	1.01600200

G[4.4.1] O+
Energy: -520.223741 au
Sum of electronic and thermal Energies: -519.934435 au
Geometry:

C	0.60566500	1.68436000	-0.26385700

C	0.54060400	-1.31452400	0.28162200
C	2.06304200	-1.19116200	0.13382000
H	0.38883400	1.53837500	-1.32796400
H	0.41200300	2.73569200	-0.02910500
H	2.39898300	-2.08656400	-0.40170200
H	2.50495700	-1.23884300	1.13650700
C	-1.81836100	1.30395200	0.26101900
H	-2.43481000	1.05191000	1.12193000
H	-1.87601900	2.38013700	0.08869600
C	-0.26032300	-1.35252400	-1.06672700
H	-0.14874000	-2.36787600	-1.46264500
H	0.22315100	-0.67953600	-1.78165000
H	0.35548200	-2.25297800	0.82156000
C	-0.22417600	-0.25541600	1.01208100
N	-0.39475400	0.95736300	0.54647200
O	-1.09986000	-0.63034000	1.92803800
C	-2.18775400	0.49058700	-0.99707700
H	-3.27541500	0.55128200	-1.11646300
H	-1.75519300	0.97248100	-1.88123600
C	2.06139600	1.35724900	0.04715600
H	2.21361900	1.35411900	1.13465600
H	2.64546800	2.19634900	-0.34543900
C	2.56759600	0.05923200	-0.58031400
H	3.66157500	0.04516800	-0.54316700
H	2.29960800	0.03884200	-1.64320300
C	-1.78019300	-1.00888900	-1.00605100
H	-2.26446000	-1.53940200	-0.17684000
H	-2.21990700	-1.42963900	-1.91598000
H	-0.97195900	-1.56551500	2.14240400

G[4.4.1] amine
Energy: -445.965505 au
Sum of electronic and thermal Energies: -445.671661 au
Geometry:

C	-0.48164200	-1.60936000	-0.47315600
C	-0.38744200	1.27097200	0.64132200
C	-1.87400800	1.27987800	0.25444400
H	-0.14878800	-1.17151200	-1.43158500
H	-0.37260500	-2.69801500	-0.57724500
H	-2.12682500	2.25299400	-0.18932600
H	-2.46265100	1.19601900	1.17887700
C	1.78845300	-1.25882200	0.33838900
H	2.33054700	-1.14455000	1.28651300
H	2.00587200	-2.27016500	-0.03254400
C	0.52958000	1.57473800	-0.55431400
H	0.42891700	2.64332200	-0.78620500
H	0.17675500	1.04013800	-1.44478200
H	-0.25148300	2.08628700	1.36978700
C	-0.02342300	-0.01889500	1.40438200
N	0.36465800	-1.19981600	0.64543300
C	2.34032400	-0.23594500	-0.66983800
H	3.42996700	-0.37282700	-0.70777100
H	1.96790000	-0.46076400	-1.67788200
C	-1.96334700	-1.26277000	-0.30348500
H	-2.28425100	-1.47573500	0.72385900
H	-2.52737800	-1.94503000	-0.95132000

C	-2.32237300	0.17421000	-0.71096400
H	-3.41208700	0.24885800	-0.81899400
H	-1.90771700	0.35745200	-1.71082500
C	2.01393100	1.22898200	-0.35046100
H	2.32429200	1.47450600	0.67528400
H	2.61474300	1.86344200	-1.01376400
H	0.81577000	0.18727000	2.07869900
H	-0.87389600	-0.27090700	2.05328300

G[4.4.1] ketone
Energy: -503.849871 au
Sum of electronic and thermal Energies: -503.562607 au
Geometry:

C	-0.48909400	-1.57962700	-0.75734400
C	-0.38348700	1.26421200	0.46647400
C	-1.89541800	1.22876600	0.15891500
H	-0.13332200	-1.05315300	-1.64920000
H	-0.36234700	-2.64922400	-0.96827100
H	-2.18988900	2.22581800	-0.19567400
H	-2.42549000	1.06214700	1.10600100
C	1.89542000	-1.22876400	0.15890200
H	2.42548400	-1.06215900	1.10599500
H	2.18990200	-2.22580900	-0.19570200
C	0.48910200	1.57964900	-0.75730800
H	0.36235700	2.64925300	-0.96820100
H	0.13333400	1.05320300	-1.64918300
H	-0.22936000	2.06273200	1.20382700
C	-0.00000600	-0.00001900	1.21834800
C	2.36105300	-0.18753300	-0.86667100
H	3.45405200	-0.26142000	-0.93224000
H	1.98102200	-0.44407800	-1.86402300
C	-1.98281200	-1.26940500	-0.56194200
H	-2.28543100	-1.53001600	0.46267800
H	-2.56463400	-1.91505700	-1.23077200
C	-2.36104600	0.18755400	-0.86667900
H	-3.45404400	0.26144300	-0.93225400
H	-1.98100800	0.44411700	-1.86402300
C	1.98281700	1.26942000	-0.56190800
H	2.28543400	1.53001100	0.46271700
H	2.56464200	1.91508400	-1.23072400
C	0.38348800	-1.26422900	0.46645000
H	0.22935900	-2.06276800	1.20378200
O	-0.00002000	-0.00003300	2.44397900

G[4.4.1] hydrocarbon
Energy: -429.956402 au
Sum of electronic and thermal Energies: -429.650512 au
Geometry:

C	0.50492800	1.59591200	-0.53756600
C	0.39357300	-1.26407800	0.66623600
C	1.88481900	-1.25774700	0.28885700
H	0.14808200	1.07658900	-1.43495900
H	0.38949100	2.66763600	-0.74792800
H	2.14786000	-2.24352900	-0.12077800
H	2.46458100	-1.14226300	1.21560100
C	-1.88481800	1.25774800	0.28885900

H	-2.46457600	1.14226900	1.21560600
H	-2.14786200	2.24352800	-0.12078200
C	-0.50492800	-1.59591000	-0.53755900
H	-0.38948400	-2.66763300	-0.74792600
H	-0.14808800	-1.07658200	-1.43495200
H	0.27321600	-2.09399000	1.37949300
C	0.00000500	0.00000200	1.45048700
C	-2.34584200	0.18754800	-0.70973300
H	-3.43610300	0.27615600	-0.80475300
H	-1.93955300	0.40370700	-1.70671700
C	1.99437700	1.26516200	-0.35739700
H	2.31486800	1.49754500	0.66786000
H	2.57784900	1.91891600	-1.01777700
C	2.34584300	-0.18755000	-0.70974000
H	3.43610300	-0.27615300	-0.80475700
H	1.93955400	-0.40371200	-1.70672300
C	-1.99438500	-1.26516900	-0.35739800
H	-2.31488500	-1.49756300	0.66785300
H	-2.57784600	-1.91891500	-1.01779500
H	-0.84039200	-0.23862800	2.11614500
H	0.84039800	0.23863700	2.11614700
C	-0.39356900	1.26408000	0.66623000
H	-0.27321400	2.09399500	1.37948100

H[5.2.1]
Energy: -480.686368 au
Sum of electronic and thermal Energies: -480.440699 au
Geometry:

