Supporting Information for:

Fine-tuning Strain and Electronic Activation of Strain-promoted 1,3-Dipolar Cycloadditions with Endocyclic Sulfamates in SNO-OCTs

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I. Computational Coordinates.

Computational details. A thorough conformational search was conducted on the sulfamate utilized experimentally (alkyl = Me). Subsequent calculations varying substitution at the X and Y positions were carried out on geometries resembling those of the lowest energy TS for each regioisomer.

Starting compounds

Methyl azide

C	-1.52790300	0.29436300	0.00000500
N	0.71295700	-0.11104800	-0.00001500
N	1.76599200	0.28596200	0.00000600
H	-1.51600100	0.92328700	0.89261000
H	-1.51611700	0.92319000	-0.89268500
H	-2.42926900	-0.31119700	0.00006300
N	-0.38911900	-0.64655000	0.00000600

HF: -204.0628394
Sum of electronic and zero-point Energies: -204.011715
Sum of electronic and thermal Energies: -204.007389
Sum of electronic and thermal Enthalpies: -204.006445
Sum of electronic and thermal Free Energies: -204.037991

Diazoacetamide

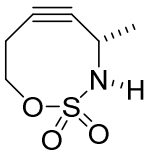
C	0.30806000	0.03534700	-0.00001900
N	-2.02530000	-0.22367900	0.00000900
N	-2.99787600	0.33351300	0.00002900
O	0.22170600	1.26335000	-0.00002500
N	1.49451000	-0.60990800	-0.00003500
H	1.51486900	-1.61736800	0.00009300
C	2.74532500	0.12776300	0.00003400
H	2.82065500	0.76026900	0.88636600
H	3.56613900	-0.58550400	-0.00024100
H	2.82044600	0.76070200	-0.88599900
C	-0.87129000	-0.83215300	-0.00001600
H	-0.88766200	-1.91012000	-0.00003600

HF: -356.7293083
Sum of electronic and zero-point Energies: -356.640393
Sum of electronic and thermal Energies: -356.633411
Sum of electronic and thermal Enthalpies: -356.632467
Sum of electronic and thermal Free Energies: -356.671727

Azidoacetamide

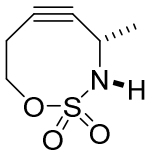
C	0.66205700	0.07181400	-0.03242000
N	-2.25048600	-0.12620900	-0.00981600
N	-2.89770000	-0.96938600	0.35051200
O	0.33873700	-1.08296600	-0.27370500
N	-1.65271000	0.83685500	-0.49007700
C	-0.38883500	1.16437300	0.17059900
H	-0.52828100	1.30574500	1.24816900
H	-0.05378200	2.10845500	-0.25433200
N	1.93526500	0.46650300	0.11639600
H	2.13573200	1.43852800	0.29507700
C	3.03435000	-0.48285000	0.03963700
H	3.08079200	-0.93651700	-0.95165800
H	3.96355800	0.04627000	0.23566000
H	2.90607300	-1.27311900	0.78071600

HF: -412.0638592
Sum of electronic and zero-point Energies: -411.956482
Sum of electronic and thermal Energies: -411.947925
Sum of electronic and thermal Enthalpies: -411.946981
Sum of electronic and thermal Free Energies: -411.990718



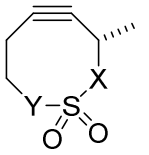
C	0.96113400	1.50110400	0.24613800
C	-0.06416600	2.09951100	0.05638800
C	-1.48516700	2.27692200	-0.22962700
H	-1.96680000	3.01695000	0.41213400
H	-1.63736800	2.57619700	-1.26819800
C	1.84180000	0.32834900	0.35710900
C	-2.11227400	0.90124400	0.03896900
H	-3.13100500	0.84503800	-0.34045500
H	-2.09705200	0.67299900	1.10372000
N	1.16125300	-0.81375700	-0.30900600
S	-0.40181300	-1.18500300	0.05162600
O	-0.67882600	-2.43018800	-0.62032300
O	-0.55814000	-1.05042300	1.48107500
O	-1.38153200	-0.13003800	-0.67768500
C	3.21666400	0.49466700	-0.27688300
H	3.74954500	1.30117700	0.22593400
H	3.78787700	-0.42807200	-0.17521000
H	3.12191300	0.74737300	-1.33479200
H	1.95010900	0.05982600	1.40961600
H	1.32304500	-0.86072700	-1.31282700

HF: -912.4680104
Sum of electronic and zero-point Energies: -912.311816
Sum of electronic and thermal Energies: -912.301562
Sum of electronic and thermal Enthalpies: -912.300618
Sum of electronic and thermal Free Energies: -912.347039



C	-0.24175200	-1.80697500	-0.36979600
C	0.94743200	-1.90672700	-0.22615500
C	2.32536100	-1.45412500	-0.05775100
H	2.88465000	-2.02925900	0.68229400
H	2.86464700	-1.50288700	-1.00550000
C	-1.54639500	-1.14910600	-0.52258600
C	2.20578400	-0.00180600	0.42741300
H	3.15876500	0.52042900	0.36174800
H	1.83126900	0.03149000	1.44927600
N	-1.29581300	0.29660800	-0.79566700
S	-0.18189500	1.17763800	0.03060700
O	-0.31476200	2.52623200	-0.46315700
O	-0.32383700	0.87779700	1.43659900
O	1.30204200	0.74117100	-0.43320500
C	-2.46699000	-1.34055700	0.67855800
H	-1.99326400	-0.97340100	1.58805000
H	-3.39902100	-0.80022900	0.51207100
H	-2.68596800	-2.40268100	0.79571800
H	-2.05104200	-1.50649500	-1.42178100
H	-1.27720800	0.53873600	-1.78191500

HF: -912.4671542
Sum of electronic and zero-point Energies: -912.310856
Sum of electronic and thermal Energies: -912.300621
Sum of electronic and thermal Enthalpies: -912.299676
Sum of electronic and thermal Free Energies: -912.346033



X = CH_2, Y = CH_2

C	1.02544200	1.41499600	0.23201200
C	0.02330600	2.06487500	0.09050600
C	-1.37915400	2.40819200	-0.13246300
H	-1.73621900	3.16620400	0.56626500
H	-1.51474100	2.80104100	-1.14342500
C	1.94042100	0.27330300	0.31856500
C	-2.17660500	1.10141500	0.05074900
H	-3.21153900	1.26877400	-0.25440600
H	-2.19002400	0.82753400	1.10818600
S	-0.46243200	-1.20536000	0.07204300
O	-0.75916400	-2.53515200	-0.48055000
O	-0.56810000	-1.03357900	1.52476900
C	3.33126900	0.53061600	-0.26737000
H	3.83102900	1.32417200	0.28869400
H	3.93957800	-0.37335500	-0.20762000
H	3.25544500	0.83419000	-1.31329100
H	2.03660000	-0.01562000	1.36890900
C	-1.63831600	-0.07705800	-0.76394800
H	-2.43844700	-0.78095800	-0.99835500
H	-1.16364200	0.22331900	-1.70054200
C	1.24952800	-0.87102200	-0.43606500
H	1.74176000	-1.83073700	-0.26181100
H	1.21187400	-0.68085000	-1.51096200

HF: -860.5267921
Sum of electronic and zero-point Energies: -860.335564
Sum of electronic and thermal Energies: -860.324669

Sum of electronic and thermal Enthalpies: -860.323725
Sum of electronic and thermal Free Energies: -860.371467

X = NH, Y = CH_2

C	0.80828300	1.56968000	0.22736900
C	-0.27566100	2.07032500	0.08242900
C	-1.71302000	2.20276500	-0.13563300
H	-2.17623900	2.89699300	0.56681400
H	-1.91058300	2.57061600	-1.14568400
C	1.82879100	0.51688100	0.33311700
C	-2.29585900	0.78595500	0.04877000
H	-3.34227800	0.78671800	-0.26322100
H	-2.27292000	0.51665500	1.10680300
N	1.29095500	-0.71233300	-0.29813900
S	-0.24553600	-1.24605300	0.07363500
O	-0.31569300	-2.57391400	-0.52745700
O	-0.38264800	-1.10353200	1.51675500
C	3.16112900	0.85261500	-0.32528500
H	3.59347600	1.72918600	0.15657600
H	3.85040700	0.01424700	-0.22222200
H	3.01845500	1.07439900	-1.38488100
H	1.98949300	0.28654000	1.38818900
H	1.45279300	-0.75634400	-1.30197100
C	-1.57051400	-0.29228200	-0.76352500
H	-2.25477300	-1.10063900	-1.02283600
H	-1.12810500	0.08873700	-1.68658000

HF: -876.5645119
Sum of electronic and zero-point Energies: -876.384888
Sum of electronic and thermal Energies: -876.374063
Sum of electronic and thermal Enthalpies: -876.373118
Sum of electronic and thermal Free Energies: -876.420819

X = NH_2^+, Y = CH_2

C	0.94637000	1.46600200	0.26071600
C	-0.10055400	2.03198500	0.10072200
C	-1.50717700	2.33028700	-0.13198100
H	-1.89102700	3.06351600	0.57782000
H	-1.64378100	2.73261700	-1.13808900
C	1.91674700	0.37879600	0.32051800
C	-2.26233400	0.99601200	0.03158600
H	-3.28781700	1.11931000	-0.32068300
H	-2.31481100	0.72385900	1.08717800
N	1.25111800	-0.74947400	-0.45478700
S	-0.47486600	-1.22805900	0.10304900
O	-0.54951800	-2.55645100	-0.44599300
O	-0.43921100	-0.98797500	1.51922700
C	3.28335500	0.67187600	-0.28123500
H	3.74973200	1.45776400	0.31240300
H	3.91887000	-0.21281000	-0.24769000
H	3.18900500	1.02164900	-1.30979200
H	2.00790500	0.00957300	1.34331200
H	1.22753800	-0.52629400	-1.45733400
C	-1.67037700	-0.16259000	-0.77201000
H	-2.42615500	-0.91952300	-0.99576000
H	-1.19972900	0.13208500	-1.71235100
H	1.78394700	-1.62529300	-0.36004700

HF: -876.972742
Sum of electronic and zero-point Energies: -876.778945
Sum of electronic and thermal Energies: -876.768002
Sum of electronic and thermal Enthalpies: -876.767058
Sum of electronic and thermal Free Energies: -876.814804

X = O, Y = CH_2

C	0.65558800	1.62643800	0.28451500
C	-0.47061300	2.02081800	0.14038600
C	-1.90660700	2.02443900	-0.11491100
H	-2.45520800	2.63528500	0.60288500
H	-2.11056000	2.41694700	-1.11396900
C	1.75031500	0.65596500	0.32640100
C	-2.35169500	0.54933800	-0.00681100
H	-3.37417100	0.46017800	-0.37795700
H	-2.35946100	0.24846100	1.04257900
S	-0.11513700	-1.24305500	0.07609800
O	0.00464400	-2.57423800	-0.48439000
O	-0.26420500	-1.08901100	1.51122100
C	3.01964000	1.06981600	-0.38816400
H	3.43841000	1.94531800	0.10901800
H	3.74567200	0.25811600	-0.35199800
H	2.80044800	1.31978200	-1.42645700
H	1.95288700	0.36289800	1.35826000
C	-1.48633600	-0.42944700	-0.80944100
H	-2.07217200	-1.29823300	-1.11083600
H	-1.03946600	0.01173400	-1.70226700
O	1.26631900	-0.53372600	-0.38166600

HF: -896.4304908
Sum of electronic and zero-point Energies: -896.263368
Sum of electronic and thermal Energies: -896.252745
Sum of electronic and thermal Enthalpies: -896.251801
Sum of electronic and thermal Free Energies: -896.299116

X = CH_2, Y = O

C	1.13603600	1.34221800	0.26331500
C	0.19550500	2.06963100	0.08380300
C	-1.18769200	2.43259100	-0.21723400
H	-1.57794500	3.22346400	0.42610000
H	-1.28148800	2.76267200	-1.25358400
C	1.92553800	0.10884800	0.33924200
C	-2.00343600	1.15485200	0.02099100
H	-3.01179600	1.24730900	-0.37805300
H	-2.04436100	0.91654300	1.08312000
S	-0.59136300	-1.13459500	0.05444600
O	-1.06890100	-2.36117700	-0.54999300
O	-0.71013200	-0.95954500	1.48980200
O	-1.41449700	0.03598400	-0.69353200
C	3.34401900	0.22418600	-0.22501700
H	3.91278800	0.95739300	0.34692000
H	3.85408100	-0.73830500	-0.16157500
H	3.31744400	0.54150400	-1.26910800
H	1.97516700	-0.21492400	1.38254400
C	1.12915500	-0.93784900	-0.45862700
H	1.54378100	-1.94069200	-0.33537300
H	1.08762500	-0.69041000	-1.52118500

HF: -896.4318069
Sum of electronic and zero-point Energies: -896.264044
Sum of electronic and thermal Energies: -896.253573
Sum of electronic and thermal Enthalpies: -896.252629
Sum of electronic and thermal Free Energies: -896.299530

X = CH_2, Y = NH

C	1.09496300	1.39043200	0.22568600
C	0.13688900	2.09282000	0.03719400
C	-1.25807700	2.43814700	-0.21975600
H	-1.62169300	3.24890000	0.41430300
H	-1.39507400	2.73983600	-1.26082100
C	1.92685400	0.18853300	0.33320000
C	-2.06098100	1.15362500	0.08696200
H	-3.10272000	1.28279900	-0.20990100
H	-2.03739400	0.95584200	1.15826200
S	-0.55062700	-1.16831700	0.05441300
O	-0.91097300	-2.43270100	-0.57927900
O	-0.63985500	-1.03911100	1.50335000
C	3.34501200	0.34640800	-0.22261200
H	3.88308800	1.11221000	0.33651200
H	3.89041100	-0.59484500	-0.13748400
H	3.31404700	0.64068400	-1.27353500
H	1.98119000	-0.10673000	1.38490500
C	1.17746400	-0.90668400	-0.43963400
H	1.63245100	-1.88756100	-0.28526900
H	1.14655400	-0.69092600	-1.50978700
N	-1.56497100	-0.04614400	-0.58565800
H	-1.69215700	-0.12931200	-1.58698900

HF: -876.5673778
Sum of electronic and zero-point Energies: -876.387745
Sum of electronic and thermal Energies: -876.376830
Sum of electronic and thermal Enthalpies: -876.375886
Sum of electronic and thermal Free Energies: -876.423587

X = CH_2, Y = NH_2^+

C	1.01867600	1.38776900	0.25748100
C	0.01644800	2.03820300	0.13070800
C	-1.38467300	2.38191800	-0.09780700
H	-1.77286400	3.08023800	0.64436000
H	-1.52029900	2.83347700	-1.08315800
C	1.96025000	0.26742400	0.32641400
C	-2.17080400	1.07034900	0.01493100
H	-3.18330400	1.17439800	-0.36992700
H	-2.20795500	0.71825100	1.04495100
S	-0.39938400	-1.24950500	0.12271900
O	-0.83911500	-2.48894600	-0.45943000
O	-0.60256300	-0.93743700	1.50951300
C	3.32971400	0.54864000	-0.29975500
H	3.82429500	1.34865800	0.25021800
H	3.95437100	-0.34435800	-0.25612200
H	3.21948300	0.85539900	-1.34088200
H	2.08831600	-0.02256800	1.37244300
C	1.28853000	-0.89119700	-0.42514300
H	1.78016800	-1.85240700	-0.24872500
H	1.22661300	-0.71965500	-1.50215100
N	-1.51504500	-0.02801000	-0.79162500
H	-0.99842500	0.36029900	-1.58983700
H	-2.23036100	-0.65116700	-1.18494100

HF: -876.9743355
Sum of electronic and zero-point Energies: -876.780152
Sum of electronic and thermal Energies: -876.769264
Sum of electronic and thermal Enthalpies: -876.768320
Sum of electronic and thermal Free Energies: -876.815916

X = NH, Y = NH

C	0.89310500	1.55231500	0.20063900
C	-0.15159400	2.11449500	0.00262200
C	-1.58554100	2.25333400	-0.23099400
H	-2.05007900	3.01231000	0.40107500
H	-1.78748800	2.51240500	-1.27286400
C	1.82579400	0.42405300	0.34734600
C	-2.17500400	0.86716300	0.11435200
H	-3.23336900	0.83036500	-0.14821600
H	-2.08295300	0.69000300	1.18536900
S	-0.34597900	-1.21748100	0.05191900
O	-0.49163800	-2.47769100	-0.65416200
O	-0.45893400	-1.13181200	1.49476200
C	3.20468900	0.65296100	-0.25971000
H	3.68288100	1.49862700	0.23410400
H	3.82328200	-0.23448800	-0.12512300
H	3.12084300	0.87583700	-1.32543400
H	1.92700100	0.18586500	1.40831500
N	-1.51738900	-0.24856300	-0.56602900
H	-1.63069000	-0.33737600	-1.56873500

N	1.22204800	-0.76331400	-0.30254100
H	1.36951400	-0.78060700	-1.30953200

HF: -892.6045456
Sum of electronic and zero-point Energies: -892.436387
Sum of electronic and thermal Energies: -892.425636
Sum of electronic and thermal Enthalpies: -892.424692
Sum of electronic and thermal Free Energies: -892.472081

X = NH, Y = NH_2^+

C	0.82554100	1.54027900	0.27751900
C	-0.25944600	2.03872700	0.14769500
C	-1.68936600	2.18314700	-0.10807900
H	-2.18778900	2.80632500	0.63518100
H	-1.86553300	2.62714500	-1.09004400
C	1.86698900	0.50947800	0.35253400
C	-2.28417500	0.76986700	-0.02898500
H	-3.28464900	0.73488700	-0.45638600
H	-2.31646000	0.41274500	0.99869000
N	1.27740700	-0.72671500	-0.25032700
S	-0.17653100	-1.27019300	0.13221900
O	-0.40153300	-2.53851900	-0.49448800
O	-0.47574000	-0.97788600	1.49972700
C	3.14927600	0.83267600	-0.40081400
H	3.61008600	1.70966700	0.05181500
H	3.84366800	-0.00495400	-0.33362600
H	2.93257300	1.05041800	-1.44751400
H	2.08750000	0.28156200	1.39647000
H	1.60609200	-1.01190900	-1.17067500
N	-1.44948400	-0.22741000	-0.80359800
H	-2.06238500	-0.94123100	-1.21157000
H	-0.96879300	0.22350000	-1.59150800

HF: -893.013291
Sum of electronic and zero-point Energies: -892.830654
Sum of electronic and thermal Energies: -892.819845
Sum of electronic and thermal Enthalpies: -892.818901
Sum of electronic and thermal Free Energies: -892.866422

X = O, Y = NH

C	0.73220400	1.61468100	0.26927300
C	-0.36241600	2.07018100	0.07137700
C	-1.79203100	2.08042900	-0.21347800
H	-2.35419000	2.75418100	0.43506100
H	-1.97720300	2.37286500	-1.24926100
C	1.75574700	0.57019300	0.34267800
C	-2.25453200	0.62625400	0.04158000
H	-3.27638800	0.48909500	-0.31254600
H	-2.23215700	0.41792900	1.11040400
S	-0.20969200	-1.22214700	0.05472700
O	-0.16280800	-2.51039700	-0.59415600
O	-0.33225100	-1.10113500	1.48969500
C	3.07076100	0.89516600	-0.33471500
H	3.53674800	1.73755600	0.17749800
H	3.73658100	0.03415700	-0.28285000
H	2.89865700	1.16245600	-1.37748900
H	1.90826500	0.26511600	1.38007900
N	-1.43275800	-0.39193200	-0.61815500
H	-1.50699400	-0.50657000	-1.62209600
O	1.21414200	-0.58475800	-0.37899300

HF: -912.4698945
Sum of electronic and zero-point Energies: -912.314226
Sum of electronic and thermal Energies: -912.303726
Sum of electronic and thermal Enthalpies: -912.302782
Sum of electronic and thermal Free Energies: -912.349699

X = O, Y = O

C	0.83093800	1.55946200	0.30964200
C	-0.23899300	2.06858100	0.11021300
C	-1.65841800	2.14048800	-0.21882100
H	-2.22123500	2.81201400	0.43167100
H	-1.79875900	2.46503900	-1.25109200
C	1.78827100	0.45475200	0.35677000
C	-2.17704500	0.70873300	-0.01766000
H	-3.15907500	0.57309200	-0.46522700
H	-2.20552900	0.45200600	1.03990500
S	-0.28771700	-1.19196400	0.05124700
O	-0.39650600	-2.47240200	-0.58529700
O	-0.45509700	-1.04611200	1.47470800
C	3.10624000	0.69534800	-0.34547300
H	3.63512700	1.49896300	0.16804500
H	3.71407200	-0.20820900	-0.31500800
H	2.93178700	0.98761100	-1.38089900
H	1.93484600	0.11577000	1.38366000
O	1.15254800	-0.66178300	-0.37721900
O	-1.31766000	-0.24333300	-0.71207300

HF: -932.3303258
Sum of electronic and zero-point Energies: -932.186412
Sum of electronic and thermal Energies: -932.176390
Sum of electronic and thermal Enthalpies: -932.175446
Sum of electronic and thermal Free Energies: -932.221489

X = O, Y = NH_2^+

C	0.72922900	1.58575600	0.32542400
C	-0.38357200	2.01469700	0.18836200
C	-1.81447400	2.06874700	-0.08722600
H	-2.36702600	2.62461800	0.67098000
H	-2.00597700	2.53339100	-1.05610300
C	1.80888000	0.60610900	0.34724400
C	-2.30433400	0.61292700	-0.06522300
H	-3.27791600	0.51563700	-0.54126900
H	-2.35444300	0.22460600	0.95006700
S	-0.09582900	-1.26028700	0.13037200
O	-0.18732800	-2.55060100	-0.46707600
O	-0.38632500	-0.98796300	1.50011100
C	3.04771900	0.94879300	-0.44255300
H	3.52521100	1.80697500	0.03170700
H	3.73768900	0.10646100	-0.43201900
H	2.78459100	1.20647000	-1.46785800
H	2.03682400	0.28669200	1.36411000
N	-1.36608600	-0.30707100	-0.83096600
H	-1.91368800	-1.04555500	-1.28916900
H	-0.87525800	0.19624800	-1.58229200
O	1.23680000	-0.60689000	-0.34722300

HF: -912.8680847
Sum of electronic and zero-point Energies: -912.697782
Sum of electronic and thermal Energies: -912.687307
Sum of electronic and thermal Enthalpies: -912.686363
Sum of electronic and thermal Free Energies: -912.733255

X = NH_2^+, Y = NH

H	-1.50590600	2.66839200	-1.27815800
C	1.90791000	0.28326700	0.34480000
C	-2.12537600	1.07140800	0.07957800
H	-3.16185600	1.12818100	-0.24874000
H	-2.10847200	0.87823300	1.15090300
N	1.17504300	-0.80451000	-0.42774400
S	-0.58604100	-1.18442900	0.08249700
O	-0.72589100	-2.45208200	-0.57147800
O	-0.52679700	-1.00484700	1.50154400
C	3.30038500	0.46379400	-0.24343100
H	3.81626500	1.22701400	0.33854500
H	3.86883900	-0.46419000	-0.18259500
H	3.24473000	0.79612300	-1.28081900
H	1.95883100	-0.07703100	1.37353100
H	1.16208200	-0.57179400	-1.42801000
H	1.66749900	-1.70241400	-0.33652700
N	-1.54532200	-0.10950000	-0.59145600
H	-1.80869100	-0.32101200	-1.54982500

HF: -893.0167672
Sum of electronic and zero-point Energies: -892.834087
Sum of electronic and thermal Energies: -892.823337
Sum of electronic and thermal Enthalpies: -892.822393
Sum of electronic and thermal Free Energies: -892.869767

X = NH_2^+, Y = O

C	1.06500700	1.40742500	0.30723200
C	0.08236200	2.05953000	0.08426100
C	-1.30248600	2.37711300	-0.24043600
H	-1.72235100	3.16065500	0.39288100
H	-1.39276900	2.68903600	-1.28173600
C	1.90130400	0.21428900	0.35755500
C	-2.07743700	1.08461100	0.01737100
H	-3.06974000	1.09741600	-0.42436800
H	-2.12573500	0.85002700	1.07860400
N	1.10930200	-0.81496100	-0.45882000
S	-0.61219100	-1.15436700	0.07844200
O	-0.86455300	-2.40435000	-0.55646500
O	-0.59667700	-0.96276900	1.49249900
C	3.29365800	0.34688600	-0.23996100
H	3.84342100	1.07250700	0.35890700
H	3.82263400	-0.60544100	-0.20314700
H	3.24545900	0.70833000	-1.26772500
H	1.94099600	-0.19121600	1.36958400
H	1.07190800	-0.52109500	-1.44482500
H	1.57652800	-1.73217400	-0.43693700
O	-1.40562700	-0.04445200	-0.67362200

HF: -912.8677595
Sum of electronic and zero-point Energies: -912.697761
Sum of electronic and thermal Energies: -912.687241
Sum of electronic and thermal Enthalpies: -912.686296
Sum of electronic and thermal Free Energies: -912.733304

X = NH_2^+, Y = NH_2^+

C	0.93629700	1.45354700	0.25937400
C	-0.10695000	2.02715600	0.11432400
C	-1.51749200	2.30489000	-0.12125700
H	-1.93399300	2.99552200	0.61281900
H	-1.67140900	2.73206600	-1.11400000
C	1.92883700	0.39198100	0.33452600
C	-2.24126300	0.96367600	0.02500200
H	-3.24990300	0.99677800	-0.38236200
H	-2.27481700	0.62379200	1.05823900
N	1.26442500	-0.78880700	-0.41893900
S	-0.40136000	-1.25038800	0.13977000
O	-0.63354700	-2.52584400	-0.43145200
O	-0.47715200	-0.88522400	1.50542800
C	3.27546200	0.67352700	-0.31044000
H	3.73299900	1.48832800	0.25097000
H	3.92673800	-0.19739800	-0.24849000
H	3.15937700	0.98713100	-1.34756900
H	2.04114600	0.03876700	1.36073300
H	1.27061300	-0.62421200	-1.43899100
H	1.81152500	-1.65636500	-0.27446000
N	-1.53055300	-0.13307500	-0.77573900
H	-2.22871400	-0.79537800	-1.14978900
H	-1.06265600	0.27023600	-1.60166200

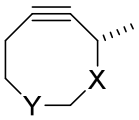
HF: -893.3733801
Sum of electronic and zero-point Energies: -893.176309

Sum of electronic and thermal Energies: -893.165671
Sum of electronic and thermal Enthalpies: -893.164727
Sum of electronic and thermal Free Energies: -893.211650

X = NBoc, Y = O

C	2.12769900	0.87057600	1.32027700
C	2.52314700	-0.20085600	1.69531400
C	2.69368800	-1.65109400	1.71835700
H	3.71397800	-1.96393300	1.94861500
H	2.02628600	-2.09988400	2.45647900
C	1.33113300	1.81410800	0.52248800
C	2.34259400	-2.13359300	0.30404900
H	2.20395800	-3.21227100	0.27564000
H	3.11165600	-1.83563100	-0.40602700
N	0.36866800	0.95434100	-0.25448500
S	0.97025800	-0.34884500	-1.14276000
O	-0.00995900	-0.70283200	-2.13106300
O	2.30060800	0.02065400	-1.55623600
O	1.06050900	-1.58847700	-0.12941600
C	2.13228700	2.77581600	-0.34629900
H	2.82858500	2.24774900	-0.99284800
H	1.44738600	3.37034600	-0.95187100
H	2.69200200	3.44522700	0.30874700
H	0.68040000	2.39850900	1.17158100
C	-0.97595900	0.97579000	0.19950000
O	-1.44237300	1.96677000	0.69911300
O	-1.56877300	-0.18139200	0.01707900
C	-3.02235200	-0.34589900	0.21983400
C	-3.77409600	0.61885400	-0.68619900
H	-3.64142200	1.65288700	-0.37102000
H	-3.43530600	0.50744000	-1.71860500
H	-4.83798200	0.37687400	-0.64634600
C	-3.35608800	-0.15623700	1.69294300
H	-3.20901500	0.87601000	2.00639600
H	-4.40255600	-0.42523100	1.85076800
H	-2.73642300	-0.81267700	2.30765900
C	-3.24671400	-1.78706000	-0.21094300
H	-2.64930300	-2.46338500	0.40330100
H	-4.30088300	-2.04205300	-0.09077800
H	-2.96829800	-1.91906400	-1.25788100

HF: -1258.2459219
Sum of electronic and zero-point Energies: -1257.963420
Sum of electronic and thermal Energies: -1257.944621
Sum of electronic and thermal Enthalpies: -1257.943677
Sum of electronic and thermal Free Energies: -1258.010918



X = CH_2, Y = CH_2

C	0.58650400	-1.10143700	-0.25543100
C	-0.54544400	-1.48056500	-0.09427300
C	-1.98549100	-1.38520800	0.14572400
H	-2.56345700	-2.07437800	-0.47325200
H	-2.20186900	-1.62694200	1.19063500
C	1.70962800	-0.16911600	-0.39841100
C	-2.38117300	0.08032300	-0.15321200
H	-3.40058000	0.23243500	0.21211500
H	-2.40956100	0.22065500	-1.23819500
C	2.98700800	-0.60575000	0.31964000
H	3.37073600	-1.54137200	-0.09066100
H	3.75776800	0.16069000	0.21120200
H	2.79264700	-0.75075100	1.38500300
H	1.92522500	-0.05456700	-1.46688500
C	-0.21519900	1.59926000	-0.36437200
H	-0.33209200	1.26879700	-1.40264200
H	-0.23141600	2.69142600	-0.39751700
C	1.18493500	1.18587200	0.13804500
H	1.91572000	1.95184000	-0.14078500
H	1.17914100	1.13873800	1.23311300
C	-1.44640000	1.13922700	0.47166100
H	-2.05694100	2.02386400	0.66891700
H	-1.11153000	0.78392800	1.45272800

HF: -351.2432209
Sum of electronic and zero-point Energies: -351.034275
Sum of electronic and thermal Energies: -351.025171
Sum of electronic and thermal Enthalpies: -351.024227
Sum of electronic and thermal Free Energies: -351.067673

X = NH, Y = CH_2

C	0.57063100	-1.13074000	-0.25260900
C	-0.57012900	-1.48119500	-0.08563400
C	-2.00590400	-1.35073100	0.15460100
H	-2.60166100	-2.02493400	-0.46359300
H	-2.23010100	-1.58020700	1.20036200
C	1.67333300	-0.15753200	-0.39905800
C	-2.35032900	0.12515700	-0.15624200
H	-3.36686400	0.31785000	0.19752200
H	-2.36337700	0.25776300	-1.24252500
N	1.20652500	1.14864300	0.09137700
C	2.95235600	-0.55803300	0.32596000
H	3.33302100	-1.50230200	-0.06498400
H	3.71203400	0.21343800	0.19215200
H	2.75911400	-0.68175800	1.39456900
H	1.88964000	-0.04757600	-1.46704400
H	1.23095800	1.13842300	1.10794200
C	-1.38176700	1.15296600	0.46847200
H	-1.95781600	2.06234400	0.65685000
H	-1.05684600	0.79646900	1.45264500
C	-0.12917500	1.57962000	-0.36017400
H	-0.24251300	1.26103500	-1.40086600
H	-0.10535600	2.67187900	-0.37456300

HF: -367.2783898
Sum of electronic and zero-point Energies: -367.080434
Sum of electronic and thermal Energies: -367.071467
Sum of electronic and thermal Enthalpies: -367.070523
Sum of electronic and thermal Free Energies: -367.113697

X = NH_2^+, Y = CH_2

C	0.57124800	-1.14830600	-0.28140600
C	-0.57448000	-1.46045500	-0.09590500
C	-2.00658100	-1.37320800	0.15739300
H	-2.58256000	-2.05411600	-0.47036600
H	-2.21227700	-1.62393100	1.20109300
C	1.68636500	-0.21756500	-0.40866800
C	-2.39094700	0.09729000	-0.13603300
H	-3.39201300	0.26810300	0.26401000
H	-2.45206300	0.23849500	-1.21836700
N	1.13879600	1.09890500	0.13965700
C	2.95597200	-0.59293700	0.33900100
H	3.35824100	-1.50552200	-0.09961900
H	3.70586400	0.19409000	0.24812600
H	2.74552700	-0.78058700	1.39304200
H	1.90272800	-0.02135200	-1.46068900
H	1.08450800	1.02180400	1.16054200
C	-1.43463600	1.14944600	0.46060700
H	-2.00813900	2.06448000	0.61327400
H	-1.11106800	0.83537400	1.45873100
H	1.82946000	1.83054400	-0.04841800
C	-0.21157100	1.55110000	-0.39557100
H	-0.13483700	2.63522000	-0.44004100
H	-0.27716300	1.17286900	-1.41542400

HF: -367.7293556
Sum of electronic and zero-point Energies: -367.516255
Sum of electronic and thermal Energies: -367.507100
Sum of electronic and thermal Enthalpies: -367.506156
Sum of electronic and thermal Free Energies: -367.549979

X = O, Y = CH_2

C	0.56394800	-1.14365200	-0.27726800
C	-0.58313200	-1.46621300	-0.10491400
C	-2.01340400	-1.32420800	0.15212700
H	-2.62293700	-1.97822500	-0.47373300
H	-2.22931200	-1.56916600	1.19576600
C	1.65566500	-0.16043900	-0.38827100
C	-2.33702600	0.16309000	-0.13176800
H	-3.33943800	0.36866500	0.25213600
H	-2.37766700	0.30895800	-1.21557700
C	2.91989900	-0.52773100	0.36628000
H	3.34576600	-1.44490900	-0.04257200
H	3.65137700	0.27570100	0.27176100
H	2.69214500	-0.68302700	1.42196400
H	1.88638500	-0.00629500	-1.45073300
C	-1.33815900	1.17047300	0.47633000
H	-1.88399400	2.10165500	0.64679400
H	-1.00685900	0.82719600	1.46149000
C	-0.08129900	1.53335500	-0.35835200
H	-0.19585700	1.20219600	-1.39708800
H	0.02646000	2.61901800	-0.36985200
O	1.16687200	1.06377300	0.16183300

HF: -387.1463089
Sum of electronic and zero-point Energies: -386.961162
Sum of electronic and thermal Energies: -386.952318
Sum of electronic and thermal Enthalpies: -386.951374
Sum of electronic and thermal Free Energies: -386.994376

X = CH_2, Y = O

C	-0.55917700	-1.10772000	0.28430100
C	0.56970400	-1.49179000	0.11313600
C	1.99389700	-1.31672600	-0.17109700
H	2.64430300	-1.93540300	0.45079200
H	2.20550400	-1.55396400	-1.21657400
C	-1.67155600	-0.15829200	0.40548000
C	2.27820100	0.17839700	0.11030600
H	3.26084300	0.44111900	-0.28853700
H	2.28954000	0.34052100	1.19258000
C	-2.95551100	-0.59465300	-0.30060800
H	-3.34860300	-1.51566900	0.13262800
H	-3.71638200	0.18335500	-0.20772900
H	-2.76473200	-0.76648500	-1.36244900
H	-1.88466000	-0.01042100	1.46997800
C	0.27629500	1.57423400	0.30301500
H	0.41990300	1.28530400	1.34982200
H	0.36671300	2.66236200	0.24132700
O	1.32890700	1.03274900	-0.50247500
C	-1.12646700	1.17213500	-0.17228900
H	-1.82715100	1.97146200	0.08927900
H	-1.10884900	1.10231700	-1.26478400

HF: -387.1478408
Sum of electronic and zero-point Energies: -386.962429
Sum of electronic and thermal Energies: -386.953652
Sum of electronic and thermal Enthalpies: -386.952708
Sum of electronic and thermal Free Energies: -386.995512

X = CH_2, Y = NH

C	0.56840200	-1.10942300	-0.27345800
C	-0.56046300	-1.49577800	-0.10720500
C	-1.98884500	-1.34765700	0.15994600
H	-2.61668000	-1.99182000	-0.45966800
H	-2.20410300	-1.58722800	1.20533900
C	1.68322100	-0.16649900	-0.40356400
C	-2.32340600	0.14570200	-0.12855400
H	-3.33737700	0.33269500	0.23871400
H	-2.34179800	0.29173300	-1.21100000
C	2.96822300	-0.60626300	0.29914500
H	3.35463300	-1.53192800	-0.13045100
H	3.73321100	0.16686400	0.19901200
H	2.78122500	-0.77151000	1.36282100
H	1.89273500	-0.02473600	-1.46978700
C	-0.24832300	1.60585800	-0.32661800
H	-0.37626200	1.30416100	-1.37099700
H	-0.25988700	2.70077800	-0.31767400
N	-1.41962000	1.13909100	0.43681200
H	-1.17243800	0.91508500	1.39380000
C	1.14818100	1.16957000	0.16750200
H	1.87027800	1.95370600	-0.08247600
H	1.13186500	1.09550700	1.26152300

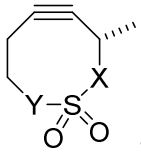
HF: -367.2785128
Sum of electronic and zero-point Energies: -367.080845
Sum of electronic and thermal Energies: -367.071773
Sum of electronic and thermal Enthalpies: -367.070829
Sum of electronic and thermal Free Energies: -367.114187

X = CH_2, Y = NH_2^+

H	-2.23931400	-1.66109400	1.13890300
C	1.72106200	-0.18903500	-0.40505100
C	-2.35403700	0.10369900	-0.12961400
H	-3.31841400	0.34601400	0.31250400
H	-2.38004300	0.33217800	-1.19278900
C	2.97708400	-0.61961200	0.35182100
H	3.35622800	-1.56630900	-0.03428400
H	3.75586800	0.13717500	0.23992000
H	2.75894500	-0.73999600	1.41498600
H	1.95445000	-0.10519300	-1.47138100
C	-0.19674300	1.56252700	-0.40035300
H	-0.31350000	2.64337200	-0.41105900
H	-0.38269900	1.18458800	-1.40436500
N	-1.32918300	1.03833700	0.48941500
H	-0.92116600	0.57722500	1.30852900
H	-1.83135300	1.84781000	0.85698700
C	1.20486000	1.18593300	0.08953600
H	1.89300500	1.96138600	-0.25430100
H	1.23405600	1.21016500	1.18420500

HF: -367.7320745
Sum of electronic and zero-point Energies: -367.518157
Sum of electronic and thermal Energies: -367.509226
Sum of electronic and thermal Enthalpies: -367.508282
Sum of electronic and thermal Free Energies: -367.551453

Transition states



+methyl azide (*anti*-TSs)

X = CH_2, Y = CH_2

C	-0.71650800	0.64918500	0.08550300
C	-1.04566800	-0.53608600	-0.03247200
N	-3.25432700	0.67738900	0.49271900
N	-2.62728200	1.63591200	0.59437600
C	-0.80018000	-1.97974800	-0.22289600
H	-1.49706300	-2.56717100	0.37775800
H	-0.98049100	-2.24421900	-1.27038400
C	0.26514400	1.75801800	0.08966200
C	0.62903200	-2.36021400	0.17317100
H	0.75853500	-3.43117100	0.00245300
H	0.77814500	-2.18657700	1.24152800
S	2.38458400	-0.11602800	0.11465200
O	3.77322600	-0.03524500	-0.36321200
O	2.16341800	-0.12576400	1.56518400
C	-0.23080500	3.03086500	-0.60841100
H	-1.08906300	3.44593000	-0.08503900
H	0.56378100	3.77924200	-0.62777900
H	-0.52509000	2.80902700	-1.63698500
H	0.50105300	1.99595300	1.13160400
N	-3.13860400	-0.55790700	0.35376800
C	-4.05031200	-1.23480900	-0.57452700
H	-3.65809600	-2.24119000	-0.70714100
H	-5.05109600	-1.30748400	-0.14688400
C	1.55654100	1.31866400	-0.60157000
H	2.32465000	2.09254300	-0.52865200
H	1.39468800	1.08352900	-1.65610700
C	1.72471200	-1.64462100	-0.60989000
H	2.63258500	-2.24990600	-0.64434900
H	1.44194800	-1.40162200	-1.63688400
H	-4.09121300	-0.72765300	-1.54081600

HF: -1064.5660302
Sum of electronic and zero-point Energies: -1064.322630
Sum of electronic and thermal Energies: -1064.306917
Sum of electronic and thermal Enthalpies: -1064.305972
Sum of electronic and thermal Free Energies: -1064.366489
Frequencies: -477.0801

X = NH, Y = CH_2

C	-0.71527600	0.63773400	0.14007100
C	-1.07114900	-0.54107900	0.05271800
N	-3.27237100	0.74484100	0.38629800
N	-2.65043600	1.70518800	0.47871900
C	-0.84114300	-1.99189200	-0.07786000
H	-1.51139300	-2.54477800	0.58345900
H	-1.06941700	-2.30881500	-1.10115500
C	0.32485600	1.69290800	0.16374500
C	0.60856300	-2.34367700	0.26856400
H	0.74501600	-3.41867400	0.13238400
H	0.80207600	-2.12759800	1.32164600
N	1.58287700	1.24151700	-0.47108500
S	2.37923600	-0.10783800	0.05963900
O	3.69987800	-0.03250400	-0.55726700
O	2.26750800	-0.10174800	1.51303100
C	-0.07317200	2.99076500	-0.53466700
H	-0.92513700	3.43961000	-0.02955300
H	0.76490600	3.68794400	-0.51533900
H	-0.35172500	2.79334100	-1.57275800
H	0.56720700	1.90900100	1.20677800
N	-3.17843400	-0.49730300	0.32339700
C	-4.03669800	-1.20596600	-0.63263400
H	-3.69995900	-2.24045000	-0.63656800
H	-5.07698800	-1.18093500	-0.30658300
H	1.57547000	1.29341600	-1.48694700
C	1.65470100	-1.64139300	-0.59446700
H	2.54795800	-2.25979700	-0.69424400
H	1.29766100	-1.40011900	-1.59838500
H	-3.94809800	-0.78682200	-1.63718700

HF: -1080.6069538
Sum of electronic and zero-point Energies: -1080.374950
Sum of electronic and thermal Energies: -1080.359462
Sum of electronic and thermal Enthalpies: -1080.358518
Sum of electronic and thermal Free Energies: -1080.418322
Frequencies: -460.9212

X = NH_2^+, Y = CH_2

C	-0.67901800	0.62512700	0.08227000
C	-1.05890200	-0.54373700	-0.02132300
N	-3.19595900	0.77561200	0.50232800
N	-2.56099500	1.72623500	0.58908000
C	-0.84187900	-1.98856900	-0.22409500
H	-1.51133200	-2.57162500	0.41090900
H	-1.07542400	-2.24865400	-1.26187600
C	0.34755600	1.67437200	0.06682800
C	0.60758900	-2.36824100	0.10118200
H	0.74865100	-3.42459300	-0.13523200
H	0.78800400	-2.25262100	1.17197700
S	2.32845000	-0.11279100	0.13886400
O	3.70407700	0.03211400	-0.29775900
O	2.04021700	-0.13574300	1.56176200
C	0.01323800	2.88647800	-0.78195800
H	-0.85216000	3.39398200	-0.35905800
H	0.86181000	3.57023600	-0.79319500
H	-0.21834000	2.57685100	-1.80194400
H	0.58603000	1.96998800	1.09091400
N	-3.13375200	-0.46421100	0.38871100
C	-4.05831400	-1.11538800	-0.54779900
H	-3.75306400	-2.15793700	-0.60342100
H	-5.07955800	-1.07148800	-0.16870700
C	1.66440900	-1.58580900	-0.67839000
H	2.56710200	-2.18269200	-0.81354600
H	1.32357600	-1.24790700	-1.65904200
O	1.58463200	1.14668700	-0.52661100
H	-4.00504300	-0.66222300	-1.53985000

HF: -1081.0165865
Sum of electronic and zero-point Energies: -1080.770271
Sum of electronic and thermal Energies: -1080.754752
Sum of electronic and thermal Enthalpies: -1080.753808
Sum of electronic and thermal Free Energies: -1080.812727
Frequencies: -459.0719

X = O, Y = CH_2

C	-0.71262900	0.63929200	0.05285300
C	-1.05543300	-0.53934400	-0.09090200
N	-3.19231200	0.68067900	0.57684000
N	-2.57878500	1.64351500	0.68523400
C	-0.80968800	-1.97383000	-0.34508800
H	-1.52573000	-2.58563600	0.20471200
H	-0.95643000	-2.18259700	-1.40931300
C	0.24711500	1.74602100	0.03575500
C	0.59840900	-2.39041500	0.08670900
H	0.72906300	-3.45004500	-0.14070200
H	0.70904100	-2.28259200	1.16758300
N	1.52758500	1.24434100	-0.62170300
S	2.36243300	-0.18620700	0.20319400
O	3.72982400	0.03845700	-0.18931100
O	1.93936000	-0.08890000	1.57356400
C	-0.20109100	2.98225100	-0.73706100
H	-1.06309200	3.41062800	-0.23066300
H	0.59330400	3.72920300	-0.76477300
H	-0.49037000	2.71602800	-1.75519000
H	0.53825500	2.01053100	1.05417500

N	-3.08608600	-0.54695800	0.38862200
C	-4.03486800	-1.18963000	-0.53069200
H	-3.66452500	-2.19856700	-0.69707000
H	-5.02117800	-1.25350200	-0.07110800
H	1.34717000	1.01079100	-1.60571300
C	1.73863400	-1.66760300	-0.62171400
H	2.65264900	-2.26752200	-0.61738200
H	1.52931700	-1.38994900	-1.65744500
H	2.24746700	1.98064800	-0.62354500
H	-4.09284400	-0.65605300	-1.48081200

HF: -1100.4757055
Sum of electronic and zero-point Energies: -1100.256389
Sum of electronic and thermal Energies: -1100.241027
Sum of electronic and thermal Enthalpies: -1100.240083
Sum of electronic and thermal Free Energies: -1100.299319
Frequencies: -448.7326

X = CH_2, Y = O

C	-0.69898100	0.64255300	0.07517400
C	-1.03233900	-0.53602200	-0.07134700
N	-3.23271800	0.63564500	0.54517000
N	-2.62957600	1.60502600	0.66304800
C	-0.72890800	-1.95834200	-0.31716200
H	-1.38991500	-2.61805600	0.25004700
H	-0.85845800	-2.19363400	-1.37716000
C	0.28233600	1.74985100	0.08331400
C	0.70255200	-2.25164000	0.11170100
H	0.99696100	-3.26416700	-0.15930200
H	0.82877600	-2.10673600	1.18430300
S	2.35894600	-0.14634000	0.11824700
O	3.72354500	-0.19321500	-0.36667300
O	2.11815000	-0.20356100	1.54846600
O	1.62387000	-1.38591400	-0.59723400
C	-0.21127100	3.01438900	-0.63042400
H	-1.08790000	3.41568600	-0.12639100
H	0.57216300	3.77454600	-0.63178500
H	-0.47862400	2.78636900	-1.66480600
H	0.50753600	1.99783300	1.12517300
N	-3.11814200	-0.59409700	0.37051500
C	-4.02472100	-1.23472400	-0.58987100
H	-3.63286500	-2.23603900	-0.75659700
H	-5.02838100	-1.32049300	-0.17203300
C	1.58368400	1.30590400	-0.59452200
H	2.35451400	2.07461900	-0.50687300
H	1.43405000	1.06621100	-1.64923400
H	-4.05658200	-0.69102100	-1.53610000

HF: -1100.4749197
Sum of electronic and zero-point Energies: -1100.255076
Sum of electronic and thermal Energies: -1100.239799
Sum of electronic and thermal Enthalpies: -1100.238855
Sum of electronic and thermal Free Energies: -1100.297894
Frequencies: -459.6684