C	-1.57366900	-1.28904200	0.04946000
C	1.66192300	0.20713800	0.35513300
C	1.10346100	1.63819600	0.18915400
H	-1.84453500	-1.40929700	1.10178200
H	-1.94863800	-2.15758600	-0.50376100
H	1.87399600	2.24050600	-0.31099900
H	0.96621200	2.06125800	1.19250500
C	0.56573500	-1.20299500	-1.29206400
H	0.69606200	-2.21420700	-1.69392900
H	-0.01185900	-0.62633900	-2.02199200
C	1.91532500	-0.52680400	-0.96523100
H	2.68989300	-1.28661300	-0.82542800
H	2.23628600	0.14413400	-1.76789600
H	2.54333200	0.24346200	1.00118700
C	0.53915200	-0.57873600	0.99920800
N	-0.12146200	-1.25600900	-0.00674500
O	0.17694800	-0.51378200	2.16610200
C	-0.21645600	1.80534600	-0.59725100
C	-1.54024300	1.31076000	0.05546300
C	-2.17066000	0.01649000	-0.50560700
H	-0.31734500	2.88588000	-0.75661400
H	-1.41257500	1.21629700	1.13996800
H	-2.28352600	2.10224200	-0.09488200
H	-3.24190800	0.00895400	-0.26658900
H	-2.10619200	0.03032600	-1.60132300
H	-0.11195900	1.38118500	-1.60321700

H[5.2.1] N+

Energy: -481.037368 au
Sum of electronic and thermal Energies: -480.778064 au
Geometry:

C	-1.59692500	-1.28471900	-0.00453700
C	1.61514400	0.29777800	0.30267900
C	1.04436100	1.73766000	0.27469000
H	-1.81381400	-1.46819700	1.05203700
H	-2.03926500	-2.08886100	-0.59965300
H	1.81515000	2.36092900	-0.19223400
H	0.94776000	2.07438100	1.31391500
C	0.53578100	-1.07203100	-1.43292800
H	0.68619700	-1.97802000	-2.02237200
H	-0.15233600	-0.41697300	-1.96107400
C	1.84790900	-0.35598700	-1.06590700
H	2.66497500	-1.08060000	-0.99931400
H	2.11201100	0.37856600	-1.83028900
H	2.52803900	0.31394100	0.90623900
C	0.64528400	-0.60054300	1.00175200
N	-0.09730800	-1.43542300	-0.12287700
O	0.34903500	-0.79525500	2.13374800
C	-0.29075300	1.96055700	-0.44799500
C	-1.55159200	1.33981400	0.20652300
C	-2.13346400	0.07207100	-0.44996500
H	-0.42915400	3.04626000	-0.47318500
H	-1.38971100	1.17641000	1.27993000
H	-2.34491800	2.09082000	0.14861800
H	-3.20119200	0.01546200	-0.20647800
H	-2.09374900	0.16640000	-1.54067100
H	-0.21797600	1.66331200	-1.50155900
H	0.12240200	-2.41142800	0.11036600

H[5.2.1] O+
Energy: -481.045750 au
Sum of electronic and thermal Energies: -480.786443 au
Geometry:

C	-1.62510200	-1.26854100	0.04407500
C	1.68611400	0.17104100	0.33360400
C	1.13454000	1.62088200	0.16862800
H	-1.90272600	-1.40291300	1.09093200
H	-1.94810900	-2.14262700	-0.52553300
H	1.92788100	2.19172500	-0.32816000
H	1.00670500	2.07100000	1.16227900
C	0.56202000	-1.23087200	-1.31648200
H	0.65413600	-2.27902900	-1.61064000
H	-0.01954600	-0.70272900	-2.07282800
C	1.91676600	-0.56309600	-1.00066500
H	2.69431800	-1.32051800	-0.88057400
H	2.22295800	0.12519200	-1.79115900
H	2.57013200	0.17989700	0.97827000
C	0.53858700	-0.58187400	0.89965100
N	-0.16160900	-1.17206400	-0.02734800
O	0.08092400	-0.51856400	2.12986100
C	-0.17637000	1.78974200	-0.63263500
C	-1.52358300	1.33623100	0.00916800
C	-2.18720000	0.04755500	-0.52833300
H	-0.25122900	2.86767100	-0.81048900

H	-1.43353200	1.28263700	1.10117200
H	-2.24523800	2.13752800	-0.17720600
H	-3.25472700	0.06236500	-0.28291800
H	-2.12715000	0.03390300	-1.62243100
H	-0.06496900	1.35281200	-1.63176700
H	0.70033700	-0.03036200	2.69153100

H[5.2.1] amine
Energy: -406.761006 au
Sum of electronic and thermal Energies: -406.497603 au
Geometry:

C	-1.32436400	-1.48156800	0.31741200
C	1.56801200	0.48450000	0.50128800
C	0.78722000	1.78568500	0.27353400
H	-1.61490200	-1.56331000	1.37188800
H	-1.65096900	-2.41451000	-0.16415800
H	1.46634000	2.48410800	-0.23547000
H	0.57064300	2.23119800	1.25556300
C	0.74548000	-1.22730100	-1.03433100
H	1.08139300	-2.18005600	-1.46360600
H	0.03306500	-0.78719200	-1.74359800
C	1.93112700	-0.27281300	-0.78932100
H	2.84531600	-0.85370900	-0.62503200
H	2.10703600	0.39744700	-1.63771800
H	2.48151200	0.75703900	1.04510500
C	0.80269700	-0.59214300	1.27955200
N	0.12882200	-1.43322500	0.28152300
C	-0.52029300	1.74542800	-0.53242300
C	-1.75255600	1.09656900	0.14092500
C	-2.11084000	-0.32336100	-0.32333400
H	-0.77025600	2.79196900	-0.74656000
H	-1.63932100	1.11852800	1.23324000
H	-2.61894500	1.73109600	-0.08055900
H	-3.16819900	-0.51620700	-0.09523800
H	-2.03266700	-0.36540200	-1.41728800
H	-0.34603900	1.28349700	-1.51218800
H	1.51363600	-1.20153700	1.85724500
H	0.08170100	-0.17036600	1.98790300

H[5.2.1] ketone
Energy: -464.647204 au
Sum of electronic and thermal Energies: -464.390553 au
Geometry:

C	-1.61161600	-1.31396900	0.02700000
C	1.61517100	0.29756600	0.29215600
C	1.02708500	1.72174600	0.25053400
H	-1.88424200	-1.46257000	1.07968100
H	-2.10571800	-2.10905200	-0.54628900
H	1.77790000	2.37256900	-0.21675000
H	0.90800600	2.06307700	1.28743600
C	0.55560400	-1.12681500	-1.42428300
H	0.76933800	-2.01379300	-2.02814700
H	-0.11627200	-0.49862900	-2.01319000
C	1.85258800	-0.34983200	-1.08031500
H	2.69113500	-1.05180500	-1.00559000
H	2.10964400	0.38613100	-1.84983500

H	2.52764900	0.33647000	0.89727800
C	0.62520700	-0.63521000	0.96977400
O	0.41992800	-0.69700300	2.16863500
C	-0.30952000	1.91267700	-0.48311000
C	-1.57100100	1.31033300	0.19015600
C	-2.16522000	0.03814800	-0.44812800
H	-0.45646800	2.99663800	-0.56159200
H	-1.38342400	1.14000500	1.25791300
H	-2.35421500	2.07570000	0.14473500
H	-3.24119100	0.02039000	-0.23326100
H	-2.08679900	0.12061300	-1.53972600
H	-0.22802600	1.55673700	-1.51732900
C	-0.09020100	-1.49209600	-0.07651500
H	0.14466600	-2.53173800	0.19196100

H[5.2.1] hydrocarbon
Energy: -390.751554 au
Sum of electronic and thermal Energies: -390.476139 au
Geometry:

C	-1.42550000	-1.47787300	0.29273600
C	1.57101500	0.47534100	0.50433800
C	0.81695400	1.79466400	0.28926400
H	-1.75597400	-1.56243100	1.33764300
H	-1.80973900	-2.37093500	-0.22019300
H	1.50897900	2.48550200	-0.21289400
H	0.61149700	2.23139200	1.27767600
C	0.75487100	-1.20595000	-1.09207500
H	1.07696600	-2.11315900	-1.61412500
H	0.03294900	-0.70941100	-1.74511400
C	1.94085800	-0.26866500	-0.79295400
H	2.84235000	-0.86768700	-0.61287600
H	2.16237400	0.41469500	-1.62146900
H	2.48747800	0.74280200	1.04643200
C	0.79493000	-0.58630800	1.30344100
C	-0.49365600	1.79172600	-0.51009400
C	-1.72908200	1.13911800	0.15372800
C	-2.11771000	-0.26392100	-0.34352500
H	-0.73364100	2.84657900	-0.69355000
H	-1.61261700	1.13590400	1.24545600
H	-2.58750700	1.79024300	-0.05058800
H	-3.19291900	-0.40041400	-0.16812100
H	-1.99642300	-0.28991700	-1.43413500
H	-0.33096500	1.35529300	-1.50334000
C	0.11036200	-1.53436200	0.28008100
H	0.37499300	-2.56355600	0.55222100
H	0.07890700	-0.14099400	2.00269500
H	1.50504300	-1.16652700	1.90464200

I[5.3.1]
Energy: -519.875327 au
Sum of electronic and thermal Energies: -519.599569 au
Geometry:

C	-1.22703300	-1.72939000	-0.00113600
C	1.08087500	1.04532800	0.57903600
C	0.23047300	1.76942300	-0.50492200
H	-1.22467100	-2.30378800	-0.93409600

H	-1.39226900	-2.42705500	0.82803900
H	0.46751200	1.34447600	-1.48778800
H	0.57902100	2.80992800	-0.53801000
C	1.05757700	-1.25677100	-0.98127300
H	1.07455700	-2.31602000	-1.26402700
H	0.76993900	-0.68618500	-1.87711100
C	2.45123800	0.62469200	0.00684300
H	3.23228400	0.74565600	0.76445300
H	2.70594600	1.29677500	-0.82211900
H	1.20026500	1.70770200	1.44112100
C	0.23383900	-0.11762300	1.03972000
N	0.09051000	-1.10814100	0.10177200
O	-0.43452200	-0.08856700	2.07245200
C	2.43515800	-0.83662000	-0.47499700
H	2.68575900	-1.49825500	0.36216000
H	3.18297200	-0.99815700	-1.25880300
C	-2.35098200	-0.68126700	-0.03961100
H	-2.57000800	-0.34095700	0.97573700
H	-3.25058600	-1.19114000	-0.40711400
C	-2.06842400	0.54281900	-0.93631800
C	-1.30292100	1.75091800	-0.32969600
H	-3.04660600	0.92418700	-1.25361700
H	-1.56177800	0.22012500	-1.85796000
H	-1.68140600	2.64605300	-0.83803700
H	-1.56713200	1.86312800	0.72927300

I[5.3.1] N+
Energy: -520.232229 au
Sum of electronic and thermal Energies: -519.942471 au
Geometry:

C	-0.84720200	-1.65230900	-0.57454200
C	0.68668800	1.28201200	0.33038100
C	-0.41459600	1.57780200	-0.71212300
H	-0.76870100	-1.30476700	-1.60629400
H	-0.82754200	-2.74536600	-0.58128600
H	-0.31134300	0.90597600	-1.57449300
H	-0.20292800	2.58208700	-1.09399900
C	1.63836900	-1.18340100	-0.84076700
H	2.00846600	-2.20426400	-0.96648300
H	1.25600300	-0.82789700	-1.80011300
C	2.11979600	1.20731900	-0.27559400
H	2.78879300	1.85923800	0.29141800
H	2.08233800	1.59011300	-1.30140500
H	0.63417800	2.05180600	1.10604400
C	0.36565000	0.00752000	1.02915500
N	0.46025800	-1.24709100	0.11182000
O	0.07904100	-0.21417600	2.16770400
C	2.67796200	-0.22207100	-0.28464300
H	2.97282000	-0.53426000	0.72606000
H	3.57668400	-0.27856100	-0.90559900
C	-2.12429100	-1.11951700	0.07943500
H	-2.03515100	-1.11038700	1.17101300
H	-2.89489400	-1.86489200	-0.14701400
C	-2.62739800	0.22921400	-0.46262900
C	-1.84077400	1.50576000	-0.12973700
H	-3.64683400	0.36154300	-0.08440500

H	-2.71658700	0.14665300	-1.55427800
H	-2.42074400	2.34570600	-0.52431500
H	-1.80722900	1.65215000	0.95815800
H	0.65331700	-1.97581200	0.80900900

I[5.3.1] O+
Energy: -520.239186 au
Sum of electronic and thermal Energies: -519.949611 au
Geometry:

C	-1.26610700	-1.73385700	0.06874600
C	1.13044600	1.03725200	0.55625300
C	0.27634000	1.78604600	-0.53037500
H	-1.22763600	-2.39839100	-0.79690700
H	-1.41049600	-2.33916000	0.96778900
H	0.55702700	1.38513600	-1.51034100
H	0.62001500	2.82624200	-0.51609400
C	1.05056300	-1.30732100	-0.95942700
H	1.01237300	-2.37777600	-1.17753600
H	0.74584300	-0.76399300	-1.85943200
C	2.48890700	0.57000700	-0.02012500
H	3.27598600	0.69621200	0.72754200
H	2.73744600	1.22060800	-0.86410800
H	1.27809200	1.69305500	1.42155300
C	0.25701100	-0.09516200	0.94763400
N	0.05902000	-1.07615800	0.11496300
O	-0.53310500	-0.04080900	2.00276400
C	2.43282300	-0.90252400	-0.45899400
H	2.67878000	-1.55073700	0.38954800
H	3.16795800	-1.10140100	-1.24334100
C	-2.37042100	-0.67328200	-0.09866700
H	-2.69063300	-0.30325800	0.87810300
H	-3.23159300	-1.19730400	-0.52636300
C	-2.01323400	0.52006100	-1.01463500
C	-1.26544000	1.74930200	-0.41920700
H	-2.96969200	0.90193000	-1.38564900
H	-1.47779800	0.16494900	-1.90645700
H	-1.61051000	2.61907500	-0.98809100
H	-1.59987500	1.93290000	0.61055800
H	-0.32891600	0.74835800	2.52515100

I[5.3.1] amine
Energy: -445.955253 au
Sum of electronic and thermal Energies: -445.661452 au
Geometry:

C	-0.83078700	-1.67774200	-0.26826100
C	0.72875100	1.24367600	0.46470600
C	-0.34449000	1.51074000	-0.59844600
H	-0.80450000	-1.45121600	-1.35110800
H	-0.86559000	-2.77432000	-0.19110000
H	-0.25406800	0.76404800	-1.39872300
H	-0.12582700	2.48020700	-1.06480500
C	1.53657500	-1.27597800	-0.57874800
H	1.90511200	-2.30812000	-0.66360700
H	1.20483300	-0.97615700	-1.59293400
C	2.14780800	1.12569900	-0.15222100
H	2.85656600	1.76090800	0.39133400