X = CH_2, Y = NH

C	-0.71923700	0.64110300	0.10716900
C	-1.05394000	-0.53910000	-0.03077900
N	-3.27388000	0.65535700	0.47710500
N	-2.66702100	1.62278200	0.59865400
C	-0.76624800	-1.97251200	-0.22263100
H	-1.45690500	-2.59664800	0.34899600
H	-0.88162500	-2.24184900	-1.27724300
C	0.27300000	1.73993700	0.12214000
C	0.65960300	-2.28120400	0.24568800
H	0.87521500	-3.34108700	0.10002900
H	0.76024800	-2.06305700	1.30886500
S	2.38950100	-0.14309100	0.07778900
O	3.72178300	-0.11204800	-0.51802900
O	2.25321600	-0.12826100	1.52908700
C	-0.22208600	3.03252100	-0.53909800
H	-1.07466300	3.43618200	0.00257200
H	0.57493200	3.77842400	-0.54538900
H	-0.52658900	2.83880700	-1.57033200
H	0.52539300	1.95421100	1.16549000
N	-3.15368800	-0.57808100	0.33117300
C	-4.03340700	-1.24207100	-0.63737400
H	-3.63223200	-2.24425900	-0.77503500
H	-5.04664200	-1.32576000	-0.24251400
C	1.55262400	1.30462800	-0.59735600
H	2.31540600	2.08405400	-0.53510600
H	1.36654100	1.07484000	-1.64916900
N	1.69999800	-1.53130200	-0.45189500
H	1.83522200	-1.70515100	-1.44087200
H	-4.04601700	-0.71789800	-1.59519100

HF: -1080.6088447
Sum of electronic and zero-point Energies: -1080.377084
Sum of electronic and thermal Energies: -1080.361374
Sum of electronic and thermal Enthalpies: -1080.360429
Sum of electronic and thermal Free Energies: -1080.420734
Frequencies: -464.6964

X = CH_2, Y = NH_2^+

C	-0.69861600	0.65420900	0.03168000
C	-1.04579300	-0.52658200	-0.08682800
N	-3.18861500	0.67265000	0.58003500
N	-2.55239700	1.62553300	0.66886800
C	-0.80242400	-1.96510200	-0.32011800
H	-1.45788000	-2.57974600	0.29912100
H	-1.01546700	-2.21964200	-1.36324500
C	0.24962800	1.79000200	0.03718900
C	0.62495900	-2.35300700	0.03740400
H	0.83082600	-3.38576300	-0.23851200
H	0.82462200	-2.21940800	1.10015200
S	2.36057700	-0.04593400	0.22097100
O	3.74298100	-0.14429500	-0.16551800
O	1.92945900	-0.23163900	1.57849800
C	-0.24101800	3.00132800	-0.76916000
H	-1.15223000	3.39792100	-0.32802200
H	0.51807600	3.78525600	-0.76911000
H	-0.44787300	2.71174300	-1.80136700
H	0.40895600	2.09679000	1.07497700
N	-3.08354700	-0.55832100	0.40126900
C	-4.04135800	-1.20901400	-0.50142600
H	-3.67772500	-2.22265500	-0.65565300
H	-5.02550700	-1.26273300	-0.03543100
C	1.60026400	1.38191300	-0.55634000
H	2.36492500	2.14935900	-0.40382800
H	1.54803000	1.15882300	-1.62425500
N	1.63098400	-1.50715500	-0.69965100
H	2.46420200	-2.06411400	-0.92365700
H	1.25425900	-1.18473300	-1.59896500
H	-4.10476900	-0.69012100	-1.45962800

HF: -1081.0151038
Sum of electronic and zero-point Energies: -1080.768697
Sum of electronic and thermal Energies: -1080.753045
Sum of electronic and thermal Enthalpies: -1080.752101
Sum of electronic and thermal Free Energies: -1080.811623
Frequencies: -481.2252

X = NH, Y = NH

C	-0.71090800	0.62920100	0.13796300
C	-1.06754000	-0.54543500	0.01899600
N	-3.27275200	0.71489600	0.40868500
N	-2.66544800	1.68101100	0.52230100
C	-0.79272200	-1.98494400	-0.13203700
H	-1.47045900	-2.58503700	0.47959800
H	-0.93697800	-2.29104400	-1.17281000
C	0.32967800	1.68308000	0.17189800
C	0.64626100	-2.27393800	0.30962000
H	0.86609000	-3.33582600	0.18543600
H	0.77062700	-2.02709300	1.36387900
N	1.58622700	1.23850600	-0.47076200
S	2.36569400	-0.13249200	0.04162000
O	3.63669000	-0.09505500	-0.66049700
O	2.29776400	-0.10468800	1.49038800
C	-0.07310400	2.98666000	-0.51307400
H	-0.93113200	3.42296200	-0.00682300
H	0.75958200	3.68977200	-0.48200400
H	-0.34543000	2.79929200	-1.55468900
H	0.57488100	1.88918700	1.21652500
N	-3.17746900	-0.52432700	0.31229300
C	-4.02820000	-1.20239300	-0.67305400
H	-3.68594700	-2.23429000	-0.71249000
H	-5.07009700	-1.19377200	-0.35132500
H	1.55214200	1.27135300	-1.48726500
H	-3.93671200	-0.74680800	-1.66129700
N	1.66444200	-1.53484700	-0.43249700
H	1.76090400	-1.72093300	-1.42380300

HF: -1096.6488042
Sum of electronic and zero-point Energies: -1096.428276
Sum of electronic and thermal Energies: -1096.412862
Sum of electronic and thermal Enthalpies: -1096.411918
Sum of electronic and thermal Free Energies: -1096.471189
Frequencies: -450.3311

X = NH, Y = NH_2^+

C	-0.68652000	0.64106900	0.04794200
C	-1.05801400	-0.53023200	-0.06705800
N	-3.17380500	0.73566600	0.56511100
N	-2.53378700	1.68355400	0.65503500
C	-0.82948000	-1.96822500	-0.31081500
H	-1.47367500	-2.58294600	0.32009700
H	-1.06659900	-2.21451500	-1.35061100
C	0.28569400	1.74858800	0.05723300
C	0.60848600	-2.35696500	0.01100200
H	0.81427800	-3.37871000	-0.30317900
H	0.82066200	-2.25828800	1.07413800
N	1.63717800	1.26958000	-0.36545600
S	2.33585700	-0.02802600	0.22826900
O	3.69691900	-0.11105000	-0.21321900
O	1.90992900	-0.26553700	1.57350600
C	-0.07847700	2.89216300	-0.88451700
H	-1.02122500	3.32954500	-0.56384100
H	0.69574600	3.65968000	-0.85589200
H	-0.19023200	2.52027100	-1.90455100
H	0.38989900	2.12712100	1.07609000
N	-3.10193200	-0.49838000	0.40516300
C	-4.06390000	-1.13562700	-0.50377900
H	-3.73305200	-2.16421700	-0.62857300
H	-5.05798700	-1.14337000	-0.05645400
H	2.01749400	1.59172700	-1.25232200
H	-4.08914500	-0.63448400	-1.47310600
N	1.59844200	-1.47664400	-0.71034300
H	1.19570900	-1.10589300	-1.57912000
H	2.42021200	-2.02587100	-0.98390000

HF: -1097.0584806
Sum of electronic and zero-point Energies: -1096.823613
Sum of electronic and thermal Energies: -1096.808006
Sum of electronic and thermal Enthalpies: -1096.807062
Sum of electronic and thermal Free Energies: -1096.866542

Frequencies: -457.0526

X = NH, Y = O

C	-0.69879500	0.63080100	0.11809600
C	-1.05100600	-0.54358500	-0.00689300
N	-3.24803000	0.69626200	0.46145100
N	-2.64933200	1.66668500	0.57569900
C	-0.75621100	-1.97386100	-0.20461300
H	-1.40440000	-2.60833500	0.40466800
H	-0.90985700	-2.25222600	-1.25080700
C	0.33215900	1.69077100	0.14458700
C	0.68671200	-2.24190300	0.20383700
H	0.98140200	-3.26367700	-0.03075400
H	0.83610400	-2.04961400	1.26583100
N	1.60733500	1.22738100	-0.45934600
S	2.34413400	-0.13243300	0.07124300
O	3.64521400	-0.16599400	-0.55110700
O	2.20108900	-0.17254400	1.50844700
O	1.58717100	-1.40250700	-0.56250200
C	-0.06055600	2.96697200	-0.59396400
H	-0.93354300	3.41095500	-0.12079200
H	0.76511600	3.67846200	-0.56565500
H	-0.30731600	2.74255100	-1.63437600
H	0.55608800	1.93156000	1.18634000
N	-3.15285700	-0.54022900	0.34151800
C	-4.02091600	-1.20062400	-0.64176500
H	-3.67863700	-2.23105500	-0.70753900
H	-5.05631300	-1.19911700	-0.30017200
H	1.63691800	1.29065100	-1.47434300
H	-3.94764200	-0.72498100	-1.62195100

HF: -1116.5140204
Sum of electronic and zero-point Energies: -1116.305677
Sum of electronic and thermal Energies: -1116.290521
Sum of electronic and thermal Enthalpies: -1116.289577
Sum of electronic and thermal Free Energies: -1116.348436
Frequencies: -443.3478

X = O, Y = NH

C	-0.68790900	0.61913900	0.12198300
C	-1.06800400	-0.54575100	-0.00992100
N	-3.22790500	0.74654800	0.47079400
N	-2.61789000	1.70851500	0.58712400
C	-0.80397800	-1.98098100	-0.20965000
H	-1.47864500	-2.59861900	0.38725900
H	-0.95593800	-2.24996900	-1.25925900
C	0.35303100	1.65462000	0.12129200
C	0.63651700	-2.29009100	0.21687500
H	0.86501000	-3.33914400	0.02449100
H	0.75718100	-2.10856000	1.28430900
S	2.33272400	-0.13649100	0.07997600
O	3.63617900	-0.03155800	-0.53216600
O	2.17457400	-0.11837500	1.51737900
C	0.01304600	2.90712000	-0.66442700
H	-0.83329500	3.40665700	-0.19567300
H	0.87049700	3.57981300	-0.67009700
H	-0.25140900	2.64546400	-1.68988900
H	0.62468600	1.90366800	1.14988300
N	-3.15559900	-0.49120100	0.34787300
C	-4.03439300	-1.13273300	-0.63892400
H	-3.71190000	-2.16941500	-0.70567600
H	-5.07002200	-1.11122100	-0.29903400
H	-3.94917800	-0.65647500	-1.61778800
N	1.65406300	-1.49999100	-0.47656100
H	1.79060900	-1.65094000	-1.46932100
O	1.56428300	1.13712700	-0.52856400

HF: -1116.5168388
Sum of electronic and zero-point Energies: -1116.308572
Sum of electronic and thermal Energies: -1116.293435
Sum of electronic and thermal Enthalpies: -1116.292491
Sum of electronic and thermal Free Energies: -1116.350800
Frequencies: -436.2270

X = O, Y = O

C	-0.67831300	0.62596300	0.12283800
C	-1.05115100	-0.54055500	-0.01011400
N	-3.21305300	0.72632000	0.49315700
N	-2.62211900	1.69863100	0.61047800
C	-0.76694800	-1.96742300	-0.24401500
H	-1.40967000	-2.61314800	0.35889100
H	-0.93390700	-2.21930800	-1.29458800
C	0.35364100	1.66530300	0.11345800
C	0.67843300	-2.25095300	0.14464300
H	0.97834400	-3.25665800	-0.14252800
H	0.83551000	-2.10592600	1.21246100
S	2.31012500	-0.13589200	0.09118200
O	3.63015700	-0.11144800	-0.47209300
O	2.11118900	-0.17468900	1.51869700
C	0.02321100	2.89710700	-0.70463400
H	-0.83005200	3.40165700	-0.25355800
H	0.87774700	3.57313100	-0.71440900
H	-0.23090000	2.61209700	-1.72617100
H	0.62640500	1.93291800	1.13640700
N	-3.13029600	-0.50952300	0.36376900
C	-4.00673200	-1.15278200	-0.62515500
H	-3.68114600	-2.18821900	-0.69385500
H	-5.04198000	-1.13484700	-0.28443300
H	-3.92262700	-0.67332400	-1.60241900
O	1.58339700	1.13069200	-0.52068000
O	1.57722100	-1.37231000	-0.58950600

HF: -1136.3791682
Sum of electronic and zero-point Energies: -1136.183190
Sum of electronic and thermal Energies: -1136.168359
Sum of electronic and thermal Enthalpies: -1136.167415
Sum of electronic and thermal Free Energies: -1136.22534
Frequencies: -427.4809

X = O, Y = NH_2^+

C	-0.67681300	0.63514900	0.06707900
C	-1.07640200	-0.52808400	-0.03723900
N	-3.16640100	0.76489300	0.55267200
N	-2.55566600	1.72794200	0.64131000
C	-0.84321400	-1.96451000	-0.28643700
H	-1.46808200	-2.58457500	0.35860200
H	-1.09719500	-2.21317200	-1.32146600
C	0.30097600	1.71287000	0.04300700
C	0.60408200	-2.33615000	0.01121800
H	0.82254200	-3.34965700	-0.31881700
H	0.83223000	-2.24489000	1.07161500
S	2.31972200	-0.03379300	0.22421800
O	3.68323600	-0.07686100	-0.19149200
O	1.89487900	-0.22481400	1.57383900
C	0.00702500	2.83992700	-0.92133900
H	-0.89374700	3.35227100	-0.58559600
H	0.83799500	3.54379400	-0.93297500
H	-0.15896100	2.44249700	-1.92269900
H	0.51566300	2.07571400	1.04858700
N	-3.08883000	-0.47114300	0.41430800
C	-4.03293100	-1.12420500	-0.50489200
H	-3.74080300	-2.17037400	-0.55533500
H	-5.04498800	-1.06478800	-0.10562600
H	-3.99003900	-0.67642700	-1.49937100
N	1.57800100	-1.43431900	-0.71987100
H	1.15412600	-1.03759600	-1.56926900
O	1.62929200	1.16757700	-0.46638800
H	2.39037400	-1.98090900	-1.03012200

HF: -1116.9171262
Sum of electronic and zero-point Energies: -1116.694768
Sum of electronic and thermal Energies: -1116.679541
Sum of electronic and thermal Enthalpies: -1116.678596
Sum of electronic and thermal Free Energies: -1116.736991
Frequencies: -434.6102

X = NH_2^+, Y = NH

C	-0.71739500	0.62950300	0.08163900
C	-1.06892200	-0.54278200	-0.08146100
N	-3.22407000	0.66184400	0.54052600
N	-2.63128100	1.63274800	0.67333500
C	-0.78353200	-1.97073200	-0.32022000
H	-1.48808900	-2.61047500	0.21415400
H	-0.87100500	-2.19913600	-1.38581200
C	0.25561600	1.72494000	0.08866200
C	0.62020100	-2.30521600	0.18419700
H	0.86360800	-3.34852200	-0.01282500
H	0.69210500	-2.13206700	1.25700400
S	2.37650100	-0.22737200	0.15180300
O	3.68640300	-0.05438000	-0.40468300
O	2.06984800	-0.08990100	1.54400400
C	-0.18719200	2.98901100	-0.64138600
H	-1.04413600	3.40703400	-0.11805500
H	0.61252200	3.73096300	-0.64856500
H	-0.48299400	2.75805400	-1.66637000
H	0.55547100	1.95563200	1.11280700
N	-3.11150300	-0.56434400	0.35004100
C	-4.02701100	-1.19968900	-0.60813600
H	-3.64409400	-2.20367200	-0.77712100
H	-5.02664200	-1.27660100	-0.18035800
H	-4.05915600	-0.65267800	-1.55185000
N	1.53008500	1.23759500	-0.59215700
H	1.33440900	1.01819500	-1.57633000
N	1.67527000	-1.51027100	-0.46659300
H	2.02638600	-1.79146400	-1.37778800
H	2.23748300	1.98372500	-0.58813600

HF: -1097.0628934
Sum of electronic and zero-point Energies: -1096.828115
Sum of electronic and thermal Energies: -1096.812576
Sum of electronic and thermal Enthalpies: -1096.811632
Sum of electronic and thermal Free Energies: -1096.870967
Frequencies: -444.5636

X = NH_2^+, Y = O

C	-0.70055000	0.63416700	0.06848400
C	-1.05667000	-0.53346200	-0.10890800
N	-3.18988900	0.64751800	0.60012900
N	-2.61004100	1.62355200	0.73888000
C	-0.75574200	-1.94653100	-0.40796000
H	-1.43916400	-2.62602000	0.10599200
H	-0.84308700	-2.13397100	-1.48081000
C	0.27188700	1.72564200	0.05829100
C	0.64343500	-2.27802800	0.07543300
H	0.96525900	-3.26797200	-0.23602300
H	0.73998900	-2.16231700	1.15319600
S	2.34446500	-0.22833200	0.18273900
O	3.68755200	-0.14110500	-0.28554900
O	1.97877900	-0.15341500	1.56080500
C	-0.15749000	2.96368900	-0.72009300
H	-1.02279600	3.39362300	-0.21965300
H	0.63937600	3.70810500	-0.73790400
H	-0.43990200	2.70004700	-1.74065800

H	0.57000900	1.98776900	1.07509600
N	-3.08200100	-0.57375300	0.38207700
C	-4.01562600	-1.18613400	-0.57494100
H	-3.64513800	-2.19101700	-0.76392700
H	-5.00993100	-1.25967700	-0.13487200
H	-4.05359800	-0.62335500	-1.50892700
N	1.55818700	1.20504700	-0.60309900
H	1.36744100	0.95326900	-1.58259100
H	2.27628800	1.94279500	-0.61548700
O	1.61798800	-1.37555100	-0.57588000

HF: -1116.9165576
Sum of electronic and zero-point Energies: -1116.694306
Sum of electronic and thermal Energies: -1116.679004
Sum of electronic and thermal Enthalpies: -1116.678060
Sum of electronic and thermal Free Energies: -1116.737016
Frequencies: -431.9051

X = NH_2^+, Y = NH_2^+

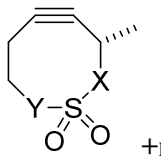
C	-0.70829400	0.64019400	0.05911500
C	-1.08718200	-0.53325400	-0.04710700
N	-3.19269400	0.69370700	0.53922100
N	-2.60348400	1.66876400	0.64172400
C	-0.83777200	-1.97246000	-0.27366400
H	-1.48749600	-2.58314100	0.35582900
H	-1.05365400	-2.23727900	-1.31314200
C	0.22680200	1.75895700	0.06856500
C	0.58326400	-2.35803500	0.09546200
H	0.80248500	-3.38780000	-0.18087400
H	0.78946600	-2.21635500	1.15490700
S	2.35642600	-0.12214300	0.22207200
O	3.70891900	-0.10388200	-0.20114100
O	1.86965600	-0.16492400	1.55130400
C	-0.18822700	2.98847800	-0.72896200
H	-1.07145500	3.40578400	-0.25010700
H	0.59865400	3.74334100	-0.71706400
H	-0.44047000	2.72395600	-1.75655600
H	0.49490200	2.02801000	1.09186800
N	-3.06546900	-0.53642100	0.37760700
C	-3.99022500	-1.21472100	-0.54479100
H	-3.65912700	-2.24805700	-0.61279300
H	-4.99880300	-1.20019000	-0.13358400
H	-3.97366600	-0.75026900	-1.53200400
N	1.57520700	1.28772100	-0.56276100
H	1.46081300	1.12934300	-1.57601300
N	1.61024000	-1.52302400	-0.66685600
H	1.23368400	-1.22549800	-1.57977500
H	2.28423500	2.03858700	-0.48805700
H	2.43221100	-2.10587600	-0.89135600

HF: -1097.420407
Sum of electronic and zero-point Energies: -1097.171484
Sum of electronic and thermal Energies: -1097.156001
Sum of electronic and thermal Enthalpies: -1097.155057
Sum of electronic and thermal Free Energies: -1097.213834
Frequencies: -452.6108

X = NBoc, Y = O

C	1.80852700	-0.17025500	0.57921200
C	2.23382600	0.01773300	-0.56051600
N	4.05716300	-1.39369400	0.57613400
N	3.42929100	-1.38003800	1.53512400
C	2.11202100	0.55879400	-1.92536700
H	3.07402100	0.89991900	-2.31609400
H	1.74005900	-0.21723800	-2.60003200
C	0.77140000	-0.11512400	1.62436900
C	1.16548600	1.75323900	-1.92516700
H	0.93409900	2.07281600	-2.93940200
H	1.58524600	2.58408700	-1.36107200
N	-0.51665400	0.36177500	1.00824100
S	-0.50857400	1.80227900	0.14621000
O	-1.84502300	2.32723100	0.10283200
O	0.55142000	2.60513000	0.70365600
O	-0.12594400	1.39633800	-1.35287000
N	4.16879000	-0.90953900	-0.56552600
C	4.50219500	-1.81979700	-1.66814600
H	4.35459400	-1.25374500	-2.58549400
H	5.54827700	-2.12265900	-1.61136600
C	1.16243600	0.66130000	2.87818000
H	0.31294100	0.69445800	3.56177800
H	1.98392600	0.13403000	3.36499700
H	1.48009100	1.67392500	2.64277500
H	0.53081200	-1.13380900	1.92656200
C	-1.50519400	-0.62912100	0.79160200
O	-2.29415500	-0.31987000	-0.21261100
O	-1.55134700	-1.62059100	1.47452600
C	-3.49960100	-1.11344000	-0.52285600
C	-4.42168500	-1.14187500	0.68839000
H	-5.37058800	-1.59376200	0.39238600
H	-3.99793900	-1.72656200	1.50348000
H	-4.61970700	-0.12522300	1.03524300
C	-4.12319500	-0.32173200	-1.66210300
H	-5.03408500	-0.82138100	-1.99581100
H	-4.37584600	0.68703800	-1.33113100
H	-3.43065900	-0.25627000	-2.50333600
C	-3.08783400	-2.50421600	-0.98515700
H	-2.36411600	-2.43083900	-1.79975000
H	-2.65730200	-3.08496700	-0.17109600
H	-3.97248100	-3.02501700	-1.35738300
H	3.85580600	-2.69971900	-1.67135300

HF: -1462.2929029
Sum of electronic and zero-point Energies: -1461.958149
Sum of electronic and thermal Energies: -1461.935479
Sum of electronic and thermal Enthalpies: -1461.934535
Sum of electronic and thermal Free Energies: -1462.009375
Frequencies: -439.5630



+methyl azide (*syn*-TSs)

X = CH_2, Y = CH_2

C	0.90665800	-0.03278200	-0.10606900
C	0.80512500	1.19461900	-0.03417800
N	3.33294400	0.81333800	0.12687900
N	2.86204400	1.86445600	0.13459200
C	0.07978300	2.47705800	-0.01785900
H	0.53227700	3.16507700	0.69900800
H	0.17623800	2.94581100	-1.00274500
C	0.42051200	-1.42093300	-0.23946100
C	-1.39852100	2.27799700	0.32625600
H	-1.90602700	3.24294800	0.26114500
H	-1.49961600	1.93181100	1.35760200
S	-2.25607900	-0.41299300	-0.03845900
O	-3.52452200	-0.90695500	-0.59490800
O	-2.09154400	-0.45580800	1.41856200
N	3.01609200	-0.39153100	0.18299400
C	3.77984600	-1.36083000	-0.60508100
H	4.80880400	-1.42323900	-0.24873900
H	3.30543400	-2.32826000	-0.45003100
C	0.52496400	-2.20428400	1.07421400
H	-0.06325800	-1.72512500	1.85602300
H	0.15945800	-3.22320600	0.92996100
H	1.56678900	-2.24733300	1.39440200
H	1.03176200	-1.93583700	-0.98874400
C	-0.99069600	-1.42756600	-0.83914400
H	-0.98935200	-1.09661800	-1.87937300
H	-1.43073600	-2.42691600	-0.79490300
C	-2.12925600	1.31209400	-0.60189900
H	-3.18773300	1.56720300	-0.67848600
H	-1.71416000	1.28073900	-1.61189600
H	3.76785800	-1.11315400	-1.66901900

HF: -1064.5664759
Sum of electronic and zero-point Energies: -1064.322820
Sum of electronic and thermal Energies: -1064.307363
Sum of electronic and thermal Enthalpies: -1064.306419
Sum of electronic and thermal Free Energies: -1064.365032
Frequencies: -473.1997

X = NH, Y = CH_2

C	0.89111000	-0.01905600	-0.06325500
C	0.81068800	1.20849800	0.01068700
N	3.33176600	0.77187400	0.11018500
N	2.88927100	1.83345500	0.14242400
C	0.09010500	2.49203000	0.02750600
H	0.51989200	3.16662300	0.77066300
H	0.21595800	2.97766500	-0.94564700
C	0.36103100	-1.39451800	-0.17924000
C	-1.39791500	2.27733800	0.32096300
H	-1.91465100	3.23587800	0.23698400
H	-1.52913000	1.93114600	1.34850600
N	-1.03480800	-1.39925700	-0.67703700
S	-2.22794200	-0.42591000	-0.06715100
O	-3.44842500	-0.92422400	-0.69504200
O	-2.10882300	-0.45940800	1.38450800
N	3.00240900	-0.42953800	0.16004700
C	3.70801400	-1.38414300	-0.69993300
H	4.75753600	-1.45812800	-0.41279400
H	3.23944500	-2.35304600	-0.53740700
H	-1.11349800	-1.46073300	-1.68723800
C	0.49224400	-2.18535100	1.12203200
H	-0.04254900	-1.68391300	1.92761200
H	0.07724200	-3.18415300	0.98202700
H	1.54564600	-2.26633500	1.39289900
H	0.90859000	-1.92408900	-0.96280200
C	-2.08218700	1.29902100	-0.63274800
H	-3.13328100	1.55716800	-0.76686700
H	-1.61336600	1.25564100	-1.61848800
H	3.62821700	-1.10874700	-1.75416500

HF: -1080.6064951
Sum of electronic and zero-point Energies: -1080.374143
Sum of electronic and thermal Energies: -1080.358791
Sum of electronic and thermal Enthalpies: -1080.357847
Sum of electronic and thermal Free Energies: -1080.416294
Frequencies: -461.4977

X = NH_2^+, Y = CH_2

C	0.92257200	-0.02639700	-0.10675900
C	0.78500300	1.19845400	-0.03901300
N	3.28385200	0.82420000	0.20956200
N	2.79829700	1.86677800	0.23563900
C	0.06131200	2.48111400	-0.06727000
H	0.49729900	3.17918900	0.64868500
H	0.19412700	2.92542800	-1.05866500
C	0.46156400	-1.41170200	-0.25952700

C	-1.42843600	2.31273100	0.23776900
H	-1.93017700	3.26945300	0.08178600
H	-1.57552500	2.04552400	1.28580500
N	-0.95618200	-1.37549200	-0.82211300
S	-2.26075000	-0.36612000	0.03434800
O	-3.44357500	-1.01217100	-0.47221500
O	-1.90563000	-0.41480200	1.42557000
N	2.98486000	-0.38711900	0.20744300
C	3.75236400	-1.29278500	-0.65700700
H	4.79405300	-1.32593000	-0.33786900
H	3.32582800	-2.28600300	-0.52994500
H	-0.92895600	-1.07081300	-1.80215800
C	0.52790300	-2.24787000	1.01307600
H	-0.00107000	-1.76650200	1.83228600
H	0.11893100	-3.24439200	0.83884100
H	1.57778700	-2.34919900	1.28696100
H	1.01966800	-1.91158100	-1.05536800
C	-2.13711700	1.30208000	-0.65769700
H	-3.20061100	1.52687300	-0.76870800
H	-1.70695100	1.20475600	-1.65718800
H	-1.35570900	-2.32410300	-0.83120300
H	3.69017000	-0.99130300	-1.70483500

HF: -1081.0140106
Sum of electronic and zero-point Energies: -1080.767692
Sum of electronic and thermal Energies: -1080.752120
Sum of electronic and thermal Enthalpies: -1080.751176
Sum of electronic and thermal Free Energies: -1080.810182
Frequencies: -471.4238

X = O, Y = CH_2

C	0.87064500	-0.00999200	-0.07914300
C	0.78745400	1.21621500	0.00721300
N	3.29097000	0.75625900	0.20333700
N	2.85361300	1.81828200	0.25445000
C	0.06835500	2.50047100	-0.01475100
H	0.46889300	3.18301100	0.73683600
H	0.23508300	2.97217200	-0.98850700
C	0.34152900	-1.36887000	-0.26360200
C	-1.43251900	2.29409500	0.21930600
H	-1.94753000	3.24159100	0.04946200
H	-1.61194600	2.01317400	1.25892600
S	-2.18383400	-0.42396200	-0.02529200
O	-3.40972700	-1.00863200	-0.53371600
O	-1.95819200	-0.40659900	1.40855300
N	2.96318600	-0.44655500	0.19592700
C	3.67433900	-1.34924200	-0.71754600
H	4.72221700	-1.43652100	-0.42914200
H	3.20724400	-2.32667500	-0.61472500
C	0.45354500	-2.26361600	0.96090100
H	-0.00957600	-1.79533900	1.82739300
H	-0.03147800	-3.21864300	0.75607600
H	1.50867500	-2.43976600	1.17399300
H	0.83087500	-1.84461100	-1.11563800
C	-2.06743100	1.25405700	-0.70394300
H	-3.11695500	1.48291700	-0.89055700
H	-1.55755500	1.15365600	-1.66391000
O	-1.04266100	-1.30056900	-0.74599100
H	3.59815400	-1.00977700	-1.75291800

HF: -1100.4733649
Sum of electronic and zero-point Energies: -1100.253562
Sum of electronic and thermal Energies: -1100.238432
Sum of electronic and thermal Enthalpies: -1100.237487
Sum of electronic and thermal Free Energies: -1100.295592
Frequencies: -456.9498

X = CH_2, Y = O

C	0.89359800	-0.02950300	-0.11975800
C	0.79511000	1.19712800	-0.06482600
N	3.31717000	0.81435700	0.17359400
N	2.86844000	1.87258800	0.17120100
C	0.01589500	2.44448000	-0.11055400
H	0.41337700	3.19921000	0.57225300
H	0.06213600	2.86458700	-1.11885600
C	0.39348300	-1.41110300	-0.26631700
C	-1.43004800	2.15936800	0.27345600
H	-2.06725800	3.02529400	0.10113500
H	-1.50785600	1.84734700	1.31447200
S	-2.24778300	-0.37234400	-0.03177500
O	-3.53610200	-0.73843400	-0.58544300
O	-2.07242000	-0.39309300	1.40884800
O	-1.96914500	1.11459200	-0.57705000
N	3.00690500	-0.39122600	0.22329100
C	3.76726400	-1.34410700	-0.59008700
H	4.79821000	-1.41296500	-0.24088600
H	3.29346100	-2.31446600	-0.45272900
C	0.49154700	-2.21638500	1.03405000
H	-0.07729600	-1.73775800	1.83056500
H	0.10415800	-3.22527800	0.87787900
H	1.53483000	-2.28512200	1.34416400
H	0.99221000	-1.92314300	-1.02763300
C	-1.02134700	-1.38984000	-0.86455600
H	-1.02141100	-1.01577500	-1.88946300
H	-1.46787900	-2.38641500	-0.85022500
H	3.74857300	-1.07279600	-1.64816400

HF: -1100.4751451
Sum of electronic and zero-point Energies: -1100.254891
Sum of electronic and thermal Energies: -1100.239874
Sum of electronic and thermal Enthalpies: -1100.238929
Sum of electronic and thermal Free Energies: -1100.296609
Frequencies: -454.5608

X = CH_2, Y = NH

C	0.90662300	-0.02524000	-0.12231600
C	0.82282300	1.20345300	-0.08118800
N	3.34686500	0.79988300	0.12980000
N	2.90111200	1.86027300	0.11270200
C	0.05916500	2.46065600	-0.09240100
H	0.50831800	3.20907900	0.56463400
H	0.06217600	2.88038900	-1.10286300
C	0.39919100	-1.40607200	-0.24225100
C	-1.37938200	2.19867200	0.36673600
H	-1.95832300	3.12312600	0.32848800
H	-1.38478100	1.84444900	1.39743900
S	-2.27227300	-0.37453800	-0.04817400
O	-3.51840300	-0.79890600	-0.67898400
O	-2.13719300	-0.47000400	1.39982200
N	3.02333800	-0.40118800	0.20466000
C	3.78100800	-1.38399500	-0.57330000
H	4.80712300	-1.45656600	-0.21058400
H	3.29359400	-2.34452300	-0.41570100
C	0.49113800	-2.18113900	1.07706700
H	-0.07744100	-1.68085200	1.86004100
H	0.09690300	-3.19090100	0.94404100
H	1.53385700	-2.24998600	1.38975300
H	1.00211200	-1.93794900	-0.98685700
C	-1.01052600	-1.39337000	-0.84853900
H	-0.99606000	-1.03801100	-1.88057800
H	-1.44800100	-2.39413600	-0.82944600
N	-2.09325100	1.20739000	-0.43450900
H	-2.28301900	1.41967800	-1.40704800
H	3.77799300	-1.14221200	-1.63865200

HF: -1080.6091081
Sum of electronic and zero-point Energies: -1080.376862
Sum of electronic and thermal Energies: -1080.361445
Sum of electronic and thermal Enthalpies: -1080.360501
Sum of electronic and thermal Free Energies: -1080.418871
Frequencies: -459.6333

X = CH_2, Y = NH_2^+

C	0.90686800	-0.04436200	-0.10281800
C	0.78256400	1.18069700	-0.00537800
N	3.28953900	0.83928200	0.16236600
N	2.80640800	1.88305400	0.20060700
C	0.05541200	2.46171900	0.00722900
H	0.43931200	3.12440700	0.78460800
H	0.21346400	2.97441900	-0.94642700
C	0.44429300	-1.44172200	-0.24767000
C	-1.43212600	2.26136500	0.26075300
H	-1.99419700	3.17703600	0.08534700
H	-1.62537600	1.90851500	1.27290600
S	-2.21434200	-0.50640100	0.01228600
O	-3.51843500	-0.84140600	-0.49484900
O	-1.95599200	-0.35764300	1.41774300
N	2.98712900	-0.36990800	0.17413900
C	3.75605800	-1.30112000	-0.65684900
H	4.79273500	-1.34226900	-0.32198600
H	3.31243300	-2.28490500	-0.51546100
C	0.57465800	-2.24106500	1.05404800
H	0.00167200	-1.77826500	1.85711000
H	0.21928100	-3.26173800	0.90252500
H	1.62173600	-2.27508800	1.35474100
H	1.04935000	-1.93550700	-1.01554500
C	-0.96855400	-1.48227600	-0.84198400
H	-1.00898900	-1.15011800	-1.88115700
H	-1.40554100	-2.48414300	-0.78867000
N	-1.99904800	1.22427400	-0.67515900
H	-1.45125700	1.17710500	-1.54279400
H	-2.95651200	1.47292300	-0.95024300
H	3.71353600	-1.02387800	-1.71233900

HF: -1081.0161463
Sum of electronic and zero-point Energies: -1080.769445
Sum of electronic and thermal Energies: -1080.754030
Sum of electronic and thermal Enthalpies: -1080.753086
Sum of electronic and thermal Free Energies: -1080.811488
Frequencies: -475.4574

X = NH, Y = NH

C	0.88982900	-0.01294400	-0.08032100
C	0.81806700	1.21544600	-0.03970000
N	3.33841700	0.77028500	0.10750300
N	2.91346900	1.83816200	0.11182200
C	0.05831300	2.47363000	-0.04556200
H	0.48944200	3.20674200	0.64019200
H	0.08995400	2.91534600	-1.04602400
C	0.34601800	-1.38411900	-0.17777900
C	-1.39153800	2.19600800	0.36855300
H	-1.97922300	3.11412400	0.31092100
H	-1.42562100	1.84164900	1.39840600
N	-1.04574800	-1.37958900	-0.68691500
S	-2.23418500	-0.39102300	-0.08139300
O	-3.42114700	-0.82710600	-0.79657900
O	-2.14857700	-0.47741800	1.36350500
N	3.00794400	-0.42875200	0.17914300
C	3.71577500	-1.39863400	-0.66219700
H	4.76100300	-1.47910900	-0.36137100
H	3.23601400	-2.36122100	-0.49515100
H	-1.10496000	-1.40166200	-1.70038400
C	0.46243300	-2.15789100	1.13488600
H	-0.06767400	-1.64058700	1.93326000

H	0.03689200	-3.15399800	1.00746500
H	1.51430400	-2.24700800	1.40905000
H	0.89226700	-1.93227100	-0.94976300
H	3.65120800	-1.13378700	-1.72007900
N	-2.06991800	1.19680300	-0.45517900
H	-2.19138600	1.39700500	-1.44153600

HF: -1096.6480441
Sum of electronic and zero-point Energies: -1096.427020
Sum of electronic and thermal Energies: -1096.411781
Sum of electronic and thermal Enthalpies: -1096.410837
Sum of electronic and thermal Free Energies: -1096.468941
Frequencies: -447.7817

X = NH, Y = NH_2^+

C	0.89916900	-0.03279300	-0.06928600
C	0.77898500	1.19107600	0.02313800
N	3.28523300	0.80904300	0.17040000
N	2.82640700	1.86075000	0.22868800
C	0.04933500	2.46944400	0.01100300
H	0.41851900	3.14227500	0.78688400
H	0.22157300	2.97028700	-0.94631000
C	0.40070700	-1.41526600	-0.21920600
C	-1.44299000	2.26772000	0.24294000
H	-2.00029500	3.18093000	0.04101100
H	-1.65046700	1.93681600	1.25859800
N	-1.02067200	-1.39142500	-0.67652000
S	-2.17420100	-0.52889800	-0.00205500
O	-3.44440800	-0.88906700	-0.56059300
O	-1.93568200	-0.34767900	1.39734400
N	2.97925600	-0.39926100	0.16790700
C	3.69975500	-1.29827000	-0.74250800
H	4.75319800	-1.35081200	-0.46726000
H	3.26302800	-2.28687600	-0.61554700
H	-1.23248700	-1.70314300	-1.62044200
C	0.56049700	-2.26320100	1.03979700
H	0.05691700	-1.79576800	1.88529700
H	0.14033100	-3.25398000	0.86677400
H	1.62067400	-2.35729900	1.27466800
H	0.91490600	-1.89956700	-1.05160300
H	3.59880300	-0.97711600	-1.78139800
N	-2.00248000	1.21078500	-0.67763500
H	-1.46196400	1.15558700	-1.54944500
H	-2.96174800	1.45350800	-0.94750300

HF: -1097.0586348
Sum of electronic and zero-point Energies: -1096.823086
Sum of electronic and thermal Energies: -1096.807805
Sum of electronic and thermal Enthalpies: -1096.806861
Sum of electronic and thermal Free Energies: -1096.864982
Frequencies: -461.0124

X = NH, Y = O

C	0.88108100	-0.01751400	-0.08143500
C	0.79450900	1.20898600	-0.02887200
N	3.31381500	0.78289000	0.14951400
N	2.88718500	1.84887600	0.16594500
C	0.01722000	2.45647800	-0.06747500
H	0.40273400	3.19977000	0.63440300
H	0.07794100	2.89321700	-1.06775300
C	0.34099800	-1.38745800	-0.20458200
C	-1.43285900	2.15458300	0.29016600
H	-2.07563400	3.01617200	0.11573500
H	-1.52392000	1.83104300	1.32635200
N	-1.06102300	-1.36343000	-0.69906200
S	-2.21282200	-0.38784500	-0.06772600
O	-3.44747600	-0.76336400	-0.71347000
O	-2.08873300	-0.41128500	1.37136400
O	-1.94925700	1.11377900	-0.57945100
N	2.99579400	-0.42033800	0.19729800
C	3.70672000	-1.36089500	-0.67581600
H	4.75522400	-1.43654200	-0.38587400
H	3.23924500	-2.33276900	-0.52956000
H	-1.15025000	-1.41084500	-1.70946900
C	0.46225700	-2.19477200	1.08639300
H	-0.05475400	-1.69293700	1.90322100
H	0.02856200	-3.18424700	0.93799900
H	1.51585900	-2.29801600	1.34804100
H	0.87446500	-1.91654700	-0.99778700
H	3.62945700	-1.06826600	-1.72538800

HF: -1116.5132594
Sum of electronic and zero-point Energies: -1116.304183
Sum of electronic and thermal Energies: -1116.289358
Sum of electronic and thermal Enthalpies: -1116.288413
Sum of electronic and thermal Free Energies: -1116.345649
Frequencies: -441.6855

X = O, Y = NH

C	0.87741300	-0.00275200	-0.07911500
C	0.81436100	1.22538700	-0.03431900
N	3.31580300	0.74162500	0.17037900
N	2.90533400	1.81407500	0.18881900
C	0.06012300	2.48545500	-0.07450900
H	0.46952700	3.22377400	0.61832100
H	0.12635200	2.91515300	-1.07819700
C	0.32513700	-1.35580600	-0.22711200
C	-1.40303000	2.21342400	0.29654200
H	-1.99847000	3.11839500	0.16834100
H	-1.47470500	1.90710800	1.33946600
S	-2.20338500	-0.38369500	-0.05975500
O	-3.38362200	-0.89620400	-0.71556800
O	-2.06793100	-0.43880800	1.37854300
N	2.97893300	-0.45698100	0.20626100
C	3.67109100	-1.39432800	-0.68686700
H	4.71941000	-1.49030000	-0.40249100
H	3.18938700	-2.36111300	-0.55495500
C	0.40887900	-2.21070100	1.02802100
H	-0.05552400	-1.70825100	1.87438400
H	-0.08735600	-3.16545600	0.85040700
H	1.45979200	-2.39374300	1.25641300
H	0.81766200	-1.86883200	-1.05536700
H	3.59344600	-1.08175900	-1.73062800
N	-2.03683400	1.16611800	-0.50615100
H	-2.17868600	1.33086400	-1.49616700
O	-1.04759400	-1.27807000	-0.73603300

HF: -1116.5143134
Sum of electronic and zero-point Energies: -1116.305755
Sum of electronic and thermal Energies: -1116.290782
Sum of electronic and thermal Enthalpies: -1116.289837
Sum of electronic and thermal Free Energies: -1116.347289
Frequencies: -441.7386

X = O, Y = O

C	0.87022600	-0.01073100	-0.08786800
C	0.79139000	1.21571400	-0.03486500
N	3.28902200	0.75675700	0.21325300
N	2.87204400	1.82549500	0.23984300
C	0.01866100	2.46391900	-0.10553800
H	0.39019000	3.21659000	0.59333900
H	0.09971600	2.88389600	-1.11123800
C	0.32224700	-1.36120800	-0.25606900
C	-1.43709800	2.16709600	0.23089300
H	-2.08387800	3.01189600	0.00307100
H	-1.55126500	1.88101200	1.27520000
S	-2.18289800	-0.37960300	-0.04734100
O	-3.41086400	-0.82350200	-0.64335400
O	-2.01444600	-0.38200200	1.38422400
N	2.97068900	-0.44666000	0.22505500
C	3.67780900	-1.35243800	-0.69026000
H	4.72592100	-1.44148800	-0.40358700
H	3.20786800	-2.32808200	-0.58477600
C	0.40570700	-2.24478300	0.97653400
H	-0.04762100	-1.75833300	1.83824800
H	-0.09713500	-3.19197200	0.77980200
H	1.45693600	-2.43931600	1.19322600
H	0.79405700	-1.85656400	-1.10602100
H	3.59965800	-1.01285700	-1.72525700
O	-1.07007000	-1.26688600	-0.74628900
O	-1.92762200	1.08417900	-0.61190100

HF: -1136.3766548
Sum of electronic and zero-point Energies: -1136.180307
Sum of electronic and thermal Energies: -1136.165688
Sum of electronic and thermal Enthalpies: -1136.164743
Sum of electronic and thermal Free Energies: -1136.221663
Frequencies: -433.4570

X = O, Y = NH_2^+

C	0.89236100	-0.02632400	-0.08321300
C	0.78241300	1.19765500	0.01703400
N	3.26429400	0.77662000	0.24247700
N	2.81293900	1.83020500	0.31206400
C	0.04968500	2.47297200	-0.01930600
H	0.39920100	3.15377500	0.75852700
H	0.23865100	2.96404700	-0.97820300
C	0.38473400	-1.38567600	-0.27738400
C	-1.44589200	2.26476900	0.18608900
H	-2.00851900	3.16155000	-0.06568000
H	-1.67753400	1.97017300	1.20745100
S	-2.14910600	-0.51299300	0.02320900
O	-3.41577200	-0.93315800	-0.47843600
O	-1.86275100	-0.33740300	1.41054300
N	2.96074100	-0.43063000	0.19742000
C	3.68569900	-1.28851500	-0.75181400
H	4.73601400	-1.35590100	-0.46887100
H	3.24502100	-2.28022400	-0.67596800
C	0.48616800	-2.30538900	0.92136600
H	0.05433500	-1.84763400	1.80962800
H	-0.01281700	-3.24913000	0.70263300
H	1.54288300	-2.49897800	1.10962200
H	0.82117700	-1.84412000	-1.16479800
H	3.59373300	-0.91493200	-1.77346900
N	-1.97895700	1.16734100	-0.71259300
H	-1.41812100	1.08082600	-1.57137300
O	-1.04881600	-1.29331100	-0.74211400
H	-2.93374900	1.39771800	-1.01300100

HF: -1116.9147269
Sum of electronic and zero-point Energies: -1116.691761
Sum of electronic and thermal Energies: -1116.676781
Sum of electronic and thermal Enthalpies: -1116.675837
Sum of electronic and thermal Free Energies: -1116.733384
Frequencies: -448.4674

X = NH_2^+, Y = NH

C	0.93035600	-0.02005700	-0.10922000
C	0.82611700	1.20764500	-0.08373900
N	3.31968200	0.79541400	0.17420900
N	2.86802200	1.85198000	0.16961700
C	0.06893100	2.46728000	-0.12324100
H	0.51380400	3.21917900	0.53126200
H	0.08870500	2.87000800	-1.13929800

C	0.43351600	-1.39597700	-0.21967100
C	-1.37067200	2.22421200	0.32906200
H	-1.97095800	3.12777000	0.22961200
H	-1.39742800	1.90724000	1.37062900
S	-2.30073400	-0.30854300	-0.00097900
O	-3.43830800	-0.86090000	-0.67731800
O	-2.04484000	-0.46259700	1.39895000
N	3.00795200	-0.41023000	0.21413700
C	3.75279800	-1.35013100	-0.63351400
H	4.79449900	-1.40135800	-0.31619400
H	3.30268600	-2.32991000	-0.48519300
C	0.47824500	-2.18811200	1.08075100
H	-0.03675700	-1.66421100	1.88259600
H	0.04151100	-3.17844900	0.94206800
H	1.52564000	-2.30844600	1.35682200
H	0.98366000	-1.93638200	-0.99469900
H	3.69449600	-1.06889300	-1.68719200
N	-0.97869800	-1.34775100	-0.79558300
H	-0.93062800	-1.03870000	-1.77350400
N	-2.05254700	1.18723100	-0.46565300
H	-2.42550600	1.41812100	-1.38264200
H	-1.37340200	-2.29697100	-0.81131100

HF: -1097.0604246
Sum of electronic and zero-point Energies: -1096.825003
Sum of electronic and thermal Energies: -1096.809711
Sum of electronic and thermal Enthalpies: -1096.808767
Sum of electronic and thermal Free Energies: -1096.866951
Frequencies: -455.7701

X = NH_2^+, Y = O

C	0.91947100	-0.02368100	-0.12503300
C	0.80315100	1.20211400	-0.09658800
N	3.28625900	0.79971700	0.24204300
N	2.83860400	1.85640800	0.23935400
C	0.02954100	2.44924900	-0.18669300
H	0.44153900	3.23158000	0.45448400
H	0.05775800	2.81952800	-1.21416000
C	0.41637900	-1.39162300	-0.28031300
C	-1.40272400	2.20110600	0.24644000
H	-2.05736700	3.04011100	0.02722700
H	-1.47189400	1.92285600	1.29615400
S	-2.26461600	-0.30842400	0.03130800
O	-3.47117500	-0.80810500	-0.53909800
O	-1.94796900	-0.39783300	1.42009900
N	2.98654400	-0.40888900	0.25432600
C	3.74851000	-1.31928100	-0.61249500
H	4.78703100	-1.36899200	-0.28545800
H	3.30573600	-2.30634600	-0.49536500
C	0.45778800	-2.24366500	0.98079600
H	-0.03502900	-1.74950600	1.81460500
H	0.00357500	-3.21919500	0.80166800
H	1.50623400	-2.39476500	1.23700200
H	0.94474700	-1.90379000	-1.08880900
H	3.69762100	-1.00819400	-1.65790600
N	-1.00987400	-1.29652400	-0.84557700
H	-0.96748000	-0.91593500	-1.80105800
H	-1.41600400	-2.23907800	-0.92318300
O	-1.96911100	1.09671400	-0.56273000

HF: -1116.9137543
Sum of electronic and zero-point Energies: -1116.690867
Sum of electronic and thermal Energies: -1116.675833
Sum of electronic and thermal Enthalpies: -1116.674889
Sum of electronic and thermal Free Energies: -1116.732750
Frequencies: -444.9043

X = NH_2^+, Y = NH_2^+

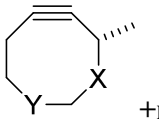
C	0.92885900	-0.04149100	-0.09124400
C	0.78488200	1.18277800	-0.00053900
N	3.25962800	0.83435200	0.20916700
N	2.76271900	1.86955800	0.26600400
C	0.05769600	2.46240400	-0.02087200
H	0.43333500	3.13610100	0.75095400
H	0.23379700	2.95519600	-0.98144400
C	0.48157400	-1.43171600	-0.21870500
C	-1.43135800	2.28444700	0.22124800
H	-1.99348000	3.18446100	-0.02168000
H	-1.65745800	1.98445600	1.24230800
S	-2.21923500	-0.43974800	0.04826200
O	-3.45552800	-0.90369400	-0.46710200
O	-1.83286200	-0.33628000	1.40631200
N	2.97754100	-0.37924800	0.17656300
C	3.73766700	-1.24914800	-0.73380900
H	4.78784400	-1.25994400	-0.44371900
H	3.34153300	-2.25551600	-0.61500900
C	0.56365700	-2.25100200	1.06129000
H	0.05270900	-1.76099600	1.88716500
H	0.16300900	-3.25379100	0.90796100
H	1.61995200	-2.33822500	1.31516700
H	1.00972200	-1.93955200	-1.02935600
H	3.63540900	-0.92241600	-1.77040000
N	-0.96942900	-1.43128800	-0.78108800
H	-0.96468500	-1.20316100	-1.78651200
N	-2.00210600	1.20430600	-0.69433100
H	-1.46332800	1.14897100	-1.57290900
H	-1.35485300	-2.39120000	-0.73161400
H	-2.96494400	1.44999000	-0.97520700

HF: -1097.4179226
Sum of electronic and zero-point Energies: -1097.168046
Sum of electronic and thermal Energies: -1097.152928
Sum of electronic and thermal Enthalpies: -1097.151984
Sum of electronic and thermal Free Energies: -1097.209351
Frequencies: -465.0242

X = NBoc, Y = O

C	-1.88760400	-0.11294600	0.03072700
C	-2.04165900	0.57627000	1.03857900
N	-4.11438700	-0.93699500	0.99188200
N	-3.97755700	-0.15520100	1.81984800
C	-1.60249600	1.60458600	1.99526600
H	-2.44598900	2.14881600	2.42701100
H	-1.07109100	1.12566800	2.82209900
C	-1.10879800	-0.57987600	-1.13480300
C	-0.69466300	2.61421600	1.30448000
H	-0.25086300	3.30245500	2.02137800
H	-1.23411000	3.17247000	0.54137400
N	0.28177900	-0.03019300	-1.00973000
S	0.48239900	1.63902200	-0.87928500
O	1.79952700	1.98232900	-1.33762600
O	-0.66782400	2.23792200	-1.50838800
O	0.44901200	1.95260200	0.68709400
N	-3.66621400	-1.33358200	-0.10099700
C	-3.55355100	-2.78325900	-0.30686600
H	-4.54245100	-3.23731300	-0.37842300
H	-3.04290300	-2.92257600	-1.25771900
C	-1.75444200	-0.31865300	-2.49261100
H	-1.07307800	-0.63466300	-3.28369100
H	-2.66769900	-0.91158400	-2.55859400
H	-2.00933600	0.72899000	-2.62644500
H	-0.94522900	-1.65370900	-1.04582700
C	1.24396300	-0.92223400	-0.46845700
O	2.24748000	-0.27678000	0.07994600
O	1.09554900	-2.11580700	-0.53275000
C	3.41829800	-0.98750900	0.63123200
C	4.08349500	-1.81330400	-0.46096100
H	5.03113600	-2.19643600	-0.07666600
H	3.46452800	-2.65657800	-0.76269800
H	4.29496800	-1.18832100	-1.33137800
C	4.31567600	0.16105000	1.06674200
H	5.22741600	-0.23883600	1.51337700
H	4.58594600	0.77854100	0.20829000
H	3.80580200	0.78261200	1.80508300
C	2.98346300	-1.82621400	1.82473400
H	2.44954900	-1.20480200	2.54686900
H	2.34588100	-2.65442100	1.51947200
H	3.87388400	-2.23029800	2.31078400
H	-2.98014500	-3.25746800	0.49266200

HF: -1462.2928217
Sum of electronic and zero-point Energies: -1461.957608
Sum of electronic and thermal Energies: -1461.934188
Sum of electronic and thermal Enthalpies: -1461.933243
Sum of electronic and thermal Free Energies: -1462.011031
Frequencies: -441.0202



+methyl azide (*anti*-TSs)

X = CH_2, Y = CH_2

C	0.00455800	0.61937000	-0.17234200
C	0.40329300	-0.54111900	-0.04610600
N	2.57522000	0.82866200	-0.44018700
N	1.89521500	1.74784100	-0.55950500
C	0.21690400	-1.99173400	0.14549400
H	0.96945000	-2.55806600	-0.40828700
H	0.35817900	-2.23155300	1.20566900
C	-1.06659000	1.63939200	-0.22170400
C	-1.18861600	-2.42444400	-0.29824600
H	-1.30235500	-3.48124200	-0.03950300
H	-1.25164800	-2.36066700	-1.38960400
C	-0.74864800	2.89221500	0.59847300
H	0.13034300	3.40783300	0.21388800
H	-1.59788200	3.57910500	0.57042100
H	-0.56123300	2.62248200	1.64132700
H	-1.19083000	1.93642400	-1.27076500
N	2.54983900	-0.41508900	-0.33377900
C	3.44878000	-1.03527800	0.64410400
H	3.14491900	-2.07778200	0.71687100
H	4.48366200	-0.99916400	0.30021700
C	-2.38866300	1.00973700	0.25715500
H	-3.17814800	1.74755300	0.08029600
H	-2.32928900	0.87365000	1.34366700
C	-2.34359600	-1.62242600	0.32386300
H	-3.21189200	-2.28533700	0.35899600
H	-2.10007200	-1.39410900	1.36816900
C	-2.77349300	-0.32374500	-0.40644500
H	-2.39151000	-0.37765300	-1.43365800
H	-3.86259000	-0.34087300	-0.49426600
H	3.36540700	-0.56231700	1.62537900

HF: -555.283997
Sum of electronic and zero-point Energies: -555.022942
Sum of electronic and thermal Energies: -555.009054
Sum of electronic and thermal Enthalpies: -555.008110
Sum of electronic and thermal Free Energies: -555.063793

Frequencies: -462.8835

X = NH, Y = CH_2

C	0.00271600	0.60592700	-0.16141200
C	0.41422600	-0.54913600	-0.03256700
N	2.56292600	0.84538700	-0.45380500
N	1.88358400	1.76321800	-0.57538800
C	0.22011400	-1.99722200	0.16138000
H	0.96752000	-2.57185900	-0.39050800
H	0.35350800	-2.23829300	1.22205200
C	-1.10266100	1.59859100	-0.21532000
C	-1.19078600	-2.40412000	-0.29073900
H	-1.33184000	-3.45745400	-0.03207500
H	-1.24410800	-2.34053000	-1.38263600
N	-2.38674700	1.01372900	0.18918200
C	-0.83346900	2.82981500	0.64559500
H	0.07397500	3.33703900	0.32221500
H	-1.67596600	3.51950100	0.57469800
H	-0.70862300	2.53538100	1.69152000
H	-1.20623100	1.91964400	-1.25864900
N	2.55474200	-0.39694100	-0.34091000
C	3.45869900	-0.99988800	0.64381800
H	3.16552000	-2.04485100	0.72389200
H	4.49334900	-0.95480000	0.30081300
H	-2.39539900	0.92175600	1.20155100
C	-2.33187800	-1.57341400	0.32050100
H	-3.21567700	-2.21544300	0.35978800
H	-2.09119600	-1.33213400	1.36284600
C	-2.74790700	-0.27290900	-0.42045200
H	-2.35150700	-0.28081400	-1.44051400
H	-3.83706300	-0.28102200	-0.51411600
H	3.36788900	-0.51974000	1.62073900

HF: -571.3210885
Sum of electronic and zero-point Energies: -571.071219
Sum of electronic and thermal Energies: -571.057417
Sum of electronic and thermal Enthalpies: -571.056473
Sum of electronic and thermal Free Energies: -571.111907
Frequencies: -453.2022

X = NH_2^+, Y = CH_2

C	0.04218900	0.61263200	-0.19922200
C	0.44257500	-0.54499800	-0.05474700
N	2.57187400	0.83701400	-0.44097800
N	1.92515200	1.77325400	-0.57477200
C	0.25054800	-1.99219000	0.15485700
H	1.00450200	-2.56337600	-0.38983800
H	0.38399700	-2.21650300	1.21855500
C	-1.02684700	1.61238600	-0.23255800
C	-1.14896300	-2.42542100	-0.30272500
H	-1.27335500	-3.47640600	-0.03306900
H	-1.20205400	-2.37321200	-1.39424200
N	-2.29915800	0.94039300	0.27093300
C	-0.77603100	2.85262900	0.61451800
H	0.07962800	3.38688600	0.20691400
H	-1.64190400	3.51656500	0.59548300
H	-0.55120800	2.57617900	1.64652300
H	-1.24861100	1.89671400	-1.26422900
N	2.53665100	-0.40259500	-0.32569400
C	3.42478800	-1.03097900	0.66040400
H	3.12777200	-2.07583900	0.71637500
H	4.46094100	-0.98137900	0.32516900
H	-2.18274400	0.75247300	1.27146600
C	-2.31588500	-1.62952000	0.29851500
H	-3.19860800	-2.27048200	0.27904100
H	-2.12728500	-1.42491700	1.35845800
H	-3.06029200	1.62075900	0.20303500
C	-2.71549000	-0.33485600	-0.42995700
H	-2.29863300	-0.28394600	-1.43574700
H	-3.79867000	-0.27229400	-0.50766100
H	3.32357800	-0.56578900	1.64283700

HF: -571.775591
Sum of electronic and zero-point Energies: -571.509891
Sum of electronic and thermal Energies: -571.496168
Sum of electronic and thermal Enthalpies: -571.495224
Sum of electronic and thermal Free Energies: -571.550275
Frequencies: -440.1775

X = O, Y = CH_2

C	0.00426300	0.60281400	-0.18166700
C	0.41342000	-0.55195200	-0.05385400
N	2.55737000	0.85265900	-0.43969700
N	1.89410600	1.78037100	-0.55897100
C	0.21282800	-1.99783300	0.14636300
H	0.94746700	-2.57904900	-0.41550900
H	0.35912600	-2.23658900	1.20561000
C	-1.11155500	1.57235600	-0.20647700
C	-1.20809700	-2.39191500	-0.28768000
H	-1.35819600	-3.44125800	-0.01950800
H	-1.27095500	-2.33655600	-1.37957300
C	-0.87413500	2.79999800	0.65687400
H	-0.01338300	3.35829100	0.29082600
H	-1.75614500	3.44142700	0.63047600
H	-0.68520000	2.49682000	1.68864300
H	-1.27613900	1.88358100	-1.24806500
N	2.54990100	-0.38973800	-0.34356200
C	3.43923100	-1.00463800	0.64807800
H	3.14829400	-2.05150400	0.70782100
H	4.47876600	-0.95041900	0.32219300
C	-2.33836400	-1.54850300	0.32495100
H	-3.23777100	-2.16971900	0.33806000
H	-2.11357900	-1.31427300	1.37085100
C	-2.70885500	-0.23328200	-0.39445100
H	-2.32113200	-0.23021400	-1.42011500
H	-3.79664300	-0.16098900	-0.45463500
O	-2.30205000	0.95540400	0.27952400
H	3.32983200	-0.53809200	1.62952200

HF: -591.1913715
Sum of electronic and zero-point Energies: -590.953996
Sum of electronic and thermal Energies: -590.940438
Sum of electronic and thermal Enthalpies: -590.939494
Sum of electronic and thermal Free Energies: -590.994349
Frequencies: -440.9608

X = CH_2, Y = O

C	-0.01983600	0.60204500	-0.16852700
C	0.42124400	-0.54084800	-0.03651800
N	2.54960900	0.87414500	-0.45479300
N	1.86225100	1.78564500	-0.57444200
C	0.22739100	-1.98637500	0.17006400
H	0.93937100	-2.58280400	-0.40653300
H	0.37376700	-2.23358700	1.22614100
C	-1.12950000	1.57984400	-0.21777800
C	-1.19825800	-2.35783200	-0.25943600
H	-1.40282400	-3.39460500	0.01959100
H	-1.28248700	-2.27379500	-1.34791900
O	-2.17325700	-1.54822500	0.37014900
C	-0.86305000	2.83893300	0.61029200
H	0.00455700	3.38139000	0.23621700
H	-1.73239000	3.49977400	0.57471200
H	-0.67901900	2.57105800	1.65408700
H	-1.25998600	1.87811800	-1.26541500
N	2.56017900	-0.36845800	-0.34698700
C	3.46084300	-0.95837700	0.64918100
H	3.18039400	-2.00707900	0.72708000
H	4.49851600	-0.89982400	0.31786400
C	-2.43016800	0.89738500	0.25122000
H	-3.26322000	1.57454200	0.03598500
H	-2.39635200	0.76808600	1.33834100
C	-2.72994600	-0.46454800	-0.37516300
H	-2.37108200	-0.49762800	-1.40983300
H	-3.81232400	-0.62020500	-0.39228800
H	3.35254600	-0.47833200	1.62432700

HF: -591.1910657
Sum of electronic and zero-point Energies: -590.953702
Sum of electronic and thermal Energies: -590.940150
Sum of electronic and thermal Enthalpies: -590.939206
Sum of electronic and thermal Free Energies: -590.994042
Frequencies: -452.0594

X = CH_2, Y = NH

C	-0.00450700	0.60873200	-0.16142000
C	0.41729900	-0.54070400	-0.02088000
N	2.56370700	0.84777900	-0.46624500
N	1.88036500	1.76264400	-0.58970500
C	0.21473700	-1.98391000	0.18700600
H	0.95268700	-2.57988000	-0.35661900
H	0.33372800	-2.22153800	1.25007800
C	-1.09708800	1.60366500	-0.21212800
C	-1.20018800	-2.38483100	-0.28022900
H	-1.34037400	-3.44325100	-0.03714800
H	-1.24758400	-2.30063800	-1.36899600
C	-0.80893200	2.85760200	0.61712800
H	0.06969400	3.38384700	0.24559700
H	-1.66547100	3.53479400	0.57962400
H	-0.63229100	2.58607000	1.66132400
H	-1.22370000	1.90512100	-1.25945100
N	2.55971900	-0.39401300	-0.34475700
C	3.46528400	-0.98462900	0.64602000
H	3.17043300	-2.02800300	0.74140200
H	4.49924800	-0.94583600	0.30028200
C	-2.40718800	0.94177100	0.25655800
H	-3.21914600	1.65396700	0.07544800
H	-2.35743000	0.79988800	1.34329900
N	-2.30983700	-1.62098000	0.27126900
H	-2.19533100	-1.46904400	1.26691900
C	-2.76777300	-0.39951200	-0.40575300
H	-2.39030400	-0.41585400	-1.43313900
H	-3.85959900	-0.44569700	-0.47704300
H	3.37787900	-0.49105600	1.61666800

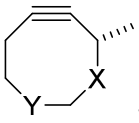
HF: -571.3206962
Sum of electronic and zero-point Energies: -571.071204
Sum of electronic and thermal Energies: -571.057298
Sum of electronic and thermal Enthalpies: -571.056354
Sum of electronic and thermal Free Energies: -571.112077
Frequencies: -457.0268

X = CH_2, Y = NH_2^+

C	0.00126100	0.61935400	-0.15479500
C	0.44906500	-0.52682300	-0.05302700
N	2.54100500	0.89273700	-0.44405600
N	1.83603900	1.79410300	-0.54450100
C	0.29716100	-1.98300200	0.13223200
H	0.99792500	-2.54350600	-0.48917200
H	0.50870800	-2.24941400	1.17275700
C	-1.07813700	1.63081900	-0.22113500
C	-1.11252400	-2.43392300	-0.24400600
H	-1.30038900	-3.44281900	0.11827400

H	-1.26829600	-2.40897300	-1.32035800
C	-0.82638200	2.84514700	0.67567500
H	0.06943200	3.38211200	0.36848500
H	-1.67861100	3.52628200	0.62364900
H	-0.70310100	2.52720800	1.71388500
H	-1.13640500	1.97236400	-1.26098500
N	2.54787900	-0.35152200	-0.34921600
C	3.47075800	-0.96294100	0.61442600
H	3.20562300	-2.01708200	0.66422900
H	4.49992400	-0.88146300	0.26340400
C	-2.42961300	0.98509900	0.14437200
H	-3.23053000	1.65444300	-0.17761600
H	-2.51828600	0.91167500	1.23444300
N	-2.16056700	-1.53283300	0.36851200
H	-2.95887200	-2.11023200	0.63613800
H	-1.79282800	-1.15632100	1.24741200
C	-2.68243900	-0.38075700	-0.48530300
H	-2.20608000	-0.46654900	-1.46074900
H	-3.74806900	-0.56092800	-0.60383100
H	3.37446700	-0.51202900	1.60423800

HF: -571.7747783
Sum of electronic and zero-point Energies: -571.508657
Sum of electronic and thermal Energies: -571.494993
Sum of electronic and thermal Enthalpies: -571.494049
Sum of electronic and thermal Free Energies: -571.548881
Frequencies: -463.2412



+methyl azide (*syn*-TSs)

X = CH_2, Y = CH_2

C	-0.28622400	0.09818900	-0.07235100
C	0.08536200	-1.07421200	-0.00080400
N	-2.48792900	-1.28721700	0.13274900
N	-1.80305500	-2.21188800	0.13757800
C	1.12502400	-2.11813900	0.00225200
H	0.86381100	-2.93040000	0.68505500
H	1.17755000	-2.55922100	-0.99940400
C	-0.08903600	1.55530200	-0.18922600
C	2.49088700	-1.52358400	0.37670900
H	3.23972500	-2.31229300	0.25805800
H	2.48405500	-1.25518800	1.43838400
N	-2.46621200	-0.04307900	0.20917100
C	-3.40711400	0.72490000	-0.60788300
H	-4.43583500	0.55275200	-0.28708600
H	-3.16717200	1.77435000	-0.44599000
C	-0.38154800	2.26799700	1.13578900
H	0.29436700	1.92303200	1.92150500
H	-0.25368500	3.34639500	1.01720300
H	-1.40450500	2.06818600	1.46009700
H	-0.77796400	1.95254400	-0.94254500
C	1.34732700	1.81670900	-0.69328000
H	1.40351100	1.53670700	-1.75005100
H	1.51115200	2.89832100	-0.64842000
C	2.47159200	1.09558100	0.07494400
H	2.20233700	1.01258800	1.13346300
H	3.34807200	1.74761700	0.04642500
C	2.90584500	-0.29642900	-0.45519700
H	3.99710500	-0.30076000	-0.51487200
H	2.54997600	-0.42533300	-1.48411600
H	-3.30481400	0.48810900	-1.66990800

HF: -555.2850031
Sum of electronic and zero-point Energies: -555.024229
Sum of electronic and thermal Energies: -555.011078
Sum of electronic and thermal Enthalpies: -555.010134
Sum of electronic and thermal Free Energies: -555.063620
Frequencies: -455.0757

X = NH, Y = CH_2

C	0.27910900	-0.08524400	-0.04513000
C	-0.08907000	1.08790600	0.02626400
N	2.48629400	1.27196900	0.14722100
N	1.81715600	2.20662200	0.16679700
C	-1.13612800	2.12265500	0.01787600
H	-0.90250900	2.92809500	0.71833200
H	-1.17176800	2.57580100	-0.97896000
C	0.04691200	-1.54439900	-0.17802900
C	-2.49863100	1.49740600	0.35378600
H	-3.26439500	2.26710500	0.22100400
H	-2.51174400	1.22295300	1.41392300
N	2.45898500	0.02744800	0.21266400
C	3.36189000	-0.73288100	-0.65544000
H	4.40433900	-0.55022500	-0.39073000
H	3.14098700	-1.78451800	-0.48255500
C	0.35456300	-2.27870400	1.12822300
H	-0.30047200	-1.93547900	1.93156700
H	0.20876000	-3.35089800	0.98928100
H	1.38560800	-2.09010600	1.43177600
H	0.71042500	-1.94296100	-0.95149100
H	-1.37714800	-1.63410900	-1.63274700
C	-2.41811300	-1.12542000	0.04799900
H	-2.15919300	-1.04267900	1.10704700
H	-3.28468800	-1.78969400	-0.00030200
C	-2.85870800	0.26323400	-0.49347000
H	-2.47097600	0.39281900	-1.51090200
H	-3.94716900	0.23759000	-0.58971100
N	-1.32102900	-1.82559400	-0.63791900
H	3.19915200	-0.49412600	-1.70934400

HF: -571.3212893
Sum of electronic and zero-point Energies: -571.071338
Sum of electronic and thermal Energies: -571.057556
Sum of electronic and thermal Enthalpies: -571.056612
Sum of electronic and thermal Free Energies: -571.111697

X = NH_2^+, Y = CH_2

C	0.33872300	-0.07336700	-0.07519800
C	-0.07448600	1.08598600	-0.03126200
N	2.47007200	1.28520300	0.20340800
N	1.78694400	2.20796700	0.21072000
C	-1.11696900	2.12442700	-0.06816800
H	-0.85214700	2.96392900	0.57717100
H	-1.17098800	2.51681400	-1.08895400
C	0.13184700	-1.52017800	-0.18887700
C	-2.47832500	1.54743300	0.34459400
H	-3.23306200	2.31919700	0.17831800
H	-2.47302600	1.34135700	1.41894600
N	2.46004000	0.03923600	0.23855500
C	3.37316400	-0.68306400	-0.65642500
H	4.41004500	-0.48717600	-0.38261200
H	3.17413500	-1.74323100	-0.51276400
C	0.39017600	-2.29027500	1.09921700
H	-0.20327900	-1.90203600	1.92705400
H	0.18038200	-3.35202700	0.96278500
H	1.44216900	-2.17332900	1.35829900
H	0.73515300	-1.94289600	-0.99565600
H	-1.37482000	-1.39708700	-1.62003200
H	-1.48365100	-2.73154000	-0.68865700
C	-2.39591400	-1.05700900	0.16363900
H	-2.00803400	-0.94075700	1.17402300
H	-3.20672900	-1.78118800	0.19436400
C	-2.90094900	0.27885100	-0.41108600
H	-2.62962900	0.36396500	-1.46936700
H	-3.99032000	0.22479500	-0.39165600
N	-1.30608800	-1.72430700	-0.65253900
H	3.20342400	-0.41230900	-1.70088100

HF: -571.7740241
Sum of electronic and zero-point Energies: -571.508550
Sum of electronic and thermal Energies: -571.494726
Sum of electronic and thermal Enthalpies: -571.493782
Sum of electronic and thermal Free Energies: -571.548976
Frequencies: -450.8004

X = O, Y = CH_2

C	0.27935800	-0.07451600	-0.05825100
C	-0.11307800	1.08972800	0.01062500
N	2.45515600	1.28714900	0.19913000
N	1.78475200	2.21906500	0.22536400
C	-1.17366400	2.11010300	-0.02613600
H	-0.95735000	2.93286300	0.65901600
H	-1.20448800	2.53954300	-1.03330500
C	0.05355800	-1.52534600	-0.22191000
C	-2.53212500	1.47415300	0.31105600
H	-3.30816200	2.22260200	0.12879200
H	-2.56247800	1.24875900	1.38226700
N	2.44205300	0.04142200	0.23397800
C	3.34057200	-0.68107600	-0.67283100
H	4.38371100	-0.50340900	-0.40852300
H	3.12546200	-1.73951500	-0.53957700
C	0.39001900	-2.32448800	1.03525000
H	-0.19751500	-1.98418300	1.88968800
H	0.18474500	-3.38133800	0.85875800
H	1.44554600	-2.20131900	1.28233100
H	0.66534800	-1.89800600	-1.04840300
C	-2.32640900	-1.13249600	0.10355800
H	-2.00584600	-0.98856000	1.14016800
H	-3.13436200	-1.86627200	0.11187900
C	-2.85706700	0.19604700	-0.48133700
H	-2.49579000	0.28680800	-1.51089100
H	-3.94500700	0.11217900	-0.54417700
O	-1.28767100	-1.75075200	-0.65788800
H	3.16683900	-0.40025200	-1.71436500

HF: -591.1900279
Sum of electronic and zero-point Energies: -590.952916
Sum of electronic and thermal Energies: -590.939264
Sum of electronic and thermal Enthalpies: -590.938320
Sum of electronic and thermal Free Energies: -590.993295
Frequencies: -443.2803

X = CH_2, Y = O

C	-0.26867400	0.09036400	-0.08961400
C	0.07167600	-1.09069300	-0.01939400
N	-2.50198900	-1.24009200	0.16123000
N	-1.85600600	-2.19040400	0.16580600
C	1.12742100	-2.11549000	-0.03744700
H	0.92355000	-2.93164900	0.66074100
H	1.18972900	-2.55530800	-1.03736000
C	-0.02319500	1.54072400	-0.21095600
C	2.46494800	-1.45660000	0.32573600
H	3.27685600	-2.17263200	0.17464900
H	2.45424800	-1.16966900	1.38246900
N	-2.45237400	0.00262600	0.22329200
C	-3.38262600	0.78136700	-0.59683200
H	-4.40493600	0.68175400	-0.22864500

H	-3.08010500	1.82211300	-0.49502800
C	-0.30568300	2.27023800	1.10729000
H	0.35236000	1.90955200	1.90147800
H	-0.14342400	3.34318700	0.98396300
H	-1.33653900	2.10341300	1.42410000
H	-0.68676300	1.95689600	-0.97616600
C	1.43016500	1.75227200	-0.69273900
H	1.51042200	1.48191100	-1.74928100
H	1.65781100	2.82054300	-0.61716200
C	2.50361500	0.96845900	0.06726200
H	2.24669600	0.87975400	1.12813000
H	3.45023900	1.51217100	0.00107700
O	2.73649400	-0.32756600	-0.48455600
H	-3.33539700	0.48972900	-1.64864700

HF: -591.1919896
Sum of electronic and zero-point Energies: -590.954597
Sum of electronic and thermal Energies: -590.941095
Sum of electronic and thermal Enthalpies: -590.940151
Sum of electronic and thermal Free Energies: -590.994476
Frequencies: -442.3930

X = CH_2, Y = NH

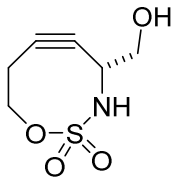
C	-0.27780900	0.09093400	-0.08802800
C	0.06580800	-1.08958200	-0.02187400
N	-2.50951200	-1.24663900	0.15072300
N	-1.85520300	-2.19205300	0.14964500
C	1.11416400	-2.12055100	-0.02970700
H	0.88214300	-2.94415800	0.65105400
H	1.18410000	-2.55394700	-1.03339900
C	-0.03974600	1.54138700	-0.20520900
C	2.46849600	-1.49320900	0.36023600
H	3.23505100	-2.26909800	0.26101300
H	2.43714600	-1.21116000	1.41590200
N	-2.46200500	-0.00372500	0.22047600
C	-3.39937200	0.77828100	-0.58779200
H	-4.41937000	0.67269800	-0.21506500
H	-3.09964800	1.81928600	-0.47975500
C	-0.31549500	2.26557900	1.11710300
H	0.34610300	1.90158600	1.90656800
H	-0.15415500	3.33916100	0.99726000
H	-1.34508700	2.09767700	1.43775200
H	-0.71210800	1.95746700	-0.96321000
C	1.40614300	1.76173900	-0.70163700
H	1.46882700	1.47378300	-1.75656200
H	1.60707300	2.83746700	-0.66184400
N	2.87690200	-0.32017200	-0.40139800
H	2.67027100	-0.43128400	-1.38756200
C	2.51700600	1.02388800	0.07083300
H	2.25701000	0.95219900	1.13122100
H	3.41381300	1.65027600	0.01931100
H	-3.35760900	0.49537600	-1.64235700

HF: -571.3216952
Sum of electronic and zero-point Energies: -571.072113
Sum of electronic and thermal Energies: -571.058224
Sum of electronic and thermal Enthalpies: -571.057280
Sum of electronic and thermal Free Energies: -571.112548
Frequencies: -447.8901

X = CH_2, Y = NH_2^+

C	-0.31178600	0.10167500	-0.05406700
C	0.07366500	-1.06596700	0.04504400
N	-2.46854300	-1.29940000	0.13243000
N	-1.78500100	-2.22275200	0.17139800
C	1.11447800	-2.10710600	0.07055900
H	0.92021800	-2.85312300	0.84339600
H	1.11862200	-2.64109400	-0.88417700
C	-0.12590500	1.56415400	-0.16249200
C	2.48863800	-1.49559900	0.33793200
H	3.28102100	-2.20569900	0.10924200
H	2.59010700	-1.17181100	1.37170000
N	-2.45070500	-0.05507500	0.18006500
C	-3.37038100	0.69963100	-0.67541300
H	-4.40626900	0.49162000	-0.40536100
H	-3.17047300	1.75303500	-0.48908100
C	-0.43675800	2.25735100	1.16925500
H	0.23986300	1.91619300	1.95657400
H	-0.32972000	3.33848200	1.06227800
H	-1.45651100	2.03175900	1.48435200
H	-0.80422400	1.96150400	-0.92288600
C	1.31153500	1.85323600	-0.64442400
H	1.39411500	1.65705200	-1.71756800
H	1.51041100	2.91952200	-0.51437300
N	2.71605900	-0.27168400	-0.52344500
H	2.17549300	-0.37469200	-1.38795700
H	3.69426600	-0.26590200	-0.81542200
C	2.40475200	1.08698100	0.09748700
H	2.13886000	0.90216000	1.13687400
H	3.33955400	1.64173200	0.07816900
H	-3.20742800	0.47550800	-1.73218200

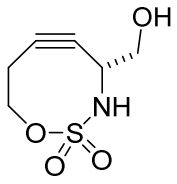
HF: -571.7760822
Sum of electronic and zero-point Energies: -571.510050
Sum of electronic and thermal Energies: -571.496380
Sum of electronic and thermal Enthalpies: -571.495436
Sum of electronic and thermal Free Energies: -571.550177
Frequencies: -457.5580



+methyl azide (*anti*-TSs)

C	-0.67697000	0.38840600	0.46144400
C	-0.99238900	-0.78057100	0.23074200
C	-3.87229200	-1.57442500	-0.71502300
N	-3.26337900	0.40234000	0.37239700
N	-2.72418900	1.39661800	0.56364700
C	-0.66174000	-2.18351000	-0.06887800
H	-1.21676700	-2.87264900	0.57269900
H	-0.91624700	-2.41970400	-1.10591400
C	0.36037600	1.43611800	0.60650200
C	0.82834300	-2.39232500	0.16524600
H	1.14859300	-3.38124100	-0.15850100
H	1.08805700	-2.24483500	1.21307600
N	1.53751300	1.14746300	-0.24091000
S	2.39982400	-0.22470400	-0.02258500
O	3.56273900	-0.11854700	-0.86802700
O	2.52275800	-0.43135300	1.40242700
O	1.58064600	-1.45720200	-0.65036600
C	-0.11677100	2.83326900	0.21215500
H	-0.90391500	3.14637600	0.90031600
H	0.72015800	3.52777800	0.28304000
H	0.70403000	1.46702500	1.64336800
H	1.37080500	1.34148800	-1.22732900
O	-0.55899200	2.85615100	-1.13114100
H	-1.39319600	2.37345100	-1.17410500
N	-3.10804700	-0.82640700	0.28989400
H	-3.73285700	-1.15608700	-1.71367600
H	-3.49650200	-2.59462000	-0.68707700
H	-4.93116700	-1.58597200	-0.45600400

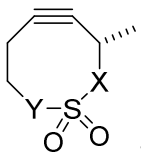
HF: -1191.7371488
Sum of electronic and zero-point Energies: -1191.522659
Sum of electronic and thermal Energies: -1191.506869
Sum of electronic and thermal Enthalpies: -1191.505925
Sum of electronic and thermal Free Energies: -1191.566011
Frequencies: -433.9149



+methyl azide (*syn*-TSs)

C	0.79565800	0.09273800	-0.02886000
C	0.65442000	1.25561600	-0.41069800
C	3.45025500	-0.60186800	1.56004500
N	3.16919200	1.07423600	-0.01348100
N	2.69289900	2.03059900	-0.43138300
C	-0.19237000	2.40105800	-0.77871100
H	0.24478200	3.34767400	-0.45258700
H	-0.30499600	2.44890900	-1.86482900
C	0.26856900	-1.25766800	0.27065800
C	-1.55488400	2.24005900	-0.11768700
H	-2.24363900	3.02437100	-0.42772500
H	-1.46753800	2.23231800	0.96847100
N	-1.14653000	-1.38038000	-0.13692400
S	-2.27085100	-0.30444300	0.37451200
O	-3.55658600	-0.86478700	0.03979000
O	-1.94075300	0.05438100	1.73428600
O	-2.17458000	1.00337500	-0.55432700
C	1.01039300	-2.36223700	-0.49017700
H	2.04566300	-2.40642500	-0.15021100
H	0.52534800	-3.31710400	-0.28813900
H	0.32848700	-1.46180900	1.34264000
H	-1.24876600	-1.58365700	-1.13070200
O	0.93410600	-2.15046100	-1.88540900
H	1.44576500	-1.36022800	-2.09733600
N	2.94303600	-0.12072700	0.26487400
H	3.14628100	0.05714700	2.37562200
H	3.02550500	-1.59137300	1.71459600
H	4.53679100	-0.69107500	1.53425600

HF: -1191.7359903
Sum of electronic and zero-point Energies: -1191.521560
Sum of electronic and thermal Energies: -1191.505748
Sum of electronic and thermal Enthalpies: -1191.504804
Sum of electronic and thermal Free Energies: -1191.564819
Frequencies: -444.9963



+diazoacetamide (*anti*-TSs)

X = CH_2, Y = CH_2

C	0.17657700	0.92591600	0.23006900
C	-0.43561200	-0.13880900	0.39278200
C	-3.29625900	0.06260500	-0.05252400
N	-2.11407800	1.69615600	1.20525200
N	-1.28224200	2.44554100	0.98694500
O	-3.42642200	0.81807500	-1.00800800
N	-3.84699100	-1.16411300	0.00282200
H	-3.75339600	-1.71622900	0.84094400
C	-4.60220400	-1.69770500	-1.11826800
H	-3.98382700	-1.71669800	-2.01714900
H	-4.91200600	-2.71095000	-0.87441600
H	-5.48571800	-1.08780000	-1.31455900
C	-2.42584400	0.40033100	1.11170300
H	-2.55374900	-0.10314800	2.06424000
C	-0.50021200	-1.62071300	0.36429400
H	-1.19920500	-1.99936700	1.11283300
H	-0.88507900	-1.94541700	-0.60890100
C	1.33526500	1.76487700	-0.14591300
C	0.86541700	-2.25843100	0.62847400
H	0.73955800	-3.34352700	0.63008000
H	1.22133900	-1.97662600	1.62237000
S	3.00932000	-0.51127600	-0.05487900
O	4.28909300	-0.82056100	-0.71046000
O	3.02963500	-0.25497100	1.38976300
C	0.95472700	2.96690500	-1.02239000
H	0.29186600	3.63997000	-0.48265900
H	1.85046500	3.51957300	-1.31216100
H	0.44610000	2.62882600	-1.92828200
H	1.79866700	2.13332500	0.77490600
C	1.94067200	-1.93610600	-0.40236700
H	2.68529500	-2.73345100	-0.44567900
H	1.54691500	-1.78874700	-1.41062000
C	2.37654100	0.94459000	-0.91025600
H	3.28287300	1.52705500	-1.09313600
H	1.99110600	0.58946400	-1.86885500

HF: -1217.2333656
Sum of electronic and zero-point Energies: -1216.951436
Sum of electronic and thermal Energies: -1216.932265
Sum of electronic and thermal Enthalpies: -1216.931321
Sum of electronic and thermal Free Energies: -1217.000314
Frequencies: -505.7019

X = NH, Y = CH_2

C	-0.18075600	0.91920100	-0.27309100
C	0.45120500	-0.12646400	-0.47014000
C	3.28875800	0.08009100	0.09220600
N	2.13420600	1.76941300	-1.11397600
N	1.29796100	2.50948200	-0.89089600
O	3.37838500	0.78599000	1.08918900
N	3.84928700	-1.13917500	-0.00623100
H	3.77281600	-1.65759200	-0.86755600
C	4.55866100	-1.72871900	1.11693900
H	3.89965500	-1.80816400	1.98325200
H	4.89576400	-2.72132600	0.82907200
H	5.42224300	-1.11969400	1.38883200
C	2.46017000	0.47469100	-1.08504000
H	2.63130000	0.03085800	-2.05985900
C	0.52427500	-1.60593500	-0.51128500
H	1.17384000	-1.94339300	-1.32237100
H	0.97194400	-1.97181100	0.41946500
C	-1.37908600	1.70627000	0.08964600
C	-0.85957700	-2.22949900	-0.71104600
H	-0.74539700	-3.31551800	-0.73675900
H	-1.26518700	-1.92777900	-1.67939700
N	-2.41509600	0.89095100	0.76344500
S	-2.98924600	-0.50625700	0.09146100
O	-4.19336400	-0.82318400	0.85327800
O	-3.09628000	-0.25999600	-1.34136600
C	-1.08676500	2.87984100	1.02397000
H	-0.41684700	3.58650300	0.53953100
H	-2.01701200	3.38836600	1.27917000
H	-0.61088500	2.52305400	1.94079400
H	-1.83016900	2.08596700	-0.83039200
H	-2.27158600	0.78507100	1.76478400
C	-1.87068100	-1.90748700	0.38640700
H	-2.58666000	-2.72200000	0.50312700
H	-1.40755200	-1.72155500	1.35833200

HF: -1233.2746942
Sum of electronic and zero-point Energies: -1233.003759
Sum of electronic and thermal Energies: -1232.984919
Sum of electronic and thermal Enthalpies: -1232.983975
Sum of electronic and thermal Free Energies: -1233.051419
Frequencies: -487.9046

X = NH_2^+, Y = CH_2

C	0.18238000	0.90193500	0.22779400
C	-0.44622200	-0.15519500	0.37803300
C	-3.28312300	0.07621300	-0.04600100
N	-2.07305800	1.67861600	1.22144400
N	-1.26848300	2.45216400	1.01315100
O	-3.38205100	0.83779000	-0.99787900
N	-3.88216600	-1.12486500	0.01706100
H	-3.83915100	-1.66217000	0.86924400
C	-4.69324500	-1.61239800	-1.08714100
H	-4.11068100	-1.60632400	-2.00895400
H	-5.00332700	-2.63019700	-0.86402500
H	-5.57663700	-0.98631600	-1.22546500
C	-2.38492300	0.38304100	1.11458500
H	-2.51342600	-0.12490300	2.06515200
C	-0.52752200	-1.63532300	0.30275900
H	-1.22984900	-2.02832200	1.03902200
H	-0.91553300	-1.92080800	-0.68068800
C	1.31895400	1.74398500	-0.14159700
C	0.82515200	-2.30308500	0.55346200
H	0.69141600	-3.38468000	0.48679700
H	1.17044800	-2.08936600	1.56701200
N	2.34637900	0.89147000	-0.88802800
S	2.99799600	-0.58195000	0.01020300
O	4.27785600	-0.74787900	-0.62910300
O	2.88418100	-0.21629400	1.39605800
C	0.98389900	2.92238500	-1.05200400
H	0.34268000	3.61037600	-0.50540200
H	1.88924600	3.45462300	-1.34649800
H	0.45279600	2.58067800	-1.94212900
H	1.84145500	2.08325200	0.75518600
H	1.96672800	0.59549500	-1.79613200
C	1.91772200	-1.95444200	-0.44974800
H	2.66466500	-2.74965000	-0.52015400
H	1.55601000	-1.75050700	-1.46012200
H	3.18819900	1.44669200	-1.09494400

HF: -1233.684609
Sum of electronic and zero-point Energies: -1233.400483
Sum of electronic and thermal Energies: -1233.381208
Sum of electronic and thermal Enthalpies: -1233.380264
Sum of electronic and thermal Free Energies: -1233.449482
Frequencies: -480.8635

X = O, Y = CH_2

C	0.21517700	0.89061300	0.24405200
C	-0.43687000	-0.14538600	0.41804500
C	-3.28461600	0.11363000	-0.06394400
N	-2.06390400	1.77103500	1.12264000
N	-1.23370400	2.51414500	0.89930200
O	-3.36601600	0.81583900	-1.06359800
N	-3.88999500	-1.08126000	0.05784200
H	-3.84430300	-1.57839700	0.93390800
C	-4.66461700	-1.64119800	-1.03721600
H	-4.04910000	-1.71168400	-1.93517100
H	-4.99840400	-2.63531200	-0.75078400
H	-5.53316800	-1.01770700	-1.25670400
C	-2.41331200	0.48313600	1.09182400
H	-2.56208900	0.03491800	2.06829800
C	-0.53395800	-1.62360000	0.38714600
H	-1.19419900	-1.99367800	1.17426100
H	-0.97931200	-1.93309600	-0.56483000
C	1.40604100	1.65991000	-0.12602600
C	0.84078600	-2.27679300	0.56185800
H	0.71628600	-3.35945200	0.49109300
H	1.22700800	-2.06455000	1.56107400
S	2.97156100	-0.50105900	-0.04224500
O	4.24249100	-0.73836900	-0.69984700
O	2.95426100	-0.26287400	1.39033500
C	1.15842000	2.77078000	-1.13088100
H	0.50163900	3.51945100	-0.69076200
H	2.10465900	3.23970100	-1.40021000
H	0.68691100	2.36438000	-2.02658500
H	1.88789900	2.04909800	0.77383000
C	1.88168000	-1.87663100	-0.48234300
H	2.60241600	-2.68032600	-0.63697700
H	1.45076500	-1.60904300	-1.44930900
O	2.38661900	0.79021000	-0.79549000

HF: -1253.143959
Sum of electronic and zero-point Energies: -1252.885790
Sum of electronic and thermal Energies: -1252.867072
Sum of electronic and thermal Enthalpies: -1252.866128
Sum of electronic and thermal Free Energies: -1252.933657
Frequencies: -469.7710

X = CH_2, Y = O

C	-0.18730800	0.94267800	-0.27791500
C	0.42825200	-0.11409200	-0.46663000
C	3.26574200	0.03428800	0.07753300
N	2.14917200	1.72054200	-1.16523400
N	1.33347900	2.48492300	-0.94844700
O	3.37604700	0.76338400	1.05546900
N	3.78708600	-1.20457600	0.01314000
H	3.69840700	-1.74167300	-0.83528100
C	4.47832100	-1.78583000	1.15183700
H	3.81489600	-1.83193700	2.01720100
H	4.79337900	-2.79199900	0.88679200
H	5.35463600	-1.19095800	1.41397100
C	2.45044700	0.42166900	-1.11124400
H	2.61149500	-0.04768300	-2.07573600
C	0.45257600	-1.59541400	-0.46005500
H	1.08308100	-2.00131100	-1.25587700
H	0.86087100	-1.95754100	0.48834900
C	-1.35517300	1.75421000	0.13097900

C	-0.95059100	-2.14261000	-0.67083300
H	-0.96877100	-3.22797300	-0.58510800
H	-1.34581300	-1.84351800	-1.64133900
S	-2.96093200	-0.55110900	0.09106500
O	-4.13218800	-1.01550400	0.80693100
O	-3.05971100	-0.31392100	-1.33759600
O	-1.83380400	-1.66257100	0.37171300
C	-0.98366200	2.97005300	0.99133800
H	-0.36613900	3.66285000	0.42368400
H	-1.88565700	3.49287900	1.31476000
H	-0.42745700	2.65269000	1.87641700
H	-1.85995400	2.10553000	-0.77461100
C	-2.34990200	0.90675300	0.93413200
H	-3.25634600	1.47212400	1.16079700
H	-1.91483600	0.53871500	1.86572200

HF: -1253.1427901
Sum of electronic and zero-point Energies: -1252.883979
Sum of electronic and thermal Energies: -1252.865372
Sum of electronic and thermal Enthalpies: -1252.864427
Sum of electronic and thermal Free Energies: -1252.931893
Frequencies: -487.1576

X = CH_2, Y = NH

C	0.18034000	0.91927700	0.22648400
C	-0.43879800	-0.14302400	0.36788000
C	-3.31332000	0.05324100	-0.05329700
N	-2.12100200	1.67628000	1.20803900
N	-1.29756800	2.43682000	1.00197000
O	-3.45411100	0.81729600	-1.00040700
N	-3.85796300	-1.17670000	-0.00564700
H	-3.76650800	-1.73130700	0.83107300
C	-4.63273600	-1.69656200	-1.11986500
H	-4.03291100	-1.69452000	-2.03116500
H	-4.92864800	-2.71675200	-0.88774700
H	-5.52543300	-1.09113700	-1.28708400
C	-2.43671700	0.38353100	1.10748500
H	-2.55202500	-0.12862800	2.05684900
C	-0.46180400	-1.62339600	0.32301200
H	-1.17001700	-2.04501900	1.04022600
H	-0.77927100	-1.96048600	-0.66916000
C	1.34612700	1.75261700	-0.13780600
C	0.92308000	-2.18643200	0.65497600
H	0.88548800	-3.27725600	0.65727700
H	1.23030800	-1.86116600	1.64888900
S	3.00673900	-0.53852500	-0.06911200
O	4.22270000	-0.89464900	-0.79395000
O	3.08139200	-0.27799100	1.36341300
C	0.97407600	2.96386400	-1.00521900
H	0.30706900	3.63129300	-0.46319900
H	1.87200200	3.51913900	-1.28280000
H	0.47183600	2.63538300	-1.91821000
H	1.80941800	2.11196700	0.78682000
C	2.38538100	0.93148400	-0.90661700
H	3.28654000	1.51955100	-1.09384600
H	1.99102600	0.57712400	-1.86207700
N	1.97939600	-1.79787600	-0.27355300
H	1.91962900	-2.12631700	-1.23036600

HF: -1233.2763928
Sum of electronic and zero-point Energies: -1233.006119
Sum of electronic and thermal Energies: -1232.986907
Sum of electronic and thermal Enthalpies: -1232.985963
Sum of electronic and thermal Free Energies: -1233.055463
Frequencies: -491.7442

X = CH_2, Y = NH_2^+

C	0.18934000	0.91285800	0.22221200
C	-0.43399900	-0.14517600	0.39504000
C	-3.28058700	0.07065400	-0.03919400
N	-2.07440800	1.67604000	1.23087400
N	-1.24618400	2.42568600	1.00841600
O	-3.38613500	0.83320000	-0.98994500
N	-3.86086200	-1.14147900	0.01351800
H	-3.82545800	-1.67608900	0.86780300
C	-4.65957400	-1.63418500	-1.09722500
H	-4.07597900	-1.60291300	-2.01780400
H	-4.94566100	-2.66186800	-0.88745200
H	-5.55762200	-1.02790400	-1.23017000
C	-2.39246400	0.38188400	1.12548000
H	-2.52575300	-0.12670000	2.07513800
C	-0.50595000	-1.62680800	0.34809000
H	-1.14525500	-2.02631300	1.13739300
H	-0.94827200	-1.95093600	-0.59992300
C	1.32540200	1.78044200	-0.15507600
C	0.85808200	-2.27102600	0.53958100
H	0.79637100	-3.35287500	0.43563700
H	1.28697500	-2.02778100	1.51115700
S	3.02542800	-0.43626700	-0.01009500
O	4.24720200	-0.90917000	-0.60488700
O	2.86399700	-0.31557500	1.41208000
C	0.92291700	2.94480400	-1.07327500
H	0.22972000	3.60530300	-0.55793400
H	1.80448400	3.52117400	-1.35861700
H	0.44192100	2.56602800	-1.97722400
H	1.76129000	2.18791400	0.76202500
C	2.41220900	0.99601400	-0.89652300
H	3.32557300	1.58293500	-1.03257200
H	2.08749200	0.63710100	-1.87632700
N	1.84237800	-1.80194300	-0.49934500
H	1.36145700	-1.53415000	-1.36593500
H	2.48263000	-2.56519300	-0.75054500