H	2.12409600	1.49289900	-1.18700500
H	0.70387400	2.07835000	1.18126800
C	0.41430900	-0.04705100	1.22017900
N	0.41481500	-1.22816300	0.36271900
C	2.65369400	-0.32818500	-0.15160000
H	3.01353300	-0.61113200	0.84392200
H	3.50173100	-0.43447100	-0.83697800
C	-2.14591800	-1.10870800	0.27744100
H	-2.13714900	-1.07430600	1.37283700
H	-2.92232900	-1.83889600	0.01536400
C	-2.59790800	0.23313300	-0.32521800
C	-1.78329900	1.50617900	-0.04381300
H	-3.62835700	0.41447800	0.00838900
H	-2.64919500	0.10338100	-1.41570700
H	-2.33990800	2.33697100	-0.49430700
H	-1.76539300	1.71125700	1.03548300
H	-0.54890100	0.02230300	1.72619700
H	1.15535900	-0.18962000	2.01832500

I[5.3.1] ketone
Energy: -503.841592 au
Sum of electronic and thermal Energies: -503.554404 au
Geometry:

C	-0.84685300	-1.66767000	-0.55108700
C	0.70922500	1.25426300	0.31199100
C	-0.38285200	1.54628300	-0.73874900
H	-0.77890600	-1.31121900	-1.58649000
H	-0.89483700	-2.76134200	-0.61246600
H	-0.28106400	0.84793200	-1.57897200
H	-0.17609300	2.54338600	-1.14698800
C	1.67984700	-1.24329900	-0.77148800
H	2.11354700	-2.24229400	-0.89552100
H	1.34633800	-0.91898300	-1.76652800
C	2.13182000	1.17666900	-0.30791100
H	2.79771700	1.87461100	0.21070100
H	2.08302100	1.49958300	-1.35629300
H	0.66203300	2.03978100	1.07415300
C	0.35735500	-0.03890700	1.00876200
O	-0.01835200	-0.06927500	2.17455400
C	2.71724000	-0.24245900	-0.25702000
H	2.99161400	-0.49818400	0.77572600
H	3.63533500	-0.28740600	-0.85343300
C	-2.15135600	-1.13035400	0.06648300
H	-2.06617400	-1.07979200	1.15801900
H	-2.94872800	-1.85197700	-0.14876000
C	-2.62206300	0.22291200	-0.49583100
C	-1.81402700	1.48907000	-0.16355100
H	-3.64664900	0.38934300	-0.13853000
H	-2.69046200	0.13287600	-1.58985600
H	-2.38427400	2.33973200	-0.55545200
H	-1.77579700	1.62218600	0.92541200
C	0.47298200	-1.31480500	0.18982600
H	0.65228200	-2.09424700	0.94029600

I[5.3.1] hydrocarbon
Energy: -429.947573 au

Sum of electronic and thermal Energies: -429.641709 au
Geometry:

C	0.85294900	1.64910200	-0.36288900
C	-0.69929600	-1.24101600	0.46300000
C	0.39581500	-1.51338200	-0.58022500
H	0.78929900	1.27799800	-1.39366300
H	0.89995700	2.74225900	-0.45143800
H	0.30628400	-0.79837600	-1.40754600
H	0.19389600	-2.50015900	-1.01746500
C	-1.65209900	1.25978200	-0.60063000
H	-2.09036000	2.25815000	-0.71895400
H	-1.28621700	0.96296900	-1.59349400
C	-2.11305500	-1.17647000	-0.17991100
H	-2.79426800	-1.86480900	0.33438300
H	-2.04897300	-1.52051700	-1.22135200
H	-0.67046800	-2.08177900	1.17066400
C	-0.43214200	0.03774300	1.25587800
C	-2.71036500	0.24160800	-0.17016900
H	-3.08326200	0.49138400	0.83090700
H	-3.57457900	0.28087400	-0.84354700
C	2.17507500	1.13795600	0.23711400
H	2.12683500	1.11479200	1.33295600
H	2.96180000	1.86239100	-0.00895800
C	2.64954900	-0.21787300	-0.31385000
C	1.82878200	-1.48227500	-0.00916700
H	3.67188500	-0.38975300	0.04901400
H	2.72632800	-0.12134400	-1.40669900
H	2.39288600	-2.32598400	-0.42555400
H	1.79626200	-1.65353300	1.07544300
C	-0.45973500	1.31003900	0.39040100
H	-0.63917200	2.13878700	1.08939700
H	-1.20524500	0.13088500	2.02931600
H	0.51424700	-0.03551400	1.79928700

J[6.2.1]
Energy: -519.882995 au
Sum of electronic and thermal Energies: -519.606993 au
Geometry:

C	-1.56780000	-1.50206200	-0.13255100
C	1.81233400	-0.11229500	0.50565800
C	1.67982700	1.41420200	0.34160100
H	-1.78644200	-2.26382600	0.62532600
H	-1.79602900	-1.92674000	-1.11626000
H	2.63647100	1.78428100	-0.05080800
H	1.54503400	1.86368600	1.33373100
C	0.69334900	-1.31671900	-1.31169100
H	0.70992400	-2.35335100	-1.67047700
H	0.30873100	-0.68830400	-2.12411700
C	2.08121300	-0.85414100	-0.81465700
H	2.71379900	-1.72665300	-0.62798400
H	2.58368000	-0.22195500	-1.55306400
H	2.57792200	-0.32172000	1.25881000
C	0.47646700	-0.67465200	0.96633100
N	-0.14432500	-1.20501000	-0.12744700
O	-0.01710800	-0.58893300	2.08708700
C	0.53800800	1.88167700	-0.58069400

C	-0.88017100	1.85368900	0.05243200
C	-1.95629900	0.99437400	-0.66662500
C	-2.42483500	-0.25183200	0.11058300
H	0.76834000	2.90959300	-0.88455200
H	-0.80570300	1.52625300	1.09431000
H	-1.24526700	2.88593400	0.09674900
H	-2.83769700	1.62106800	-0.84408700
H	-1.60041900	0.69654900	-1.66253400
H	-2.43456000	-0.02439700	1.18094500
H	-3.45367000	-0.50590300	-0.17416000
H	0.55046900	1.29857700	-1.50871300

J[6.2.1] N+
Energy: -520.224501 au
Sum of electronic and thermal Energies: -519.935169 au
Geometry:

C	-1.79996200	-1.33512000	-0.21649600
C	1.75097400	-0.29096100	0.44543200
C	1.81232400	1.25473500	0.41433200
H	-2.23309000	-2.07324800	0.46317400
H	-2.08390200	-1.59484400	-1.24067100
H	2.82911300	1.49643200	0.08452800
H	1.71789400	1.61931000	1.44408200
C	0.46549300	-1.21826400	-1.41051900
H	0.36723000	-2.04314200	-2.11887900
H	0.01386400	-0.32325600	-1.83305000
C	1.89566700	-0.97318100	-0.92386400
H	2.42697800	-1.92550800	-0.82529900
H	2.44789600	-0.35385300	-1.63466300
H	2.52255200	-0.62963200	1.14648200
C	0.44803700	-0.79153400	1.00581700
N	-0.29807400	-1.54527000	-0.16396700
O	-0.05386700	-0.75940200	2.08091800
C	0.80069000	1.98811500	-0.47539100
C	-0.64053200	2.09714000	0.08578600
C	-1.77690200	1.29123200	-0.59811300
C	-2.30115300	0.05492300	0.16454600
H	1.19367400	3.00354100	-0.58910500
H	-0.63477900	1.87555900	1.16081000
H	-0.92396600	3.15109100	0.01857500
H	-2.63319800	1.96599600	-0.68698600
H	-1.51509000	1.04080400	-1.63388500
H	-2.18292400	0.20701300	1.24105700
H	-3.38180500	-0.02621400	-0.00393700
H	0.80068800	1.57789800	-1.49289900
H	-0.14149400	-2.53836100	0.05191200