HF: -1233.6829926
Sum of electronic and zero-point Energies: -1233.397817
Sum of electronic and thermal Energies: -1233.379713
Sum of electronic and thermal Enthalpies: -1233.378769
Sum of electronic and thermal Free Energies: -1233.444102
Frequencies: -503.7825

X = NH, Y = NH

C	0.20276100	1.00978800	0.38569500
C	-0.45865100	-0.00979100	0.61867600
C	-3.24276800	0.04840400	-0.19780000
N	-2.21267300	1.91151500	0.85431600
N	-1.37829700	2.64721000	0.61914400
O	-3.22545200	0.59148300	-1.29548500
N	-3.82907400	-1.14053400	0.03195100
H	-3.85421800	-1.51398800	0.96801800
C	-4.44142700	-1.89199900	-1.05101500
H	-3.70817300	-2.09225300	-1.83418300
H	-4.80961400	-2.83437700	-0.65282900
H	-5.27276500	-1.33419000	-1.48528000
C	-2.52414100	0.61970500	0.97866100
H	-2.77590600	0.31225000	1.98810900
C	-0.52988100	-1.47875200	0.77632700
H	-1.14429300	-1.75812600	1.63666200
H	-1.00042900	-1.92810900	-0.10475000
C	1.47559200	1.68426600	0.02894400
C	0.87071900	-2.06080700	0.98042000
H	0.80385200	-3.14192000	1.11758800
H	1.32843100	-1.63815000	1.87480600
S	2.90639100	-0.62786700	-0.19537500
O	3.86776800	-1.07013100	-1.18987800
O	3.29958900	-0.36021100	1.17528900
C	1.31226400	2.99060600	-0.74418000
H	0.79534600	3.72521300	-0.13081000
H	2.29332900	3.37905400	-1.01821500
H	0.72532300	2.82619000	-1.65127800
H	2.02572700	1.88403200	0.95186200
N	1.78768400	-1.82286200	-0.13170500
H	1.52512800	-2.17718700	-1.04446300
N	2.34937100	0.81519100	-0.79007400
H	2.02489300	0.70613600	-1.74843200

HF: -1249.3169349
Sum of electronic and zero-point Energies: -1249.057202
Sum of electronic and thermal Energies: -1249.038584
Sum of electronic and thermal Enthalpies: -1249.037640
Sum of electronic and thermal Free Energies: -1249.104883
Frequencies: -474.9820

X = NH, Y = NH_2^+

C	0.20447500	0.91467000	0.26949400
C	-0.43930600	-0.12481300	0.46619600
C	-3.27396500	0.09145100	-0.08374400
N	-2.08876600	1.76005300	1.12330500
N	-1.25862300	2.50371900	0.90097700
O	-3.31553200	0.78124400	-1.09298600
N	-3.89801400	-1.09294400	0.03937700
H	-3.91239700	-1.56156200	0.93220800
C	-4.66847000	-1.64732900	-1.06224800
H	-4.04819700	-1.70550900	-1.95729800
H	-4.99629500	-2.64619400	-0.78557900
H	-5.53998900	-1.02687700	-1.27956000
C	-2.42048500	0.46625000	1.08934000
H	-2.59251600	0.02315800	2.06495000
C	-0.53214700	-1.60490300	0.46577000
H	-1.11487300	-1.96951100	1.31428500
H	-1.05001200	-1.94535900	-0.43695400
C	1.37566600	1.73556300	-0.08336700
C	0.83772300	-2.26103400	0.56951600
H	0.76148100	-3.33929900	0.44180800
H	1.31258700	-2.04624200	1.52501200
N	2.46115200	0.90447800	-0.69209200
S	3.00845000	-0.43371200	-0.03573200
O	4.16501500	-0.90575100	-0.73906400
O	2.90247900	-0.37738300	1.39034600
C	1.08421100	2.84120300	-1.09438400
H	0.37469600	3.54547700	-0.66662200
H	2.00389500	3.37424800	-1.33807500
H	0.65525900	2.41736800	-2.00429000
H	1.79043500	2.16961600	0.82921700
H	2.64438400	0.99624500	-1.68843500
N	1.77522200	-1.76605600	-0.50192200
H	2.36661600	-2.53519700	-0.83492500
H	1.25102500	-1.42693100	-1.31734200

HF: -1249.7268535
Sum of electronic and zero-point Energies: -1249.452960
Sum of electronic and thermal Energies: -1249.434111
Sum of electronic and thermal Enthalpies: -1249.433166
Sum of electronic and thermal Free Energies: -1249.501131
Frequencies: -478.2725

X = NH, Y = O

C	0.20404900	0.96723400	0.33797900
C	-0.43945200	-0.06679500	0.55151400
C	-3.24881200	0.04878000	-0.14003800
N	-2.17456700	1.82731600	1.00800000
N	-1.35641400	2.58356600	0.78445300
O	-3.28194200	0.68039100	-1.18850000
N	-3.81333400	-1.16255700	0.01529800

H	-3.80405700	-1.60870500	0.91937500
C	-4.46960400	-1.82704500	-1.09866800
H	-3.76697300	-1.97001400	-1.92125200
H	-4.82847500	-2.79551300	-0.75937800
H	-5.31307800	-1.23449200	-1.45659600
C	-2.48578800	0.53105800	1.04913800
H	-2.69425600	0.14711900	2.04177600
C	-0.48466300	-1.54453600	0.62042300
H	-1.08862500	-1.89555800	1.46178000
H	-0.93576600	-1.94935300	-0.29048500
C	1.43462300	1.69491800	-0.04404600
C	0.92204300	-2.09425200	0.80058500
H	0.92860900	-3.18294900	0.77231000
H	1.36178200	-1.74765900	1.73536700
N	2.38460200	0.82752900	-0.78796000
S	2.92019800	-0.57625000	-0.14446200
O	3.97096100	-1.05392300	-1.00981100
O	3.15643800	-0.34882300	1.26290200
O	1.76211200	-1.67952200	-0.30458000
C	1.19423100	2.91853900	-0.92456900
H	0.61477400	3.65878700	-0.37764700
H	2.14885800	3.35671800	-1.21692300
H	0.63742000	2.63727900	-1.82172400
H	1.95307500	2.00383100	0.86677300
H	2.16122500	0.71713100	-1.77451200

HF: -1269.1822489
Sum of electronic and zero-point Energies: -1268.935181
Sum of electronic and thermal Energies: -1268.916708
Sum of electronic and thermal Enthalpies: -1268.915764
Sum of electronic and thermal Free Energies: -1268.983910
Frequencies: -468.9808

X = O, Y = NH

C	0.21282600	0.91480600	0.29573600
C	-0.44619800	-0.11600200	0.46859200
C	-3.27696800	0.08958400	-0.10447400
N	-2.11617200	1.79447800	1.07392300
N	-1.29771600	2.55194800	0.86229400
O	-3.33473700	0.76330300	-1.12509700
N	-3.86581300	-1.11247900	0.02876000
H	-3.84404100	-1.58465900	0.91944800
C	-4.58742200	-1.71712000	-1.07876100
H	-3.93245700	-1.81431900	-1.94588500
H	-4.92672100	-2.70319200	-0.77176900
H	-5.44977300	-1.10897700	-1.35736500
C	-2.45316000	0.50427800	1.06991200
H	-2.62431000	0.08030800	2.05319600
C	-0.50638600	-1.59408100	0.47067300
H	-1.16670100	-1.97506300	1.25353600
H	-0.90780400	-1.95030400	-0.48358400
C	1.42314900	1.65202200	-0.08096600
C	0.89180700	-2.17201700	0.71277400
H	0.85035300	-3.26201900	0.69638800
H	1.25910200	-1.86305600	1.69090300
S	2.94230000	-0.54478700	-0.10178400
O	4.08973300	-0.84652500	-0.92463200
O	3.08471700	-0.28132200	1.31349200
C	1.19590900	2.80914000	-1.03715200
H	0.60057300	3.57571900	-0.54372400
H	2.15480500	3.23564200	-1.33125400
H	0.66502400	2.46217900	-1.92480500
H	1.94512300	1.98855900	0.81821700
N	1.89430300	-1.77078900	-0.27373500
H	1.77233000	-2.07259100	-1.23366200
O	2.34830400	0.76987000	-0.80723800

HF: -1269.1852146
Sum of electronic and zero-point Energies: -1268.938592
Sum of electronic and thermal Energies: -1268.919927
Sum of electronic and thermal Enthalpies: -1268.918982
Sum of electronic and thermal Free Energies: -1268.986612
Frequencies: -459.3148

X = O, Y = O

C	0.22834200	0.92494900	0.29175600
C	-0.43269500	-0.10330200	0.46886100
C	-3.25916200	0.08320700	-0.09523000
N	-2.10301600	1.79847700	1.07256200
N	-1.29930000	2.56844200	0.85807900
O	-3.31723300	0.75034300	-1.11962900
N	-3.84375000	-1.11970900	0.04622100
H	-3.82709000	-1.58282200	0.94187200
C	-4.56478500	-1.73264800	-1.05740300
H	-3.90983600	-1.83219600	-1.92421200
H	-4.90039900	-2.71816500	-0.74474800
H	-5.42918600	-1.12860100	-1.33845500
C	-2.43482000	0.50730200	1.07651800
H	-2.60119400	0.08807400	2.06264600
C	-0.49238700	-1.58177300	0.44076700
H	-1.12634800	-1.98605300	1.23386400
H	-0.91237600	-1.91969900	-0.51117800
C	1.43418000	1.65932200	-0.09057500
C	0.90557300	-2.15012600	0.63457100
H	0.91812600	-3.23032900	0.50311900
H	1.30483900	-1.88931400	1.61374800
S	2.91661200	-0.55082500	-0.08857000
O	4.06417100	-0.94383900	-0.85589500
O	3.01524800	-0.33476800	1.33392400
C	1.21491400	2.78938000	-1.07762500
H	0.61269000	3.56412800	-0.60535300
H	2.17464000	3.21289900	-1.37274800
H	0.69178300	2.41913600	-1.96009900
H	1.95933200	2.01013400	0.80049100
O	2.37678300	0.75493300	-0.79896000
O	1.79937300	-1.63946100	-0.39315300

HF: -1289.0478714
Sum of electronic and zero-point Energies: -1288.813430
Sum of electronic and thermal Energies: -1288.795114
Sum of electronic and thermal Enthalpies: -1288.794169
Sum of electronic and thermal Free Energies: -1288.861045
Frequencies: -447.6135

X = O, Y = NH_2^+

C	0.22056200	0.89801400	0.26348900
C	-0.44906900	-0.12429200	0.46221900
C	-3.26296500	0.09490000	-0.07196500
N	-2.06977900	1.76478400	1.12022100
N	-1.27807600	2.54226600	0.90093200
O	-3.30305900	0.78286800	-1.08150700
N	-3.89740200	-1.08142100	0.06191300
H	-3.91195400	-1.54522800	0.95740300
C	-4.68638900	-1.62924000	-1.03049400
H	-4.07701300	-1.69230200	-1.93251100
H	-5.01912300	-2.62517200	-0.74962000
H	-5.55476000	-1.00083200	-1.23670500
C	-2.39382900	0.46772500	1.09409500
H	-2.56080600	0.03277200	2.07431200
C	-0.53602400	-1.60483200	0.43162500
H	-1.11341700	-1.99213600	1.27346100
H	-1.05015000	-1.92922000	-0.47857900
C	1.36623400	1.70302200	-0.11324800
C	0.84082000	-2.24744400	0.52304000
H	0.78047800	-3.32132600	0.35916900
H	1.31032100	-2.05658100	1.48606300
S	2.99663400	-0.42410100	-0.01429700
O	4.19082000	-0.85466600	-0.66586200
O	2.86074500	-0.33112600	1.40460900
C	1.12475900	2.73977500	-1.18786900
H	0.45446400	3.49992000	-0.78848200
H	2.06681400	3.20807300	-1.46978800
H	0.66269700	2.27785500	-2.06036900
H	1.85964600	2.12456300	0.76331500
N	1.78354100	-1.71160700	-0.53344500
H	2.36802500	-2.47390300	-0.89626800
H	1.26350300	-1.33572800	-1.33755000
O	2.43431100	0.80678900	-0.75821300

HF: -1269.5864649
Sum of electronic and zero-point Energies: -1269.325650
Sum of electronic and thermal Energies: -1269.306971
Sum of electronic and thermal Enthalpies: -1269.306027
Sum of electronic and thermal Free Energies: -1269.373254
Frequencies: -449.7780

X = NH_2^+, Y = NH

C	0.18270200	0.92185300	0.26868000
C	-0.45687700	-0.12857400	0.41046300
C	-3.28785300	0.05572900	-0.08307800
N	-2.12311400	1.70777700	1.16548500
N	-1.32793700	2.49236700	0.96999800
O	-3.36227100	0.78033600	-1.06564400
N	-3.87866600	-1.14812100	0.00691200
H	-3.86534400	-1.64751900	0.88287100
C	-4.64955600	-1.68571800	-1.10265300
H	-4.03849200	-1.70453700	-2.00561900
H	-4.95305900	-2.69919900	-0.85253600
H	-5.53633600	-1.07783600	-1.29152600
C	-2.42777700	0.41013900	1.09107500
H	-2.57028400	-0.07133500	2.05307600
C	-0.50286000	-1.60948600	0.35907700
H	-1.20867000	-2.02176700	1.08253000
H	-0.83366600	-1.93520100	-0.63162500
C	1.34289800	1.73250100	-0.10309800
C	0.87114500	-2.19189500	0.68277000
H	0.84638500	-3.28054500	0.65301500
H	1.19299700	-1.88294300	1.67649200
N	2.32540100	0.86013400	-0.88377000
S	2.98351100	-0.63525500	-0.03168000
O	4.15567900	-0.87168900	-0.82379200
O	3.01093000	-0.22775200	1.34105000
C	1.03317300	2.94102800	-0.98270200
H	0.43655400	3.64469800	-0.40632500
H	1.95195900	3.44050700	-1.29328400
H	0.46406500	2.64020300	-1.86386400
H	1.89232400	2.03723300	0.78991500
H	1.89081500	0.55168000	-1.76269900
H	3.15461500	1.41071300	-1.13887600
N	1.91353900	-1.78129700	-0.27121300
H	2.01072400	-2.27671100	-1.15266800

HF: -1249.731306
Sum of electronic and zero-point Energies: -1249.457585
Sum of electronic and thermal Energies: -1249.438653
Sum of electronic and thermal Enthalpies: -1249.437709
Sum of electronic and thermal Free Energies: -1249.505696
Frequencies: -465.1473

X = NH_2^+, Y = O

C	0.19405500	0.91647700	0.26703200
C	-0.44537600	-0.13278100	0.40963600
C	-3.27476300	0.05182900	-0.06642300
N	-2.10536900	1.69045400	1.19131700

N	-1.32664800	2.48915200	0.99738300
O	-3.34606300	0.78552100	-1.04194100
N	-3.86817700	-1.15110800	0.01341000
H	-3.86319300	-1.65476300	0.88711500
C	-4.64609600	-1.67286800	-1.09917800
H	-4.03946000	-1.68008700	-2.00514500
H	-4.94919600	-2.68933600	-0.86104400
H	-5.53306200	-1.06131000	-1.27495500
C	-2.41238700	0.39442900	1.11086000
H	-2.55195900	-0.09303200	2.07031400
C	-0.47964000	-1.61195100	0.31948900
H	-1.16058000	-2.05895900	1.04709900
H	-0.82203600	-1.91817900	-0.67277000
C	1.34704100	1.72199100	-0.12344400
C	0.89539800	-2.18141400	0.60370600
H	0.93766000	-3.25657300	0.45172900
H	1.24708800	-1.91957500	1.60004800
N	2.33111400	0.82404200	-0.89942400
S	2.96593800	-0.62228500	-0.01920200
O	4.15025700	-0.94075500	-0.74586600
O	2.95838200	-0.26014300	1.36213500
C	1.03598100	2.90595300	-1.03246200
H	0.43881700	3.61959900	-0.46843300
H	1.95270500	3.40148600	-1.35474600
H	0.46431700	2.58419800	-1.90422100
H	1.90778400	2.04290100	0.75639900
H	1.88628600	0.48864500	-1.76555900
H	3.15909800	1.36729000	-1.17812700
O	1.85854900	-1.65131400	-0.38364800

HF: -1269.5854765
Sum of electronic and zero-point Energies: -1269.324493
Sum of electronic and thermal Energies: -1269.305791
Sum of electronic and thermal Enthalpies: -1269.304846
Sum of electronic and thermal Free Energies: -1269.372506
Frequencies: -449.2907

X = NH_2^+, Y = NH_2^+

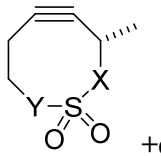
C	0.18524600	0.87222700	0.25146700
C	-0.47896400	-0.15673400	0.45588100
C	-3.25767800	0.06063000	-0.07199500
N	-2.08868300	1.66696600	1.22241800
N	-1.32161700	2.47151300	1.02374300
O	-3.28926900	0.80707600	-1.03760800
N	-3.89873100	-1.11619900	-0.00477000
H	-3.93229700	-1.62107000	0.86781800
C	-4.70326600	-1.58643100	-1.12275500
H	-4.10267300	-1.59301000	-2.03241800
H	-5.03908900	-2.59689200	-0.90460600
H	-5.56913000	-0.93991800	-1.27670000
C	-2.37908300	0.36239200	1.11552100
H	-2.55200800	-0.12901100	2.06836000
C	-0.53432900	-1.64206700	0.43063500
H	-1.12055300	-2.03646400	1.26281700
H	-1.01971800	-1.98790800	-0.48715300
C	1.27594400	1.75674300	-0.10887300
C	0.84507600	-2.25990300	0.57320100
H	0.81819900	-3.33906900	0.43926000
H	1.30419100	-2.02590400	1.53189700
N	2.41003300	0.93790700	-0.84584100
S	3.01674300	-0.50729500	0.00446200
O	4.21816500	-0.88504100	-0.64691300
O	2.82782800	-0.27301900	1.38864800
C	0.93727300	2.88490600	-1.07571100
H	0.25386100	3.56245100	-0.56797300
H	1.83026600	3.44682800	-1.35172500
H	0.44672400	2.49691200	-1.96941300
H	1.77746100	2.13434100	0.78422600
H	2.11093800	0.69903200	-1.80490500
H	3.24695900	1.53458100	-0.96529500
N	1.79265900	-1.74713400	-0.50925100
H	2.37496400	-2.51942200	-0.86981400
H	1.25328100	-1.40283800	-1.31708700

HF: -1250.0898827
Sum of electronic and zero-point Energies: -1249.802492
Sum of electronic and thermal Energies: -1249.783648
Sum of electronic and thermal Enthalpies: -1249.782704
Sum of electronic and thermal Free Energies: -1249.849773
Frequencies: -461.4719

X = NBoc, Y = O

C	1.10392700	-1.11573800	-0.62257600
C	1.72843200	-0.68085400	0.34946200
C	3.96489800	1.05977400	-0.31122800
N	3.52037000	-0.91596100	-1.54612000
N	2.68752000	-1.30024800	-2.21810600
O	3.52639000	1.77400200	-1.20409000
N	4.53161000	1.53845000	0.81135100
H	4.94297000	0.90187800	1.47647500
C	4.62696500	2.96961000	1.04642200
H	3.63907300	3.42723100	0.97818700
H	5.03034000	3.12964000	2.04324200
H	5.28269800	3.44091700	0.31189100
C	3.82131000	-0.42533300	-0.34453600
H	4.44668500	-1.06600800	0.26748900
C	1.73194100	-0.18873400	1.74461300
H	2.65352100	-0.44802300	2.27249100
H	1.65936300	0.90322500	1.74728000
C	-0.11988100	-1.48225500	-1.35562600
C	0.57857700	-0.79351700	2.53258000
H	0.50603900	-0.34967300	3.52387000
H	0.68523100	-1.87367000	2.61817900
H	-0.18709300	-0.86022500	-2.24799200
N	-1.32220600	-1.04515500	-0.56202100
S	-1.47106600	-1.57691900	1.02331700
O	-2.85400800	-1.51437000	1.40742200
O	-0.76926400	-2.83424800	1.09896600
O	-0.70250300	-0.49184600	1.90879700
C	-0.18711400	-2.93932300	-1.80448200
H	0.59454500	-3.10441800	-2.54727300
H	-0.03990600	-3.62587400	-0.97502800
H	-1.15564700	-3.13019200	-2.26891000
C	-1.95269600	0.14562800	-1.00031700
O	-1.89926400	0.49187700	-2.15288400
O	-2.55020700	0.77179900	-0.01113000
C	-3.40194900	1.95326900	-0.24617500
C	-4.54014400	1.58674100	-1.18877400
H	-4.18089600	1.39532600	-2.19881900
H	-5.06778900	0.70531500	-0.81759700
H	-5.24521300	2.41962300	-1.22195700
C	-2.54873600	3.10115000	-0.76776700
H	-2.17863300	2.90020000	-1.77176500
H	-3.15910900	4.00636400	-0.79296800
H	-1.70371100	3.27568300	-0.09821300
C	-3.92817400	2.25442500	1.14891100
H	-3.10123200	2.45892300	1.83166700
H	-4.57722100	3.13090300	1.11143800
H	-4.50132000	1.40717500	1.52982000

HF: -1614.9615414
Sum of electronic and zero-point Energies: -1614.587657
Sum of electronic and thermal Energies: -1614.560811
Sum of electronic and thermal Enthalpies: -1614.559867
Sum of electronic and thermal Free Energies: -1614.645875
Frequencies: -453.9978



+diazoacetamide (*syn*-TSs)

X = CH_2, Y = CH_2

C	0.26898400	0.40687800	0.28737700
C	-0.20146300	1.53052800	0.06150400
C	3.15171700	0.04418400	-0.23661500
N	2.26527400	2.07508100	0.63444100
N	1.50345500	2.86333700	0.31625000
O	3.28519200	0.50771100	-1.36263800
N	3.58448700	-1.18231300	0.11460600
H	3.52373500	-1.47652700	1.07718000
C	4.21842800	-2.05977900	-0.85541500
H	5.15434800	-1.62923200	-1.21587500
H	4.42223700	-3.01395300	-0.37574300
H	3.55553900	-2.21918800	-1.70720900
C	2.39679100	0.75649800	0.83308600
C	-1.23106900	2.51991700	-0.30126500
H	-1.13535200	3.40995900	0.32529600
H	-1.05013000	2.84870400	-1.33040200
C	0.13206400	-1.06947400	0.35635700
C	-2.65082100	1.96366200	-0.17388100
H	-3.35457900	2.72721300	-0.51291400
H	-2.88287200	1.75949900	0.87409200
S	-2.68668200	-0.87832700	-0.14478800
O	-3.61414000	-1.80600800	-0.80996200
O	-2.85070300	-0.67212700	1.29808700
H	2.54271400	0.48334300	1.87333600
C	0.08328400	-1.58590800	1.79991900
H	-0.03810000	-2.67121700	1.80366900
H	1.01329400	-1.34711700	2.31787900
H	-0.74532400	-1.13639800	2.34518400
H	1.00182100	-1.52905100	-0.12630800
C	-2.90623300	0.70839300	-1.00130200
H	-3.95725300	0.63257800	-1.28603800
H	-2.30333500	0.65636900	-1.91107100
C	-1.04629200	-1.54909600	-0.49715900
H	-0.88323300	-1.34238400	-1.55669500
H	-1.20425100	-2.62352900	-0.37437500

HF: -1217.2332586
Sum of electronic and zero-point Energies: -1216.951023
Sum of electronic and thermal Energies: -1216.932032
Sum of electronic and thermal Enthalpies: -1216.931087
Sum of electronic and thermal Free Energies: -1216.998793
Frequencies: -502.1286

X = NH, Y = CH_2

C	0.24842400	0.44227200	0.32644300
C	-0.20829800	1.56596100	0.08255500
C	3.11296900	0.02154300	-0.25833600
N	2.27651500	2.07578300	0.60605400
N	1.52677900	2.87534800	0.29033000
O	3.21937400	0.46759700	-1.39366600
N	3.53243600	-1.20856100	0.09712800
H	3.51237800	-1.48185100	1.06779400
C	4.12966700	-2.10598500	-0.87832600
H	5.07137800	-1.70205900	-1.25458200
H	4.31413800	-3.06385500	-0.39816400
H	3.44948100	-2.24952900	-1.71888500
C	2.40360100	0.76200100	0.82414900

C	-1.24293000	2.54113900	-0.29764500
H	-1.17905600	3.42811100	0.33731200
H	-1.04700200	2.87949000	-1.32076300
C	0.08112000	-1.02944700	0.42866500
C	-2.64950400	1.94465700	-0.20287300
H	-3.36746600	2.68404400	-0.56487000
H	-2.90052400	1.74040600	0.84040500
N	-1.09415100	-1.51948100	-0.32737300
S	-2.62152800	-0.90665200	-0.16322900
O	-3.46701000	-1.85008100	-0.88990000
O	-2.84813300	-0.69929800	1.26123000
H	2.57168100	0.50296100	1.86447600
H	-0.89973500	-1.72949200	-1.30128200
C	0.05233700	-1.51597300	1.87827700
H	-0.10644100	-2.59475100	1.89537700
H	1.00455100	-1.29457400	2.36206800
H	-0.74628100	-1.02640800	2.43300000
H	0.91552900	-1.52447200	-0.07512400
C	-2.84308300	0.67635300	-1.03057100
H	-3.87854900	0.58203500	-1.36032300
H	-2.20035400	0.63388400	-1.91308600

HF: -1233.2739449
Sum of electronic and zero-point Energies: -1233.002576
Sum of electronic and thermal Energies: -1232.983858
Sum of electronic and thermal Enthalpies: -1232.982914
Sum of electronic and thermal Free Energies: -1233.049770
Frequencies: -485.3674

X = NH_2^+, Y = CH_2

C	0.28380000	0.40611600	0.30856300
C	-0.20212800	1.51893600	0.06018300
C	3.14567000	0.06273100	-0.22583900
N	2.23423800	2.05049000	0.71122100
N	1.47896900	2.84094600	0.38969300
O	3.25995100	0.57000900	-1.33190200
N	3.58505900	-1.17301100	0.08063600
H	3.59433400	-1.47267000	1.04410800
C	4.26399400	-1.98993600	-0.91375300
H	5.23714200	-1.56630600	-1.17004100
H	4.39959700	-2.98844700	-0.50572000
H	3.65695900	-2.04767200	-1.81718700
C	2.38305100	0.73079400	0.87580800
C	-1.21567500	2.50681200	-0.34504100
H	-1.12111400	3.40911900	0.26225400
H	-1.00916500	2.80655900	-1.37764200
C	0.16076600	-1.06013000	0.35494700
C	-2.64546900	1.97873300	-0.22622900
H	-3.33332900	2.73604500	-0.60710800
H	-2.90504900	1.81290800	0.82115500
N	-1.03552000	-1.47603700	-0.49895000
S	-2.73244100	-0.83303600	-0.11506100
O	-3.52978000	-1.85623200	-0.74123500
O	-2.73992900	-0.63060400	1.30731100
H	2.53752700	0.42977300	1.90758100
H	-0.83879200	-1.25573400	-1.48265700
C	0.06941300	-1.65191100	1.75745300
H	-0.11696200	-2.72613200	1.71098000
H	1.03082100	-1.50479700	2.24869400
H	-0.70314500	-1.16697300	2.34856600
H	0.99345000	-1.53176600	-0.17555100
C	-2.91359000	0.71268400	-1.03089900
H	-3.96714300	0.62316100	-1.30937200
H	-2.31858800	0.61799100	-1.94197800
H	-1.15762900	-2.49754800	-0.45786400

HF: -1233.6822028
Sum of electronic and zero-point Energies: -1233.397230
Sum of electronic and thermal Energies: -1233.378365
Sum of electronic and thermal Enthalpies: -1233.377421
Sum of electronic and thermal Free Energies: -1233.444394
Frequencies: -486.3924

X = O, Y = CH_2

C	0.22266600	0.41964700	0.33000000
C	-0.22138400	1.54943900	0.09308500
C	3.08834000	0.03883100	-0.23196100
N	2.23193800	2.02552700	0.75053500
N	1.49429300	2.83924000	0.44401700
O	3.19775900	0.56250600	-1.33245200
N	3.51011200	-1.21045200	0.04234800
H	3.50229400	-1.54208500	0.99469700
C	4.12519100	-2.03333700	-0.98670200
H	5.08737700	-1.62002200	-1.29543800
H	4.27331800	-3.03312500	-0.58619700
H	3.47142400	-2.08684500	-1.85784100
C	2.36718400	0.70416000	0.89452800
C	-1.22825900	2.52874100	-0.34638000
H	-1.20180700	3.41578700	0.29022100
H	-0.96364200	2.86276600	-1.35526700
C	0.06496800	-1.04556900	0.35322300
C	-2.64122000	1.93772300	-0.34369200
H	-3.32261500	2.65708000	-0.80226400
H	-2.98014700	1.78607200	0.68296800
S	-2.59884200	-0.87887900	-0.12816800
O	-3.45809200	-1.88347600	-0.72577100
O	-2.75358300	-0.57607000	1.28326400
H	2.52321900	0.37957900	1.91807300
C	0.05699900	-1.66273600	1.74419900
H	-0.16151500	-2.72822600	1.66462500
H	1.04292200	-1.54709000	2.19654800
H	-0.68352400	-1.18379300	2.38170200
H	0.84925800	-1.51289400	-0.24568500
C	-2.76655500	0.62741700	-1.11909400
H	-3.76936700	0.50683000	-1.52985800
H	-2.04351400	0.53073600	-1.93134500
O	-1.12410600	-1.45156100	-0.40701600

HF: -1253.1414068
Sum of electronic and zero-point Energies: -1252.882688
Sum of electronic and thermal Energies: -1252.864235
Sum of electronic and thermal Enthalpies: -1252.863291
Sum of electronic and thermal Free Energies: -1252.929503
Frequencies: -473.4616

X = CH_2, Y = O

C	0.25479700	0.39984900	0.24787800
C	-0.19634400	1.52495000	0.00179600
C	3.14868900	0.04485600	-0.20420400
N	2.24614100	2.06550100	0.66803000
N	1.50869500	2.86645300	0.33101800
O	3.30655000	0.52404300	-1.32028200
N	3.55904100	-1.19271600	0.13512300
H	3.48402900	-1.49873700	1.09295300
C	4.20494400	-2.05964200	-0.83664600
H	5.16093300	-1.64140300	-1.15711100
H	4.37229400	-3.03013600	-0.37592700
H	3.56568700	-2.18170400	-1.71223600
C	2.38540400	0.75024300	0.86332000
C	-1.25322500	2.45898400	-0.41945300
H	-1.20177900	3.40081100	0.13336100
H	-1.12206500	2.70212900	-1.47770500
C	0.10705700	-1.07572400	0.29699800
C	-2.62640800	1.84568400	-0.19160100
H	-3.41615200	2.47090600	-0.60507700
H	-2.81186100	1.67333700	0.86808500
S	-2.69890500	-0.82795500	-0.13883000
O	-3.69121600	-1.63631300	-0.81856100
O	-2.83708100	-0.59949800	1.28780900
O	-2.72788900	0.58589000	-0.90288800
H	2.50570300	0.46816000	1.90391200
C	0.07976900	-1.62309900	1.72921200
H	-0.06158100	-2.70566200	1.71260700
H	1.02561900	-1.41371700	2.23050600
H	-0.72576300	-1.17048700	2.30601900
H	0.96194200	-1.53357600	-0.21358300
C	-1.09433400	-1.52769500	-0.54509700
H	-0.95911400	-1.28772100	-1.60083700
H	-1.25756300	-2.60301200	-0.44472500

HF: -1253.1423797
Sum of electronic and zero-point Energies: -1252.883839
Sum of electronic and thermal Energies: -1252.865222
Sum of electronic and thermal Enthalpies: -1252.864278
Sum of electronic and thermal Free Energies: -1252.931475
Frequencies: -478.2278

X = CH_2, Y = NH

C	0.26997100	0.41870200	0.25808200
C	-0.17534900	1.54428300	0.00113100
C	3.16111400	0.02508000	-0.22106800
N	2.28572800	2.07404400	0.61233300
N	1.54616500	2.87155200	0.26932700
O	3.31159300	0.47505500	-1.35058500
N	3.57121400	-1.20498200	0.14505900
H	3.49595800	-1.49091700	1.10901200
C	4.19861900	-2.10043800	-0.81265000
H	5.14003300	-1.68365600	-1.17507000
H	4.39110500	-3.05106400	-0.32137800
H	3.53697300	-2.26293200	-1.66493400
C	2.41109400	0.76073200	0.83466700
C	-1.23163700	2.49317000	-0.38462700
H	-1.13566300	3.43459000	0.16277000
H	-1.13151200	2.73704700	-1.44723500
C	0.10898600	-1.05307700	0.34879900
C	-2.61786400	1.90446900	-0.10891100
H	-3.39015700	2.61401200	-0.41206900
H	-2.74220700	1.71222400	0.95689200
S	-2.71205700	-0.84435400	-0.16138600
O	-3.61994700	-1.70687100	-0.91147300
O	-2.89387100	-0.69871200	1.27732500
H	2.53898800	0.50119600	1.88040800
C	0.05043800	-1.54670300	1.79984300
H	-0.10556000	-2.62741800	1.82063900
H	0.99039500	-1.33023400	2.30968800
H	-0.76044600	-1.06365600	2.34314800
H	0.97234800	-1.53364800	-0.12564000
C	-1.07435200	-1.52721400	-0.50381100
H	-0.90843800	-1.31703000	-1.56229600
H	-1.22674500	-2.60226200	-0.38230600
N	-2.88603000	0.65113300	-0.80924700
H	-2.88000900	0.66138100	-1.82262800

HF: -1233.2761377
Sum of electronic and zero-point Energies: -1233.005557
Sum of electronic and thermal Energies: -1232.986542
Sum of electronic and thermal Enthalpies: -1232.985598
Sum of electronic and thermal Free Energies: -1233.053412
Frequencies: -485.9600

X = CH_2, Y = NH_2^+

C	0.28080700	0.37700700	0.36150200
C	-0.19481500	1.49760000	0.12556400
C	3.12208100	0.04419100	-0.25923200

N	2.25480200	2.03543200	0.70573000
N	1.50086000	2.83465700	0.40311600
O	3.19867300	0.54707100	-1.37172000
N	3.59205500	-1.18152200	0.03905000
H	3.61785300	-1.48498200	1.00077100
C	4.23382800	-2.00271900	-0.97525100
H	5.19110600	-1.57430800	-1.27891700
H	4.39640300	-2.99573900	-0.56350600
H	3.58894300	-2.07587400	-1.85115300
C	2.38760500	0.71122300	0.86161200
C	-1.19713600	2.49450400	-0.28540100
H	-1.19306600	3.34996300	0.39352700
H	-0.92841400	2.88522800	-1.27189400
C	0.13388000	-1.09682100	0.47694200
C	-2.61319300	1.93675700	-0.31066700
H	-3.30218200	2.62787300	-0.79321200
H	-2.97972100	1.70759700	0.68895200
S	-2.63610800	-0.93757800	-0.11280800
O	-3.61544800	-1.72017200	-0.81934300
O	-2.83840000	-0.50761500	1.24339300
H	2.56822500	0.40280500	1.88682600
C	0.01492900	-1.56163300	1.93391100
H	-0.12055400	-2.64408700	1.97126100
H	0.92724000	-1.31423300	2.47669100
H	-0.82173000	-1.07877900	2.43627400
H	1.01572000	-1.58282200	0.04520000
C	-0.99712800	-1.60960700	-0.41844900
H	-0.81086600	-1.43143200	-1.47952300
H	-1.17507400	-2.67988300	-0.27766100
N	-2.67337300	0.65271500	-1.09756800
H	-1.93498200	0.62312600	-1.81128400
H	-3.56532600	0.58053100	-1.60153800

HF: -1233.6833708
Sum of electronic and zero-point Energies: -1233.397927
Sum of electronic and thermal Energies: -1233.379088
Sum of electronic and thermal Enthalpies: -1233.378144
Sum of electronic and thermal Free Energies: -1233.445384
Frequencies: -499.5792

X = NH, Y = NH

C	0.24728300	0.45378400	0.30851700
C	-0.19283100	1.57437600	0.02849100
C	3.11923800	0.00691400	-0.24610800
N	2.28951700	2.08010100	0.57204300
N	1.55853100	2.88503900	0.23084500
O	3.23123000	0.43152200	-1.38918700
N	3.53043500	-1.21931300	0.13181500
H	3.50687100	-1.47672000	1.10667200
C	4.12477500	-2.13576900	-0.82762400
H	5.06539500	-1.73905800	-1.21405200
H	4.31079000	-3.08398600	-0.32944700
H	3.44257500	-2.29577700	-1.66353100
C	2.41408000	0.77333800	0.82022600
C	-1.25550200	2.50829300	-0.37059800
H	-1.19187400	3.44365100	0.19160000
H	-1.13706600	2.76765800	-1.42740500
C	0.05991900	-1.01319200	0.44047200
C	-2.63052200	1.87785900	-0.13219400
H	-3.41650000	2.56094800	-0.46026100
H	-2.77868300	1.68354700	0.92999300
S	-2.63493900	-0.87704000	-0.18836300
O	-3.43414500	-1.75743800	-1.02284400
O	-2.89695500	-0.73844000	1.23131600
H	2.56845900	0.53422400	1.86719600
C	0.00035300	-1.46611400	1.89953300
H	-0.17842600	-2.54124900	1.93924200
H	0.95054700	-1.25063400	2.38983200
H	-0.79544100	-0.95037800	2.43404000
H	0.89708300	-1.52995300	-0.03686800
N	-2.83565400	0.61485300	-0.83837400
H	-2.76625100	0.62478000	-1.84967800
N	-1.10619100	-1.50483000	-0.32949400
H	-0.89671900	-1.66745000	-1.30994100

HF: -1249.3158094
Sum of electronic and zero-point Energies: -1249.056014
Sum of electronic and thermal Energies: -1249.037419
Sum of electronic and thermal Enthalpies: -1249.036475
Sum of electronic and thermal Free Energies: -1249.102806
Frequencies: -470.1596

X = NH, Y = NH_2^+

C	0.26032200	0.38505500	0.39784700
C	-0.19786800	1.50642100	0.14223000
C	3.08819600	0.03074700	-0.26808400
N	2.25523600	2.00454500	0.74900900
N	1.51811400	2.81838800	0.44769300
O	3.14849000	0.56328100	-1.36699400
N	3.54469700	-1.20945800	-0.01282500
H	3.59533400	-1.53519500	0.94058700
C	4.16830600	-2.00296700	-1.06041400
H	5.12357700	-1.56989600	-1.36393400
H	4.33102700	-3.00857100	-0.68077100
H	3.51136000	-2.04627600	-1.92908800
C	2.38887100	0.68083000	0.88667700
C	-1.18342700	2.49593800	-0.32074900
H	-1.20766900	3.36085900	0.34551000
H	-0.87445100	2.87126600	-1.30131800
C	0.08334000	-1.08167200	0.52369800
C	-2.59657500	1.93198200	-0.39616000
H	-3.25823500	2.60597000	-0.93787600
H	-3.01102300	1.74091800	0.59154500
N	-1.10770200	-1.53836000	-0.25351500
S	-2.57512600	-0.94696200	-0.11126200
O	-3.50338500	-1.75443500	-0.84762300
O	-2.81589100	-0.45896000	1.21268400
H	2.58686400	0.35357700	1.90227900
H	-0.95546200	-2.06890600	-1.10692900
C	0.00355000	-1.55865700	1.97287000
H	-0.16432400	-2.63553200	1.99271000
H	0.94247600	-1.34110400	2.48160900
H	-0.80212300	-1.05343800	2.50332000
H	0.90503500	-1.59912600	0.02421600
N	-2.62238300	0.61843400	-1.13685300
H	-3.49781400	0.52829300	-1.66391800
H	-1.86029400	0.56855800	-1.82433400

HF: -1249.7265559
Sum of electronic and zero-point Energies: -1249.452160
Sum of electronic and thermal Energies: -1249.433541
Sum of electronic and thermal Enthalpies: -1249.432597
Sum of electronic and thermal Free Energies: -1249.499016
Frequencies: -477.7370

X = NH, Y = O

C	0.23851600	0.43576500	0.30128600
C	-0.20670000	1.55620600	0.03153600
C	3.11156300	0.02252700	-0.23222500
N	2.26123400	2.07109900	0.62504200
N	1.53305300	2.87990600	0.28968800
O	3.23474000	0.47700400	-1.36223000
N	3.51373800	-1.21477500	0.11786800
H	3.48318300	-1.49507300	1.08619100
C	4.11595500	-2.10827700	-0.85835900
H	5.06675600	-1.71001200	-1.21730200
H	4.28390900	-3.07277500	-0.38557800
H	3.44621900	-2.23606800	-1.70975300
C	2.39819000	0.76202600	0.84809700
C	-1.26935100	2.47480500	-0.40403800
H	-1.24746100	3.41177900	0.15875700
H	-1.12267300	2.72953200	-1.45732800
C	0.05919400	-1.03414800	0.39279100
C	-2.63085400	1.82461200	-0.20602800
H	-3.42846400	2.42799800	-0.63702100
H	-2.83431700	1.64625800	0.84921600
N	-1.13326400	-1.49513200	-0.36499400
S	-2.62611900	-0.85664500	-0.16949000
O	-3.51896200	-1.68661300	-0.94125000
O	-2.84394200	-0.63948900	1.24209000
O	-2.68316300	0.56322100	-0.92043600
H	2.54836700	0.50201400	1.89045700
H	-0.95470600	-1.68370200	-1.34669700
C	0.02950000	-1.54401300	1.83330300
H	-0.15262500	-2.61912600	1.83407400
H	0.99112100	-1.35227000	2.31070200
H	-0.75097100	-1.04575500	2.40599200
H	0.88077800	-1.53419500	-0.12667800

HF: -1269.1811879
Sum of electronic and zero-point Energies: -1268.933715
Sum of electronic and thermal Energies: -1268.915357
Sum of electronic and thermal Enthalpies: -1268.914413
Sum of electronic and thermal Free Energies: -1268.980565
Frequencies: -460.4564

X = O, Y = NH

C	0.22397200	0.44686300	0.30198100
C	-0.20794800	1.57234100	0.03164100
C	3.09826400	0.02532800	-0.22448400
N	2.24890000	2.05394000	0.67775800
N	1.52576300	2.86930200	0.34580700
O	3.21894800	0.50533000	-1.34371300
N	3.50282100	-1.21806800	0.09894000
H	3.48079200	-1.51609100	1.06214500
C	4.10486500	-2.09007400	-0.89678700
H	5.06213500	-1.69141700	-1.23791500
H	4.25972900	-3.06887900	-0.44948400
H	3.43995400	-2.18743700	-1.75587200
C	2.38204200	0.74056600	0.87239700
C	-1.25288100	2.50454900	-0.41364700
H	-1.21556900	3.44180200	0.14690800
H	-1.08628900	2.75686800	-1.46536600
C	0.05534200	-1.01582100	0.34994900
C	-2.63707100	1.87469000	-0.23023600
H	-3.40586900	2.53047900	-0.64111300
H	-2.84909700	1.73047300	0.82851200
S	-2.60794600	-0.86156300	-0.15453200
O	-3.41735400	-1.81501500	-0.87721100
O	-2.79273900	-0.65285000	1.26418000
H	2.52615500	0.45413200	1.90874100
C	0.03437000	-1.60550800	1.75290000
H	-0.19540300	-2.67008300	1.69487500
H	1.02101400	-1.49046200	2.20388900
H	-0.70147300	-1.10633200	2.37991500
H	0.84243900	-1.49979700	-0.23201900
N	-2.78996000	0.57465200	-0.88514300
H	-2.73328000	0.53367600	-1.89645500
O	-1.12591700	-1.42600300	-0.41801400

HF: -1269.1825523
Sum of electronic and zero-point Energies: -1268.935466
Sum of electronic and thermal Energies: -1268.917068
Sum of electronic and thermal Enthalpies: -1268.916124

Sum of electronic and thermal Free Energies: -1268.982122
Frequencies: -456.7712

X = O, Y = O

C	0.21075100	0.42957600	0.26594900
C	-0.23445200	1.55299600	0.01254300
C	3.09870100	0.05017200	-0.20177800
N	2.20141900	2.05059000	0.71910700
N	1.48186800	2.86917200	0.39102900
O	3.23733500	0.55412200	-1.30783100
N	3.50466600	-1.19692200	0.10576800
H	3.48042100	-1.50728500	1.06518300
C	4.14874700	-2.03839600	-0.89030800
H	5.12220400	-1.63386900	-1.17441900
H	4.27897100	-3.03252100	-0.46986600
H	3.52243800	-2.10230200	-1.78058500
C	2.35284200	0.73800500	0.89339900
C	-1.29135200	2.46537400	-0.44813300
H	-1.28335700	3.40781500	0.10503100
H	-1.12632600	2.70686100	-1.50156900
C	0.06146500	-1.03373200	0.26540700
C	-2.65363600	1.81301200	-0.26365200
H	-3.44344500	2.38657800	-0.74457500
H	-2.88652300	1.67030200	0.79032600
S	-2.60188400	-0.84939900	-0.12975500
O	-3.50564100	-1.74252400	-0.79810500
O	-2.73052700	-0.59000500	1.28255500
H	2.46943800	0.43370300	1.92805900
C	0.09575200	-1.69180400	1.63458800
H	-0.14188700	-2.75115100	1.53361200
H	1.10221200	-1.60449900	2.04526600
H	-0.60633200	-1.22001500	2.31910200
H	0.81767800	-1.48601100	-0.37900700
O	-1.16480200	-1.42222000	-0.46671500
O	-2.67685400	0.51958800	-0.93239300

HF: -1289.0451908
Sum of electronic and zero-point Energies: -1288.810397
Sum of electronic and thermal Energies: -1288.792313
Sum of electronic and thermal Enthalpies: -1288.791369
Sum of electronic and thermal Free Energies: -1288.856837
Frequencies: -444.6424

X = O, Y = NH_2^+

C	0.24197200	0.38882900	0.35108300
C	-0.21711800	1.51460500	0.12098100
C	3.09183600	0.05497500	-0.23142500
N	2.20736300	1.99573400	0.81291100
N	1.47340000	2.81388600	0.51749000
O	3.17671800	0.61706600	-1.31284200
N	3.53837500	-1.19225100	0.00354800
H	3.56490100	-1.54267200	0.94913000
C	4.18221900	-1.96248900	-1.04973400
H	5.14757800	-1.52830300	-1.31724900
H	4.32833100	-2.97887800	-0.69288600
H	3.54606000	-1.97730900	-1.93470800
C	2.36184100	0.67433600	0.92237200
C	-1.21352100	2.49070900	-0.34543700
H	-1.24668500	3.36058900	0.31363600
H	-0.91217500	2.85888000	-1.33080500
C	0.10051700	-1.07090800	0.36487600
C	-2.62040100	1.90968000	-0.40594600
H	-3.29004300	2.56024500	-0.96516300
H	-3.03360100	1.73609700	0.58531400
S	-2.56188200	-0.93222900	-0.06801200
O	-3.51441500	-1.78773600	-0.69643300
O	-2.69341300	-0.45374300	1.27068100
H	2.52566900	0.32436700	1.93651500
C	0.07316500	-1.72616100	1.73092600
H	-0.16566500	-2.78411400	1.62371700
H	1.06513600	-1.64366700	2.17616400
H	-0.64534400	-1.24296400	2.39048600
H	0.84409000	-1.54383000	-0.27742500
N	-2.63882600	0.57432600	-1.12046100
H	-3.51939300	0.46864300	-1.63849500
H	-1.88226600	0.51071700	-1.81514200
O	-1.14410500	-1.45626900	-0.40584200

HF: -1269.583637
Sum of electronic and zero-point Energies: -1269.321810
Sum of electronic and thermal Energies: -1269.303496
Sum of electronic and thermal Enthalpies: -1269.302552
Sum of electronic and thermal Free Energies: -1269.368071
Frequencies: -454.3573

X = NH_2^+, Y = NH

C	0.28239800	0.43309900	0.29689000
C	-0.18133700	1.54577600	0.01627000
C	3.14894600	0.03675800	-0.22636200
N	2.26320700	2.06846900	0.63966400
N	1.52389200	2.86439400	0.29801200
O	3.26318300	0.49955300	-1.35203700
N	3.57110700	-1.19362900	0.12342600
H	3.57612000	-1.46106300	1.09634800
C	4.22138700	-2.06190900	-0.84601500
H	5.19001300	-1.65741300	-1.14603400
H	4.36172600	-3.04023300	-0.39306200
H	3.59291900	-2.16032100	-1.73132400
C	2.40724900	0.75775600	0.85394600
C	-1.22751500	2.49040700	-0.40289100
H	-1.14197300	3.43455100	0.13976000
H	-1.10064400	2.72126000	-1.46440500
C	0.13819400	-1.02892700	0.38363400
C	-2.61852800	1.91356200	-0.14615900
H	-3.39365800	2.58633800	-0.51149600
H	-2.78056000	1.75098200	0.91869400
N	-1.04890800	-1.45607800	-0.47745600
S	-2.75228000	-0.80035800	-0.14626500
O	-3.50800200	-1.75871600	-0.89945000
O	-2.79117700	-0.69058900	1.28034700
H	2.55624200	0.49371300	1.89622100
H	-0.84043100	-1.22746500	-1.45671000
C	0.02420300	-1.57083300	1.80424800
H	-0.19873600	-2.63896000	1.79456700
H	0.98909900	-1.43723100	2.29264300
H	-0.73369300	-1.04143100	2.37542400
H	0.97201400	-1.52702700	-0.12016700
H	-1.15348200	-2.47806200	-0.43537300
N	-2.83587100	0.62781400	-0.83005900
H	-3.05448700	0.61517700	-1.82220000

HF: -1249.7288443
Sum of electronic and zero-point Energies: -1249.454568
Sum of electronic and thermal Energies: -1249.435851
Sum of electronic and thermal Enthalpies: -1249.434907
Sum of electronic and thermal Free Energies: -1249.502098
Frequencies: -467.1771

X = NH_2^+, Y = O

C	0.27257900	0.42066500	0.29890400
C	-0.18356700	1.53458600	0.01473200
C	3.13661000	0.03925500	-0.20748100
N	2.24394100	2.04909200	0.69612600
N	1.51645500	2.85397200	0.35359800
O	3.25188500	0.52860800	-1.32123400
N	3.55264200	-1.20081200	0.11378300
H	3.56578500	-1.48668800	1.08145800
C	4.20394600	-2.04631600	-0.87541200
H	5.17860700	-1.64193000	-1.15552900
H	4.33160500	-3.03865500	-0.45011100
H	3.58161400	-2.11267800	-1.76786600
C	2.39565900	0.73767600	0.88936300
C	-1.22372500	2.46248200	-0.45374800
H	-1.17546600	3.41849800	0.07373800
H	-1.07061300	2.67225800	-1.51542600
C	0.12426800	-1.04073400	0.35166500
C	-2.60360400	1.87894500	-0.22569000
H	-3.38909100	2.46123200	-0.69973400
H	-2.81962800	1.73053400	0.83057200
N	-1.08517500	-1.43486600	-0.51444700
S	-2.73617800	-0.77837000	-0.12876100
O	-3.58132400	-1.68455900	-0.83333600
O	-2.77401100	-0.59883000	1.28655000
H	2.53834600	0.45262500	1.92671700
H	-0.89483200	-1.16562400	-1.48925700
C	0.01874100	-1.63175700	1.75204700
H	-0.19646100	-2.70046700	1.70753000
H	0.98666300	-1.50908600	2.23715000
H	-0.73562100	-1.12504200	2.34833700
H	0.94280600	-1.53043500	-0.18423200
H	-1.19435900	-2.45858100	-0.50985000
O	-2.68542400	0.56571100	-0.90485800

HF: -1269.5826114
Sum of electronic and zero-point Energies: -1269.321067
Sum of electronic and thermal Energies: -1269.302657
Sum of electronic and thermal Enthalpies: -1269.301713
Sum of electronic and thermal Free Energies: -1269.367697
Frequencies: -452.9666

X = NH_2^+, Y = NH_2^+

C	0.29693300	0.36621400	0.38539000
C	-0.19277300	1.47621300	0.12702300
C	3.11754100	0.06133100	-0.25129800
N	2.22540700	2.00007500	0.78857700
N	1.47808500	2.80114000	0.48265100
O	3.16847000	0.61390900	-1.33828000
N	3.60060600	-1.17022300	-0.00659700
H	3.67611300	-1.49469300	0.94624600
C	4.27020500	-1.92584600	-1.05558600
H	5.22859700	-1.47117000	-1.31385400
H	4.43316900	-2.93973400	-0.69899600
H	3.64105600	-1.95067200	-1.94474700
C	2.38083900	0.67636200	0.90687600
C	-1.17201200	2.47185200	-0.33296600
H	-1.16427300	3.34722600	0.31992300
H	-0.87463000	2.82564400	-1.32457300
C	0.15803300	-1.09255700	0.49475200
C	-2.60136000	1.95821000	-0.36408900
H	-3.25900600	2.63477700	-0.90793600
H	-3.00998800	1.78207600	0.62865700
N	-1.02216900	-1.54382900	-0.41303400
S	-2.65932200	-0.87006400	-0.10033500
O	-3.55413600	-1.75921400	-0.74699900
O	-2.69350200	-0.44637100	1.25017200
H	2.57180200	0.33833000	1.92107500
H	-0.76868300	-1.39828800	-1.40224000
C	-0.01300900	-1.62458600	1.91162100
H	-0.25498700	-2.68802400	1.90300000
H	0.94226700	-1.51018200	2.42242400
H	-0.76629800	-1.07173000	2.46622100
H	0.98668600	-1.61125400	0.00309300
H	-1.15807100	-2.56666000	-0.32405000

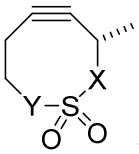
N	-2.69551900	0.63614600	-1.11887800
H	-3.61260200	0.56383000	-1.58761400
H	-1.99991200	0.59862700	-1.87977500

HF: -1250.0869802
Sum of electronic and zero-point Energies: -1249.798524
Sum of electronic and thermal Energies: -1249.780009
Sum of electronic and thermal Enthalpies: -1249.779065
Sum of electronic and thermal Free Energies: -1249.844550
Frequencies: -471.1944

X = NBoc, Y = O

C	1.40309400	-0.94799600	0.02537500
C	1.17366300	-1.58224800	1.05966800
C	3.37485200	1.18566600	0.24833500
N	3.67455000	-0.91498200	1.31825700
N	3.13112600	-1.51282800	2.11908000
O	3.03479200	1.73214200	1.28933600
N	3.52223100	1.84062100	-0.91988000
H	3.90101200	1.35908900	-1.72097300
C	3.23140300	3.26206900	-1.01964800
H	3.88386000	3.83811500	-0.36141300
H	3.39188400	3.57389100	-2.04874500
H	2.19299700	3.45192000	-0.74245900
C	3.54657100	-0.29180600	0.14614000
H	4.10814900	-0.73865400	-0.66660500
C	0.29893700	-2.31859800	1.98581000
H	0.83627300	-3.12071100	2.49898300
H	-0.06689400	-1.63500800	2.75744100
C	0.88751200	-0.28979800	-1.19937100
C	-0.87572200	-2.94231000	1.24586100
H	-1.58082000	-3.39924600	1.93786700
H	-0.53956400	-3.67978200	0.51868900
H	1.16936700	0.76224600	-1.18099100
N	-0.60669800	-0.21007200	-1.10801800
S	-1.48558500	-1.64669300	-1.00325100
O	-2.80521200	-1.42627200	-1.52515900
O	-0.65704500	-2.67624100	-1.57866400
O	-1.66087900	-1.92339200	0.56020900
C	1.40271200	-0.86985500	-2.51394000
H	2.45820100	-0.61063200	-2.61422100
H	1.30388700	-1.95042800	-2.55629500
H	0.86249600	-0.41896500	-3.34763400
C	-1.09349700	0.96270300	-0.46826600
O	-0.40358300	1.94111500	-0.33775500
O	-2.33817300	0.81471800	-0.07635900
C	-3.03667200	1.86034700	0.69579900
C	-3.14910400	3.13368600	-0.13065400
H	-2.18074200	3.61215100	-0.26551900
H	-3.58343400	2.91223800	-1.10791200
H	-3.81354800	3.82656000	0.38984900
C	-2.31096400	2.07330900	2.01713500
H	-1.33423900	2.53186100	1.86816700
H	-2.91337700	2.73191100	2.64607400
H	-2.18822500	1.11936700	2.53530400
C	-4.40518000	1.23410800	0.91870100
H	-4.30752000	0.28735100	1.45325900
H	-5.02309600	1.91065700	1.51129300
H	-4.90060200	1.05174900	-0.03673600

HF: -1614.9617493
Sum of electronic and zero-point Energies: -1614.587305
Sum of electronic and thermal Energies: -1614.560675
Sum of electronic and thermal Enthalpies: -1614.559731
Sum of electronic and thermal Free Energies: -1614.644346
Frequencies: -454.7516



+azidoacetamide (*anti*-TSs)

X = CH_2, Y = CH_2

C	-0.47421600	0.89589100	-0.31098900
C	0.03160800	-0.19694200	-0.58552100
N	1.76705000	1.54557000	-1.39919900
N	0.99856600	2.33654600	-1.07627000
C	0.08117400	-1.66865200	-0.69085900
H	0.63362900	-1.97068900	-1.58228900
H	0.62004100	-2.07446400	0.17249700
C	-1.54841800	1.76477100	0.22298400
C	-1.32469400	-2.27234500	-0.76128700
H	-1.22937700	-3.35984200	-0.79523700
H	-1.81459500	-1.96503400	-1.68827700
S	-3.28483700	-0.46705800	0.23912100
O	-4.49426100	-0.76482200	1.02112000
O	-3.45485900	-0.15526800	-1.18422300
C	-1.03517800	2.92276700	1.08866400
H	-0.42488700	3.60150300	0.49744000
H	-1.87717800	3.47963500	1.50439900
H	-0.43008700	2.53964700	1.91358300
H	-2.09978100	2.17732900	-0.62772600
N	1.86627000	0.30981400	-1.56434600
C	3.13286200	-0.35244400	-1.30534800
H	2.97587000	-1.40764700	-1.52859100
H	3.90775000	0.01404500	-1.98537400
C	3.61527900	-0.16126000	0.13183500
O	3.34097100	0.84914500	0.76425300
N	4.37687300	-1.15301900	0.61855000
C	4.98038300	-1.06314900	1.93856300
H	5.52467900	-1.98353100	2.13497300
H	5.66950400	-0.21839900	1.98937400
H	4.20956900	-0.93147000	2.69896900
H	4.55414300	-1.96711800	0.05039300
C	-2.52351700	0.94313200	1.06846500
H	-3.38984500	1.54018700	1.36301400
H	-2.04967100	0.54742000	1.96975300
C	-2.22678700	-1.93421000	0.42038800
H	-2.98378000	-2.70711700	0.56403000
H	-1.68568300	-1.81169100	1.36139600

HF: -1272.5671116
Sum of electronic and zero-point Energies: -1272.267675
Sum of electronic and thermal Energies: -1272.247517
Sum of electronic and thermal Enthalpies: -1272.246573
Sum of electronic and thermal Free Energies: -1272.318847
Frequencies: -465.9172

X = NH, Y = CH_2

C	-0.47263800	0.97223600	-0.35471700
C	0.06769100	-0.05791400	-0.76575200
N	1.83065700	1.78673400	-1.17786200
N	1.05907900	2.53785000	-0.78409800
C	0.13608400	-1.49639200	-1.08051200
H	0.61649100	-1.65145800	-2.04881100
H	0.75172200	-2.00722700	-0.33158200
C	-1.61603100	1.69295500	0.25340800
C	-1.26754800	-2.10856300	-1.11710200
H	-1.17274500	-3.17863800	-1.31330100
H	-1.83478000	-1.67990300	-1.94642800
N	-2.50518500	0.77909300	1.00380400
S	-3.20048200	-0.53621800	0.28148900
O	-4.24235600	-0.96577200	1.20928900
O	-3.57069200	-0.11441900	-1.06389000
C	-1.22153100	2.80701000	1.21945400
H	-0.66953900	3.58036400	0.69060300
H	-2.11821500	3.24304900	1.66063200
H	-0.58531500	2.41168700	2.01506400
H	-2.21933900	2.11566800	-0.55325400
N	1.94481700	0.59650000	-1.54161600
C	3.18505100	-0.11737300	-1.28446000
H	3.05583500	-1.11336500	-1.70777600
H	4.01924600	0.35688000	-1.80989000
C	3.52411900	-0.18550000	0.20442300
O	3.19306800	0.70934700	0.96966100
N	4.23090200	-1.26086800	0.58424400
C	4.70295000	-1.41245900	1.95144800
H	5.29385500	-2.32292400	2.01450600
H	5.32127800	-0.55994200	2.23620600
H	3.86134000	-1.48056000	2.64255300
H	4.45501900	-1.97180800	-0.09462700
H	-2.17774800	0.55919700	1.94126300
C	-2.06381900	-1.95183500	0.17677500
H	-2.76162000	-2.78083800	0.30197300
H	-1.43577800	-1.90209300	1.06949100

HF: -1288.6081614
Sum of electronic and zero-point Energies: -1288.319935
Sum of electronic and thermal Energies: -1288.299972
Sum of electronic and thermal Enthalpies: -1288.299028
Sum of electronic and thermal Free Energies: -1288.370713
Frequencies: -450.6076

X = NH_2^+, Y = CH_2

C	-0.44914500	0.89297000	-0.34003200
C	0.06487100	-0.19854500	-0.60588400
N	1.75430500	1.54553600	-1.42535500
N	1.01195000	2.35915100	-1.11005300
C	0.11871600	-1.67264700	-0.67656700
H	0.67843900	-1.99039500	-1.55707100
H	0.65147100	-2.05460900	0.20046300
C	-1.49954400	1.74615500	0.22446900
C	-1.27821500	-2.29285000	-0.75887300
H	-1.17151500	-3.37929100	-0.76838600
H	-1.75943800	-2.01370500	-1.69818800
N	-2.39982800	0.85939300	1.07615100
S	-3.25990500	-0.52112100	0.18962300
O	-4.44356600	-0.66362900	0.99765200
O	-3.32136300	-0.07449000	-1.17508500
C	-1.01246000	2.88483900	1.11483800
H	-0.45131700	3.58482800	0.50024700
H	-1.85565800	3.41224000	1.56271000
H	-0.35585100	2.50681800	1.90002200
H	-2.14695400	2.12553700	-0.56867600
N	1.84450700	0.31059300	-1.58596600
C	3.10325800	-0.36373900	-1.30790700
H	2.94280500	-1.41791400	-1.53164200
H	3.88437800	-0.00178600	-1.98214400
C	3.56299900	-0.16456000	0.13601000
O	3.25470200	0.83939300	0.76257200
N	4.33786000	-1.13989300	0.63156700
C	4.92076900	-1.03787800	1.96039700
H	5.47219400	-1.95128600	2.16857500
H	5.59939700	-0.18517200	2.01790400
H	4.13656900	-0.91221200	2.70780400
H	4.54561900	-1.94710700	0.06348000
H	-1.86289200	0.47310200	1.86263500
C	-2.20618300	-1.97277300	0.40713900
H	-2.98060800	-2.73596100	0.52033900
H	-1.70976500	-1.86173000	1.37420900

H	-3.16853000	1.40710000	1.48669200

HF: -1289.0175196
Sum of electronic and zero-point Energies: -1288.715475
Sum of electronic and thermal Energies: -1288.695338
Sum of electronic and thermal Enthalpies: -1288.694393
Sum of electronic and thermal Free Energies: -1288.767237
Frequencies: -448.8373

X = O, Y = CH_2

C	-0.42846900	0.94990500	-0.32402200
C	0.11354000	-0.06677000	-0.76324200
N	1.81055700	1.81314400	-1.22621300
N	1.05204800	2.56100400	-0.80702500
C	0.18104700	-1.50791000	-1.06823000
H	0.65224100	-1.67282900	-2.03918400
H	0.80325300	-2.00969800	-0.31863700
C	-1.52113800	1.64824900	0.36438700
C	-1.22309000	-2.12280500	-1.08696200
H	-1.12525300	-3.20053200	-1.23133400
H	-1.78329500	-1.73506300	-1.94043900
S	-3.13509700	-0.47438300	0.21451900
O	-4.26352100	-0.82174000	1.05631500
O	-3.38240700	0.00936400	-1.13205500
C	-1.08311500	2.59444000	1.46638600
H	-0.50952000	3.41186600	1.03299500
H	-1.96039100	2.99845800	1.97118800
H	-0.45903000	2.06464400	2.18739000
H	-2.14809800	2.16452000	-0.36588200
N	1.93313600	0.62639400	-1.59940500
C	3.17052100	-0.08709000	-1.30825900
H	3.06555700	-1.07231600	-1.76129600
H	4.02037400	0.40880100	-1.78500200
C	3.43590900	-0.17578000	0.19388300
O	3.19114000	0.77211500	0.92793100
N	3.96891600	-1.32817100	0.62535900
C	4.33086800	-1.51677300	2.02120100
H	4.79776600	-2.49263200	2.12956900
H	5.03168900	-0.74348900	2.33848400
H	3.44497400	-1.46855400	2.65668000
H	4.12194200	-2.08037700	-0.02827300
C	-2.03271000	-1.91031700	0.19179200
H	-2.74247800	-2.72511200	0.33859500
H	-1.41843400	-1.82303500	1.09031900
O	-2.37552700	0.66875800	1.05054800

HF: -1308.4768353
Sum of electronic and zero-point Energies: -1308.201285
Sum of electronic and thermal Energies: -1308.181524
Sum of electronic and thermal Enthalpies: -1308.180579
Sum of electronic and thermal Free Energies: -1308.251453
Frequencies: -444.1019

X = CH_2, Y = O

C	-0.42623400	0.97658000	-0.31034300
C	0.09235800	-0.06488000	-0.71945100
N	1.84028000	1.73939200	-1.29132000
N	1.09391700	2.51170400	-0.89116000
C	0.10111200	-1.51733600	-0.97444300
H	0.59404600	-1.75953000	-1.91909100
H	0.64125200	-2.03650100	-0.17699100
C	-1.50141100	1.73617100	0.36739800
C	-1.33342000	-2.02139200	-1.05064500
H	-1.37130600	-3.10707400	-1.12062000
H	-1.85802200	-1.57805800	-1.89649500
S	-3.15469900	-0.53515400	0.22972100
O	-4.22256500	-1.08890100	1.03779800
O	-3.45316500	-0.08623000	-1.11790500
O	-2.03714600	-1.69087400	0.17197600
C	-0.98627200	2.82158000	1.32052500
H	-0.43922800	3.58250800	0.76818600
H	-1.82309100	3.29686200	1.83555000
H	-0.31712700	2.38634900	2.06635000
H	-2.12269300	2.20718500	-0.40058600
N	1.93469700	0.53531900	-1.61569600
C	3.16538900	-0.18584600	-1.31792300
H	3.04031800	-1.18564700	-1.73233300
H	4.01541200	0.27881000	-1.82542900
C	3.45869900	-0.22575500	0.18083500
O	3.24357300	0.74997200	0.88732400
N	3.98624800	-1.37000100	0.64092200
C	4.38097400	-1.51333600	2.03310900
H	4.84418800	-2.48822500	2.16376500
H	5.09469500	-0.73464200	2.30530100
H	3.51201000	-1.43641100	2.68891500
H	4.10973200	-2.14826100	0.01216500
C	-2.38656900	0.78003000	1.17712600
H	-3.23668700	1.30623400	1.61668800
H	-1.82763400	0.27733400	1.96919300

HF: -1308.4760204
Sum of electronic and zero-point Energies: -1308.199737
Sum of electronic and thermal Energies: -1308.180101
Sum of electronic and thermal Enthalpies: -1308.179157
Sum of electronic and thermal Free Energies: -1308.249489
Frequencies: -451.9888

X = CH_2, Y = NH

C	-0.41928100	0.98097000	-0.32126600
C	0.10356300	-0.06250300	-0.72189800
N	1.86143100	1.74738900	-1.27097800
N	1.10539200	2.51407200	-0.87580300
C	0.11863500	-1.50944900	-1.00338700
H	0.65022500	-1.72848100	-1.93230500
H	0.63618200	-2.04316400	-0.19938000
C	-1.50579100	1.74174300	0.33742600
C	-1.31809600	-2.02293900	-1.14306000
H	-1.31052900	-3.09616200	-1.34021000
H	-1.80826800	-1.53199000	-1.98366300
S	-3.17741700	-0.54291200	0.24687100
O	-4.22577800	-1.02774000	1.13946500
O	-3.53532400	-0.05902700	-1.08100400
C	-1.00791900	2.85482700	1.26806200
H	-0.46865800	3.61204200	0.70316200
H	-1.85296400	3.32874500	1.77087100
H	-0.33576900	2.44441400	2.02541500
H	-2.12854700	2.18899600	-0.44377200
N	1.95766500	0.54339900	-1.59642000
C	3.18894000	-0.17685700	-1.30258700
H	3.06479500	-1.17540800	-1.72039800
H	4.03867600	0.29011600	-1.80865600
C	3.48420700	-0.22347300	0.19545500
O	3.26633600	0.74718600	0.90810900
N	4.01758400	-1.36800000	0.64853200
C	4.41832400	-1.51622500	2.03842500
H	4.87918900	-2.49285500	2.16438600
H	5.13563700	-0.74049200	2.30990500
H	3.55258400	-1.43852800	2.69832500
H	4.14478300	-2.14165900	0.01489800
C	-2.38496300	0.79484100	1.16035000
H	-3.22972400	1.33151600	1.59798400
H	-1.82124700	0.31178900	1.96201800
N	-2.15619500	-1.80670100	0.03251200
H	-1.91642400	-2.29236700	0.88889900

HF: -1288.6099101
Sum of electronic and zero-point Energies: -1288.321717
Sum of electronic and thermal Energies: -1288.301642
Sum of electronic and thermal Enthalpies: -1288.300698
Sum of electronic and thermal Free Energies: -1288.371966
Frequencies: -457.5419

X = CH_2, Y = NH_2^+

C	-0.46946400	0.85557900	-0.32114500
C	0.03279800	-0.24812900	-0.56106500
N	1.73155700	1.41991700	-1.49005800
N	0.97350400	2.23249800	-1.20117000
C	0.05987100	-1.72421400	-0.59450600
H	0.54002600	-2.08695200	-1.50485400
H	0.63900100	-2.11015300	0.25067200
C	-1.50350200	1.78884800	0.17883600
C	-1.34635600	-2.30630800	-0.58062200
H	-1.32243800	-3.38827500	-0.46601600
H	-1.89599600	-2.05317400	-1.48637000
S	-3.31487900	-0.34821000	0.21758100
O	-4.48393400	-0.76437400	0.94547200
O	-3.30549200	-0.23145200	-1.21376700
C	-0.93964700	2.92193900	1.04847100
H	-0.27717700	3.54966300	0.45764000
H	-1.75313600	3.53755100	1.43605000
H	-0.37718500	2.51068000	1.88901100
H	-2.01241600	2.22539600	-0.68553900
N	1.82083000	0.17533300	-1.57700400
C	3.08653800	-0.47771600	-1.28650300
H	2.91595400	-1.54702900	-1.41262900
H	3.84515300	-0.18215700	-2.01728300
C	3.60212000	-0.16394400	0.11867100
O	3.25656100	0.85001800	0.70806800
N	4.46794400	-1.05525500	0.62449600
C	5.10167200	-0.83933800	1.91576900
H	5.72252900	-1.70142200	2.14643300
H	5.72240000	0.05813300	1.89563300
H	4.34431300	-0.72308000	2.69192300
H	4.71345300	-1.87236400	0.08634800
C	-2.54576700	1.05497100	1.02758500
H	-3.41297800	1.68503800	1.24640400
H	-2.14918200	0.68156200	1.97491400
N	-2.14932900	-1.77267100	0.57683300
H	-2.78529900	-2.49645300	0.93221400
H	-1.53715100	-1.51803000	1.36135300

HF: -1289.0161145
Sum of electronic and zero-point Energies: -1288.713504
Sum of electronic and thermal Energies: -1288.693456
Sum of electronic and thermal Enthalpies: -1288.692512
Sum of electronic and thermal Free Energies: -1288.763721
Frequencies: -469.8358

X = NH, Y = NH

C	-0.46190800	1.06794900	-0.36011300
C	0.09997000	0.09322800	-0.86441400
N	1.89623500	1.94161200	-0.97630900
N	1.13254300	2.66065200	-0.51738800
C	0.14851700	-1.30484500	-1.32286000
H	0.60853400	-1.37975300	-2.31141800
H	0.75337800	-1.90901400	-0.63828000
C	-1.63396800	1.67633200	0.31500500
C	-1.27706500	-1.86123800	-1.40385000
H	-1.25006100	-2.90609400	-1.71841900
H	-1.85446600	-1.30438500	-2.14186800
S	-3.08150600	-0.63804300	0.28530800
O	-3.92015600	-1.25533300	1.29779900
O	-3.63738900	-0.11485100	-0.94806700
C	-1.29772600	2.79069500	1.30137400

H	-0.83078700	3.62178500	0.77745800
H	-2.21023500	3.13710700	1.78700800
H	-0.60002300	2.42932900	2.06079800
H	-2.30443600	2.06892000	-0.45313200
N	2.00954900	0.80830600	-1.49072800
C	3.21265200	0.02714600	-1.24221400
H	3.09381800	-0.89847500	-1.80497300
H	4.09484800	0.54161500	-1.63412000
C	3.42952000	-0.24399200	0.24575200
O	3.13810800	0.59524000	1.08688900
N	3.98201100	-1.42902500	0.54483800
C	4.31950500	-1.77950000	1.91533900
H	4.76502200	-2.77115200	1.91993700
H	5.03049800	-1.06226600	2.32846200
H	3.42414300	-1.78379300	2.53870200
H	4.18050700	-2.08518700	-0.19450600
N	-2.01651900	-1.80782500	-0.14450300
H	-1.65027300	-2.32829700	0.64426600
N	-2.41234600	0.66473600	1.06232100
H	-1.96817600	0.37406800	1.93047100

HF: -1304.6499734
Sum of electronic and zero-point Energies: -1304.372984
Sum of electronic and thermal Energies: -1304.353294
Sum of electronic and thermal Enthalpies: -1304.352350
Sum of electronic and thermal Free Energies: -1304.422529
Frequencies: -442.0691

X = NH, Y = NH_2^+

C	-0.47077900	0.84105700	-0.34169600
C	0.03988100	-0.25303300	-0.59467400
N	1.73496200	1.45494300	-1.46164700
N	0.98602200	2.27151700	-1.16911100
C	0.06604800	-1.72758400	-0.63228500
H	0.53400400	-2.08998500	-1.54921300
H	0.65423200	-2.11472700	0.20588400
C	-1.52107200	1.74413500	0.16215800
C	-1.34523500	-2.30172800	-0.59895400
H	-1.32272500	-3.38258400	-0.47345100
H	-1.89857200	-2.05598900	-1.50345900
N	-2.59451200	0.96862900	0.85647200
S	-3.29680600	-0.30962900	0.22568500
O	-4.42130300	-0.70822900	1.01964000
O	-3.30855300	-0.22655400	-1.20263000
C	-1.02108900	2.77715700	1.16668100
H	-0.29260000	3.42177400	0.68071900
H	-1.85342000	3.38672000	1.52029400
H	-0.54287500	2.28079800	2.01317300
H	-1.99528400	2.24771100	-0.68276300
N	1.83529100	0.21633700	-1.58541900
C	3.09959200	-0.43872100	-1.29101300
H	2.93232900	-1.50555200	-1.43977300
H	3.86564500	-0.12677400	-2.00687700
C	3.59516200	-0.14944600	0.12649900
O	3.22816900	0.84648400	0.73341400
N	4.46756300	-1.03959100	0.62216700
C	5.08690100	-0.84133800	1.92337900
H	5.70483300	-1.70669500	2.14944600
H	5.70795600	0.05618700	1.92281500
H	4.32034300	-0.73568800	2.69179400
H	4.73430900	-1.83857400	0.06695900
H	-2.67787400	1.04753200	1.86745300
N	-2.14201500	-1.75255600	0.55795300
H	-2.76908600	-2.47696300	0.92379700
H	-1.52647200	-1.48467000	1.33537600

HF: -1305.0594331
Sum of electronic and zero-point Energies: -1304.768033
Sum of electronic and thermal Energies: -1304.748219
Sum of electronic and thermal Enthalpies: -1304.747274
Sum of electronic and thermal Free Energies: -1304.817669
Frequencies: -442.8302

X = NH, Y = O

C	0.55652500	1.07552100	-0.07512600
C	-0.07613900	0.25252300	-0.73859200
N	-1.75341700	2.18008500	-0.40114600
N	-0.94939600	2.71547800	0.21440600
C	-0.22392700	-1.05259700	-1.40281500
H	-1.21454000	-1.48744800	-1.24409800
H	-0.08097200	-0.94781200	-2.48133000
C	1.77511700	1.50037700	0.65060000
C	0.80223400	-2.01396400	-0.81686200
H	0.81197300	-2.96037000	-1.35517000
H	0.61139700	-2.19278600	0.24078800
N	2.96615300	0.73690700	0.20082100
S	2.99265000	-0.89722900	0.26040200
O	4.34367600	-1.29722500	-0.04725900
O	2.35435500	-1.29711700	1.49361400
O	2.13592100	-1.46978100	-0.97502000
C	2.12223800	2.97812200	0.49765600
H	1.32450600	3.58709500	0.91708900
H	3.05346800	3.19473200	1.02157000
H	2.23474900	3.23515300	-0.55823100
H	1.64397100	1.26872800	1.71019900
N	-1.93528200	1.22057000	-1.17901600
C	-3.21009500	0.52019600	-1.16303900
H	-4.02963600	1.20896400	-1.38706900
H	-3.17022000	-0.21180100	-1.96954500
C	-3.48642400	-0.14430400	0.18606100
O	-3.05550400	0.33573900	1.22496600
N	-4.24522600	-1.24978500	0.14024400
C	-4.65878300	-1.93141100	1.35654000
H	-5.23289600	-2.81292000	1.08238500
H	-3.78498200	-2.23534700	1.93425000
H	-5.27573900	-1.27629600	1.97410500
H	-4.56421800	-1.59609700	-0.75153500
H	3.37884800	1.07937500	-0.66395400

HF: -1324.5148987
Sum of electronic and zero-point Energies: -1324.250050
Sum of electronic and thermal Energies: -1324.230628
Sum of electronic and thermal Enthalpies: -1324.229684
Sum of electronic and thermal Free Energies: -1324.299752
Frequencies: -431.0922

X = O, Y = NH

C	-0.43101000	0.94340600	-0.33162900
C	0.11368200	-0.07844100	-0.75187100
N	1.82535900	1.78179800	-1.23894300
N	1.08212600	2.54902300	-0.83075400
C	0.12855800	-1.52147100	-1.04472800
H	0.62952800	-1.73194400	-1.99238100
H	0.67001000	-2.06026200	-0.26070800
C	-1.53020300	1.63766600	0.35000000
C	-1.31689400	-2.02546300	-1.14307400
H	-1.32629100	-3.10373000	-1.30611300
H	-1.81789600	-1.55104000	-1.98619200
S	-3.12591900	-0.50208100	0.24737600
O	-4.14841300	-0.91115500	1.18139000
O	-3.46627400	0.00437100	-1.06399400
C	-1.09928000	2.61205900	1.43012700
H	-0.53844000	3.42723300	0.97584300
H	-1.97863400	3.01557800	1.93171000
H	-0.46392900	2.10595300	2.15833600
H	-2.16917300	2.13079200	-0.38640700
N	1.94227000	0.59244900	-1.60180900
C	3.17610500	-0.12485100	-1.30563100
H	3.06046100	-1.11731800	-1.73973000
H	4.02600900	0.35577400	-1.79790600
C	3.45455800	-0.18953800	0.19506200
O	3.20840600	0.76649300	0.91797900
N	4.00471400	-1.32987100	0.63651700
C	4.38790600	-1.49320600	2.02984800
H	4.87003400	-2.46071800	2.14577200
H	5.08186600	-0.70542200	2.32569400
H	3.51034100	-1.44797100	2.67698600
H	4.15368000	-2.09147900	-0.00707500
N	-2.12973000	-1.76708100	0.04599100
H	-1.88709600	-2.23950600	0.90934800
O	-2.36615300	0.66056200	1.05826800

HF: -1324.5178918
Sum of electronic and zero-point Energies: -1324.253500
Sum of electronic and thermal Energies: -1324.233882
Sum of electronic and thermal Enthalpies: -1324.232938
Sum of electronic and thermal Free Energies: -1324.303008
Frequencies: -430.2851

X = O, Y = O

C	-0.43556100	0.95034600	-0.32384900
C	0.10341400	-0.06854400	-0.75717000
N	1.81414500	1.78015900	-1.24741400
N	1.08703100	2.55766100	-0.83311700
C	0.10696200	-1.51598100	-1.03227800
H	0.57433800	-1.74544400	-1.99289700
H	0.66243400	-2.04832500	-0.25487700
C	-1.51983600	1.63945700	0.37905600
C	-1.33507600	-2.00476000	-1.08368100
H	-1.38842900	-3.08985900	-1.14201000
H	-1.86993100	-1.55811700	-1.92054500
S	-3.09959700	-0.49624600	0.23721300
O	-4.13277100	-0.98440600	1.10549100
O	-3.40651100	-0.01769300	-1.08798400
C	-1.07701500	2.56852500	1.49138400
H	-0.50630800	3.38962700	1.06024000
H	-1.94970600	2.96823700	2.00712400
H	-0.44639000	2.02987000	2.19962700
H	-2.16452900	2.15677700	-0.33452600
N	1.92177500	0.59161000	-1.61481300
C	3.15056200	-0.13567400	-1.31750600
H	3.02780800	-1.12735500	-1.75128400
H	4.00313600	0.33901300	-1.81066100
C	3.42743200	-0.19930400	0.18368200
O	3.18417200	0.75961700	0.90366000
N	3.97153700	-1.34110600	0.62797300
C	4.34952600	-1.50401500	2.02289100
H	4.82902900	-2.47251000	2.14130800
H	5.04423900	-0.71749400	2.32017400
H	3.46971700	-1.45617100	2.66679300
H	4.11736200	-2.10505000	-0.01361400
O	-2.37272900	0.64011400	1.06641900
O	-2.02129700	-1.66286100	0.15318600

HF: -1344.380071
Sum of electronic and zero-point Energies: -1344.127914
Sum of electronic and thermal Energies: -1344.108638
Sum of electronic and thermal Enthalpies: -1344.107694
Sum of electronic and thermal Free Energies: -1344.177256
Frequencies: -420.9609

X = O, Y = NH_2^+

C	-0.47539300	0.84795200	-0.33822700
C	0.06205400	-0.22323700	-0.63057200

N	1.72484200	1.52643000	-1.42446000
N	0.99955300	2.35225600	-1.11231300
C	0.09223300	-1.69721500	-0.68637700
H	0.53836500	-2.04877100	-1.61832900
H	0.69734000	-2.09376700	0.13478400
C	-1.51439100	1.70228200	0.21777300
C	-1.31905200	-2.26974600	-0.63198800
H	-1.29777400	-3.34941000	-0.50071300
H	-1.88653300	-2.02585100	-1.52793800
S	-3.26275200	-0.32204600	0.21128000
O	-4.40735300	-0.69599800	0.97525900
O	-3.27153100	-0.16840700	-1.20805200
C	-1.06390400	2.66303700	1.29480300
H	-0.38804300	3.38942200	0.84491600
H	-1.92526100	3.18313300	1.71170700
H	-0.53669500	2.12459300	2.08250000
H	-2.07973500	2.20131100	-0.56968600
N	1.82027200	0.29303900	-1.59442300
C	3.08040800	-0.37777000	-1.31011500
H	2.91452000	-1.43646600	-1.50818700
H	3.85446600	-0.03460400	-2.00198700
C	3.55337600	-0.14781500	0.12594000
O	3.17337300	0.82166000	0.76657600
N	4.41832800	-1.05735800	0.59721000
C	5.01938200	-0.91254400	1.91422700
H	5.61460200	-1.79771400	2.12383100
H	5.65924500	-0.02906900	1.95239300
H	4.24108600	-0.81441200	2.67147800
H	4.69904500	-1.82854700	0.01049900
N	-2.10472400	-1.71958800	0.54122700
H	-2.70902700	-2.45526600	0.92655300
H	-1.48132000	-1.42975300	1.30699200
O	-2.53529100	0.83334200	0.94087300

HF: -1324.9180439
Sum of electronic and zero-point Energies: -1324.639519
Sum of electronic and thermal Energies: -1324.619875
Sum of electronic and thermal Enthalpies: -1324.618931
Sum of electronic and thermal Free Energies: -1324.689283
Frequencies: -421.9973

X = NH_2^+, Y = NH

C	-0.44010100	0.95541300	-0.34913800
C	0.10822600	-0.09064400	-0.70818000
N	1.81165400	1.72023600	-1.29265800
N	1.07114400	2.51060000	-0.92492600
C	0.14926200	-1.54973800	-0.92009600
H	0.68435000	-1.80087400	-1.83779300
H	0.67090700	-2.03554300	-0.09010300
C	-1.52038300	1.72580000	0.27526900
C	-1.27386200	-2.09013600	-1.05182800
H	-1.27061000	-3.17397400	-1.15807600
H	-1.76303900	-1.65987900	-1.92464900
N	-2.37738000	0.76850200	1.09799500
S	-3.18925800	-0.62834300	0.20514700
O	-4.21032900	-0.95813300	1.15676300
O	-3.44533500	-0.06326300	-1.08571700
C	-1.07178600	2.83965300	1.21594600
H	-0.56299200	3.60263000	0.63150700
H	-1.93038800	3.29579500	1.71064700
H	-0.37751400	2.45487000	1.96477200
H	-2.19503500	2.11599300	-0.48951700
N	1.90775100	0.50906400	-1.58129400
C	3.14802300	-0.20075600	-1.30114800
H	3.01673600	-1.21227400	-1.68388100
H	3.97652700	0.25320300	-1.85158700
C	3.48866700	-0.20318400	0.18918600
O	3.14822200	0.72199300	0.91282500
N	4.20092700	-1.25659200	0.61379200
C	4.66940400	-1.34822800	1.98785000
H	5.24064700	-2.26651800	2.09796300
H	5.30466100	-0.49551200	2.23206800
H	3.82455200	-1.36465400	2.67783100
H	4.43619900	-1.99124000	-0.03572400
H	-1.81529700	0.36891200	1.85980800
H	-3.14864700	1.28656900	1.53858100
N	-2.11410500	-1.79225200	0.11967200
H	-2.04803200	-2.37479100	0.94960600

HF: -1305.0639156
Sum of electronic and zero-point Energies: -1304.772556
Sum of electronic and thermal Energies: -1304.752653
Sum of electronic and thermal Enthalpies: -1304.751708
Sum of electronic and thermal Free Energies: -1304.822459
Frequencies: -438.7902

X = NH_2^+, Y = O

C	-0.44242300	0.88300800	-0.35631800
C	0.07915100	-0.20077300	-0.62957700
N	1.77235400	1.51423500	-1.46192400
N	1.06280200	2.35667800	-1.15887000
C	0.06619100	-1.67489900	-0.68577700
H	0.59754600	-2.05245700	-1.56215700
H	0.54644700	-2.09231700	0.20298300
C	-1.48289900	1.72293800	0.23674300
C	-1.36611500	-2.16288400	-0.79141700
H	-1.44584700	-3.24174600	-0.69096700
H	-1.84534300	-1.82514400	-1.70855400
N	-2.39084700	0.81628500	1.08532100
S	-3.22326800	-0.53861800	0.21505400
O	-4.31248500	-0.84350000	1.08244400
O	-3.38330300	-0.08429200	-1.12905100
C	-0.97995500	2.82982500	1.15572800
H	-0.40858100	3.53311900	0.55358700
H	-1.81257500	3.36237800	1.61688600
H	-0.32622200	2.42324800	1.92871600
H	-2.14069400	2.12676800	-0.53523300
N	1.85085100	0.27882300	-1.62020500
C	3.09547500	-0.40941600	-1.30642500
H	2.92273800	-1.46444100	-1.51631400
H	3.89296300	-0.06990600	-1.97295500
C	3.53130900	-0.18941700	0.14189500
O	3.23099800	0.83461400	0.73904500
N	4.27704400	-1.16759000	0.67415800
C	4.83431500	-1.04513000	2.01246700
H	5.38890800	-1.95144300	2.24173500
H	5.50544900	-0.18670900	2.07002500
H	4.03663000	-0.91576100	2.74500000
H	4.47737200	-1.99363400	0.13095800
H	-1.84475600	0.39848600	1.85156600
H	-3.14168500	1.37210000	1.51790100
O	-2.14093300	-1.64597100	0.35664800

HF: -1324.9175223
Sum of electronic and zero-point Energies: -1324.638991
Sum of electronic and thermal Energies: -1324.620241
Sum of electronic and thermal Enthalpies: -1324.619296
Sum of electronic and thermal Free Energies: -1324.686667
Frequencies: -422.8954

X = NH_2^+, Y = NH_2^+

C	-0.43839000	0.80075900	-0.38886500
C	0.07465800	-0.30892800	-0.57013100
N	1.73913200	1.28880500	-1.58375800
N	1.02564100	2.15475400	-1.36622000
C	0.05349900	-1.78289100	-0.49447500
H	0.55991000	-2.22663700	-1.35376000
H	0.57699700	-2.12806800	0.40204900
C	-1.40675400	1.77913800	0.08298000
C	-1.36517000	-2.32224400	-0.53346200
H	-1.38257800	-3.40089000	-0.38683600
H	-1.87778600	-2.07672000	-1.46196500
N	-2.47097200	1.04927500	0.95882700
S	-3.30645800	-0.35420600	0.21673000
O	-4.45861800	-0.57086700	1.01439700
O	-3.24765000	-0.16122000	-1.18495700
C	-0.83661200	2.87566100	0.97547800
H	-0.17955200	3.48886600	0.36240200
H	-1.62681700	3.51101100	1.37652100
H	-0.25238900	2.44338500	1.78910600
H	-1.98113100	2.19613200	-0.74568500
N	1.80250400	0.04035200	-1.58493800
C	3.05647000	-0.60944300	-1.22969700
H	2.86843800	-1.68271100	-1.26098600
H	3.81546500	-0.39395800	-1.98624500
C	3.56569900	-0.18365600	0.14989700
O	3.10281100	0.79276300	0.72096600
N	4.55163100	-0.94234500	0.64724300
C	5.17823500	-0.62932900	1.92254000
H	5.96899400	-1.35269000	2.10479500
H	5.60458600	0.37456700	1.90056100
H	4.44733400	-0.68366400	2.73075100
H	4.87997000	-1.73776600	0.12077600
H	-2.06332800	0.80073800	1.87384700
H	-3.24823500	1.69873100	1.17807000
N	-2.22954500	-1.77120800	0.59770100
H	-2.92322200	-2.48909300	0.86549200
H	-1.67420800	-1.61116600	1.45259700

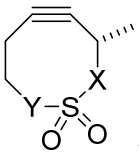
HF: -1305.4213803
Sum of electronic and zero-point Energies: -1305.116414
Sum of electronic and thermal Energies: -1305.097321
Sum of electronic and thermal Enthalpies: -1305.096377
Sum of electronic and thermal Free Energies: -1305.164507
Frequencies: -449.0380

X = NBoc, Y = O

C	0.88657100	-1.39447600	-0.60920000
C	1.46589700	-1.11421500	0.43926300
N	3.34179500	-1.24751200	-1.33018000
N	2.54107700	-1.52891800	-2.09844100
C	1.49482000	-0.76464100	1.86932200
H	2.33982500	-1.22921300	2.38393600
H	1.59569600	0.31902300	1.98418100
C	-0.32169800	-1.56288100	-1.43533300
C	0.21943100	-1.25304900	2.54670700
H	0.14045300	-0.86874500	3.56170100
H	0.17615200	-2.34053300	2.55752000
N	-1.50473500	-1.03442100	-0.66982300
S	-1.80785800	-1.65206000	0.86422400
O	-3.19246700	-1.44130200	1.18329800
O	-1.27004800	-2.98963900	0.87755700
O	-0.96456300	-0.73860900	1.87151600
N	3.55197500	-1.11467000	-0.10667900
C	4.40509400	-0.02709200	0.35585300
H	4.48113000	-0.14005800	1.43670100
H	5.41154300	-0.12326700	-0.06047900
C	3.84291100	1.33852100	-0.03454800
O	3.32452300	1.51016900	-1.12951000
N	3.98267900	2.31051600	0.87892300
C	3.55202600	3.67193200	0.60286900
H	3.81661200	4.29797000	1.45131200
H	4.04481400	4.05006600	-0.29383400
H	2.47200200	3.70834500	0.45021100

H	4.39872300	2.09715700	1.77218100
C	-0.52610900	-2.97028100	-1.98722400
H	-1.47593700	-3.01692800	-2.52161800
H	0.28195100	-3.17700700	-2.69054600
H	-0.51289400	-3.72016400	-1.20072400
H	-0.26210600	-0.88164700	-2.28306000
C	-1.93469900	0.26768200	-1.03373500
O	-2.51538900	0.88657500	-0.03089400
O	-1.74911000	0.69721500	-2.14344700
C	-3.12411700	2.22175200	-0.19387900
C	-4.21887400	2.16395600	-1.25013200
H	-4.76681900	3.10827700	-1.23580200
H	-3.80769200	2.01550000	-2.24728600
H	-4.91994200	1.35802700	-1.02259600
C	-3.71102300	2.47947400	1.18572000
H	-4.17889900	3.46509200	1.20369500
H	-4.46517800	1.72772100	1.42536300
H	-2.92621100	2.44918200	1.94398800
C	-2.03712500	3.23580600	-0.52277400
H	-1.23832700	3.18439700	0.22042900
H	-1.61917000	3.06756000	-1.51405900
H	-2.47174400	4.23704300	-0.49102100

HF: -1670.294165
Sum of electronic and zero-point Energies: -1669.903071
Sum of electronic and thermal Energies: -1669.875156
Sum of electronic and thermal Enthalpies: -1669.874211
Sum of electronic and thermal Free Energies: -1669.963260
Frequencies: -431.7374



+azidoacetamide (*syn*-TSs)

X = CH_2, Y = CH_2

C	-0.09555800	0.46701400	0.37131400
C	-0.49663700	1.52905500	-0.11021100
N	1.84920200	2.13546700	0.73644000
N	1.16463600	2.88725500	0.19894600
C	-1.45231500	2.40127400	-0.81466900
H	-1.46279600	3.39779900	-0.36866800
H	-1.11239200	2.52620000	-1.84793100
C	-0.15553000	-0.96423700	0.72932900
C	-2.86622200	1.81433500	-0.79364600
H	-3.51860200	2.45075600	-1.39541000
H	-3.26010100	1.82470200	0.22522300
S	-2.88408000	-0.95637900	-0.14214900
O	-3.73088800	-2.02321500	-0.69641500
O	-3.22878100	-0.43566800	1.18502100
N	1.80863000	0.99413800	1.24736300
C	2.98828900	0.14832100	1.20305900
H	3.83834600	0.63980700	1.68519400
H	2.75291500	-0.74120600	1.78842900
C	3.38535400	-0.22332400	-0.22667000
O	3.13946200	0.51930400	-1.16649200
N	4.03695000	-1.38961300	-0.35552500
C	4.55262700	-1.83040300	-1.64193500
H	5.03706600	-2.79462600	-1.50891800
H	3.74014300	-1.93272500	-2.36265000
H	5.27709200	-1.11312200	-2.03128000
H	4.20070400	-1.95827400	0.46106800
C	-0.33985200	-1.18629100	2.23507100
H	-1.27888800	-0.75182100	2.57600400
H	-0.34312900	-2.25590200	2.45484700
H	0.48080900	-0.71879800	2.78073700
H	0.78491800	-1.44192300	0.42971600
C	-1.22078700	-1.66906800	-0.11970500
H	-0.92906400	-1.72331800	-1.17023700
H	-1.40366300	-2.68367700	0.24242200
C	-2.96049500	0.39816100	-1.35592100
H	-3.94245000	0.21433200	-1.79492800
H	-2.20314500	0.18074500	-2.11281600