J[6.2.1] O+
Energy: -520.245252 au
Sum of electronic and thermal Energies: -519.955570 au
Geometry:

C	-1.62118200	-1.47929500	-0.14839000
C	1.81988500	-0.16104500	0.46812300
C	1.70884300	1.38271400	0.35995700
H	-1.82393400	-2.23605000	0.61525700
H	-1.83640800	-1.90918800	-1.12929200

H	2.68205100	1.72456900	-0.01054800
H	1.59022300	1.81743600	1.36155000
C	0.65915500	-1.29834900	-1.37037800
H	0.62559500	-2.33359400	-1.71952200
H	0.23540500	-0.65197000	-2.14140200
C	2.05713700	-0.86357100	-0.88779800
H	2.69322800	-1.74020800	-0.74735500
H	2.54150100	-0.19688100	-1.60412100
H	2.58652900	-0.42127100	1.20631400
C	0.48829500	-0.70954200	0.85460600
N	-0.17390000	-1.19536100	-0.15233300
O	-0.08301300	-0.65251200	2.03737300
C	0.58657700	1.89920200	-0.55749400
C	-0.84513800	1.88448100	0.04862500
C	-1.92885200	1.04086400	-0.68134000
C	-2.43594800	-0.19962100	0.08285800
H	0.84706100	2.93072500	-0.81353300
H	-0.80340400	1.58026900	1.10129200
H	-1.19659800	2.91978500	0.07856900
H	-2.79814700	1.68177100	-0.85373700
H	-1.58196700	0.75223400	-1.68241800
H	-2.48062600	0.02390500	1.15299000
H	-3.45883100	-0.43625400	-0.22868400
H	0.60678100	1.36046800	-1.51170900
H	0.52031500	-0.25315300	2.68107800

J[6.2.1] amine
Energy: -445.957474 au
Sum of electronic and thermal Energies: -445.664572 au
Geometry:

C	-1.16206900	-1.73953400	0.00023500
C	1.78451400	0.33872300	0.66602300
C	1.26917900	1.73844300	0.28315700
H	-1.11934700	-2.60024500	0.69731700
H	-1.34919800	-2.13962800	-1.00478600
H	2.10185800	2.26613200	-0.20272700
H	1.04835700	2.29952800	1.20312500
C	1.19133300	-1.53348900	-0.80882000
H	1.51486400	-2.52183400	-0.42481500
H	0.92358500	-1.64615900	-1.86542900
C	2.28898600	-0.47108400	-0.56310400
H	3.25766700	-0.93948000	-0.36503800
H	2.40650000	0.18146900	-1.43445400
H	2.58402400	0.45806200	1.40688800
C	0.66303400	-0.55955100	1.19533000
N	0.07267700	-0.99711200	-0.05554500
C	0.03633100	1.81169900	-0.64326300
C	-1.34410500	1.64355300	0.05088800
C	-2.28027500	0.51489600	-0.45379100
C	-2.30316200	-0.78762300	0.37038800
H	0.05781000	2.80184500	-1.11715700
H	-1.20682000	1.53097800	1.13340000
H	-1.88522100	2.59088600	-0.06491700
H	-3.30410700	0.90978900	-0.46416600
H	-2.03243300	0.27386800	-1.49664100
H	-2.26464900	-0.54300700	1.43989200

H	-3.25424200	-1.31191400	0.21096600
H	0.13506500	1.07718400	-1.44837600
H	1.07151400	-1.41219400	1.77813200
H	-0.05656200	-0.03168600	1.82534800

J[6.2.1] ketone
Energy: -503.834236 au
Sum of electronic and thermal Energies: -503.547541 au
Geometry:

C	-1.80562800	-1.39377100	-0.17487400
C	1.76265300	-0.26216700	0.45502100
C	1.79330200	1.27587300	0.37667700
H	-2.28709000	-2.09699800	0.51471600
H	-2.12528900	-1.68218200	-1.18574700
H	2.79832900	1.55478800	0.03367500
H	1.68238600	1.67172600	1.39463900
C	0.50910600	-1.29279800	-1.38353800
H	0.48482600	-2.13711200	-2.07985500
H	0.07755400	-0.43448800	-1.90307000
C	1.93730700	-0.97295400	-0.89870400
H	2.48949800	-1.90935200	-0.75480700
H	2.49924400	-0.36702100	-1.61778800
H	2.53364900	-0.56096800	1.17569500
C	0.42463100	-0.77951700	0.98266300
O	0.00345200	-0.59697600	2.11144000
C	0.75370300	1.95299300	-0.52997400
C	-0.68373400	2.03287800	0.04883500
C	-1.80523400	1.21042100	-0.64326800
C	-2.35587700	0.00411000	0.15092300
H	1.11090900	2.97576900	-0.69884000
H	-0.65770300	1.77551500	1.11388000
H	-0.98578500	3.08519300	0.01245000
H	-2.64864300	1.89080400	-0.80644900
H	-1.49089500	0.90023000	-1.64726500
H	-2.22542400	0.19690100	1.22117500
H	-3.43857500	-0.05468800	-0.01680500
H	0.74835500	1.48416000	-1.52081600
C	-0.28236100	-1.58848800	-0.10115300
H	-0.08015200	-2.63595500	0.17804600

J[6.2.1] hydrocarbon
Energy: -429.937555 au
Sum of electronic and thermal Energies: -429.632052 au
Geometry:

C	-1.63467700	-1.60210000	0.06742300
C	1.79393400	-0.12052500	0.61204700
C	1.63288900	1.40138800	0.47010100
H	-2.05355100	-2.32277200	0.78306100
H	-1.95136800	-1.94663000	-0.92767300
H	2.59712400	1.79146300	0.11445300
H	1.48231200	1.82844100	1.47263300
C	0.60188400	-1.26159300	-1.17861100
H	0.61066000	-2.08454400	-1.90250800
H	0.07659800	-0.42750100	-1.64713600
C	2.00536500	-0.83802000	-0.73755500
H	2.62119100	-1.73349200	-0.58346700

H	2.52089100	-0.20504400	-1.46990100
H	2.67493800	-0.26995700	1.24883700
C	0.56857700	-0.82869900	1.24413600
C	0.54150400	1.96652000	-0.45772800
C	-0.91754300	1.98319400	0.06708000
C	-1.94835700	0.97554500	-0.50609700
C	-2.30987400	-0.25243300	0.36057900
H	0.82564600	3.01108600	-0.63602000
H	-0.91334900	1.91187200	1.16277400
H	-1.31192400	2.98202700	-0.15260400
H	-2.87990000	1.53693100	-0.64451700
H	-1.65160700	0.66017900	-1.51371900
H	-2.17052600	0.00924000	1.41716800
H	-3.38693100	-0.43293900	0.24976800
H	0.58858900	1.48872900	-1.44285000
H	0.87856300	-1.47198800	2.07500700
H	-0.12137900	-0.09348400	1.66557900
C	-0.10057500	-1.67428200	0.12940600
H	0.16526000	-2.72559700	0.30643200

K[5.4.1]
Energy: -559.059730 au
Sum of electronic and thermal Energies: -558.753955 au
Geometry:

C	1.50760200	1.66549200	0.13168800
C	-0.76068700	-1.15770400	0.76598100
C	-0.19800700	-1.74810000	-0.55278600
H	1.38027300	2.37838000	-0.69095200
H	1.86744200	2.21618500	1.01205000
H	-0.61054800	-1.20034300	-1.40574000
H	-0.56716400	-2.77919700	-0.63755400
C	-1.02068200	1.78742700	-0.01517400
H	-1.62974600	1.98191000	0.87870900
H	-0.68804800	2.76495300	-0.37783500
C	-2.24883600	-0.77228900	0.68258200
H	-2.49343600	-0.15533300	1.55709300
H	-2.84303700	-1.68858100	0.79244600
H	-0.64985600	-1.90811900	1.55687200
C	0.19078300	-0.05204300	1.16139600
N	0.19756600	1.06136000	0.34914900
O	1.07877900	-0.25102200	1.99083300
C	-1.86279200	1.11286300	-1.09868900
H	-2.52039100	1.87010800	-1.54421600
H	-1.17793600	0.79073000	-1.89065100
C	2.53757500	0.60139600	-0.28579800
H	2.94602100	0.10753400	0.59908600
H	3.36772100	1.13688600	-0.76367400
C	2.00443300	-0.46395400	-1.26896000
C	1.34094600	-1.74996300	-0.69871500
H	2.86792800	-0.79835200	-1.85718900
H	1.31521600	0.00912000	-1.98384200
H	1.58023200	-2.55958400	-1.39889100
H	1.81284700	-2.01803500	0.25514300
C	-2.72497700	-0.06659700	-0.59910000
H	-3.74168300	0.29465000	-0.40200200
H	-2.82118200	-0.80340600	-1.40412200

K[5.4.1] N+
Energy: -559.425816 au
Sum of electronic and thermal Energies: -559.105513 au
Geometry:

C	-0.89671100	-1.57683800	-0.62660300
C	0.38115900	1.24750600	0.65261700
C	-0.44378500	1.61788800	-0.58913600
H	-0.55963500	-1.11179600	-1.55061000
H	-0.89647400	-2.66108200	-0.77354800
H	-0.16640100	1.00723800	-1.45502900
H	-0.14869000	2.64235200	-0.84395900
C	1.58750200	-1.60748700	-0.07271900
H	2.23611700	-1.53972500	0.80659000
H	1.57126300	-2.64993400	-0.40620300
C	1.91601300	1.32605800	0.46991700
H	2.39854500	0.88384100	1.35121600
H	2.17923100	2.38924500	0.49512400
H	0.11363900	1.95756100	1.44416700
C	0.01183800	-0.06246700	1.27154500
N	0.17488600	-1.34674500	0.42487200
O	-0.35144500	-0.27040500	2.39510700
C	2.05163400	-0.69778900	-1.20306900
H	2.89866000	-1.21741100	-1.66424400
H	1.28790600	-0.66779500	-1.98474500
C	-2.28308400	-1.05899900	-0.22094500
H	-2.38903900	-1.03659000	0.87084900
H	-3.00373600	-1.80573000	-0.57037100
C	-2.67284200	0.29055800	-0.84464000
C	-1.96519200	1.55492100	-0.33983800
H	-3.74759800	0.42290600	-0.67935600
H	-2.53925100	0.21759900	-1.93241700
H	-2.43656300	2.40484800	-0.84335200
H	-2.16825200	1.69159800	0.73111500
C	2.49722400	0.72950900	-0.81682400
H	3.58635700	0.74479100	-0.70701100
H	2.27143900	1.39313300	-1.65710300
H	-0.00270400	-2.05175500	1.15208800

K[5.4.1] O+
Energy: -559.424063 au
Sum of electronic and thermal Energies: -559.104106 au
Geometry:

C	1.60480300	1.62814700	0.28175100
C	-0.84405000	-1.13284800	0.76434200
C	-0.30458400	-1.78581100	-0.55683100
H	1.45957000	2.47935000	-0.38515300
H	2.02626200	1.99367700	1.22260800
H	-0.82512900	-1.32757400	-1.40075700
H	-0.61509000	-2.83644000	-0.53172000
C	-0.94902500	1.83204200	0.01336700
H	-1.58003000	2.05378900	0.87940300
H	-0.54500600	2.78041200	-0.34286700
C	-2.31034700	-0.66746900	0.68885400
H	-2.51952200	-0.05312000	1.57293400
H	-2.93830400	-1.55885200	0.79328500

H	-0.78114500	-1.87548500	1.57108600
C	0.16022000	-0.08532100	1.08530300
N	0.24017500	1.08260900	0.50812900
O	1.20802300	-0.41950500	1.82128500
C	-1.74083800	1.14252400	-1.09329000
H	-2.29536200	1.92225300	-1.62627200
H	-1.03492900	0.72785600	-1.81854400
C	2.51574700	0.57728300	-0.38745100
H	3.06177100	0.00547300	0.36541100
H	3.26738900	1.15187800	-0.93901100
C	1.82307500	-0.38979100	-1.37738200
C	1.21407000	-1.72534200	-0.85376400
H	2.59968100	-0.67913400	-2.09255100
H	1.07203300	0.15212800	-1.96780000
H	1.36348400	-2.46232100	-1.65006600
H	1.80605400	-2.10152900	-0.00915100
C	-2.72964300	0.07656600	-0.58792500
H	-3.69184500	0.55429500	-0.37497400
H	-2.92275400	-0.63958600	-1.39230000
H	1.11090200	-1.32918100	2.13740400

K[5.4.1] amine
Energy: -485.152255 au
Sum of electronic and thermal Energies: -484.828597 au
Geometry:

C	1.42861600	1.70037300	0.21931500
C	-0.63803500	-1.21930400	0.84513500
C	0.08559500	-1.72772200	-0.41196900
H	1.42232600	2.32791700	-0.68068000
H	1.58771900	2.37199700	1.08769600
H	-0.21142000	-1.11876500	-1.27175200
H	-0.26331700	-2.75076700	-0.61199500
C	-1.04511400	1.77388100	0.01772200
H	-1.59519100	1.95097800	0.96001300
H	-0.75513200	2.75919500	-0.36921600
C	-2.14520900	-0.99720000	0.61974300
H	-2.54279300	-0.46650400	1.49627600
H	-2.64959400	-1.97332300	0.60588700
H	-0.53689900	-1.97791700	1.63791700
C	0.03104400	0.05421100	1.35059700
N	0.16209900	0.99583300	0.25770600
C	-1.95022400	1.10767400	-1.02424200
H	-2.75555700	1.81230700	-1.27195700
H	-1.34121600	1.00089200	-1.92964500
C	2.59706100	0.70851000	0.11481000
H	2.85723600	0.30719300	1.10196800
H	3.47699600	1.27809700	-0.21109700
C	2.36268200	-0.45875200	-0.86369500
C	1.62852100	-1.72497700	-0.35141800
H	3.35386500	-0.78908500	-1.20106700
H	1.83912500	-0.08449400	-1.75379900
H	1.97343500	-2.55261700	-0.98395300
H	1.97476600	-1.96784800	0.66414800
C	-2.58097200	-0.26679600	-0.66661200
H	-3.66809900	-0.14202500	-0.58915400
H	-2.42746600	-0.94593600	-1.51243600

H	1.02333500	-0.19097500	1.73571400
H	-0.54059500	0.48145400	2.19687200

K[5.4.1] ketone
Energy: -543.034315 au
Sum of electronic and thermal Energies: -542.716609 au
Geometry:

C	0.90400000	1.62461400	-0.54146200
C	-0.39889000	-1.24714500	0.61537800
C	0.39985100	-1.57483700	-0.65454100
H	0.58509900	1.21230300	-1.50340200
H	0.95685300	2.71116800	-0.68547700
H	0.12554300	-0.91077300	-1.48047000
H	0.10213400	-2.58512600	-0.96552100
C	-1.60187900	1.63977200	0.00848200
H	-2.31801500	1.56436900	0.83800100
H	-1.62480300	2.68808900	-0.31898300
C	-1.93020700	-1.31125400	0.44584200
H	-2.38943900	-0.87926400	1.34497300
H	-2.22059100	-2.37000800	0.44344600
H	-0.12628000	-2.00000100	1.36624000
C	0.00873200	0.06306700	1.26232900
O	0.48433700	0.05715300	2.39441400
C	-2.06200800	0.76305900	-1.16356800
H	-2.88775700	1.27619300	-1.67094000
H	-1.25993000	0.71121300	-1.90603400
C	2.30648700	1.07448100	-0.21099300
H	2.43537400	0.98459600	0.87495600
H	3.05151600	1.80476800	-0.54841800
C	2.64826400	-0.25993000	-0.89478100
C	1.92553900	-1.53025500	-0.41947800
H	3.72502700	-0.43294200	-0.76870800
H	2.48096300	-0.14551800	-1.97573700
H	2.38750400	-2.37420500	-0.94589500
H	2.13075400	-1.68675500	0.64821700
C	-2.53494300	-0.66187900	-0.80671600
H	-3.62234400	-0.65059400	-0.66162700
H	-2.35493900	-1.31292900	-1.67055900
C	-0.17500100	1.38869900	0.54255200
H	0.00897100	2.12784200	1.33237700

K[5.4.1] hydrocarbon
Energy: -469.142940 au
Sum of electronic and thermal Energies: -468.806663 au
Geometry:

C	0.93814800	1.61440400	-0.32801400
C	-0.41305900	-1.26298100	0.75091700
C	0.46907400	-1.56353900	-0.46778700
H	0.65419700	1.18743700	-1.29444000
H	0.97265700	2.70050300	-0.48876100
H	0.23568100	-0.88270800	-1.29359000
H	0.20288200	-2.56822300	-0.82438000
C	-1.56401200	1.64457700	0.17394400
H	-2.29997300	1.51944400	0.98094000
H	-1.59835200	2.70573200	-0.11040500
C	-1.91752700	-1.35556800	0.44778300

H	-2.45916000	-0.98756700	1.32964500
H	-2.19094200	-2.41520800	0.34729100
H	-0.20301300	-2.06624500	1.47606300
C	-0.05645500	0.03189200	1.48709600
C	-1.98870700	0.82052000	-1.05149600
H	-2.81497300	1.34878100	-1.54339200
H	-1.17376500	0.83036500	-1.78167400
C	2.35175700	1.10619400	0.01457300
H	2.49975500	1.07180000	1.10164900
H	3.08001700	1.83578200	-0.36117600
C	2.72220900	-0.24491900	-0.61956400
C	1.98166800	-1.51220900	-0.16245000
H	3.79529300	-0.41105400	-0.45419000
H	2.59266400	-0.14971900	-1.70761300
H	2.47058600	-2.35620800	-0.66464200
H	2.14467800	-1.67016000	0.91257100
C	-2.44174700	-0.63620900	-0.80541700
H	-3.53718000	-0.66193700	-0.74488500
H	-2.18111000	-1.22976300	-1.69019200
H	0.95401900	-0.06096700	1.90219500
H	-0.72446500	0.10147800	2.35804200
C	-0.15388300	1.36312000	0.73396300
H	0.01570900	2.12674600	1.50965700

L[6.3.1]
Energy: -559.076578 au
Sum of electronic and thermal Energies: -558.770411 au
Geometry:

C	-1.17476800	-1.86799900	0.16871800
C	1.43902100	0.82757800	0.69976400
C	0.70753600	2.11844100	0.26295100
H	-1.17661600	-2.47358000	1.08453300
H	-1.19708400	-2.54598400	-0.69136200
H	1.47321200	2.83100300	-0.07113700
H	0.20772800	2.56203900	1.13161100
C	1.07279000	-1.59276300	-0.90708800
H	1.02314400	-2.68846700	-0.93341300
H	0.82956400	-1.22545200	-1.91605100
C	2.45350200	0.38236800	-0.36982900
H	3.44627600	0.76939200	-0.11506100
H	2.18573500	0.81400400	-1.34284600
H	1.95447600	1.02256100	1.64701700
C	0.35785500	-0.19298000	1.02170900
N	0.07956200	-1.12477400	0.06039500
O	-0.33023000	-0.08276600	2.03947100
C	-0.32677600	1.88593900	-0.85815900
C	-1.74793600	1.50312200	-0.36318500
C	-2.34144800	0.17415700	-0.90123300
C	-2.41755800	-0.96993100	0.12913100
H	-0.39397800	2.80111400	-1.45766900
H	-1.75363600	1.46845300	0.73121200
H	-2.42821600	2.31685700	-0.63913600
H	-3.36120300	0.36851200	-1.25325500
H	-1.77720800	-0.15932800	-1.78389400
H	-2.59875100	-0.54965700	1.12165100
H	-3.26821000	-1.62274000	-0.10501900

H	0.04223500	1.11076200	-1.54185200
C	2.46820000	-1.13461700	-0.51093000
H	3.18483700	-1.45818500	-1.27402300
H	2.75009300	-1.60564400	0.43907000

L[6.3.1] N+
Energy: -559.423639 au
Sum of electronic and thermal Energies: -559.103669 au
Geometry:

C	-1.22724900	2.06955800	0.05556700
C	0.15142000	-1.45959000	0.62518300
C	1.69634700	-1.55304900	0.54657100
H	-1.56443100	2.66414400	0.90688700
H	-1.87280100	2.28497800	-0.79921500
H	1.92298600	-2.62098300	0.44449000
H	2.10403300	-1.23410100	1.51233400
C	-2.19528400	-0.13746800	-0.74037800
H	-3.23383600	0.20681300	-0.75057400
H	-1.71629400	0.18697000	-1.66620500
C	-0.58890500	-2.02488600	-0.59080500
H	-0.47236700	-3.11292800	-0.57685600
H	-0.13774100	-1.67401300	-1.52536900
H	-0.14080400	-2.07267900	1.49438200
C	-0.27417500	-0.08729400	1.08285100
N	-1.51625800	0.59774300	0.39154400
O	0.15754900	0.53475000	2.00488000
C	2.41206400	-0.78502500	-0.57557200
C	2.27948900	0.74356700	-0.49699200
C	0.94961300	1.26484400	-1.09314700
C	0.24622400	2.35181400	-0.24917100
H	3.47088800	-1.05563700	-0.49637000
H	2.37309700	1.05340200	0.55072700
H	3.11744700	1.20712600	-1.02608000
H	1.12453300	1.63867500	-2.10730500
H	0.28520400	0.40793700	-1.24396500
H	0.77742500	2.49399800	0.69407400
H	0.26470400	3.32020900	-0.75934400
H	2.08815700	-1.13799600	-1.56297500
C	-2.06616300	-1.64012400	-0.56737800
H	-2.60983300	-2.11953500	-1.38747300
H	-2.54333800	-1.96644200	0.36651300
H	-2.18390300	0.61377800	1.17210600

L[6.3.1] O+
Energy: -559.444066 au
Sum of electronic and thermal Energies: -559.124078 au
Geometry:

C	-1.24895500	-1.86166200	0.22404100
C	1.47084900	0.77068500	0.70055100
C	0.76559300	2.09411000	0.27161200
H	-1.27511600	-2.40833900	1.17182400
H	-1.24697900	-2.58463400	-0.59406400
H	1.57124500	2.77457600	-0.02542200
H	0.26682800	2.56343600	1.12939200
C	1.00185100	-1.59793300	-0.94237500
H	0.89320500	-2.68364000	-1.00873200

H	0.68520800	-1.15864100	-1.89447600
C	2.48038800	0.30712700	-0.36860300
H	3.48225200	0.62517300	-0.06818800
H	2.25717400	0.80387100	-1.31870000
H	1.98519200	0.93191500	1.65752100
C	0.37960000	-0.21581500	0.94776800
N	0.05808600	-1.16449300	0.11704500
O	-0.40500800	-0.08119400	2.00595900
C	-0.24472800	1.91572900	-0.87864600
C	-1.69541900	1.54853300	-0.45695200
C	-2.27086500	0.20183500	-0.97615000
C	-2.44196200	-0.90771600	0.08264200
H	-0.26997100	2.85728800	-1.43508400
H	-1.79106800	1.58030800	0.63482600
H	-2.34955500	2.34761100	-0.81720800
H	-3.26308900	0.39764000	-1.39268400
H	-1.67051000	-0.16820300	-1.81876500
H	-2.68655300	-0.45920000	1.04844100
H	-3.29115200	-1.54496000	-0.18666500
H	0.13371800	1.17257100	-1.59197400
C	2.42160700	-1.20175000	-0.57650200
H	3.09233500	-1.51113000	-1.38308700
H	2.72498400	-1.73602600	0.33181500
H	-0.12242700	0.68252000	2.52992200

L[6.3.1] amine
Energy: -485.156643 au
Sum of electronic and thermal Energies: -484.832948 au
Geometry:

C	-0.77342300	-1.97929200	0.09989100
C	1.22770500	1.10382600	0.72743300
C	0.21980900	2.19847100	0.33960600
H	-0.52128100	-2.71960600	0.88800000
H	-0.81973900	-2.52950000	-0.84995300
H	0.79804200	3.04287500	-0.06102200
H	-0.28115400	2.57193900	1.24413200
C	1.51915200	-1.60486400	-0.51124900
H	1.72790900	-2.53193800	0.05948000
H	1.37988300	-1.88894300	-1.56227100
C	2.19692100	0.81291500	-0.43859300
H	3.03307300	1.52158700	-0.41162800
H	1.68083500	0.96150500	-1.39440300
H	1.81383100	1.47301500	1.58154200
C	0.53862400	-0.20290600	1.15473300
N	0.27459800	-0.98398300	-0.04782600
C	-0.85205300	1.78425300	-0.69133500
C	-2.15748800	1.19507900	-0.09475100
C	-2.56551000	-0.22665000	-0.54771800
C	-2.15075500	-1.37943800	0.38473700
H	-1.11569100	2.67508800	-1.27371500
H	-2.11277800	1.21553100	1.00220600
H	-2.97899100	1.87220500	-0.35770700
H	-3.65956400	-0.25011000	-0.62449200
H	-2.17947000	-0.41689900	-1.55802500
H	-2.21879000	-1.04428000	1.42729100
H	-2.87256200	-2.20108500	0.29051900

H	-0.42265500	1.06380400	-1.39347300
C	2.70064400	-0.62831400	-0.36664200
H	3.44338500	-0.83082500	-1.14549000
H	3.20071500	-0.78448000	0.59667400
H	-0.40119800	0.01951000	1.66575700
H	1.16225200	-0.76999700	1.87468900

L[6.3.1] ketone
Energy: -543.033811 au
Sum of electronic and thermal Energies: -542.716630 au
Geometry:

C	-1.01351800	2.21550500	0.07990800
C	-0.02455700	-1.46110600	0.62881100
C	1.49522900	-1.71137800	0.53728400
H	-1.25064400	2.90342600	0.89816200
H	-1.61152800	2.53633000	-0.78312300
H	1.63457000	-2.79632900	0.43561500
H	1.94098500	-1.42029600	1.49525400
C	-2.21251400	0.08738700	-0.72043600
H	-3.22625700	0.50255100	-0.78323600
H	-1.72314800	0.33199300	-1.67203600
C	-0.81286900	-1.96128600	-0.58716500
H	-0.79494600	-3.05843200	-0.58707800
H	-0.33419800	-1.64213300	-1.52146500
H	-0.37338800	-2.05144200	1.49275600
C	-0.33884600	-0.02806100	1.07070500
O	0.28302300	0.45745000	2.00651200
C	2.28002800	-1.02006700	-0.59226500
C	2.32329100	0.51494100	-0.51018600
C	1.06134800	1.19405100	-1.09259500
C	0.48942300	2.34900700	-0.23934300
H	3.30506800	-1.40850500	-0.53553400
H	2.44873700	0.80291700	0.53993900
H	3.21167500	0.87834400	-1.04003000
H	1.27604000	1.54628800	-2.10894200
H	0.29556300	0.42698700	-1.23096200
H	1.03262300	2.39272800	0.70850700
H	0.65177000	3.31396200	-0.73338000
H	1.89779300	-1.32546900	-1.57566900
C	-2.24694300	-1.43233800	-0.57104500
H	-2.83087500	-1.87967600	-1.38371800
H	-2.73858000	-1.71051200	0.37238400
C	-1.47956700	0.77642800	0.44420500
H	-2.19848500	0.85916800	1.27318800

L[6.3.1] hydrocarbon
Energy: -469.130170 au
Sum of electronic and thermal Energies: -468.794105 au
Geometry:

C	-0.77677300	-2.13224100	0.29246200
C	1.22015200	0.87241300	0.96940800
C	-0.05672200	1.75451500	0.89212600
H	-0.77425800	-2.83713300	1.13567200
H	-1.01503600	-2.72499800	-0.60302700
H	0.29624100	2.76569600	1.13323000
H	-0.72013400	1.47842000	1.72295200

C	1.00919800	-0.97485300	-1.20071700
H	1.06386900	-1.77510900	-1.94973500
H	0.23648100	-0.28192800	-1.53790400
C	2.17010900	1.05451000	-0.24733100
H	3.15594700	1.38649000	0.09940100
H	1.78974000	1.85622300	-0.89139000
H	1.74153700	1.28029600	1.84582100
C	1.04663600	-0.62265800	1.31549200
C	-0.88270000	1.88564400	-0.41418400
C	-2.27933300	1.24141400	-0.45952800
C	-2.34090900	-0.27473000	-0.67514900
C	-1.89727300	-1.11557000	0.54220600
H	-1.03961200	2.95839100	-0.58166000
H	-2.82194400	1.49638400	0.46215600
H	-2.83026900	1.72113200	-1.27952600
H	-3.37661100	-0.53467600	-0.92639000
H	-1.75194500	-0.53825800	-1.56057900
H	-1.59930300	-0.45196200	1.36054900
H	-2.76568200	-1.66777200	0.92161200
H	-0.30430900	1.54972100	-1.28110500
C	2.33694200	-0.22290800	-1.09318700
H	2.72351700	0.04042900	-2.08457800
H	3.08139500	-0.88550300	-0.63046500
H	0.34731500	-0.72112900	2.15604400
H	2.01963100	-0.94957900	1.70555700
C	0.65591800	-1.58288300	0.16530200
H	1.31196000	-2.46106000	0.26196500