HF: -1272.5678958
Sum of electronic and zero-point Energies: -1272.267909
Sum of electronic and thermal Energies: -1272.247985
Sum of electronic and thermal Enthalpies: -1272.247041
Sum of electronic and thermal Free Energies: -1272.317499
Frequencies: -468.8944

X = NH, Y = CH_2

C	-0.12613300	0.49488200	0.39350000
C	-0.50522200	1.55290000	-0.11059300
N	1.85262600	2.12000100	0.72795300
N	1.18404200	2.88225100	0.18717900
C	-1.45229800	2.40872400	-0.84325300
H	-1.49630800	3.40476600	-0.39812000
H	-1.08621100	2.53895400	-1.86665500
C	-0.23626800	-0.92522800	0.78912400
C	-2.85110300	1.78427700	-0.85709100
H	-3.50051600	2.39007500	-1.49275600
H	-3.27740100	1.80503900	0.14815400
N	-1.31191200	-1.61368900	0.03732600
S	-2.83309200	-0.98156200	-0.15185400
O	-3.60278400	-2.07358100	-0.74031100
O	-3.23347100	-0.44396800	1.14171800
N	1.80237400	0.98587700	1.25185700
C	2.97127400	0.12417800	1.20246200
H	3.82625200	0.60224000	1.68945600
H	2.72357600	-0.76509000	1.78306800
C	3.36653700	-0.24328100	-0.22888600
O	3.11783700	0.50170600	-1.16596800
N	4.02049400	-1.40753300	-0.36127000
C	4.53428700	-1.84451400	-1.64982200
H	5.01581100	-2.81076900	-1.52103900
H	3.72086200	-1.94131300	-2.37016900
H	5.26068300	-1.12786300	-2.03670400
H	4.18618500	-1.97813800	0.45358900
H	-0.99944200	-2.04503300	-0.82702500
C	-0.40707500	-1.10368400	2.29761900
H	-1.30783500	-0.59698100	2.64081700
H	-0.48055400	-2.16653000	2.53040300
H	0.45472700	-0.67945000	2.81417400
H	0.66725100	-1.45737600	0.47838300
C	-2.88465200	0.35318900	-1.39272700
H	-3.83722400	0.14218300	-1.87995100
H	-2.08248200	0.14001000	-2.10278200

HF: -1288.6078021
Sum of electronic and zero-point Energies: -1288.319255
Sum of electronic and thermal Energies: -1288.299440
Sum of electronic and thermal Enthalpies: -1288.298496
Sum of electronic and thermal Free Energies: -1288.368537
Frequencies: -454.1380

X = NH_2^+, Y = CH_2

C	-0.10498100	0.38014200	0.41024300
C	-0.48324800	1.47649000	-0.00996800
N	1.81778500	1.94204700	0.96588400
N	1.15108300	2.75001900	0.49357400
C	-1.37921700	2.42869000	-0.68728100
H	-1.36537900	3.39167800	-0.17488400
H	-0.99099100	2.60392000	-1.69532000
C	-0.21411800	-1.06189900	0.66011900
C	-2.81808100	1.91446900	-0.75706500
H	-3.40894300	2.59729800	-1.37020200
H	-3.26956000	1.91065400	0.23681300
N	-1.31009900	-1.61199400	-0.24723500
S	-3.00539300	-0.84464100	-0.22228400
O	-3.76992500	-1.92622200	-0.78719300
O	-3.19009300	-0.41248400	1.13544300
N	1.76161400	0.75106900	1.34493000
C	2.94422400	-0.08665700	1.22484000
H	3.75253400	0.30611100	1.84795600
H	2.67794800	-1.06397500	1.63011000
C	3.43316200	-0.21213500	-0.22100500
O	3.03578500	0.54564000	-1.09352800
N	4.32843000	-1.18787700	-0.43496800
C	4.93677800	-1.37917700	-1.74253100
H	5.59072800	-2.24640200	-1.69706900
H	4.16649500	-1.54844700	-2.49578000
H	5.51948200	-0.50176600	-2.02836200
H	4.62283900	-1.76951100	0.33493700
H	-0.98671700	-1.60302000	-1.22189000
C	-0.46393000	-1.43791100	2.11568300
H	-1.34426000	-0.93623200	2.51059200
H	-0.57304500	-2.51890600	2.21807400
H	0.40522800	-1.12290600	2.69273200
H	0.67717300	-1.58196200	0.29730100
C	-2.95515400	0.53487900	-1.39392800
H	-3.92990400	0.39744400	-1.86830900
H	-2.18484200	0.29904300	-2.13158400
H	-1.49292600	-2.59842000	-0.01627400

HF: -1289.0149872
Sum of electronic and zero-point Energies: -1288.712377
Sum of electronic and thermal Energies: -1288.692498
Sum of electronic and thermal Enthalpies: -1288.691554
Sum of electronic and thermal Free Energies: -1288.761572
Frequencies: -463.2467

X = O, Y = CH_2

C	-0.11216000	0.49610000	0.41479300
C	-0.48001100	1.55399000	-0.09686400
N	1.84341600	2.10545700	0.81907700
N	1.18420400	2.87818000	0.28319400
C	-1.39210900	2.39807900	-0.88469300
H	-1.47505600	3.39400400	-0.44574000
H	-0.96235600	2.52910700	-1.88277500
C	-0.22377400	-0.92762900	0.76250100
C	-2.78193300	1.75884900	-0.98731100
H	-3.37588800	2.32393400	-1.70823700
H	-3.29507300	1.82755100	-0.02619200
S	-2.77936300	-0.93907700	-0.12706800
O	-3.55621400	-2.06638100	-0.60528700
O	-3.14004800	-0.32548400	1.13775200
N	1.79439900	0.96029800	1.31845300
C	2.95873000	0.09212200	1.21718300
H	3.83051400	0.56329100	1.67978300
H	2.72823500	-0.80383700	1.79355200
C	3.30018800	-0.24877300	-0.23401600
O	3.09408300	0.55261400	-1.13434500
N	3.85637700	-1.45433700	-0.42658700
C	4.30717500	-1.87666900	-1.74344500
H	4.74082800	-2.87001800	-1.65900000
H	3.46842300	-1.90727500	-2.44034900
H	5.05815600	-1.18568200	-2.12950800
H	3.98779300	-2.07120500	0.36021600
C	-0.40960700	-1.20421000	2.24635900

H	-1.27092700	-0.66560600	2.63661000
H	-0.54501200	-2.27525200	2.40049100
H	0.48302400	-0.87876200	2.78209100
H	0.64806100	-1.47165000	0.39142100
C	-2.76266200	0.30193300	-1.45064900
H	-3.67529600	0.04983600	-1.99132800
H	-1.90593400	0.05630100	-2.08103800
O	-1.29050600	-1.54568000	-0.03174700

HF: -1308.4745385
Sum of electronic and zero-point Energies: -1308.198461
Sum of electronic and thermal Energies: -1308.178910
Sum of electronic and thermal Enthalpies: -1308.177966
Sum of electronic and thermal Free Energies: -1308.247836
Frequencies: -449.1777

X = CH_2, Y = O

C	-0.09941500	0.46150900	0.34855900
C	-0.47699100	1.51352000	-0.16763400
N	1.84980100	2.13039500	0.72484800
N	1.19517000	2.88995300	0.16634300
C	-1.44665700	2.31076200	-0.93470900
H	-1.49631600	3.34371800	-0.58222500
H	-1.14144400	2.34095200	-1.98414000
C	-0.19150100	-0.96348100	0.72327400
C	-2.83012400	1.68741900	-0.80712000
H	-3.54502700	2.15674100	-1.48092400
H	-3.19558300	1.74750300	0.21742500
S	-2.90107700	-0.90885100	-0.15437600
O	-3.78643600	-1.87018700	-0.77972100
O	-3.25701400	-0.36539700	1.14357600
O	-2.77972500	0.29515800	-1.21342100
N	1.80362700	1.00076500	1.25671900
C	2.97877000	0.14661500	1.22254300
H	3.82828100	0.63418200	1.70964400
H	2.73239100	-0.73916700	1.80883000
C	3.38404700	-0.23088700	-0.20318500
O	3.15511000	0.51435000	-1.14516400
N	4.02446600	-1.40381900	-0.32544200
C	4.54741900	-1.85025800	-1.60700700
H	5.03355100	-2.81254700	-1.46636200
H	3.73928400	-1.95831700	-2.33185300
H	5.27212100	-1.13294900	-1.99566300
H	4.17298300	-1.97477100	0.49240600
C	-0.39272300	-1.16872200	2.22895200
H	-1.31734500	-0.70051500	2.56462700
H	-0.43129700	-2.23562800	2.45736500
H	0.44009800	-0.72381900	2.77470300
H	0.73896700	-1.46660800	0.43478400
C	-1.26425300	-1.65424900	-0.13387500
H	-0.97809400	-1.69276000	-1.18619700
H	-1.45370100	-2.67021600	0.21938500

HF: -1308.476532
Sum of electronic and zero-point Energies: -1308.199915
Sum of electronic and thermal Energies: -1308.180455
Sum of electronic and thermal Enthalpies: -1308.179511
Sum of electronic and thermal Free Energies: -1308.248825
Frequencies: -445.7996

X = CH_2, Y = NH

C	-0.09666300	0.47754500	0.33293100
C	-0.47025600	1.53115400	-0.18416300
N	1.87205900	2.13696000	0.68283100
N	1.21392600	2.89104800	0.11903900
C	-1.45577800	2.35249800	-0.90338700
H	-1.45348100	3.38536600	-0.54761200
H	-1.20051500	2.38103000	-1.96708000
C	-0.19166800	-0.94073000	0.72932700
C	-2.85695400	1.76216900	-0.71027900
H	-3.59037200	2.34581100	-1.26952600
H	-3.13498200	1.79542300	0.34315900
S	-2.91995500	-0.93716000	-0.16544500
O	-3.72199000	-1.96487000	-0.82163800
O	-3.29568000	-0.47983200	1.16677600
N	1.81832700	1.01182600	1.22441100
C	2.99172500	0.15599900	1.21435900
H	3.83640700	0.64633400	1.70728300
H	2.73617200	-0.72355700	1.80632100
C	3.41511100	-0.23746400	-0.20169900
O	3.19939400	0.49721700	-1.15514400
N	4.05699100	-1.41173800	-0.30263100
C	4.59720300	-1.87262900	-1.57171400
H	5.09225900	-2.82717500	-1.41097600
H	3.79824400	-2.00098000	-2.30347900
H	5.31817700	-1.15351800	-1.96383300
H	4.19179000	-1.97500500	0.52277700
C	-0.39942100	-1.11352900	2.23841300
H	-1.31875700	-0.62570400	2.55983500
H	-0.45553900	-2.17519000	2.48779000
H	0.43902800	-0.67096600	2.77780900
H	0.74182800	-1.44809200	0.45787800
C	-1.25684300	-1.64733400	-0.12075700
H	-0.95884000	-1.69685300	-1.16974300
H	-1.42901100	-2.66320100	0.24208200
N	-2.98289000	0.37360500	-1.14583600
H	-2.85455700	0.16274900	-2.12839100

HF: -1288.610501
Sum of electronic and zero-point Energies: -1288.321998
Sum of electronic and thermal Energies: -1288.302070
Sum of electronic and thermal Enthalpies: -1288.301126
Sum of electronic and thermal Free Energies: -1288.371710
Frequencies: -452.4556

X = CH_2, Y = NH_2^+

C	-0.07302200	0.46127700	0.39839600
C	-0.49576500	1.51613200	-0.08324000
N	1.82459200	2.14565100	0.74592100
N	1.13400900	2.89411700	0.21370600
C	-1.45001700	2.38193600	-0.79579700
H	-1.53226600	3.35722900	-0.31278700
H	-1.08286700	2.56584400	-1.80995300
C	-0.12172800	-0.96919000	0.76749100
C	-2.84210000	1.76727900	-0.83877100
H	-3.49893900	2.31573300	-1.51155300
H	-3.29824900	1.72383800	0.14943800
S	-2.82508800	-1.02031300	-0.07384600
O	-3.72720700	-1.94966700	-0.70007000
O	-3.15131200	-0.34254000	1.14982600
N	1.79573600	1.00214600	1.25080000
C	2.98036400	0.16161400	1.19528600
H	3.83083100	0.66639700	1.66163400
H	2.76259800	-0.72383300	1.79339500
C	3.35496500	-0.21527700	-0.23970200
O	3.06458300	0.51099800	-1.17937700
N	4.03096700	-1.36635000	-0.37100100
C	4.52780800	-1.80843900	-1.66474200
H	5.00470200	-2.77745800	-1.53977400
H	3.70391800	-1.90137600	-2.37327900
H	5.25364200	-1.09710600	-2.06261500
H	4.23800800	-1.91604300	0.44908400
C	-0.31426100	-1.18418900	2.27321300
H	-1.24975900	-0.74400300	2.61682400
H	-0.31504500	-2.25140700	2.50076200
H	0.50543400	-0.71079800	2.81389900
H	0.82008200	-1.44575700	0.47142700
C	-1.15961900	-1.70238100	-0.09026200
H	-0.88276700	-1.75725700	-1.14519600
H	-1.34097900	-2.72062300	0.26788800
N	-2.79034000	0.35034700	-1.35285100
H	-1.98418400	0.21321200	-1.97448600
H	-3.62573100	0.14414300	-1.91346000

HF: -1289.0173219
Sum of electronic and zero-point Energies: -1288.714736
Sum of electronic and thermal Energies: -1288.694679
Sum of electronic and thermal Enthalpies: -1288.693735
Sum of electronic and thermal Free Energies: -1288.765972
Frequencies: -471.8530

X = NH, Y = NH

C	-0.12070600	0.51833700	0.35791000
C	-0.48384400	1.55535400	-0.19582500
N	1.87326500	2.14415900	0.64240800
N	1.22825300	2.89698000	0.06420000
C	-1.46919800	2.34803100	-0.94415400
H	-1.49983100	3.38342800	-0.59715000
H	-1.19255700	2.37351200	-2.00241000
C	-0.25649400	-0.88219900	0.81020600
C	-2.85651000	1.71865700	-0.77169100
H	-3.59278100	2.26394500	-1.36516700
H	-3.16377400	1.76851900	0.27275700
S	-2.84250400	-0.97395700	-0.16940600
O	-3.52941200	-2.04526000	-0.86902000
O	-3.29421500	-0.50573500	1.12642300
N	1.81310400	1.03702200	1.21799800
C	2.97408400	0.16301000	1.20839000
H	3.83041300	0.64944000	1.68471100
H	2.71260800	-0.70246300	1.81831500
C	3.37570300	-0.25851300	-0.20595400
O	3.14327100	0.45705800	-1.16983000
N	4.01760300	-1.43352500	-0.29328100
C	4.53842200	-1.91876500	-1.56154200
H	5.03105800	-2.87286900	-1.39122300
H	3.72884100	-2.05536500	-2.27989700
H	5.25746500	-1.20992500	-1.97528700
H	4.16517100	-1.98065400	0.54077200
C	-0.46832200	-0.99009900	2.31973600
H	-1.36245100	-0.44622000	2.62057900
H	-0.57349500	-2.03913500	2.59853500
H	0.39334600	-0.56413100	2.83529300
H	0.64832900	-1.43842100	0.54891400
N	-2.92542300	0.31567200	-1.17713900
H	-2.71356000	0.08949900	-2.14224800
N	-1.31559900	-1.59128100	0.05431900
H	-0.98311300	-1.99043000	-0.81858000

HF: -1304.6493604
Sum of electronic and zero-point Energies: -1304.372192
Sum of electronic and thermal Energies: -1304.352452
Sum of electronic and thermal Enthalpies: -1304.351508
Sum of electronic and thermal Free Energies: -1304.421283
Frequencies: -439.6416

X = NH, Y = NH_2^+

C	-0.09908000	0.46139800	0.43835300
C	-0.49320100	1.51818000	-0.05884800
N	1.83007500	2.08989600	0.80427900
N	1.16115000	2.86135900	0.28028600
C	-1.41047500	2.37856700	-0.82303800
H	-1.52251900	3.35520900	-0.34906200
H	-0.98628400	2.55774600	-1.81524200
C	-0.20874100	-0.96130100	0.81979400

C	-2.79613300	1.75459400	-0.94421800
H	-3.40076900	2.27855900	-1.68236200
H	-3.32160800	1.74647400	0.00861700
N	-1.31389000	-1.60454900	0.04899400
S	-2.78573000	-1.01576900	-0.08523800
O	-3.63366400	-1.96592200	-0.74326300
O	-3.15928500	-0.28174400	1.08461000
N	1.78884900	0.94177900	1.29653900
C	2.96078900	0.08422000	1.20517000
H	3.81561100	0.55454400	1.69897200
H	2.72590700	-0.82313500	1.76238900
C	3.33819000	-0.23244000	-0.24387400
O	3.03889500	0.52669400	-1.15406200
N	4.02803300	-1.36886400	-0.41991800
C	4.52367300	-1.75639000	-1.73161600
H	5.00047600	-2.72998200	-1.64756400
H	3.69801100	-1.81962200	-2.44149800
H	5.24913600	-1.02941100	-2.10139500
H	4.24400200	-1.94705100	0.37791800
H	-1.07290200	-2.28710300	-0.66427600
C	-0.38253700	-1.17624100	2.32099100
H	-1.26504700	-0.65143000	2.68499100
H	-0.47939100	-2.24194300	2.52768100
H	0.49229800	-0.78575700	2.84096100
H	0.67324300	-1.50519300	0.47404500
N	-2.70672800	0.31863400	-1.40104200
H	-3.49775800	0.09360300	-2.01392000
H	-1.85561900	0.16326200	-1.95499000

HF: -1305.0595694
Sum of electronic and zero-point Energies: -1304.768240
Sum of electronic and thermal Energies: -1304.748371
Sum of electronic and thermal Enthalpies: -1304.747427
Sum of electronic and thermal Free Energies: -1304.817568
Frequencies: -452.5678

X = NH, Y = O

C	-0.12184900	0.49378600	0.36903600
C	-0.48645900	1.53278100	-0.17885200
N	1.85347400	2.12571100	0.69712700
N	1.21396100	2.88856700	0.12802300
C	-1.45484300	2.30726200	-0.96844900
H	-1.52591400	3.34278000	-0.62743200
H	-1.13780400	2.33021900	-2.01435100
C	-0.26209900	-0.91589300	0.78860700
C	-2.82702200	1.65674100	-0.84589100
H	-3.54454200	2.10029100	-1.53444000
H	-3.20393700	1.72372600	0.17383300
N	-1.34621900	-1.58886000	0.02478400
S	-2.83828400	-0.93921300	-0.16419900
O	-3.62382000	-1.94369500	-0.83868500
O	-3.25763800	-0.39185400	1.10522600
O	-2.74383000	0.25978100	-1.23126000
N	1.79957600	1.00892600	1.25317900
C	2.96365300	0.13829300	1.21919200
H	3.81932200	0.61753400	1.70370200
H	2.70666200	-0.74101200	1.81057000
C	3.36206200	-0.24954700	-0.20564000
O	3.12808600	0.48926400	-1.15122000
N	4.00246900	-1.42266600	-0.32205800
C	4.51977900	-1.87812800	-1.60287200
H	5.00402000	-2.84072800	-1.45814700
H	3.70874200	-1.98840100	-2.32405600
H	5.24484300	-1.16489000	-1.99817900
H	4.15413600	-1.98803400	0.49903200
H	-1.03728500	-2.02031500	-0.84119600
C	-0.45846700	-1.07280300	2.29530100
H	-1.34209700	-0.52947000	2.62692600
H	-0.57085300	-2.12964000	2.53898600
H	0.41348200	-0.67381500	2.81472100
H	0.63002000	-1.47550500	0.49474600

HF: -1324.5144782
Sum of electronic and zero-point Energies: -1324.249290
Sum of electronic and thermal Energies: -1324.229995
Sum of electronic and thermal Enthalpies: -1324.229051
Sum of electronic and thermal Free Energies: -1324.297670
Frequencies: -431.1292

X = O, Y = NH

C	-0.13073100	0.50268600	0.37673600
C	-0.47891400	1.55360300	-0.15884900
N	1.84644800	2.10541700	0.76258100
N	1.20864600	2.88126500	0.20826700
C	-1.42750900	2.35340900	-0.94470300
H	-1.48614600	3.38198700	-0.58243700
H	-1.08875400	2.39721400	-1.98377100
C	-0.26538300	-0.91288100	0.74605400
C	-2.81911800	1.71446500	-0.85979300
H	-3.51144300	2.22675700	-1.52913300
H	-3.20755300	1.79600400	0.15458600
S	-2.81962600	-0.93695400	-0.16826200
O	-3.52202600	-2.04153700	-0.77715700
O	-3.22211100	-0.41615800	1.11893800
N	1.78911900	0.97347500	1.28681300
C	2.95329800	0.10271000	1.22773400
H	3.80920700	0.57115700	1.72205500
H	2.69876600	-0.79111400	1.79745500
C	3.34842100	-0.24880500	-0.20743600
O	3.11621300	0.51602100	-1.13259000
N	3.98315800	-1.42133100	-0.35536600
C	4.49199000	-1.84761600	-1.64956600
H	4.96522700	-2.81940600	-1.53247100
H	3.67704700	-1.92870100	-2.37022400
H	5.22417300	-1.13252600	-2.02813000
H	4.13421400	-2.00849300	0.45055000
C	-0.47032500	-1.15939900	2.23299600
H	-1.32179600	-0.59541300	2.60857200
H	-0.63047400	-2.22427100	2.40532000
H	0.42620900	-0.84464400	2.76876600
H	0.60416300	-1.47468100	0.39713300
N	-2.84416800	0.29560100	-1.22041900
H	-2.63950700	0.03124900	-2.17726700
O	-1.32609000	-1.53131000	-0.05431400

HF: -1324.5153982
Sum of electronic and zero-point Energies: -1324.250853
Sum of electronic and thermal Energies: -1324.231362
Sum of electronic and thermal Enthalpies: -1324.230418
Sum of electronic and thermal Free Energies: -1324.299812
Frequencies: -431.2065

X = O, Y = O

C	-0.12892100	0.48428800	0.37572400
C	-0.48268800	1.53330300	-0.15863400
N	1.82774800	2.09558600	0.78506700
N	1.19327700	2.87434000	0.23294500
C	-1.42957200	2.31131300	-0.96945800
H	-1.51680100	3.34299200	-0.62162200
H	-1.07917800	2.34310000	-2.00410300
C	-0.26809400	-0.93298500	0.72793000
C	-2.80174700	1.65469600	-0.89121600
H	-3.49298800	2.07305500	-1.61987900
H	-3.22178000	1.73539100	0.10996700
S	-2.81486600	-0.91351200	-0.16553900
O	-3.59317000	-1.94888400	-0.78330100
O	-3.20567600	-0.35042500	1.10253200
N	1.77963900	0.96119900	1.30286400
C	2.95017500	0.09819600	1.23601700
H	3.80280400	0.57117900	1.73150500
H	2.70369800	-0.80038400	1.80141700
C	3.34450800	-0.24082800	-0.20225900
O	3.10687800	0.53043100	-1.12059900
N	3.98357200	-1.40949100	-0.35988500
C	4.49106500	-1.82432500	-1.65840900
H	4.96145300	-2.79862900	-1.55097000
H	3.67525600	-1.89585400	-2.37903800
H	5.22516300	-1.10771200	-2.03038400
H	4.13872000	-2.00200900	0.44136000
C	-0.47288900	-1.20917400	2.20758900
H	-1.31715400	-0.64461700	2.59842700
H	-0.63967400	-2.27593900	2.35914500
H	0.42788800	-0.91154300	2.74584500
H	0.58510200	-1.50271900	0.35471300
O	-1.35441600	-1.52734500	-0.07969900
O	-2.69303200	0.24516900	-1.24623300

HF: -1344.3775952
Sum of electronic and zero-point Energies: -1344.125154
Sum of electronic and thermal Energies: -1344.106014
Sum of electronic and thermal Enthalpies: -1344.105070
Sum of electronic and thermal Free Energies: -1344.174078
Frequencies: -421.6414

X = O, Y = NH_2^+

C	-0.11483200	0.40778100	0.44952000
C	-0.47069700	1.49814900	-0.00090500
N	1.81358000	1.96184900	0.98616200
N	1.16979800	2.77903600	0.50321400
C	-1.34887200	2.39563200	-0.76710900
H	-1.46718300	3.35817400	-0.26711600
H	-0.88686100	2.59745300	-1.73757200
C	-0.25809300	-1.02333600	0.72261700
C	-2.73728200	1.79386500	-0.95536000
H	-3.29760400	2.32507800	-1.72202200
H	-3.30914000	1.78970900	-0.02999800
S	-2.81575700	-0.95144000	-0.12828200
O	-3.68747300	-1.88959500	-0.75472300
O	-3.13900400	-0.24594400	1.06944400
N	1.75719100	0.78157000	1.39126900
C	2.92325300	-0.07737200	1.23692500
H	3.76374100	0.32177100	1.81149400
H	2.66191300	-1.03994200	1.67778000
C	3.34453700	-0.23342300	-0.22638100
O	3.00199400	0.58044800	-1.07145900
N	4.12332100	-1.29315300	-0.48683300
C	4.66644600	-1.51973900	-1.81740200
H	5.28142100	-2.41576500	-1.79235800
H	3.86097700	-1.65611700	-2.54030500
H	5.27703200	-0.67092800	-2.12884700
H	4.36243600	-1.93085200	0.25719300
C	-0.47631900	-1.39611100	2.17409500
H	-1.30686200	-0.83931900	2.60458500
H	-0.65799400	-2.46749500	2.25457100
H	0.42985600	-1.14748900	2.72788600
H	0.56452300	-1.59207800	0.28772400
N	-2.65200600	0.35253700	-1.41895100
H	-3.41709600	0.14876800	-2.07326000
H	-1.77674000	0.17948500	-1.93149800
O	-1.38580900	-1.55527900	-0.12648300

HF: -1324.9155003
Sum of electronic and zero-point Energies: -1324.636768
Sum of electronic and thermal Energies: -1324.617253

Sum of electronic and thermal Enthalpies: -1324.616308
Sum of electronic and thermal Free Energies: -1324.685491
Frequencies: -439.4076

X = NH_2^+, Y = NH

C	-0.07280800	0.46725400	0.35660100
C	-0.44892500	1.51487300	-0.17097200
N	1.84748900	2.09723900	0.75932500
N	1.18950500	2.85668400	0.20459200
C	-1.40667600	2.34723100	-0.91336500
H	-1.39264900	3.38021600	-0.56108400
H	-1.12972400	2.36154200	-1.97097200
C	-0.18074800	-0.94538500	0.73824700
C	-2.81953800	1.79163100	-0.73728700
H	-3.53843500	2.34768500	-1.33776800
H	-3.12742900	1.84578800	0.30604800
N	-1.26258000	-1.58486300	-0.12724700
S	-2.98035100	-0.86612400	-0.18641000
O	-3.64724100	-1.96712600	-0.81712200
O	-3.20637200	-0.45598000	1.16630200
N	1.80423600	0.95734700	1.26829900
C	2.98812800	0.11187100	1.22682600
H	3.82280300	0.60154800	1.73600100
H	2.74833000	-0.78767700	1.79430200
C	3.41144700	-0.22626100	-0.20440600
O	3.13764900	0.51743800	-1.13513200
N	4.11131500	-1.36196900	-0.34018500
C	4.65572600	-1.76620500	-1.62717300
H	5.15567900	-2.72391600	-1.50547700
H	3.85540700	-1.86904200	-2.36093500
H	5.37245600	-1.02818100	-1.99128400
H	4.29880600	-1.92942100	0.47234500
H	-0.93512100	-1.62279400	-1.10001400
C	-0.44029300	-1.18059400	2.22136000
H	-1.30651800	-0.62161800	2.56657900
H	-0.58073900	-2.24412000	2.42136900
H	0.43774800	-0.84003900	2.76969900
H	0.71598900	-1.49473600	0.43667800
H	-1.40363000	-2.56015100	0.16676300
N	-2.93223800	0.38437200	-1.15949900
H	-3.00160900	0.16007900	-2.14806100

HF: -1305.061351
Sum of electronic and zero-point Energies: -1304.769778
Sum of electronic and thermal Energies: -1304.749974
Sum of electronic and thermal Enthalpies: -1304.749030
Sum of electronic and thermal Free Energies: -1304.819071
Frequencies: -445.9661

X = NH_2^+, Y = O

C	-0.10723000	0.38941100	0.38311100
C	-0.45083200	1.47294300	-0.08893200
N	1.82615900	1.94802600	0.93471000
N	1.19668500	2.76323800	0.43153900
C	-1.36204400	2.34423300	-0.84450700
H	-1.36643300	3.36493000	-0.45616000
H	-1.03499600	2.39172300	-1.88588900
C	-0.25688400	-1.04227700	0.65635700
C	-2.77681500	1.80538900	-0.75665400
H	-3.45741100	2.29493000	-1.44781700
H	-3.16779100	1.84168200	0.25822500
N	-1.37075000	-1.57395000	-0.25927200
S	-3.01905500	-0.79412400	-0.23173500
O	-3.81000700	-1.78121600	-0.88842300
O	-3.23420100	-0.37080600	1.11424900
N	1.76258900	0.77341800	1.35381800
C	2.93578500	-0.08115600	1.24829500
H	3.74548500	0.30740400	1.87220300
H	2.65170200	-1.04977100	1.66205100
C	3.42971300	-0.22950900	-0.19354400
O	3.04162100	0.52011400	-1.07710200
N	4.31744800	-1.21508800	-0.39145000
C	4.92632700	-1.42905200	-1.69537900
H	5.57642600	-2.29831500	-1.63618700
H	4.15603900	-1.60600100	-2.44684600
H	5.51313700	-0.55848800	-1.99340600
H	4.60434300	-1.78978300	0.38655400
H	-1.05323900	-1.53253600	-1.23734000
C	-0.52144700	-1.39793400	2.11315600
H	-1.38052400	-0.86024900	2.50736200
H	-0.66828200	-2.47320800	2.22578800
H	0.36025100	-1.10906400	2.68506100
H	0.61402500	-1.59691900	0.29565500
H	-1.54087200	-2.56697900	-0.04794800
O	-2.78133100	0.39251300	-1.20502300

HF: -1324.9144712
Sum of electronic and zero-point Energies: -1324.635532
Sum of electronic and thermal Energies: -1324.616059
Sum of electronic and thermal Enthalpies: -1324.615115
Sum of electronic and thermal Free Energies: -1324.684214
Frequencies: -435.9113

X = NH_2^+, Y = NH_2^+

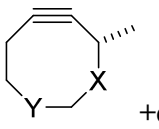
C	-0.08474500	0.39459300	0.43504400
C	-0.48137400	1.47966500	-0.00005900
N	1.80210400	1.98236900	0.92629500
N	1.12631700	2.77297800	0.43966300
C	-1.39011300	2.40792600	-0.69019400
H	-1.44943600	3.35992000	-0.15958600
H	-0.99026000	2.62780100	-1.68416300
C	-0.17201300	-1.03844500	0.72254100
C	-2.80387100	1.86111000	-0.78951800
H	-3.41343800	2.43813500	-1.48301500
H	-3.30601700	1.81030300	0.17475100
N	-1.27769000	-1.64998200	-0.18405300
S	-2.92316200	-0.91724000	-0.16132000
O	-3.75322000	-1.87762700	-0.79201500
O	-3.09886700	-0.32440300	1.11241500
N	1.76206700	0.80205600	1.33567500
C	2.95064200	-0.03073200	1.21697800
H	3.76900800	0.40388400	1.79659100
H	2.71188500	-0.99072300	1.67692000
C	3.38796900	-0.21951400	-0.23899100
O	2.88787700	0.43717000	-1.14009600
N	4.34849800	-1.13521900	-0.42487500
C	4.89753800	-1.39839600	-1.74637200
H	5.67575500	-2.15168500	-1.65253200
H	4.11956500	-1.76577600	-2.41718100
H	5.32490100	-0.48792600	-2.16866300
H	4.71021100	-1.64298300	0.36826200
H	-0.94663900	-1.72771900	-1.15949100
C	-0.41520400	-1.38999900	2.18256700
H	-1.29557800	-0.88861800	2.57855800
H	-0.50224600	-2.46976000	2.31151000
H	0.45399800	-1.04594400	2.74287700
H	0.70864000	-1.56808200	0.34875700
H	-1.45143000	-2.62633700	0.11487900
N	-2.80493000	0.44391500	-1.35941500
H	-3.65224400	0.30132200	-1.93265700
H	-2.00993200	0.30882700	-2.00213600

HF: -1305.4186574
Sum of electronic and zero-point Energies: -1305.113503
Sum of electronic and thermal Energies: -1305.093805
Sum of electronic and thermal Enthalpies: -1305.092861
Sum of electronic and thermal Free Energies: -1305.162023
Frequencies: -458.0894

X = NBoc, Y = O

C	1.21582200	-1.28696900	-0.04014600
C	1.05806700	-1.83063700	1.05177800
N	3.55214200	-1.19866800	1.02135500
N	3.09417100	-1.74500600	1.91818300
C	0.21870300	-2.43212800	2.09903500
H	0.72132700	-3.26509400	2.59692400
H	0.00465100	-1.68191000	2.86505600
C	0.71848100	-0.65903200	-1.28121700
C	-1.07870200	-2.95415500	1.49569400
H	-1.77232500	-3.28277400	2.26743500
H	-0.88993300	-3.76701700	0.79664800
N	-0.75379900	-0.42534700	-1.10882900
S	-1.74740800	-1.75227600	-0.79044200
O	-3.08397000	-1.43602000	-1.20985800
O	-1.07864400	-2.90170500	-1.34649000
O	-1.79352200	-1.88945800	0.80047700
N	3.33305500	-0.87347000	-0.16478400
C	3.81353700	0.41505800	-0.64781000
H	4.88905600	0.51331600	-0.47829200
H	3.64826700	0.42154400	-1.72503900
C	3.10191100	1.58221500	0.03955500
O	2.80028500	1.52139600	1.22375900
N	2.87632400	2.65486700	-0.73215000
C	2.23524000	3.84791700	-0.20223900
H	2.29837800	4.63604200	-0.94908600
H	1.18731900	3.64512700	0.02649600
H	2.74567600	4.17068800	0.70554700
H	3.10840000	2.61706800	-1.71276400
C	1.09813300	-1.37866500	-2.57123600
H	0.60785400	-0.89312800	-3.41609200
H	2.17874700	-1.29535200	-2.70085400
H	0.83062500	-2.43094200	-2.54771200
H	1.10386700	0.35914300	-1.34668500
C	-1.08990900	0.86097500	-0.60426700
O	-2.25999300	0.85870900	-0.00990400
O	-0.34546800	1.79810200	-0.73903600
C	-2.81513100	2.08094100	0.60572400
C	-3.00037400	3.15897300	-0.45324800
H	-3.57121700	3.98006400	-0.01481500
H	-2.04599000	3.54684100	-0.80498100
H	-3.56545700	2.76265100	-1.29964500
C	-4.15899500	1.59631800	1.12824200
H	-4.67096900	2.41867500	1.63068500
H	-4.78356400	1.24441600	0.30514200
H	-4.01972000	0.78178900	1.84150600
C	-1.91121600	2.52343700	1.74797200
H	-1.76024200	1.70149000	2.45116400
H	-0.94493500	2.86878700	1.38281600
H	-2.39744300	3.34467600	2.27859900

HF: -1670.2954048
Sum of electronic and zero-point Energies: -1669.903256
Sum of electronic and thermal Energies: -1669.875711
Sum of electronic and thermal Enthalpies: -1669.874767
Sum of electronic and thermal Free Energies: -1669.961747
Frequencies: -436.7871



+diazoacetamide (*anti*-TSs)

X = CH_2, Y = CH_2

C	0.97492400	-0.68433700	-0.31326900
C	0.20840700	0.27097600	-0.48974800
C	-2.59234100	-0.34397100	0.06879700
N	-1.22288800	-1.83467200	-1.17203600
N	-0.28044000	-2.44341200	-0.96286300
O	-2.58231500	-1.07173900	1.05572800
N	-3.31917800	0.78813300	-0.00316700
H	-3.30157200	1.34009400	-0.84644800
C	-4.08488700	1.25956700	1.13777500
H	-3.42513700	1.50816800	1.97175900
H	-4.63741000	2.14769100	0.84067500
H	-4.78725300	0.49226500	1.46565900
C	-1.73224800	-0.60172000	-1.11817200
H	-1.96768600	-0.16472700	-2.08254300
C	-0.05859300	1.72790200	-0.47471600
H	-0.77273900	2.00858200	-1.25371100
H	-0.52570300	1.99167900	0.48174400
C	2.26802600	-1.28871900	0.07437900
C	1.22883900	2.54080400	-0.66310300
H	0.95636300	3.59817000	-0.59088100
H	1.60231300	2.38401100	-1.68060800
C	2.10878100	-2.50591200	0.99116300
H	1.58100900	-3.31801300	0.49251000
H	3.09140700	-2.86926000	1.30141300
H	1.54822300	-2.22960500	1.88850300
H	2.77137900	-1.61203500	-0.84580100
C	3.32889300	1.09206000	-0.00784600
H	3.29091600	0.89403100	-1.08540000
H	4.34187600	1.44994200	0.19272700
C	3.15226800	-0.22978200	0.75755200
H	4.13288000	-0.68889500	0.92131900
H	2.73582000	-0.02473300	1.75102600
C	2.35234200	2.24219400	0.34196200
H	2.94245800	3.15725700	0.43942700
H	1.91244100	2.06457400	1.33062300

HF: -707.9513821
Sum of electronic and zero-point Energies: -707.651572
Sum of electronic and thermal Energies: -707.634362
Sum of electronic and thermal Enthalpies: -707.633418
Sum of electronic and thermal Free Energies: -707.697164
Frequencies: -494.7402

X = NH, Y = CH_2

C	0.96996700	-0.67642500	-0.31089600
C	0.20174000	0.27587200	-0.49114800
C	-2.59173200	-0.34454500	0.06582200
N	-1.21806300	-1.84074100	-1.16285800
N	-0.28159900	-2.45542500	-0.95198400
O	-2.58022900	-1.06594000	1.05712000
N	-3.31609300	0.78843100	-0.01259800
H	-3.29931300	1.33462000	-0.85967100
C	-4.07985600	1.26826700	1.12625100
H	-3.41878100	1.51803300	1.95877300
H	-4.62865600	2.15727200	0.82500000
H	-4.78539400	0.50551200	1.45791100
C	-1.73500500	-0.61158100	-1.12173400
H	-1.97105900	-0.18440400	-2.09018300
C	-0.05300900	1.73355000	-0.47710600
H	-0.75710500	2.02428700	-1.26132800
H	-0.52151300	2.00388000	0.47665200
C	2.28308900	-1.24851900	0.08482600
C	1.25251500	2.51930000	-0.65732100
H	1.00862600	3.58306800	-0.57995100
H	1.62496000	2.35860200	-1.67463100
N	3.15883200	-0.25239100	0.71153500
C	2.14325200	-2.43450400	1.03743100
H	1.58469700	-3.24513600	0.57217000
H	3.13285000	-2.79777400	1.31843500
H	1.61291600	-2.12696800	1.94330300
H	2.78334000	-1.59244300	-0.82851100
H	2.82002500	-0.07073000	1.65255300
C	2.36612100	2.18527800	0.34834600
H	2.98106200	3.08277400	0.45657500
H	1.92630700	2.00473500	1.33676100
C	3.32857900	1.02017800	-0.00119600
H	3.28706200	0.80968300	-1.07463700
H	4.34630200	1.36216500	0.20549600

HF: -723.9887872
Sum of electronic and zero-point Energies: -723.700338
Sum of electronic and thermal Energies: -723.683171
Sum of electronic and thermal Enthalpies: -723.682227
Sum of electronic and thermal Free Energies: -723.746086
Frequencies: -480.2958

X = NH_2^+, Y = CH_2

C	0.94651900	-0.69092500	-0.35598500
C	0.18036000	0.26703500	-0.51499900
C	-2.58359400	-0.33106100	0.08155200
N	-1.23636100	-1.82597000	-1.17241600
N	-0.32674400	-2.47575800	-0.97389300
O	-2.52899800	-1.04444600	1.07487000
N	-3.33948000	0.77779100	0.00268300
H	-3.38053300	1.29687800	-0.86048300
C	-4.11972500	1.23130200	1.14225500
H	-3.46532200	1.48446000	1.97824600
H	-4.68243500	2.11319400	0.84653300
H	-4.81193200	0.45183500	1.46296600
C	-1.73110700	-0.58744900	-1.12021100
H	-1.98111500	-0.15966700	-2.08549400
C	-0.08504100	1.72403100	-0.48042500
H	-0.80086800	2.01224000	-1.25324700
H	-0.54627000	1.97298700	0.48204700
C	2.22242500	-1.27924500	0.05101800
C	1.20256700	2.53330000	-0.67264700
H	0.94035500	3.59016800	-0.58388500
H	1.57026700	2.38710500	-1.69277500
N	3.03655600	-0.19706500	0.75038600
C	2.10542300	-2.46455200	1.00166100
H	1.61611900	-3.28639600	0.48317100
H	3.09120900	-2.80106400	1.32725200
H	1.50457400	-2.19973900	1.87412000
H	2.81346800	-1.55458200	-0.82575500
H	2.56691200	0.03168200	1.63214200
C	2.33337100	2.23502600	0.32052200
H	2.96282300	3.12462000	0.37803400
H	1.92552600	2.09948900	1.32852500
H	3.93850900	-0.60311600	1.01299600
C	3.27904500	1.07583100	-0.03017200
H	4.30488300	1.35523900	0.19933000
H	3.22656100	0.80749400	-1.08541400

HF: -724.443706
Sum of electronic and zero-point Energies: -724.139260
Sum of electronic and thermal Energies: -724.122202
Sum of electronic and thermal Enthalpies: -724.121258
Sum of electronic and thermal Free Energies: -724.184636
Frequencies: -464.9747

X = O, Y = CH_2

C	0.97626400	-0.67060800	-0.31161000
C	0.20430300	0.27814800	-0.48479400
C	-2.58967600	-0.35238800	0.06338000
N	-1.19936900	-1.85159900	-1.14151700
N	-0.27042300	-2.47308900	-0.92845300
O	-2.57615500	-1.06318600	1.06183700
N	-3.32251600	0.77309800	-0.03183800
H	-3.30888100	1.30836100	-0.88590400
C	-4.10151200	1.25542000	1.09580300
H	-3.45057800	1.51217300	1.93403900
H	-4.65031300	2.14062100	0.78357300
H	-4.80769100	0.49145600	1.42351800
C	-1.72477700	-0.62660900	-1.11767500
H	-1.95604400	-0.21244000	-2.09287500
C	-0.05737000	1.73406500	-0.45037400
H	-0.76435200	2.03373100	-1.22832900
H	-0.52355400	1.98691100	0.50907000
C	2.28932400	-1.21464800	0.09135900
C	1.24711800	2.52469600	-0.62410500
H	1.00494600	3.58572100	-0.51498900
H	1.60646800	2.39167300	-1.65014000
C	2.19189800	-2.37339400	1.07148800
H	1.68267900	-3.21894200	0.61053000
H	3.19403400	-2.68157500	1.37255300
H	1.63344800	-2.06427300	1.95743700
H	2.82025500	-1.54457800	-0.81334400
C	2.37672000	2.16813600	0.35485400
H	3.01891400	3.04877100	0.44166800
H	1.97036400	1.98634300	1.35551400
C	3.29054100	0.98252100	-0.01745200
H	3.22244900	0.76284300	-1.08978600
H	4.32555300	1.25698700	0.19672400
O	3.06508800	-0.20615000	0.73543300

HF: -743.8592904
Sum of electronic and zero-point Energies: -743.583324
Sum of electronic and thermal Energies: -743.566423
Sum of electronic and thermal Enthalpies: -743.565479
Sum of electronic and thermal Free Energies: -743.628500
Frequencies: -464.1100

X = CH_2, Y = O

C	0.99509500	-0.65698800	-0.29742200
C	0.20049300	0.27364200	-0.47264100
C	-2.59711700	-0.36968400	0.06210500
N	-1.19012800	-1.85621400	-1.14352200
N	-0.24652700	-2.45922200	-0.93096500
O	-2.59248700	-1.08678000	1.05655900
N	-3.32665500	0.75899200	-0.02953000
H	-3.30333100	1.30146600	-0.87880900
C	-4.10741400	1.23899300	1.09768000
H	-3.45851300	1.49226500	1.93866500
H	-4.65419700	2.12602200	0.78698400
H	-4.81568900	0.47520400	1.42118900
C	-1.72509800	-0.63556600	-1.11383000
H	-1.95050800	-0.21421400	-2.08731000
C	-0.06635700	1.72811400	-0.43132400
H	-0.74534100	2.05123500	-1.22609400
H	-0.54297800	1.98632300	0.52019000
C	2.31256400	-1.21944000	0.07344900
C	1.25051500	2.49800800	-0.57760600
H	1.06149900	3.56493600	-0.43189400
H	1.64571600	2.35708100	-1.58916000
C	2.20731800	-2.42635400	1.01072600
H	1.68513000	-3.25564900	0.53467200
H	3.20586100	-2.76322400	1.29887500
H	1.66415400	-2.15090300	1.91866300
H	2.80286000	-1.54451400	-0.85286300
C	3.24078900	1.20428800	-0.02863400
H	3.18439300	1.03795000	-1.11032400
H	4.19296500	1.69895900	0.18365100

O	2.21101400	2.10317700	0.38207200
C	3.18761700	-0.12639300	0.71862400
H	4.20482600	-0.52065800	0.81156700
H	2.82767400	0.06994600	1.73431400

HF: -743.8589275
Sum of electronic and zero-point Energies: -743.582632
Sum of electronic and thermal Energies: -743.565787
Sum of electronic and thermal Enthalpies: -743.564842
Sum of electronic and thermal Free Energies: -743.627717
Frequencies: -479.9207

X = CH_2, Y = NH

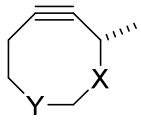
C	0.98005100	-0.67400300	-0.30786300
C	0.20092100	0.27033400	-0.48076000
C	-2.59850700	-0.35172600	0.06506000
N	-1.21654500	-1.84226900	-1.16293300
N	-0.27663000	-2.45362900	-0.95467500
O	-2.59400700	-1.07723200	1.05358300
N	-3.32020500	0.78319000	-0.01240200
H	-3.29493300	1.33422400	-0.85610700
C	-4.08812200	1.26096000	1.12444000
H	-3.43041400	1.51052200	1.95975500
H	-4.63696600	2.14968900	0.82237500
H	-4.79397000	0.49699700	1.45258600
C	-1.73624300	-0.61485000	-1.11860700
H	-1.96536900	-0.18218900	-2.08622300
C	-0.05091600	1.72652400	-0.45194700
H	-0.74859900	2.03984500	-1.23455000
H	-0.51462000	1.99648400	0.50423300
C	2.28428600	-1.25337300	0.07767300
C	1.26337000	2.51018900	-0.63281700
H	1.01945600	3.57599900	-0.56584800
H	1.64144600	2.33581500	-1.64369900
C	2.15014900	-2.47092000	0.99789200
H	1.62872200	-3.28953300	0.50297800
H	3.13973300	-2.82140400	1.30032000
H	1.59277600	-2.20120900	1.89911400
H	2.79210700	-1.57022100	-0.84212400
C	3.30614000	1.15175300	-0.00645700
H	3.27647000	0.96472500	-1.08473800
H	4.30740800	1.53829200	0.21167800
N	2.33971100	2.21363600	0.29980000
H	1.99532600	2.13542300	1.25003300
C	3.15133900	-0.17575500	0.75469600
H	4.14540700	-0.60686900	0.91483900
H	2.73895000	0.02997200	1.75033000

HF: -723.9884558
Sum of electronic and zero-point Energies: -723.699820
Sum of electronic and thermal Energies: -723.682699
Sum of electronic and thermal Enthalpies: -723.681754
Sum of electronic and thermal Free Energies: -723.745219
Frequencies: -484.8782

X = CH_2, Y = NH_2^+

C	0.98635900	-0.65714100	-0.29163200
C	0.18061500	0.26308800	-0.49272500
C	-2.59591900	-0.38791700	0.06634900
N	-1.16790200	-1.86978400	-1.12265700
N	-0.21422700	-2.44987800	-0.89310100
O	-2.55970800	-1.08125500	1.07501000
N	-3.36278100	0.71156700	-0.05064000
H	-3.39909200	1.20711300	-0.92776300
C	-4.18508300	1.16922800	1.05722400
H	-3.56164500	1.42699700	1.91516900
H	-4.73672700	2.04970600	0.73720400
H	-4.88880800	0.39142200	1.35720000
C	-1.70712200	-0.64801200	-1.10518100
H	-1.94783000	-0.24893300	-2.08536100
C	-0.14089000	1.71088900	-0.47625300
H	-0.77083300	2.00016600	-1.32007600
H	-0.70799000	1.94971200	0.42996400
C	2.29712600	-1.25966800	0.04553800
C	1.12102700	2.56824800	-0.54221000
H	0.89828100	3.60022900	-0.27854000
H	1.57118200	2.54540600	-1.53244200
C	2.18942500	-2.41231600	1.04879000
H	1.61419900	-3.24146700	0.64043200
H	3.18781700	-2.77432900	1.30407200
H	1.70437900	-2.06880000	1.96587500
H	2.71354300	-1.65192800	-0.88977600
C	3.23678200	1.13949000	-0.13653000
H	4.17992600	1.67051900	-0.03264800
H	3.02487700	1.01116600	-1.19665900
N	2.16679500	2.06773900	0.42447700
H	1.69117500	1.59177700	1.19722100
C	3.27450500	-0.19716500	0.59098800
H	4.29006700	-0.59265700	0.51817400
H	3.08833000	-0.03844400	1.65960800
H	2.63267100	2.87253400	0.84557600

HF: -724.4427056
Sum of electronic and zero-point Energies: -724.137842
Sum of electronic and thermal Energies: -724.120785
Sum of electronic and thermal Enthalpies: -724.119840
Sum of electronic and thermal Free Energies: -724.183666
Frequencies: -491.6439



+diazoacetamide (*syn*-TSs)

X = CH_2, Y = CH_2

C	-0.37980900	0.09928400	0.26226200
C	-1.08643800	1.09351000	0.05845000
C	2.53350800	0.44228700	-0.19336400
N	1.19132700	2.18532100	0.71050900
N	0.28146900	2.79697900	0.39466400
O	2.59443500	0.97334600	-1.29727400
N	3.21383100	-0.67870300	0.11987300
H	3.15390600	-1.05651000	1.05264400
C	4.01378400	-1.37099200	-0.87593100
H	4.77714800	-0.70498000	-1.28068100
H	4.49467700	-2.22296500	-0.40132800
H	3.38613000	-1.72249500	-1.69762600
C	1.63261500	0.93457100	0.88048000
C	-2.33924700	1.77528600	-0.30849300
H	-2.47035400	2.68605300	0.28239400
H	-2.26719200	2.09585400	-1.35425100
C	-0.20822900	-1.37338600	0.28217200
C	-3.55452900	0.85538300	-0.13327200
H	-4.43363800	1.39970000	-0.49152200
H	-3.71349900	0.67393300	0.93501000
H	1.81017300	0.66501800	1.91581300
C	-0.12915200	-1.91395200	1.71496600
H	0.00623900	-2.99778900	1.70016300
H	0.70881000	-1.47389900	2.25960000
H	-1.04078500	-1.68597800	2.27143700
H	0.73024300	-1.63289400	-0.22036900
C	-2.78247600	-1.66220000	-0.11195300
H	-2.82310100	-1.46642800	0.96481500
H	-3.39798700	-2.55128400	-0.27100400
C	-3.45861100	-0.49160100	-0.86845600
H	-4.48011800	-0.80079800	-1.10494300
H	-2.96141100	-0.34027800	-1.83413100
C	-1.34534100	-2.03295500	-0.52472900
H	-1.21211900	-3.11621300	-0.43271900
H	-1.20544000	-1.79141200	-1.58322200

HF: -707.9518526
Sum of electronic and zero-point Energies: -707.652206
Sum of electronic and thermal Energies: -707.634919
Sum of electronic and thermal Enthalpies: -707.633975
Sum of electronic and thermal Free Energies: -707.697753
Frequencies: -482.1961

X = NH, Y = CH_2

C	-0.39591700	0.11498600	0.29532000
C	-1.10234500	1.10688800	0.08322100
C	2.51060200	0.43862900	-0.20037000
N	1.18649200	2.18818100	0.71614000
N	0.28115000	2.80918700	0.40802800
O	2.55120600	0.96329500	-1.30772700
N	3.19274900	-0.68284900	0.10670400
H	3.16305700	-1.04602100	1.04667000
C	3.98038900	-1.37730100	-0.89766900
H	4.74476300	-0.71571500	-1.30783700
H	4.45915800	-2.23377500	-0.42930100
H	3.34281000	-1.72263600	-1.71401400
C	1.62939200	0.93962600	0.88715900
C	-2.35740400	1.76855700	-0.30685600
H	-2.52781400	2.66632400	0.29357400
H	-2.26609800	2.10514900	-1.34585900
C	-0.23835600	-1.36757900	0.29684200
C	-3.54751600	0.80915200	-0.17456700
H	-4.43398200	1.31954700	-0.56257300
H	-3.73617500	0.61986300	0.88751300
H	1.81939000	0.67393900	1.92123200
C	-0.13938000	-1.92125200	1.72012700
H	-0.01340100	-3.00423300	1.68316600
H	0.71145500	-1.48635200	2.24769700
H	-1.03776100	-1.68985600	2.29570500
H	0.68879800	-1.62687200	-0.22389300
H	-1.15283800	-1.89026600	-1.44435900
C	-2.69709100	-1.69013000	-0.12337400
H	-2.75608100	-1.49120700	0.95000300
H	-3.28964900	-2.59245300	-0.29702700
C	-3.37353400	-0.53302900	-0.90517200
H	-4.37063800	-0.88238700	-1.18592300
H	-2.83789700	-0.37117000	-1.84845900
N	-1.30750200	-2.03873700	-0.45265300

HF: -723.988643
Sum of electronic and zero-point Energies: -723.700130
Sum of electronic and thermal Energies: -723.682943
Sum of electronic and thermal Enthalpies: -723.681999
Sum of electronic and thermal Free Energies: -723.745585
Frequencies: -471.1592

X = NH_2^+, Y = CH_2

C	-0.34888800	0.12884600	0.30403400
C	-1.07025200	1.10267200	0.06103600
C	2.53319900	0.43630900	-0.19162800
N	1.19810500	2.16169200	0.75277800
N	0.30247900	2.78697600	0.43263200
O	2.53596400	0.96295000	-1.29559000

N	3.23314000	-0.67628700	0.10472800
H	3.30473100	-0.97928000	1.06420700
C	4.06397100	-1.32153500	-0.89950600
H	4.89463800	-0.67697900	-1.19377100
H	4.45430500	-2.24619200	-0.48136000
H	3.46733900	-1.54993400	-1.78316100
C	1.64964700	0.91674200	0.91241700
C	-2.30838800	1.78238800	-0.35077100
H	-2.43535900	2.71447900	0.20427400
H	-2.21147700	2.05985600	-1.40606500
C	-0.19255000	-1.33317800	0.29705700
C	-3.53833400	0.88794800	-0.15351800
H	-4.40519500	1.42323800	-0.54812900
H	-3.71611200	0.74984200	0.91734500
H	1.84564900	0.64192700	1.94332500
C	-0.15594600	-1.97490100	1.67817900
H	-0.12025400	-3.06272300	1.60002800
H	0.74684700	-1.64495300	2.19151400
H	-1.01057800	-1.67923100	2.28626100
H	0.69978600	-1.62935700	-0.26121300
H	-1.23081000	-1.55771800	-1.48445400
H	-1.21865400	-2.91572600	-0.58094400
C	-2.75471400	-1.60496500	-0.06305700
H	-2.70425800	-1.38871400	1.00248400
H	-3.29108600	-2.54245300	-0.19210300
C	-3.46986100	-0.48505000	-0.83417400
H	-4.49414800	-0.83435500	-0.97552000
H	-3.05212100	-0.39085500	-1.84309400
N	-1.34204800	-1.90182700	-0.52661200

HF: -724.4425452
Sum of electronic and zero-point Energies: -724.137743
Sum of electronic and thermal Energies: -724.120825
Sum of electronic and thermal Enthalpies: -724.119881
Sum of electronic and thermal Free Energies: -724.182311
Frequencies: -460.1053

X = O, Y = CH_2

C	-0.40037300	0.10806100	0.27573400
C	-1.11419800	1.09350400	0.06497500
C	2.50246600	0.45203100	-0.18384300
N	1.15955600	2.16152700	0.77630900
N	0.26212000	2.79345100	0.47127300
O	2.54388700	1.01398300	-1.27179400
N	3.18324300	-0.67884200	0.08807100
H	3.17502900	-1.05750500	1.02240000
C	3.99203800	-1.32658800	-0.93082500
H	4.80897300	-0.67649500	-1.24907700
H	4.40301400	-2.24265100	-0.51363600
H	3.38028500	-1.57090700	-1.80072200
C	1.61362500	0.91517900	0.91678100
C	-2.36257700	1.75191000	-0.35262700
H	-2.53550900	2.66505000	0.22249200
H	-2.25547600	2.05973100	-1.39875000
C	-0.24217700	-1.36581200	0.22467200
C	-3.56171100	0.80337900	-0.21019100
H	-4.43421900	1.30011300	-0.64383200
H	-3.77981600	0.66251700	0.85380900
H	1.79638700	0.62064900	1.94427100
C	-0.07034100	-2.00085900	1.60406300
H	-0.01329200	-3.08527800	1.49812700
H	0.85041400	-1.65039900	2.07287900
H	-0.89884600	-1.74844800	2.26756900
H	0.63439000	-1.61500700	-0.38048000
C	-2.64657600	-1.64678500	-0.04527000
H	-2.63626600	-1.36689000	1.01274300
H	-3.19037600	-2.59008000	-0.12628700
C	-3.38179500	-0.57188300	-0.87190100
H	-4.37829300	-0.96260200	-1.09450600
H	-2.87094200	-0.46750100	-1.83486200
O	-1.32640900	-1.94899300	-0.49709700

HF: -743.8579101
Sum of electronic and zero-point Energies: -743.581877
Sum of electronic and thermal Energies: -743.564930
Sum of electronic and thermal Enthalpies: -743.563985
Sum of electronic and thermal Free Energies: -743.626913
Frequencies: -459.5361

X = CH_2, Y = O

C	-0.39648200	0.10410500	0.22966300
C	-1.09140600	1.10570500	0.02705700
C	2.52453100	0.43886600	-0.17414200
N	1.17722500	2.18023500	0.72649500
N	0.28316200	2.81044000	0.40703100
O	2.60737000	0.98231400	-1.27027600
N	3.18132900	-0.69704900	0.13477200
H	3.11665300	-1.07503200	1.06719500
C	3.99613700	-1.38329700	-0.85303800
H	4.82495600	-0.75143300	-1.17666100
H	4.39166200	-2.29094200	-0.40362200
H	3.39580200	-1.64657300	-1.72566100
C	1.61659800	0.93045000	0.89378200
C	-2.35878600	1.74566300	-0.35923200
H	-2.55659200	2.64648400	0.22908200
H	-2.30404900	2.05572200	-1.40757300
C	-0.23875700	-1.37114500	0.23587700
C	-3.51462100	0.75751200	-0.17162300
H	-4.43551800	1.19477400	-0.56614700
H	-3.65942600	0.56254500	0.89641900
H	1.77532900	0.65166400	1.92945000
C	-0.13349500	-1.92462200	1.66204300
H	-0.00587700	-3.00894400	1.63554400
H	0.71777100	-1.49455800	2.19293800
H	-1.03196300	-1.69525300	2.23970500
H	0.68325800	-1.63671700	-0.29272000
C	-1.40794300	-2.01372400	-0.54060800
H	-1.30023300	-1.79928900	-1.60742300
H	-1.33020700	-3.09966000	-0.42288300
C	-2.81386100	-1.57617300	-0.12109200
H	-2.85292000	-1.35382000	0.95049600
H	-3.51092700	-2.39658700	-0.31275700
O	-3.29502200	-0.45703900	-0.86417200

HF: -743.8591132
Sum of electronic and zero-point Energies: -743.582780
Sum of electronic and thermal Energies: -743.565909
Sum of electronic and thermal Enthalpies: -743.564965
Sum of electronic and thermal Free Energies: -743.627542
Frequencies: -466.1571

X = CH_2, Y = NH

C	-0.38580700	0.11091400	0.23118700
C	-1.08229100	1.11040400	0.02365700
C	2.53629800	0.43532500	-0.17650000
N	1.19293000	2.18784600	0.70895400
N	0.29748800	2.81452200	0.38502500
O	2.62102200	0.96839300	-1.27781700
N	3.19168400	-0.69858200	0.14315700
H	3.12469400	-1.06848500	1.07865600
C	4.00444600	-1.39632600	-0.83817600
H	4.83528100	-0.77001400	-1.16750500
H	4.39727900	-2.30100200	-0.38039700
H	3.40339500	-1.66574700	-1.70850100
C	1.62793900	0.93722600	0.88571000
C	-2.34857500	1.75698500	-0.34985100
H	-2.51277500	2.67808900	0.21742100
H	-2.30667500	2.04651700	-1.40601900
C	-0.22947800	-1.36273200	0.23851000
C	-3.53495700	0.80061200	-0.12267300
H	-4.44360000	1.31646900	-0.45130400
H	-3.64349600	0.61998800	0.95022000
H	1.78520800	0.66593700	1.92362700
C	-0.13228100	-1.91807700	1.66426400
H	-0.01887400	-3.00412900	1.63764800
H	0.72555200	-1.49983300	2.19448200
H	-1.02691800	-1.67647000	2.24247100
H	0.69629300	-1.62889900	-0.28394300
C	-1.38991500	-2.00199600	-0.55135200
H	-1.27643400	-1.75187300	-1.61158200
H	-1.27571700	-3.08882800	-0.47473100
N	-3.46283600	-0.49368600	-0.78473800
H	-3.14204800	-0.40185200	-1.74216500
C	-2.81997200	-1.62873400	-0.11217000
H	-2.85031300	-1.43862700	0.96455000
H	-3.44632100	-2.51068800	-0.28280900

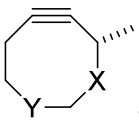
HF: -723.9887489
Sum of electronic and zero-point Energies: -723.700388
Sum of electronic and thermal Energies: -723.683159
Sum of electronic and thermal Enthalpies: -723.682215
Sum of electronic and thermal Free Energies: -723.745720
Frequencies: -471.4718

X = CH_2, Y = NH_2^+

C	-0.36335900	0.08747000	0.34366000
C	-1.06311100	1.09005400	0.14724200
C	2.51331000	0.42363800	-0.22190200
N	1.20953100	2.14427100	0.76875000
N	0.30625400	2.77692800	0.48273900
O	2.51617600	0.97721300	-1.31441300
N	3.22244900	-0.68898900	0.04556800
H	3.24264800	-1.05787000	0.98384600
C	4.02609200	-1.32712900	-0.98391600
H	4.81897100	-0.65907700	-1.32491500
H	4.46857300	-2.22813600	-0.56648100
H	3.40283400	-1.59469600	-1.83844100
C	1.64060800	0.88515400	0.89725700
C	-2.29368100	1.79563700	-0.24525900
H	-2.52666000	2.60511100	0.44990900
H	-2.14711900	2.26203700	-1.22458000
C	-0.21498900	-1.38882100	0.42618300
C	-3.49253400	0.85205600	-0.29125300
H	-4.32667100	1.31132900	-0.81823400
H	-3.81902300	0.56491400	0.70587700
H	1.85634200	0.59255200	1.91942000
C	-0.26602300	-1.86056700	1.88516100
H	-0.12961900	-2.94266000	1.93369100
H	0.52067200	-1.38862600	2.47561800
H	-1.22250300	-1.60822900	2.34862100
H	0.75193500	-1.68633900	0.01053200
C	-1.29300800	-2.07753700	-0.43316100
H	-1.05723900	-1.95640000	-1.49491100
H	-1.25269600	-3.15136800	-0.23486000
N	-3.14456700	-0.42536700	-1.02205900
H	-2.40180400	-0.22132400	-1.69773500
H	-3.95300000	-0.70160200	-1.58068000
C	-2.72658600	-1.62152500	-0.17426600
H	-2.88439500	-1.33947200	0.86530700
H	-3.42664000	-2.41632300	-0.42013800

HF: -724.443327
Sum of electronic and zero-point Energies: -724.138307
Sum of electronic and thermal Energies: -724.121298
Sum of electronic and thermal Enthalpies: -724.120354

Sum of electronic and thermal Free Energies: -724.183716
Frequencies: -479.7435



+azidoacetamide (*anti*-TSs)

X = CH_2, Y = CH_2

C	-1.19446500	0.75493700	-0.33095100
C	-0.55324100	-0.20997200	-0.75450500
N	0.97367700	1.83278900	-1.28489300
N	0.12623000	2.48576000	-0.86928700
C	-0.31257900	-1.64063400	-1.01636200
H	0.16547100	-1.78149500	-1.98908300
H	0.38447100	-2.02752700	-0.26294900
C	-2.36961100	1.33627800	0.35767800
C	-1.62640400	-2.43432400	-0.96398400
H	-1.37177300	-3.49503000	-1.04507800
H	-2.22463700	-2.18701000	-1.84697300
C	-2.01305300	2.46690500	1.32608600
H	-1.57781500	3.31828900	0.80503800
H	-2.91033900	2.79987300	1.85332900
H	-1.29151400	2.11294700	2.06768600
H	-3.03809600	1.73873800	-0.41362900
N	1.22442300	0.65824100	-1.63951900
C	2.52988600	0.08956400	-1.33072200
H	2.53300800	-0.90840800	-1.76807300
H	3.33007700	0.66554500	-1.80430400
C	2.78873700	0.04765900	0.17375800
O	2.54203500	1.01779200	0.87883400
N	3.31335100	-1.09285700	0.64799500
C	3.65217900	-1.24084500	2.05411100
H	4.12604800	-2.20885800	2.19727600
H	4.34020000	-0.45242800	2.36196600
H	2.75522500	-1.18347200	2.67343800
H	3.46867100	-1.86643700	0.02057200
C	-3.12188500	0.21758000	1.10385500
H	-4.04093600	0.66065500	1.50127600
H	-2.52072700	-0.07970800	1.97138600
C	-2.47038300	-2.20727600	0.30115200
H	-3.03942300	-3.12357600	0.47729100
H	-1.80141800	-2.10128100	1.16339000
C	-3.47540700	-1.02706400	0.27169600
H	-3.65652900	-0.72547900	-0.76654600
H	-4.43264700	-1.40205100	0.64238300

HF: -763.285372
Sum of electronic and zero-point Energies: -762.967816
Sum of electronic and thermal Energies: -762.949520
Sum of electronic and thermal Enthalpies: -762.948576
Sum of electronic and thermal Free Energies: -763.015709
Frequencies: -457.9865

X = NH, Y = CH_2

C	1.17592700	-0.75273400	-0.32518900
C	0.53656500	0.20514800	-0.76590700
N	-0.97973400	-1.84755900	-1.27503800
N	-0.14144200	-2.50468400	-0.85108800
C	0.31839300	1.63568000	-1.04198400
H	-0.14819700	1.77808400	-2.01990700
H	-0.37541900	2.04280500	-0.29652700
C	2.36293900	-1.29763700	0.38851700
C	1.65305800	2.39370600	-0.98328100
H	1.43374700	3.46150800	-1.07082400
H	2.25063800	2.12414200	-1.86019700
N	3.12233500	-0.24331900	1.07081000
C	2.00265700	-2.37443200	1.40850800
H	1.52287400	-3.22314200	0.92455500
H	2.90641000	-2.71286400	1.91739600
H	1.31101100	-1.96933800	2.15303600
H	3.02706600	-1.73803700	-0.36443300
N	-1.23188900	-0.67953000	-1.64697900
C	-2.53334300	-0.10292300	-1.33190700
H	-2.53845100	0.88817800	-1.78455100
H	-3.33934200	-0.68498400	-1.78763000
C	-2.77274300	-0.03907400	0.17500700
O	-2.53088500	-1.00478600	0.88793100
N	-3.27257100	1.11537900	0.64228000
C	-3.58738900	1.28678800	2.05134500
H	-4.03704200	2.26696600	2.18985700
H	-4.28882900	0.51825500	2.37914700
H	-2.68242900	1.21595200	2.65753000
H	-3.42834900	1.88213900	0.00678400
H	2.60709000	0.04050400	1.90021000
C	2.47939800	2.14417300	0.28955400
H	3.07178300	3.04356400	0.47592400
H	1.80543900	2.04697300	1.14909200
C	3.46537700	0.94401900	0.27666700
H	3.64028100	0.61488300	-0.75259100
H	4.42688500	1.30441400	0.65181300

HF: -779.3223608
Sum of electronic and zero-point Energies: -779.015810
Sum of electronic and thermal Energies: -778.997694
Sum of electronic and thermal Enthalpies: -778.996750
Sum of electronic and thermal Free Energies: -779.063191
Frequencies: -448.1957

X = NH_2^+, Y = CH_2

C	-1.21804500	0.67051700	-0.38473500
C	-0.63656800	-0.39723800	-0.58738900
N	0.95126500	1.41835200	-1.51114800
N	0.16421900	2.20517700	-1.24428300
C	-0.50877700	-1.86494800	-0.55194300
H	0.02924200	-2.22759300	-1.42980900
H	0.08069900	-2.14734200	0.32725400
C	-2.33388100	1.44124200	0.16593700
C	-1.89336700	-2.52583700	-0.49633600
H	-1.74096700	-3.59906700	-0.36276400
H	-2.38947500	-2.39695400	-1.46275200
N	-3.17971800	0.48825800	1.00120800
C	-1.93052500	2.61439600	1.05013500
H	-1.41278700	3.35234500	0.44120700
H	-2.81014800	3.08386500	1.49365900
H	-1.25498700	2.28435200	1.84182200
H	-2.99651100	1.77896100	-0.63449300
N	1.13359800	0.18766900	-1.61027700
C	2.43973200	-0.37154800	-1.30484400
H	2.34164000	-1.45121500	-1.42106300
H	3.18262600	-0.03115800	-2.03221700
C	2.91998200	-0.01647300	0.10343300
O	2.45056700	0.93264700	0.71461000
N	3.90000300	-0.79587100	0.58418600
C	4.50569000	-0.53527300	1.88065500
H	5.30142600	-1.25818600	2.04227100
H	4.92166600	0.47279900	1.91042300
H	3.76455400	-0.63222300	2.67565000
H	4.23147800	-1.57339400	0.03399400
H	-2.63952400	0.23323900	1.83367700
C	-2.82301900	-2.02740300	0.61870400
H	-3.54021500	-2.82256500	0.82809000
H	-2.25980500	-1.89021100	1.54870800
H	-3.98990600	1.01048900	1.34433500
C	-3.66014100	-0.77231500	0.31478300
H	-3.69645600	-0.54875200	-0.75140300
H	-4.67912600	-0.91439200	0.66832900

HF: -779.7767943
Sum of electronic and zero-point Energies: -779.454788
Sum of electronic and thermal Energies: -779.436644
Sum of electronic and thermal Enthalpies: -779.435700
Sum of electronic and thermal Free Energies: -779.502626
Frequencies: -426.6101

X = O, Y = CH_2

C	-1.17240900	0.75279300	-0.32720100
C	-0.53447700	-0.20749000	-0.76111600
N	0.97205100	1.84756700	-1.27282700
N	0.14733000	2.51739400	-0.84666200
C	-0.32042200	-1.64173300	-1.01834800
H	0.15176200	-1.79888000	-1.99110000
H	0.36450700	-2.04304400	-0.26203200
C	-2.34882800	1.27238900	0.40377600
C	-1.66237700	-2.38842100	-0.96292100
H	-1.45027800	-3.45877600	-1.03181300
H	-2.24677900	-2.12758900	-1.85143000
C	-2.00648500	2.31032100	1.45941200
H	-1.57064200	3.19369000	0.99493600
H	-2.91244100	2.59594500	1.99569700
H	-1.28811000	1.89472100	2.16916300
H	-3.04607900	1.70726200	-0.32614600
N	1.22185500	0.68232600	-1.65050500
C	2.52193500	0.09988200	-1.33836000
H	2.52083100	-0.89147400	-1.79017900
H	3.32815700	0.67818100	-1.79807600
C	2.76447500	0.03776700	0.16817100
O	2.51868000	1.00301900	0.88004200
N	3.27085600	-1.11356100	0.63489000
C	3.59001200	-1.28206600	2.04345500
H	4.04089600	-2.26162500	2.18243000
H	4.29152800	-0.51221500	2.36761300
H	2.68670400	-1.21097300	2.65194700
H	3.42887000	-1.88028100	-0.00031500
C	-2.50827400	-2.12105400	0.29246100
H	-3.14671400	-2.99483700	0.44730800
H	-1.86583100	-2.05237000	1.17671200
C	-3.43489900	-0.88562300	0.27090400
H	-3.59820900	-0.54096900	-0.75732300
H	-4.40665200	-1.17106900	0.67876600
O	-3.00563800	0.20418500	1.08347800

HF: -799.1925188
Sum of electronic and zero-point Energies: -798.898790
Sum of electronic and thermal Energies: -798.880825
Sum of electronic and thermal Enthalpies: -798.879881
Sum of electronic and thermal Free Energies: -798.946183
Frequencies: -436.9358

X = CH_2, Y = O

C	-1.18026300	0.74163800	-0.32186000
C	-0.52699300	-0.20644000	-0.76069800
N	0.97795600	1.84705300	-1.27859300
N	0.13854700	2.50186500	-0.85427700
C	-0.32251700	-1.64219400	-1.01509200
H	0.11484600	-1.82351800	-2.00081500
H	0.36579300	-2.05698100	-0.27096000
C	-2.35956800	1.28974500	0.38600300
C	-1.67898500	-2.35458400	-0.92906500
H	-1.52391900	-3.43573400	-0.96694700

H	-2.29423300	-2.06687500	-1.78785700
O	-2.35664500	-2.06355000	0.27829200
C	-2.01095100	2.39207900	1.38881900
H	-1.57495300	3.25779400	0.89235000
H	-2.91097900	2.70881600	1.92119100
H	-1.29204700	2.01797100	2.12288600
H	-3.03379600	1.71008000	-0.37024500
N	1.23993400	0.68216300	-1.65236600
C	2.54399100	0.11477100	-1.32852600
H	2.56239600	-0.87329200	-1.78711600
H	3.34831900	0.70736900	-1.77317100
C	2.76942200	0.04485900	0.18014000
O	2.52643200	1.00971300	0.89371800
N	3.25704300	-1.11424500	0.64842300
C	3.55478000	-1.29349900	2.06021700
H	3.99253600	-2.27881900	2.20025500
H	4.26053900	-0.53356000	2.39826400
H	2.64401800	-1.21514400	2.65651600
H	3.41556500	-1.87940800	0.01156900
C	-3.09799200	0.13983400	1.09927300
H	-4.04136400	0.53642000	1.48889300
H	-2.50621800	-0.18311300	1.96255300
C	-3.40271700	-1.09204300	0.24638600
H	-3.61165700	-0.80013000	-0.78904900
H	-4.29674200	-1.58402200	0.63970900

HF: -799.1922317
Sum of electronic and zero-point Energies: -798.898337
Sum of electronic and thermal Energies: -798.880347
Sum of electronic and thermal Enthalpies: -798.879403
Sum of electronic and thermal Free Energies: -798.945980
Frequencies: -446.6966

X = CH_2, Y = NH

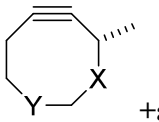
C	-1.17243400	0.75167100	-0.32026700
C	-0.52853200	-0.21058900	-0.74235500
N	0.98878100	1.82926600	-1.29929900
N	0.15132200	2.49173000	-0.88135300
C	-0.32571400	-1.64772600	-0.98408300
H	0.15204000	-1.83083200	-1.95066400
H	0.34103900	-2.05779700	-0.21610200
C	-2.34491800	1.32153100	0.37912700
C	-1.68257800	-2.38112700	-0.94536800
H	-1.48059600	-3.45319800	-1.03951400
H	-2.26384100	-2.09006200	-1.82406700
C	-1.98041900	2.42691400	1.37344400
H	-1.52702500	3.28021700	0.87092400
H	-2.87627800	2.76476400	1.89982800
H	-1.27044400	2.04701200	2.11338100
H	-3.01261900	1.74575600	-0.38091000
N	1.24102900	0.65624200	-1.65483000
C	2.54391500	0.08580400	-1.33410500
H	2.55137100	-0.90962400	-1.77689500
H	3.34871100	0.66530500	-1.79501900
C	2.78245100	0.03693100	0.17331300
O	2.54938600	1.01263700	0.87544400
N	3.27100900	-1.11689100	0.65381200
C	3.58158800	-1.27665900	2.06512800
H	4.02950600	-2.25621900	2.21339300
H	4.28322300	-0.50622300	2.38743700
H	2.67548400	-1.19914100	2.66873900
H	3.41634200	-1.89328800	0.02755100
C	-3.10079500	0.18821200	1.09918400
H	-4.02141700	0.61677900	1.50935400
H	-2.50235500	-0.13866200	1.95857300
N	-2.51240700	-2.15602800	0.22895000
H	-1.96441400	-2.18622600	1.08130000
C	-3.46877500	-1.04053000	0.24834800
H	-3.65401000	-0.73145300	-0.78546000
H	-4.42066800	-1.42504500	0.62944500

HF: -779.3219828
Sum of electronic and zero-point Energies: -779.015819
Sum of electronic and thermal Energies: -778.997552
Sum of electronic and thermal Enthalpies: -778.996608
Sum of electronic and thermal Free Energies: -779.063675
Frequencies: -451.1003

X = CH_2, Y = NH_2^+

C	-1.26182000	0.67523800	-0.33362700
C	-0.63096200	-0.34161300	-0.63632900
N	0.91011000	1.56482200	-1.40517100
N	0.07420000	2.27736600	-1.07322900
C	-0.43359700	-1.80145400	-0.70892400
H	-0.00444100	-2.10198100	-1.66654500
H	0.26618400	-2.12163700	0.07005400
C	-2.43437900	1.39879900	0.21278500
C	-1.76301000	-2.53590700	-0.54772700
H	-1.59606800	-3.59029100	-0.33775700
H	-2.38279000	-2.44484300	-1.43709100
C	-2.06303700	2.57257700	1.12217900
H	-1.52673600	3.34409300	0.57297100
H	-2.96953900	3.01074400	1.54541400
H	-1.43100700	2.22803400	1.94443000
H	-3.00005500	1.78594200	-0.64263300
N	1.13719500	0.35050500	-1.59871700
C	2.46220900	-0.18495900	-1.33673900
H	2.41150500	-1.24875800	-1.57023400
H	3.19876200	0.26020600	-2.01225300
C	2.91592700	0.03655200	0.10681300
O	2.44493600	0.93422200	0.79022800
N	3.87592700	-0.79523500	0.53993200
C	4.45556500	-0.65075300	1.86600300
H	5.22737100	-1.40605200	1.99157600
H	4.89770700	0.33978800	1.98307300
H	3.69180200	-0.78571400	2.63340500
H	4.21279100	-1.52676600	-0.06708300
C	-3.34505100	0.41862400	0.97921800
H	-4.30906200	0.90376900	1.14800900
H	-2.92317700	0.22814500	1.97327200
N	-2.56396400	-1.96825900	0.60192500
H	-3.03795300	-2.74059100	1.07172600
H	-1.91381900	-1.58670300	1.29562500
C	-3.60748600	-0.90592500	0.27077100
H	-3.60760200	-0.78736300	-0.81159600
H	-4.56378600	-1.32526600	0.57408200

HF: -779.7757724
Sum of electronic and zero-point Energies: -779.453197
Sum of electronic and thermal Energies: -779.435154
Sum of electronic and thermal Enthalpies: -779.434210
Sum of electronic and thermal Free Energies: -779.500890
Frequencies: -449.4383



+azidoacetamide (*syn*-TSs)

X = CH_2, Y = CH_2

C	-0.73407300	0.13445600	0.37020700
C	-1.35246300	1.09380800	-0.09124500
N	0.85080100	2.18601700	0.73010200
N	0.03416500	2.79227200	0.19561100
C	-2.50540900	1.69102400	-0.78612700
H	-2.75492100	2.66753100	-0.36337600
H	-2.22833500	1.86724600	-1.83138400
C	-0.51377700	-1.28501200	0.70098100
C	-3.72098500	0.75373700	-0.72171600
H	-4.50630600	1.18583800	-1.34898400
H	-4.10897800	0.74270000	0.30216000
N	1.05290800	1.07227700	1.26064600
C	2.37665000	0.47944400	1.19844700
H	3.13016800	1.15088200	1.62099000
H	2.34276100	-0.41258000	1.82475000
C	2.78842200	0.13096600	-0.23195500
O	2.42162100	0.81026500	-1.18068900
N	3.59583100	-0.93483000	-0.35635300
C	4.12638300	-1.33464800	-1.64965000
H	4.83738700	-2.14335900	-1.49942600
H	3.32521000	-1.67693500	-2.30725500
H	4.63248200	-0.49355800	-2.12516300
H	3.83878500	-1.47140500	0.46222100
C	-0.65438500	-1.53863000	2.20600400
H	-1.66680400	-1.30866900	2.54569700
H	-0.44273300	-2.58615700	2.43181600
H	0.03859200	-0.91066600	2.76929000
H	0.50194700	-1.57240600	0.40376000
C	-1.49685000	-2.13650700	-0.13302700
H	-1.15929900	-2.14266100	-1.17424300
H	-1.41425400	-3.16675800	0.22801000
C	-2.97232300	-1.69436100	-0.08861100
H	-3.20785000	-1.29115900	0.90214500
H	-3.57890100	-2.59781400	-0.18878000
C	-3.44155800	-0.69101400	-1.17569200
H	-4.36876800	-1.07980900	-1.60417500
H	-2.71688900	-0.67210900	-1.99829000

HF: -763.2865873
Sum of electronic and zero-point Energies: -762.969331
Sum of electronic and thermal Energies: -762.951006
Sum of electronic and thermal Enthalpies: -762.950062
Sum of electronic and thermal Free Energies: -763.017051
Frequencies: -447.1765

X = NH, Y = CH_2

C	-0.73480000	0.16650700	0.39663700
C	-1.34779400	1.11049900	-0.10123900
N	0.85494300	2.20893900	0.71284500
N	0.04487300	2.81245800	0.16725000
C	-2.49146200	1.66643600	-0.84207500
H	-2.78136600	2.64347000	-0.44775900
H	-2.18794000	1.82739400	-1.88229200
C	-0.53562200	-1.26043900	0.74574200
C	-3.67809900	0.69172100	-0.78835100
H	-4.45775700	1.07424600	-1.45337800
H	-4.09863600	0.69939100	0.22273800
N	1.05821700	1.10637100	1.26525300
C	2.37852000	0.50307900	1.18917500
H	3.14300900	1.18005500	1.58151900
H	2.35199100	-0.37447600	1.83555000
C	2.75684700	0.12535800	-0.24282700
O	2.42096900	0.82268200	-1.19010400
N	3.49618300	-0.98784900	-0.37041300
C	3.98785300	-1.42635800	-1.66674500
H	4.64994200	-2.27586800	-1.51793300
H	3.16038200	-1.72351300	-2.31365700
H	4.53882800	-0.62006600	-2.15240500
H	3.71139100	-1.53636000	0.44795400
C	-0.66624700	-1.49282300	2.25181200
H	-1.67196300	-1.24404300	2.59648500
H	-0.46555900	-2.54055900	2.47974700

H	0.03962200	-0.86275500	2.79566600
H	0.47159000	-1.56646500	0.44268400
H	-1.11629700	-2.21799800	-0.95669000
C	-2.87345000	-1.71347200	-0.04660200
H	-3.13003600	-1.28142100	0.92443100
H	-3.45563000	-2.63448900	-0.13198800
C	-3.33296300	-0.75658800	-1.18249600
H	-2.57686200	-0.74839400	-1.97666900
H	-4.22891300	-1.19678600	-1.62754600
N	-1.45996700	-2.12082400	-0.00690700

HF: -779.3227405
Sum of electronic and zero-point Energies: -779.016652
Sum of electronic and thermal Energies: -778.998436
Sum of electronic and thermal Enthalpies: -778.997492
Sum of electronic and thermal Free Energies: -779.064135
Frequencies: -439.3634

X = NH_2^+, Y = CH_2

C	-0.71547900	0.10861900	0.36678600
C	-1.29891700	1.10214900	-0.06493400
N	0.87951200	2.01988200	0.94110500
N	0.09558500	2.69679300	0.44803000
C	-2.40257400	1.79312800	-0.74927200
H	-2.58263600	2.77282900	-0.30273200
H	-2.10513500	1.96957200	-1.78813000
C	-0.59578400	-1.33379000	0.59217200
C	-3.68126700	0.94549700	-0.70291800
H	-4.43509800	1.44341400	-1.31676400
H	-4.06850200	0.93264700	0.32010600
N	1.05092000	0.85331100	1.35376700
C	2.36900600	0.24654700	1.25147800
H	3.10563300	0.83361200	1.80728000
H	2.30036400	-0.72717900	1.73799300
C	2.83932400	0.10685300	-0.19765800
O	2.40556300	0.83546900	-1.07797300
N	3.76876800	-0.83812500	-0.40539200
C	4.36950100	-1.03484700	-1.71548200
H	5.15529800	-1.78104500	-1.62700900
H	3.62366900	-1.38140300	-2.43293700
H	4.79784500	-0.09989500	-2.07901900
H	4.06963000	-1.41519100	0.36522900
C	-0.78686400	-1.75696600	2.04245000
H	-1.73859900	-1.40658400	2.44177900
H	-0.72228100	-2.84171600	2.14219200
H	0.00800200	-1.30546600	2.63573300
H	0.35961700	-1.71390700	0.22138300
H	-1.33811900	-1.87660100	-1.27500600
H	-1.58743900	-3.00982000	-0.12866600
C	-3.07256300	-1.54354100	-0.16671600
H	-3.19655000	-1.18126700	0.85223500
H	-3.66270800	-2.45078900	-0.27562400
C	-3.52347800	-0.49868600	-1.20277300
H	-2.86880100	-0.52440700	-2.08094300
H	-4.49865100	-0.83517300	-1.55806400
N	-1.63271000	-2.00259800	-0.30237400

HF: -779.7748509
Sum of electronic and zero-point Energies: -779.452838
Sum of electronic and thermal Energies: -779.434746
Sum of electronic and thermal Enthalpies: -779.433802
Sum of electronic and thermal Free Energies: -779.500028
Frequencies: -438.2956

X = O, Y = CH_2

C	-0.70840600	0.14858300	0.38924100
C	-1.29554700	1.10698100	-0.11000900
N	0.87719900	2.14580000	0.84051000
N	0.09047800	2.78482700	0.30354600
C	-2.39955500	1.69432400	-0.88586500
H	-2.66817500	2.68348900	-0.50831700
H	-2.05876400	1.83366200	-1.91738400
C	-0.56064400	-1.28808900	0.69869300
C	-3.61957200	0.75918000	-0.85896300
H	-4.35539600	1.14694100	-1.56877400
H	-4.08499000	0.81091400	0.13095400
N	1.06496500	1.01552600	1.33946500
C	2.37935800	0.39868700	1.22286200
H	3.14968600	1.03954600	1.66122200
H	2.33927400	-0.51964100	1.80847900
C	2.75200500	0.12233500	-0.23275800
O	2.50217800	0.93732300	-1.11043200
N	3.37965200	-1.04134800	-0.46167000
C	3.85264500	-1.39666900	-1.79015400
H	4.31015200	-2.38175900	-1.74303100
H	3.01981700	-1.41884200	-2.49431100
H	4.58940500	-0.67273900	-2.14237000
H	3.54941700	-1.67219800	0.30622100
C	-0.67624600	-1.58923200	2.19140100
H	-1.63956400	-1.26075500	2.58521200
H	-0.57012800	-2.66258400	2.35498100
H	0.10725900	-1.06468700	2.74065600
H	0.41240800	-1.64038800	0.34193700
C	-2.86454900	-1.61072800	-0.02004900
H	-3.07542900	-1.12064700	0.93572300
H	-3.43944500	-2.53807000	-0.04259100
C	-3.31131000	-0.71059100	-1.19450100
H	-2.55158500	-0.76895300	-1.98072800
H	-4.21964500	-1.15106100	-1.61331900
O	-1.50085500	-2.03539200	-0.07293100

HF: -799.1912232
Sum of electronic and zero-point Energies: -798.897596
Sum of electronic and thermal Energies: -798.879576
Sum of electronic and thermal Enthalpies: -798.878631
Sum of electronic and thermal Free Energies: -798.945503
Frequencies: -434.9803

X = CH_2, Y = O

C	-0.72424200	0.15757000	0.35490100
C	-1.32202200	1.11319200	-0.13833000
N	0.86464300	2.20652900	0.72211200
N	0.07446300	2.82587100	0.16698900
C	-2.47441200	1.64188100	-0.88438400
H	-2.79902500	2.61608900	-0.50918600
H	-2.19583900	1.77809800	-1.93359100
C	-0.53299900	-1.26109000	0.71106700
C	-3.63285900	0.64115000	-0.77569400
H	-4.44305300	0.94544400	-1.44346200
H	-4.01750700	0.63948600	0.24951700
N	1.05205500	1.10032300	1.27101600
C	2.36786700	0.48542800	1.21141000
H	3.13200200	1.15087700	1.62372200
H	2.32048700	-0.39880900	1.84731100
C	2.76634000	0.12104100	-0.21822100
O	2.48257200	0.85156000	-1.15762700
N	3.45768700	-1.02151300	-0.35422100
C	3.96651000	-1.44890200	-1.64764300
H	4.45563500	-2.41240500	-1.52673200
H	3.14827800	-1.54760700	-2.36223400
H	4.68525700	-0.72574300	-2.03710400
H	3.64868500	-1.58493400	0.45989900
C	-0.69381200	-1.48886300	2.21824600
H	-1.70605100	-1.23696200	2.54355900
H	-0.50193300	-2.53579400	2.46280500
H	0.00267100	-0.86292600	2.77901600
H	0.47836800	-1.57316800	0.42588400
C	-1.52783400	-2.10717300	-0.11601600
H	-1.19386600	-2.15311200	-1.15627200
H	-1.50556700	-3.12996400	0.27364600
C	-2.97815700	-1.61591400	-0.11809400
H	-3.24995600	-1.19173100	0.85443800
H	-3.63762800	-2.46887800	-0.30202900
O	-3.23871700	-0.66610400	-1.15161000

HF: -799.1934406
Sum of electronic and zero-point Energies: -798.899670
Sum of electronic and thermal Energies: -798.881745
Sum of electronic and thermal Enthalpies: -798.880801
Sum of electronic and thermal Free Energies: -798.946781
Frequencies: -434.6930

X = CH_2, Y = NH

C	-0.72208300	0.15862500	0.35597300
C	-1.32895800	1.11180900	-0.13113300
N	0.86302200	2.21333100	0.70947900
N	0.06357200	2.82389300	0.15665000
C	-2.48737400	1.65299400	-0.85628200
H	-2.78158400	2.63678500	-0.48034600
H	-2.21975100	1.78786200	-1.90991000
C	-0.51805300	-1.25804600	0.70633700
C	-3.67785400	0.67831900	-0.74026100
H	-4.48879800	1.06818800	-1.36469200
H	-4.04086600	0.68477500	0.29074700
N	1.05637800	1.10851200	1.26023200
C	2.37542300	0.50214500	1.20213900
H	3.13724300	1.17571200	1.60552000
H	2.33670600	-0.37656900	1.84635000
C	2.77216000	0.12354300	-0.22461500
O	2.44966800	0.82056900	-1.17678700
N	3.51249100	-0.99038000	-0.34218700
C	4.01834300	-1.43142400	-1.63211400
H	4.67516300	-2.28351600	-1.47464300
H	3.19777500	-1.72578200	-2.28906600
H	4.57857800	-0.62775100	-2.11154900
H	3.71466300	-1.54001100	0.47869300
C	-0.67002800	-1.49390100	2.21302100
H	-1.68102500	-1.24683700	2.54524100
H	-0.47305700	-2.54139100	2.45146300
H	0.02785100	-0.86858500	2.77293500
H	0.49543800	-1.56060200	0.41683000
C	-1.50581900	-2.10951100	-0.12173000
H	-1.17367900	-2.12794000	-1.16528700
H	-1.43795200	-3.13950900	0.24371000
N	-3.41555200	-0.70642800	-1.10998000
H	-2.83708900	-0.76382500	-1.94060200
C	-2.98311400	-1.67118700	-0.08938800
H	-3.23498100	-1.26087000	0.89309800
H	-3.58722200	-2.57737200	-0.20523500

HF: -779.3232252
Sum of electronic and zero-point Energies: -779.017422
Sum of electronic and thermal Energies: -778.999110
Sum of electronic and thermal Enthalpies: -778.998166
Sum of electronic and thermal Free Energies: -779.065040
Frequencies: -438.7722

X = CH_2, Y = NH_2^+

C	-0.73090200	0.09535600	0.40863100
C	-1.33072600	1.09027400	-0.00472600
N	0.85876900	2.08264100	0.87336100
N	0.05693200	2.74032700	0.38139600
C	-2.44514400	1.75843000	-0.69706500
H	-2.77078700	2.65349600	-0.16414700

H	-2.11063300	2.08674700	-1.68534500
C	-0.56145200	-1.34305600	0.70489500
C	-3.64362900	0.81884100	-0.83228800
H	-4.34437700	1.18590500	-1.57960100
H	-4.16695200	0.69409300	0.11324900
N	1.03803600	0.93128000	1.32309000
C	2.34952500	0.31530100	1.22607600
H	3.10128000	0.91773800	1.74432000
H	2.27992100	-0.63869500	1.75044000
C	2.79406600	0.11402700	-0.22368100
O	2.37071900	0.82697800	-1.12207800
N	3.69256700	-0.86427700	-0.41528000
C	4.26798000	-1.11708500	-1.72688600
H	5.03947400	-1.87656600	-1.62632500
H	3.50411000	-1.47035400	-2.42175000
H	4.70969500	-0.20365100	-2.12709400
H	3.98690700	-1.42714200	0.36813700
C	-0.73733300	-1.61929100	2.20275000
H	-1.75089300	-1.37286200	2.52857100
H	-0.55107400	-2.67392800	2.41322800
H	-0.04336500	-1.01391200	2.78749200
H	0.44392400	-1.66002100	0.41030600
C	-1.56022600	-2.15420400	-0.15064300
H	-1.19128100	-2.24311800	-1.17675200
H	-1.60806400	-3.17114600	0.24500000
N	-3.19738100	-0.56001400	-1.26669300
H	-2.33173400	-0.46404500	-1.80649100
H	-3.88644400	-0.93054700	-1.92223700
C	-2.98140400	-1.59546100	-0.16784100
H	-3.23658400	-1.11186400	0.77371500
H	-3.70584700	-2.38443800	-0.35454700

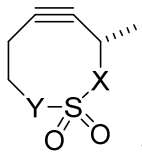
HF: -779.7775299
Sum of electronic and zero-point Energies: -779.455303
Sum of electronic and thermal Energies: -779.437210
Sum of electronic and thermal Enthalpies: -779.436266
Sum of electronic and thermal Free Energies: -779.502555
Frequencies: -448.8392

II. PUT IN THE TITLE HERE.

methyl azide

C	-1.52790300	0.29436300	0.00000500
N	0.71295700	-0.11104800	-0.00001500
N	1.76599200	0.28596200	0.00000600
H	-1.51600100	0.92328700	0.89261000
H	-1.51611700	0.92319000	-0.89268500
H	-2.42926900	-0.31119700	0.00006300
N	-0.38911900	-0.64655000	0.00000600

HF: -204.0628394
Sum of electronic and zero-point Energies: -204.011715
Sum of electronic and thermal Energies: -204.007389
Sum of electronic and thermal Enthalpies: -204.006445
Sum of electronic and thermal Free Energies: -204.037991



+methyl azide (*anti*-TSs)

X = CH_2, Y = CH_2

C	-0.71650800	0.64918500	0.08550300
C	-1.04566800	-0.53608600	-0.03247200
N	-3.25432700	0.67738900	0.49271900
N	-2.62728200	1.63591200	0.59437600
C	-0.80018000	-1.97974800	-0.22289600
H	-1.49706300	-2.56717100	0.37775800
H	-0.98049100	-2.24421900	-1.27038400
C	0.26514400	1.75801800	0.08966200
C	0.62903200	-2.36021400	0.17317100
H	0.75853500	-3.43117100	0.00245300
H	0.77814500	-2.18657700	1.24152800
S	2.38458400	-0.11602800	0.11465200
O	3.77322600	-0.03524500	-0.36321200
O	2.16341800	-0.12576400	1.56518400
C	-0.23080500	3.03086500	-0.60841100
H	-1.08906300	3.44593000	-0.08503900
H	0.56378100	3.77924200	-0.62777900
H	-0.52509000	2.80902700	-1.63698500
H	0.50105300	1.99595300	1.13160400
N	-3.13860400	-0.55790700	0.35376800
C	-4.05031200	-1.23480900	-0.57452700
H	-3.65809600	-2.24119000	-0.70714100
H	-5.05109600	-1.30748400	-0.14688400
C	1.55654100	1.31866400	-0.60157000
H	2.32465000	2.09254300	-0.52865200
H	1.39468800	1.08352900	-1.65610700
C	1.72471200	-1.64462100	-0.60989000
H	2.63258500	-2.24990600	-0.64434900
H	1.44194800	-1.40162200	-1.63688400
H	-4.09121300	-0.72765300	-1.54081600

HF: -1064.5660302
Sum of electronic and zero-point Energies: -1064.322630
Sum of electronic and thermal Energies: -1064.306917
Sum of electronic and thermal Enthalpies: -1064.305972
Sum of electronic and thermal Free Energies: -1064.366489
Frequencies: -477.0801

X = NH, Y = CH_2

C	-0.71527600	0.63773400	0.14007100
C	-1.07114900	-0.54107900	0.05271800
N	-3.27237100	0.74484100	0.38629800
N	-2.65043600	1.70518800	0.47871900
C	-0.84114300	-1.99189200	-0.07786000
H	-1.51139300	-2.54477800	0.58345900
H	-1.06941700	-2.30881500	-1.10115500
C	0.32485600	1.69290800	0.16374500
C	0.60856300	-2.34367700	0.26856400
H	0.74501600	-3.41867400	0.13238400
H	0.80207600	-2.12759800	1.32164600
N	1.58287700	1.24151700	-0.47108500
S	2.37923600	-0.10783800	0.05963900
O	3.69987800	-0.03250400	-0.55726700
O	2.26750800	-0.10174800	1.51303100
C	-0.07317200	2.99076500	-0.53466700
H	-0.92513700	3.43961000	-0.02955300
H	0.76490600	3.68794400	-0.51533900
H	-0.35172500	2.79334100	-1.57275800
H	0.56720700	1.90900100	1.20677800
N	-3.17843400	-0.49730300	0.32339700
C	-4.03669800	-1.20596600	-0.63263400
H	-3.69995900	-2.24045000	-0.63656800
H	-5.07698800	-1.18093500	-0.30658300
H	1.57547000	1.29341600	-1.48694700
C	1.65470100	-1.64139300	-0.59446700
H	2.54795800	-2.25979700	-0.69424400
H	1.29766100	-1.40011900	-1.59838500
H	-3.94809800	-0.78682200	-1.63718700

HF: -1080.6069538
Sum of electronic and zero-point Energies: -1080.374950
Sum of electronic and thermal Energies: -1080.359462
Sum of electronic and thermal Enthalpies: -1080.358518
Sum of electronic and thermal Free Energies: -1080.418322
Frequencies: -460.9212

X = NH_2^+, Y = CH_2

C	-0.67901800	0.62512700	0.08227000
C	-1.05890200	-0.54373700	-0.02132300
N	-3.19595900	0.77561200	0.50232800
N	-2.56099500	1.72623500	0.58908000
C	-0.84187900	-1.98856900	-0.22409500
H	-1.51133200	-2.57162500	0.41090900
H	-1.07542400	-2.24865400	-1.26187600
C	0.34755600	1.67437200	0.06682800
C	0.60758900	-2.36824100	0.10118200
H	0.74865100	-3.42459300	-0.13523200
H	0.78800400	-2.25262100	1.17197700
S	2.32845000	-0.11279100	0.13886400
O	3.70407700	0.03211400	-0.29775900
O	2.04021700	-0.13574300	1.56176200
C	0.01323800	2.88647800	-0.78195800
H	-0.85216000	3.39398200	-0.35905800
H	0.86181000	3.57023600	-0.79319500
H	-0.21834000	2.57685100	-1.80194400
H	0.58603000	1.96998800	1.09091400
N	-3.13375200	-0.46421100	0.38871100
C	-4.05831400	-1.11538800	-0.54779900
H	-3.75306400	-2.15793700	-0.60342100
H	-5.07955800	-1.07148800	-0.16870700
C	1.66440900	-1.58580900	-0.67839000
H	2.56710200	-2.18269200	-0.81354600
H	1.32357600	-1.24790700	-1.65904200
O	1.58463200	1.14668700	-0.52661100
H	-4.00504300	-0.66222300	-1.53985000

HF: -1081.0165865

Sum of electronic and zero-point Energies: -1080.770271
Sum of electronic and thermal Energies: -1080.754752
Sum of electronic and thermal Enthalpies: -1080.753808
Sum of electronic and thermal Free Energies: -1080.812727
Frequencies: -459.0719

X = O, Y = CH_2

C	-0.71262900	0.63929200	0.05285300
C	-1.05543300	-0.53934400	-0.09090200
N	-3.19231200	0.68067900	0.57684000
N	-2.57878500	1.64351500	0.68523400
C	-0.80968800	-1.97383000	-0.34508800
H	-1.52573000	-2.58563600	0.20471200
H	-0.95643000	-2.18259700	-1.40931300
C	0.24711500	1.74602100	0.03575500
C	0.59840900	-2.39041500	0.08670900
H	0.72906300	-3.45004500	-0.14070200
H	0.70904100	-2.28259200	1.16758300
N	1.52758500	1.24434100	-0.62170300
S	2.36243300	-0.18620700	0.20319400
O	3.72982400	0.03845700	-0.18931100
O	1.93936000	-0.08890000	1.57356400
C	-0.20109100	2.98225100	-0.73706100
H	-1.06309200	3.41062800	-0.23066300
H	0.59330400	3.72920300	-0.76477300
H	-0.49037000	2.71602800	-1.75519000
H	0.53825500	2.01053100	1.05417500
N	-3.08608600	-0.54695800	0.38862200
C	-4.03486800	-1.18963000	-0.53069200
H	-3.66452500	-2.19856700	-0.69707000
H	-5.02117800	-1.25350200	-0.07110800
H	1.34717000	1.01079100	-1.60571300
C	1.73863400	-1.66760300	-0.62171400
H	2.65264900	-2.26752200	-0.61738200
H	1.52931700	-1.38994900	-1.65744500
H	2.24746700	1.98064800	-0.62354500
H	-4.09284400	-0.65605300	-1.48081200

HF: -1100.4757055
Sum of electronic and zero-point Energies: -1100.256389
Sum of electronic and thermal Energies: -1100.241027
Sum of electronic and thermal Enthalpies: -1100.240083
Sum of electronic and thermal Free Energies: -1100.299319
Frequencies: -448.7326

X = CH_2, Y = O

C	-0.69898100	0.64255300	0.07517400
C	-1.03233900	-0.53602200	-0.07134700
N	-3.23271800	0.63564500	0.54517000
N	-2.62957600	1.60502600	0.66304800
C	-0.72890800	-1.95834200	-0.31716200
H	-1.38991500	-2.61805600	0.25004700
H	-0.85845800	-2.19363400	-1.37716000
C	0.28233600	1.74985100	0.08331400
C	0.70255200	-2.25164000	0.11170100
H	0.99696100	-3.26416700	-0.15930200
H	0.82877600	-2.10673600	1.18430300
S	2.35894600	-0.14634000	0.11824700
O	3.72354500	-0.19321500	-0.36667300
O	2.11815000	-0.20356100	1.54846600
O	1.62387000	-1.38591400	-0.59723400
C	-0.21127100	3.01438900	-0.63042400
H	-1.08790000	3.41568600	-0.12639100
H	0.57216300	3.77454600	-0.63178500
H	-0.47862400	2.78636900	-1.66480600
H	0.50753600	1.99783300	1.12517300
N	-3.11814200	-0.59409700	0.37051500
C	-4.02472100	-1.23472400	-0.58987100
H	-3.63286500	-2.23603900	-0.75659700
H	-5.02838100	-1.32049300	-0.17203300
C	1.58368400	1.30590400	-0.59452200
H	2.35451400	2.07461900	-0.50687300
H	1.43405000	1.06621100	-1.64923400
H	-4.05658200	-0.69102100	-1.53610000

HF: -1100.4749197
Sum of electronic and zero-point Energies: -1100.255076
Sum of electronic and thermal Energies: -1100.239799
Sum of electronic and thermal Enthalpies: -1100.238855
Sum of electronic and thermal Free Energies: -1100.297894
Frequencies: -459.6684

X = CH_2, Y = NH

C	-0.71923700	0.64110300	0.10716900
C	-1.05394000	-0.53910000	-0.03077900
N	-3.27388000	0.65535700	0.47710500
N	-2.66702100	1.62278200	0.59865400
C	-0.76624800	-1.97251200	-0.22263100
H	-1.45690500	-2.59664800	0.34899600
H	-0.88162500	-2.24184900	-1.27724300
C	0.27300000	1.73993700	0.12214000
C	0.65960300	-2.28120400	0.24568800
H	0.87521500	-3.34108700	0.10002900
H	0.76024800	-2.06305700	1.30886500
S	2.38950100	-0.14309100	0.07778900
O	3.72178300	-0.11204800	-0.51802900
O	2.25321600	-0.12826100	1.52908700
C	-0.22208600	3.03252100	-0.53909800
H	-1.07466300	3.43618200	0.00257200
H	0.57493200	3.77842400	-0.54538900
H	-0.52658900	2.83880700	-1.57033200
H	0.52539300	1.95421100	1.16549000
N	-3.15368800	-0.57808100	0.33117300
C	-4.03340700	-1.24207100	-0.63737400
H	-3.63223200	-2.24425900	-0.77503500
H	-5.04664200	-1.32576000	-0.24251400
C	1.55262400	1.30462800	-0.59735600
H	2.31540600	2.08405400	-0.53510600
H	1.36654100	1.07484000	-1.64916900
N	1.69999800	-1.53130200	-0.45189500
H	1.83522200	-1.70515100	-1.44087200
H	-4.04601700	-0.71789800	-1.59519100

HF: -1080.6088447
Sum of electronic and zero-point Energies: -1080.377084
Sum of electronic and thermal Energies: -1080.361374
Sum of electronic and thermal Enthalpies: -1080.360429
Sum of electronic and thermal Free Energies: -1080.420734
Frequencies: -464.6964

X = CH_2, Y = NH_2^+

C	-0.69861600	0.65420900	0.03168000
C	-1.04579300	-0.52658200	-0.08682800
N	-3.18861500	0.67265000	0.58003500
N	-2.55239700	1.62553300	0.66886800
C	-0.80242400	-1.96510200	-0.32011800
H	-1.45788000	-2.57974600	0.29912100
H	-1.01546700	-2.21964200	-1.36324500
C	0.24962800	1.79000200	0.03718900
C	0.62495900	-2.35300700	0.03740400
H	0.83082600	-3.38576300	-0.23851200
H	0.82462200	-2.21940800	1.10015200
S	2.36057700	-0.04593400	0.22097100
O	3.74298100	-0.14429500	-0.16551800
O	1.92945900	-0.23163900	1.57849800
C	-0.24101800	3.00132800	-0.76916000
H	-1.15223000	3.39792100	-0.32802200
H	0.51807600	3.78525600	-0.76911000
H	-0.44787300	2.71174300	-1.80136700
H	0.40895600	2.09679000	1.07497700
N	-3.08354700	-0.55832100	0.40126900
C	-4.04135800	-1.20901400	-0.50142600
H	-3.67772500	-2.22265500	-0.65565300
H	-5.02550700	-1.26273300	-0.03543100
C	1.60026400	1.38191300	-0.55634000
H	2.36492500	2.14935900	-0.40382800
H	1.54803000	1.15882300	-1.62425500
N	1.63098400	-1.50715500	-0.69965100
H	2.46420200	-2.06411400	-0.92365700
H	1.25425900	-1.18473300	-1.59896500
H	-4.10476900	-0.69012100	-1.45962800

HF: -1081.0151038
Sum of electronic and zero-point Energies: -1080.768697
Sum of electronic and thermal Energies: -1080.753045
Sum of electronic and thermal Enthalpies: -1080.752101
Sum of electronic and thermal Free Energies: -1080.811623
Frequencies: -481.2252

X = NH, Y = NH

C	-0.71090800	0.62920100	0.13796300
C	-1.06754000	-0.54543500	0.01899600
N	-3.27275200	0.71489600	0.40868500
N	-2.66544800	1.68101100	0.52230100
C	-0.79272200	-1.98494400	-0.13203700
H	-1.47045900	-2.58503700	0.47959800
H	-0.93697800	-2.29104400	-1.17281000
C	0.32967800	1.68308000	0.17189800
C	0.64626100	-2.27393800	0.30962000
H	0.86609000	-3.33582600	0.18543600
H	0.77062700	-2.02709300	1.36387900
N	1.58622700	1.23850600	-0.47076200
S	2.36569400	-0.13249200	0.04162000
O	3.63669000	-0.09505500	-0.66049700
O	2.29776400	-0.10468800	1.49038800
C	-0.07310400	2.98666000	-0.51307400
H	-0.93113200	3.42296200	-0.00682300
H	0.75958200	3.68977200	-0.48200400
H	-0.34543000	2.79929200	-1.55468900
H	0.57488100	1.88918700	1.21652500
N	-3.17746900	-0.52432700	0.31229300
C	-4.02820000	-1.20239300	-0.67305400
H	-3.68594700	-2.23429000	-0.71249000
H	-5.07009700	-1.19377200	-0.35132500
H	1.55214200	1.27135300	-1.48726500
H	-3.93671200	-0.74680800	-1.66129700
N	1.66444200	-1.53484700	-0.43249700
H	1.76090400	-1.72093300	-1.42380300

HF: -1096.6488042
Sum of electronic and zero-point Energies: -1096.428276
Sum of electronic and thermal Energies: -1096.412862
Sum of electronic and thermal Enthalpies: -1096.411918
Sum of electronic and thermal Free Energies: -1096.471189
Frequencies: -450.3311

X = NH, Y = NH_2^+

C	-0.68652000	0.64106900	0.04794200
C	-1.05801400	-0.53023200	-0.06705800
N	-3.17380500	0.73566600	0.56511100
N	-2.53378700	1.68355400	0.65503500
C	-0.82948000	-1.96822500	-0.31081500
H	-1.47367500	-2.58294600	0.32009700

H	-1.06659900	-2.21451500	-1.35061100
C	0.28569400	1.74858800	0.05723300
C	0.60848600	-2.35696500	0.01100200
H	0.81427800	-3.37871000	-0.30317900
H	0.82066200	-2.25828800	1.07413800
N	1.63717800	1.26958000	-0.36545600
S	2.33585700	-0.02802600	0.22826900
O	3.69691900	-0.11105000	-0.21321900
O	1.90992900	-0.26553700	1.57350600
C	-0.07847700	2.89216300	-0.88451700
H	-1.02122500	3.32954500	-0.56384100
H	0.69574600	3.65968000	-0.85589200
H	-0.19023200	2.52027100	-1.90455100
H	0.38989900	2.12712100	1.07609000
N	-3.10193200	-0.49838000	0.40516300
C	-4.06390000	-1.13562700	-0.50377900
H	-3.73305200	-2.16421700	-0.62857300
H	-5.05798700	-1.14337000	-0.05645400
H	2.01749400	1.59172700	-1.25232200
H	-4.08914500	-0.63448400	-1.47310600
N	1.59844200	-1.47664400	-0.71034300
H	1.19570900	-1.10589300	-1.57912000
H	2.42021200	-2.02587100	-0.98390000

HF: -1097.0584806
Sum of electronic and zero-point Energies: -1096.823613
Sum of electronic and thermal Energies: -1096.808006
Sum of electronic and thermal Enthalpies: -1096.807062
Sum of electronic and thermal Free Energies: -1096.866542
Frequencies: -457.0526

X = NH, Y = O

C	-0.69879500	0.63080100	0.11809600
C	-1.05100600	-0.54358500	-0.00689300
N	-3.24803000	0.69626200	0.46145100
N	-2.64933200	1.66668500	0.57569900
C	-0.75621100	-1.97386100	-0.20461300
H	-1.40440000	-2.60833500	0.40466800
H	-0.90985700	-2.25222600	-1.25080700
C	0.33215900	1.69077100	0.14458700
C	0.68671200	-2.24190300	0.20383700
H	0.98140200	-3.26367700	-0.03075400
H	0.83610400	-2.04961400	1.26583100
N	1.60733500	1.22738100	-0.45934600
S	2.34413400	-0.13243300	0.07124300
O	3.64521400	-0.16599400	-0.55110700
O	2.20108900	-0.17254400	1.50844700
O	1.58717100	-1.40250700	-0.56250200
C	-0.06055600	2.96697200	-0.59396400
H	-0.93354300	3.41095500	-0.12079200
H	0.76511600	3.67846200	-0.56565500
H	-0.30731600	2.74255100	-1.63437600
H	0.55608800	1.93156000	1.18634000
N	-3.15285700	-0.54022900	0.34151800
C	-4.02091600	-1.20062400	-0.64176500
H	-3.67863700	-2.23105500	-0.70753900
H	-5.05631300	-1.19911700	-0.30017200
H	1.63691800	1.29065100	-1.47434300
H	-3.94764200	-0.72498100	-1.62195100

HF: -1116.5140204
Sum of electronic and zero-point Energies: -1116.305677
Sum of electronic and thermal Energies: -1116.290521
Sum of electronic and thermal Enthalpies: -1116.289577
Sum of electronic and thermal Free Energies: -1116.348436
Frequencies: -443.3478

X = O, Y = NH

C	-0.68790900	0.61913900	0.12198300
C	-1.06800400	-0.54575100	-0.00992100
N	-3.22790500	0.74654800	0.47079400
N	-2.61789000	1.70851500	0.58712400
C	-0.80397800	-1.98098100	-0.20965000
H	-1.47864500	-2.59861900	0.38725900
H	-0.95593800	-2.24996900	-1.25925900
C	0.35303100	1.65462000	0.12129200
C	0.63651700	-2.29009100	0.21687500
H	0.86501000	-3.33914400	0.02449100
H	0.75718100	-2.10856000	1.28430900
S	2.33272400	-0.13649100	0.07997600
O	3.63617900	-0.03155800	-0.53216600
O	2.17457400	-0.11837500	1.51737900
C	0.01304600	2.90712000	-0.66442700
H	-0.83329500	3.40665700	-0.19567300
H	0.87049700	3.57981300	-0.67009700
H	-0.25140900	2.64546400	-1.68988900
H	0.62468600	1.90366800	1.14988300
N	-3.15559900	-0.49120100	0.34787300
C	-4.03439300	-1.13273300	-0.63892400
H	-3.71190000	-2.16941500	-0.70567600
H	-5.07002200	-1.11122100	-0.29903400
H	-3.94917800	-0.65647500	-1.61778800
N	1.65406300	-1.49999100	-0.47656100
H	1.79060900	-1.65094000	-1.46932100
O	1.56428300	1.13712700	-0.52856400

HF: -1116.5168388
Sum of electronic and zero-point Energies: -1116.308572
Sum of electronic and thermal Energies: -1116.293435
Sum of electronic and thermal Enthalpies: -1116.292491
Sum of electronic and thermal Free Energies: -1116.350800
Frequencies: -436.2270

X = O, Y = O

C	-0.67831300	0.62596300	0.12283800
C	-1.05115100	-0.54055500	-0.01011400
N	-3.21305300	0.72632000	0.49315700
N	-2.62211900	1.69863100	0.61047800
C	-0.76694800	-1.96742300	-0.24401500
H	-1.40967000	-2.61314800	0.35889100
H	-0.93390700	-2.21930800	-1.29458800
C	0.35364100	1.66530300	0.11345800
C	0.67843300	-2.25095300	0.14464300
H	0.97834400	-3.25665800	-0.14252800
H	0.83551000	-2.10592600	1.21246100
S	2.31012500	-0.13589200	0.09118200
O	3.63015700	-0.11144800	-0.47209300
O	2.11118900	-0.17468900	1.51869700
C	0.02321100	2.89710700	-0.70463400
H	-0.83005200	3.40165700	-0.25355800
H	0.87774700	3.57313100	-0.71440900
H	-0.23090000	2.61209700	-1.72617100
H	0.62640500	1.93291800	1.13640700
N	-3.13029600	-0.50952300	0.36376900
C	-4.00673200	-1.15278200	-0.62515500
H	-3.68114600	-2.18821900	-0.69385500
H	-5.04198000	-1.13484700	-0.28443300
H	-3.92262700	-0.67332400	-1.60241900
O	1.58339700	1.13069200	-0.52068000
O	1.57722100	-1.37231000	-0.58950600

HF: -1136.3791682
Sum of electronic and zero-point Energies: -1136.183190
Sum of electronic and thermal Energies: -1136.168359
Sum of electronic and thermal Enthalpies: -1136.167415
Sum of electronic and thermal Free Energies: -1136.22534
Frequencies: -427.4809

X = O, Y = NH_2^+

C	-0.67681300	0.63514900	0.06707900
C	-1.07640200	-0.52808400	-0.03723900
N	-3.16640100	0.76489300	0.55267200
N	-2.55566600	1.72794200	0.64131000
C	-0.84321400	-1.96451000	-0.28643700
H	-1.46808200	-2.58457500	0.35860200
H	-1.09719500	-2.21317200	-1.32146600
C	0.30097600	1.71287000	0.04300700
C	0.60408200	-2.33615000	0.01121800
H	0.82254200	-3.34965700	-0.31881700
H	0.83223000	-2.24489000	1.07161500
S	2.31972200	-0.03379300	0.22421800
O	3.68323600	-0.07686100	-0.19149200
O	1.89487900	-0.22481400	1.57383900
C	0.00702500	2.83992700	-0.92133900
H	-0.89374700	3.35227100	-0.58559600
H	0.83799500	3.54379400	-0.93297500
H	-0.15896100	2.44249700	-1.92269900
H	0.51566300	2.07571400	1.04858700
N	-3.08883000	-0.47114300	0.41430800
C	-4.03293100	-1.12420500	-0.50489200
H	-3.74080300	-2.17037400	-0.55533500
H	-5.04498800	-1.06478800	-0.10562600
H	-3.99003900	-0.67642700	-1.49937100
N	1.57800100	-1.43431900	-0.71987100
H	1.15412600	-1.03759600	-1.56926900
O	1.62929200	1.16757700	-0.46638800
H	2.39037400	-1.98090900	-1.03012200

HF: -1116.9171262
Sum of electronic and zero-point Energies: -1116.694768
Sum of electronic and thermal Energies: -1116.679541
Sum of electronic and thermal Enthalpies: -1116.678596
Sum of electronic and thermal Free Energies: -1116.736991
Frequencies: -434.6102

X = NH_2^+, Y = NH

C	-0.71739500	0.62950300	0.08163900
C	-1.06892200	-0.54278200	-0.08146100
N	-3.22407000	0.66184400	0.54052600
N	-2.63128100	1.63274800	0.67333500
C	-0.78353200	-1.97073200	-0.32022000
H	-1.48808900	-2.61047500	0.21415400
H	-0.87100500	-2.19913600	-1.38581200
C	0.25561600	1.72494000	0.08866200
C	0.62020100	-2.30521600	0.18419700
H	0.86360800	-3.34852200	-0.01282500
H	0.69210500	-2.13206700	1.25700400
S	2.37650100	-0.22737200	0.15180300
O	3.68640300	-0.05438000	-0.40468300
O	2.06984800	-0.08990100	1.54400400
C	-0.18719200	2.98901100	-0.64138600
H	-1.04413600	3.40703400	-0.11805500
H	0.61252200	3.73096300	-0.64856500
H	-0.48299400	2.75805400	-1.66637000
H	0.55547100	1.95563200	1.11280700
N	-3.11150300	-0.56434400	0.35004100
C	-4.02701100	-1.19968900	-0.60813600
H	-3.64409400	-2.20367200	-0.77712100
H	-5.02664200	-1.27660100	-0.18035800
H	-4.05915600	-0.65267800	-1.55185000
N	1.53008500	1.23759500	-0.59215700
H	1.33440900	1.01819500	-1.57633000
N	1.67527000	-1.51027100	-0.46659300
H	2.02638600	-1.79146400	-1.37778800

H	2.23748300	1.98372500	-0.58813600

HF: -1097.0628934
Sum of electronic and zero-point Energies: -1096.828115
Sum of electronic and thermal Energies: -1096.812576
Sum of electronic and thermal Enthalpies: -1096.811632
Sum of electronic and thermal Free Energies: -1096.870967
Frequencies: -444.5636

X = NH_2^+, Y = O

C	-0.70055000	0.63416700	0.06848400
C	-1.05667000	-0.53346200	-0.10890800
N	-3.18988900	0.64751800	0.60012900
N	-2.61004100	1.62355200	0.73888000
C	-0.75574200	-1.94653100	-0.40796000
H	-1.43916400	-2.62602000	0.10599200
H	-0.84308700	-2.13397100	-1.48081000
C	0.27188700	1.72564200	0.05829100
C	0.64343500	-2.27802800	0.07543300
H	0.96525900	-3.26797200	-0.23602300
H	0.73998900	-2.16231700	1.15319600
S	2.34446500	-0.22833200	0.18273900
O	3.68755200	-0.14110500	-0.28554900
O	1.97877900	-0.15341500	1.56080500
C	-0.15749000	2.96368900	-0.72009300
H	-1.02279600	3.39362300	-0.21965300
H	0.63937600	3.70810500	-0.73790400
H	-0.43990200	2.70004700	-1.74065800
H	0.57000900	1.98776900	1.07509600
N	-3.08200100	-0.57375300	0.38207700
C	-4.01562600	-1.18613400	-0.57494100
H	-3.64513800	-2.19101700	-0.76392700
H	-5.00993100	-1.25967700	-0.13487200
H	-4.05359800	-0.62335500	-1.50892700
N	1.55818700	1.20504700	-0.60309900
H	1.36744100	0.95326900	-1.58259100
H	2.27628800	1.94279500	-0.61548700
O	1.61798800	-1.37555100	-0.57588000

HF: -1116.9165576
Sum of electronic and zero-point Energies: -1116.694306
Sum of electronic and thermal Energies: -1116.679004
Sum of electronic and thermal Enthalpies: -1116.678060
Sum of electronic and thermal Free Energies: -1116.737016
Frequencies: -431.9051

X = NH_2^+, Y = NH_2^+

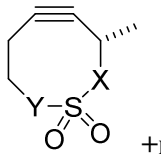
C	-0.70829400	0.64019400	0.05911500
C	-1.08718200	-0.53325400	-0.04710700
N	-3.19269400	0.69370700	0.53922100
N	-2.60348400	1.66876400	0.64172400
C	-0.83777200	-1.97246000	-0.27366400
H	-1.48749600	-2.58314100	0.35582900
H	-1.05365400	-2.23727900	-1.31314200
C	0.22680200	1.75895700	0.06856500
C	0.58326400	-2.35803500	0.09546200
H	0.80248500	-3.38780000	-0.18087400
H	0.78946600	-2.21635500	1.15490700
S	2.35642600	-0.12214300	0.22207200
O	3.70891900	-0.10388200	-0.20114100
O	1.86965600	-0.16492400	1.55130400
C	-0.18822700	2.98847800	-0.72896200
H	-1.07145500	3.40578400	-0.25010700
H	0.59865400	3.74334100	-0.71706400
H	-0.44047000	2.72395600	-1.75655600
H	0.49490200	2.02801000	1.09186800
N	-3.06546900	-0.53642100	0.37760700
C	-3.99022500	-1.21472100	-0.54479100
H	-3.65912700	-2.24805700	-0.61279300
H	-4.99880300	-1.20019000	-0.13358400
H	-3.97366600	-0.75026900	-1.53200400
N	1.57520700	1.28772100	-0.56276100
H	1.46081300	1.12934300	-1.57601300
N	1.61024000	-1.52302400	-0.66685600
H	1.23368400	-1.22549800	-1.57977500
H	2.28423500	2.03858700	-0.48805700
H	2.43221100	-2.10587600	-0.89135600

HF: -1097.420407
Sum of electronic and zero-point Energies: -1097.171484
Sum of electronic and thermal Energies: -1097.156001
Sum of electronic and thermal Enthalpies: -1097.155057
Sum of electronic and thermal Free Energies: -1097.213834
Frequencies: -452.6108

X = NBoc, Y = O

C	1.80852700	-0.17025500	0.57921200
C	2.23382600	0.01773300	-0.56051600
N	4.05716300	-1.39369400	0.57613400
N	3.42929100	-1.38003800	1.53512400
C	2.11202100	0.55879400	-1.92536700
H	3.07402100	0.89991900	-2.31609400
H	1.74005900	-0.21723800	-2.60003200
C	0.77140000	-0.11512400	1.62436900
C	1.16548600	1.75323900	-1.92516700
H	0.93409900	2.07281600	-2.93940200
H	1.58524600	2.58408700	-1.36107200
N	-0.51665400	0.36177500	1.00824100
S	-0.50857400	1.80227900	0.14621000
O	-1.84502300	2.32723100	0.10283200
O	0.55142000	2.60513000	0.70365600
O	-0.12594400	1.39633800	-1.35287000
N	4.16879000	-0.90953900	-0.56552600
C	4.50219500	-1.81979700	-1.66814600
H	4.35459400	-1.25374500	-2.58549400
H	5.54827700	-2.12265900	-1.61136600
C	1.16243600	0.66130000	2.87818000
H	0.31294100	0.69445800	3.56177800
H	1.98392600	0.13403000	3.36499700
H	1.48009100	1.67392500	2.64277500
H	0.53081200	-1.13380900	1.92656200
C	-1.50519400	-0.62912100	0.79160200
O	-2.29415500	-0.31987000	-0.21261100
O	-1.55134700	-1.62059100	1.47452600
C	-3.49960100	-1.11344000	-0.52285600
C	-4.42168500	-1.14187500	0.68839000
H	-5.37058800	-1.59376200	0.39238600
H	-3.99793900	-1.72656200	1.50348000
H	-4.61970700	-0.12522300	1.03524300
C	-4.12319500	-0.32173200	-1.66210300
H	-5.03408500	-0.82138100	-1.99581100
H	-4.37584600	0.68703800	-1.33113100
H	-3.43065900	-0.25627000	-2.50333600
C	-3.08783400	-2.50421600	-0.98515700
H	-2.36411600	-2.43083900	-1.79975000
H	-2.65730200	-3.08496700	-0.17109600
H	-3.97248100	-3.02501700	-1.35738300
H	3.85580600	-2.69971900	-1.67135300

HF: -1462.2929029
Sum of electronic and zero-point Energies: -1461.958149
Sum of electronic and thermal Energies: -1461.935479
Sum of electronic and thermal Enthalpies: -1461.934535
Sum of electronic and thermal Free Energies: -1462.009375
Frequencies: -439.5630



+methyl azide (*syn*-TSs)

X = CH_2, Y = CH_2

C	0.90665800	-0.03278200	-0.10606900
C	0.80512500	1.19461900	-0.03417800
N	3.33294400	0.81333800	0.12687900
N	2.86204400	1.86445600	0.13459200
C	0.07978300	2.47705800	-0.01785900
H	0.53227700	3.16507700	0.69900800
H	0.17623800	2.94581100	-1.00274500
C	0.42051200	-1.42093300	-0.23946100
C	-1.39852100	2.27799700	0.32625600
H	-1.90602700	3.24294800	0.26114500
H	-1.49961600	1.93181100	1.35760200
S	-2.25607900	-0.41299300	-0.03845900
O	-3.52452200	-0.90695500	-0.59490800
O	-2.09154400	-0.45580800	1.41856200
N	3.01609200	-0.39153100	0.18299400
C	3.77984600	-1.36083000	-0.60508100
H	4.80880400	-1.42323900	-0.24873900
H	3.30543400	-2.32826000	-0.45003100
C	0.52496400	-2.20428400	1.07421400
H	-0.06325800	-1.72512500	1.85602300
H	0.15945800	-3.22320600	0.92996100
H	1.56678900	-2.24733300	1.39440200
H	1.03176200	-1.93583700	-0.98874400
C	-0.99069600	-1.42756600	-0.83914400
H	-0.98935200	-1.09661800	-1.87937300
H	-1.43073600	-2.42691600	-0.79490300
C	-2.12925600	1.31209400	-0.60189900
H	-3.18773300	1.56720300	-0.67848600
H	-1.71416000	1.28073900	-1.61189600
H	3.76785800	-1.11315400	-1.66901900

HF: -1064.5664759
Sum of electronic and zero-point Energies: -1064.322820
Sum of electronic and thermal Energies: -1064.307363
Sum of electronic and thermal Enthalpies: -1064.306419
Sum of electronic and thermal Free Energies: -1064.365032
Frequencies: -473.1997

X = NH, Y = CH_2

C	0.89111000	-0.01905600	-0.06325500
C	0.81068800	1.20849800	0.01068700
N	3.33176600	0.77187400	0.11018500
N	2.88927100	1.83345500	0.14242400
C	0.09010500	2.49203000	0.02750600
H	0.51989200	3.16662300	0.77066300
H	0.21595800	2.97766500	-0.94564700
C	0.36103100	-1.39451800	-0.17924000
C	-1.39791500	2.27733800	0.32096300
H	-1.91465100	3.23587800	0.23698400
H	-1.52913000	1.93114600	1.34850600
N	-1.03480800	-1.39925700	-0.67703700
S	-2.22794200	-0.42591000	-0.06715100
O	-3.44842500	-0.92422400	-0.69504200
O	-2.10882300	-0.45940800	1.38450800
N	3.00240900	-0.42953800	0.16004700
C	3.70801400	-1.38414300	-0.69993300
H	4.75753600	-1.45812800	-0.41279400

H	3.23944500	-2.35304600	-0.53740700
H	-1.11349800	-1.46073300	-1.68723800
C	0.49224400	-2.18535100	1.12203200
H	-0.04254900	-1.68391300	1.92761200
H	0.07724200	-3.18415300	0.98202700
H	1.54564600	-2.26633500	1.39289900
H	0.90859000	-1.92408900	-0.96280200
C	-2.08218700	1.29902100	-0.63274800
H	-3.13328100	1.55716800	-0.76686700
H	-1.61336600	1.25564100	-1.61848800
H	3.62821700	-1.10874700	-1.75416500

HF: -1080.6064951
Sum of electronic and zero-point Energies: -1080.374143
Sum of electronic and thermal Energies: -1080.358791
Sum of electronic and thermal Enthalpies: -1080.357847
Sum of electronic and thermal Free Energies: -1080.416294
Frequencies: -461.4977

X = NH_2^+, Y = CH_2

C	0.92257200	-0.02639700	-0.10675900
C	0.78500300	1.19845400	-0.03901300
N	3.28385200	0.82420000	0.20956200
N	2.79829700	1.86677800	0.23563900
C	0.06131200	2.48111400	-0.06727000
H	0.49729900	3.17918900	0.64868500
H	0.19412700	2.92542800	-1.05866500
C	0.46156400	-1.41170200	-0.25952700
C	-1.42843600	2.31273100	0.23776900
H	-1.93017700	3.26945300	0.08178600
H	-1.57552500	2.04552400	1.28580500
N	-0.95618200	-1.37549200	-0.82211300
S	-2.26075000	-0.36612000	0.03434800
O	-3.44357500	-1.01217100	-0.47221500
O	-1.90563000	-0.41480200	1.42557000
N	2.98486000	-0.38711900	0.20744300
C	3.75236400	-1.29278500	-0.65700700
H	4.79405300	-1.32593000	-0.33786900
H	3.32582800	-2.28600300	-0.52994500
H	-0.92895600	-1.07081300	-1.80215800
C	0.52790300	-2.24787000	1.01307600
H	-0.00107000	-1.76650200	1.83228600
H	0.11893100	-3.24439200	0.83884100
H	1.57778700	-2.34919900	1.28696100
H	1.01966800	-1.91158100	-1.05536800
C	-2.13711700	1.30208000	-0.65769700
H	-3.20061100	1.52687300	-0.76870800
H	-1.70695100	1.20475600	-1.65718800
H	-1.35570900	-2.32410300	-0.83120300
H	3.69017000	-0.99130300	-1.70483500

HF: -1081.0140106
Sum of electronic and zero-point Energies: -1080.767692
Sum of electronic and thermal Energies: -1080.752120
Sum of electronic and thermal Enthalpies: -1080.751176
Sum of electronic and thermal Free Energies: -1080.810182
Frequencies: -471.4238

X = O, Y = CH_2

C	0.87064500	-0.00999200	-0.07914300
C	0.78745400	1.21621500	0.00721300
N	3.29097000	0.75625900	0.20333700
N	2.85361300	1.81828200	0.25445000
C	0.06835500	2.50047100	-0.01475100
H	0.46889300	3.18301100	0.73683600
H	0.23508300	2.97217200	-0.98850700
C	0.34152900	-1.36887000	-0.26360200
C	-1.43251900	2.29409500	0.21930600
H	-1.94753000	3.24159100	0.04946200
H	-1.61194600	2.01317400	1.25892600
S	-2.18383400	-0.42396200	-0.02529200
O	-3.40972700	-1.00863200	-0.53371600
O	-1.95819200	-0.40659900	1.40855300
N	2.96318600	-0.44655500	0.19592700
C	3.67433900	-1.34924200	-0.71754600
H	4.72221700	-1.43652100	-0.42914200
H	3.20724400	-2.32667500	-0.61472500
C	0.45354500	-2.26361600	0.96090100
H	-0.00957600	-1.79533900	1.82739300
H	-0.03147800	-3.21864300	0.75607600
H	1.50867500	-2.43976600	1.17399300
H	0.83087500	-1.84461100	-1.11563800
C	-2.06743100	1.25405700	-0.70394300
H	-3.11695500	1.48291700	-0.89055700
H	-1.55755500	1.15365600	-1.66391000
O	-1.04266100	-1.30056900	-0.74599100
H	3.59815400	-1.00977700	-1.75291800

HF: -1100.4733649
Sum of electronic and zero-point Energies: -1100.253562
Sum of electronic and thermal Energies: -1100.238432
Sum of electronic and thermal Enthalpies: -1100.237487
Sum of electronic and thermal Free Energies: -1100.295592
Frequencies: -456.9498

X = CH_2, Y = O

C	0.89359800	-0.02950300	-0.11975800
C	0.79511000	1.19712800	-0.06482600
N	3.31717000	0.81435700	0.17359400
N	2.86844000	1.87258800	0.17120100
C	0.01589500	2.44448000	-0.11055400
H	0.41337700	3.19921000	0.57225300
H	0.06213600	2.86458700	-1.11885600
C	0.39348300	-1.41110300	-0.26631700
C	-1.43004800	2.15936800	0.27345600
H	-2.06725800	3.02529400	0.10113500
H	-1.50785600	1.84734700	1.31447200
S	-2.24778300	-0.37234400	-0.03177500
O	-3.53610200	-0.73843400	-0.58544300
O	-2.07242000	-0.39309300	1.40884800
O	-1.96914500	1.11459200	-0.57705000
N	3.00690500	-0.39122600	0.22329100
C	3.76726400	-1.34410700	-0.59008700
H	4.79821000	-1.41296500	-0.24088600
H	3.29346100	-2.31446600	-0.45272900
C	0.49154700	-2.21638500	1.03405000
H	-0.07729600	-1.73775800	1.83056500
H	0.10415800	-3.22527800	0.87787900
H	1.53483000	-2.28512200	1.34416400
H	0.99221000	-1.92314300	-1.02763300
C	-1.02134700	-1.38984000	-0.86455600
H	-1.02141100	-1.01577500	-1.88946300
H	-1.46787900	-2.38641500	-0.85022500
H	3.74857300	-1.07279600	-1.64816400

HF: -1100.4751451
Sum of electronic and zero-point Energies: -1100.254891
Sum of electronic and thermal Energies: -1100.239874
Sum of electronic and thermal Enthalpies: -1100.238929
Sum of electronic and thermal Free Energies: -1100.296609
Frequencies: -454.5608

X = CH_2, Y = NH

C	0.90662300	-0.02524000	-0.12231600
C	0.82282300	1.20345300	-0.08118800
N	3.34686500	0.79988300	0.12980000
N	2.90111200	1.86027300	0.11270200
C	0.05916500	2.46065600	-0.09240100
H	0.50831800	3.20907900	0.56463400
H	0.06217600	2.88038900	-1.10286300
C	0.39919100	-1.40607200	-0.24225100
C	-1.37938200	2.19867200	0.36673600
H	-1.95832300	3.12312600	0.32848800
H	-1.38478100	1.84444900	1.39743900
S	-2.27227300	-0.37453800	-0.04817400
O	-3.51840300	-0.79890600	-0.67898400
O	-2.13719300	-0.47000400	1.39982200
N	3.02333800	-0.40118800	0.20466000
C	3.78100800	-1.38399500	-0.57330000
H	4.80712300	-1.45656600	-0.21058400
H	3.29359400	-2.34452300	-0.41570100
C	0.49113800	-2.18113900	1.07706700
H	-0.07744100	-1.68085200	1.86004100
H	0.09690300	-3.19090100	0.94404100
H	1.53385700	-2.24998600	1.38975300
H	1.00211200	-1.93794900	-0.98685700
C	-1.01052600	-1.39337000	-0.84853900
H	-0.99606000	-1.03801100	-1.88057800
H	-1.44800100	-2.39413600	-0.82944600
N	-2.09325100	1.20739000	-0.43450900
H	-2.28301900	1.41967800	-1.40704800
H	3.77799300	-1.14221200	-1.63865200

HF: -1080.6091081
Sum of electronic and zero-point Energies: -1080.376862
Sum of electronic and thermal Energies: -1080.361445
Sum of electronic and thermal Enthalpies: -1080.360501
Sum of electronic and thermal Free Energies: -1080.418871
Frequencies: -459.6333

X = CH_2, Y = NH_2^+

C	0.90686800	-0.04436200	-0.10281800
C	0.78256400	1.18069700	-0.00537800
N	3.28953900	0.83928200	0.16236600
N	2.80640800	1.88305400	0.20060700
C	0.05541200	2.46171900	0.00722900
H	0.43931200	3.12440700	0.78460800
H	0.21346400	2.97441900	-0.94642700
C	0.44429300	-1.44172200	-0.24767000
C	-1.43212600	2.26136500	0.26075300
H	-1.99419700	3.17703600	0.08534700
H	-1.62537600	1.90851500	1.27290600
S	-2.21434200	-0.50640100	0.01228600
O	-3.51843500	-0.84140600	-0.49484900
O	-1.95599200	-0.35764300	1.41774300
N	2.98712900	-0.36990800	0.17413900
C	3.75605800	-1.30112000	-0.65684900
H	4.79273500	-1.34226900	-0.32198600
H	3.31243300	-2.28490500	-0.51546100
C	0.57465800	-2.24106500	1.05404800
H	0.00167200	-1.77826500	1.85711000
H	0.21928100	-3.26173800	0.90252500
H	1.62173600	-2.27508800	1.35474100
H	1.04935000	-1.93550700	-1.01554500
C	-0.96855400	-1.48227600	-0.84198400
H	-1.00898900	-1.15011800	-1.88115700
H	-1.40554100	-2.48414300	-0.78867000
N	-1.99904800	1.22427400	-0.67515900
H	-1.45125700	1.17710500	-1.54279400
H	-2.95651200	1.47292300	-0.95024300
H	3.71353600	-1.02387800	-1.71233900

HF: -1081.0161463
Sum of electronic and zero-point Energies: -1080.769445
Sum of electronic and thermal Energies: -1080.754030

Sum of electronic and thermal Enthalpies: -1080.753086
Sum of electronic and thermal Free Energies: -1080.811488
Frequencies: -475.4574

X = NH, Y = NH

C	0.88982900	-0.01294400	-0.08032100
C	0.81806700	1.21544600	-0.03970000
N	3.33841700	0.77028500	0.10750300
N	2.91346900	1.83816200	0.11182200
C	0.05831300	2.47363000	-0.04556200
H	0.48944200	3.20674200	0.64019200
H	0.08995400	2.91534600	-1.04602400
C	0.34601800	-1.38411900	-0.17777900
C	-1.39153800	2.19600800	0.36855300
H	-1.97922300	3.11412400	0.31092100
H	-1.42562100	1.84164900	1.39840600
N	-1.04574800	-1.37958900	-0.68691500
S	-2.23418500	-0.39102300	-0.08139300
O	-3.42114700	-0.82710600	-0.79657900
O	-2.14857700	-0.47741800	1.36350500
N	3.00794400	-0.42875200	0.17914300
C	3.71577500	-1.39863400	-0.66219700
H	4.76100300	-1.47910900	-0.36137100
H	3.23601400	-2.36122100	-0.49515100
H	-1.10496000	-1.40166200	-1.70038400
C	0.46243300	-2.15789100	1.13488600
H	-0.06767400	-1.64058700	1.93326000
H	0.03689200	-3.15399800	1.00746500
H	1.51430400	-2.24700800	1.40905000
H	0.89226700	-1.93227100	-0.94976300
H	3.65120800	-1.13378700	-1.72007900
N	-2.06991800	1.19680300	-0.45517900
H	-2.19138600	1.39700500	-1.44153600

HF: -1096.6480441
Sum of electronic and zero-point Energies: -1096.427020
Sum of electronic and thermal Energies: -1096.411781
Sum of electronic and thermal Enthalpies: -1096.410837
Sum of electronic and thermal Free Energies: -1096.468941
Frequencies: -447.7817

X = NH, Y = NH_2^+

C	0.89916900	-0.03279300	-0.06928600
C	0.77898500	1.19107600	0.02313800
N	3.28523300	0.80904300	0.17040000
N	2.82640700	1.86075000	0.22868800
C	0.04933500	2.46944400	0.01100300
H	0.41851900	3.14227500	0.78688400
H	0.22157300	2.97028700	-0.94631000
C	0.40070700	-1.41526600	-0.21920600
C	-1.44299000	2.26772000	0.24294000
H	-2.00029500	3.18093000	0.04101100
H	-1.65046700	1.93681600	1.25859800
N	-1.02067200	-1.39142500	-0.67652000
S	-2.17420100	-0.52889800	-0.00205500
O	-3.44440800	-0.88906700	-0.56059300
O	-1.93568200	-0.34767900	1.39734400
N	2.97925600	-0.39926100	0.16790700
C	3.69975500	-1.29827000	-0.74250800
H	4.75319800	-1.35081200	-0.46726000
H	3.26302800	-2.28687600	-0.61554700
H	-1.23248700	-1.70314300	-1.62044200
C	0.56049700	-2.26320100	1.03979700
H	0.05691700	-1.79576800	1.88529700
H	0.14033100	-3.25398000	0.86677400
H	1.62067400	-2.35729900	1.27466800
H	0.91490600	-1.89956700	-1.05160300
H	3.59880300	-0.97711600	-1.78139800
N	-2.00248000	1.21078500	-0.67763500
H	-1.46196400	1.15558700	-1.54944500
H	-2.96174800	1.45350800	-0.94750300

HF: -1097.0586348
Sum of electronic and zero-point Energies: -1096.823086
Sum of electronic and thermal Energies: -1096.807805
Sum of electronic and thermal Enthalpies: -1096.806861
Sum of electronic and thermal Free Energies: -1096.864982
Frequencies: -461.0124

X = NH, Y = O

C	0.88108100	-0.01751400	-0.08143500
C	0.79450900	1.20898600	-0.02887200
N	3.31381500	0.78289000	0.14951400
N	2.88718500	1.84887600	0.16594500
C	0.01722000	2.45647800	-0.06747500
H	0.40273400	3.19977000	0.63440300
H	0.07794100	2.89321700	-1.06775300
C	0.34099800	-1.38745800	-0.20458200
C	-1.43285900	2.15458300	0.29016600
H	-2.07563400	3.01617200	0.11573500
H	-1.52392000	1.83104300	1.32635200
N	-1.06102300	-1.36343000	-0.69906200
S	-2.21282200	-0.38784500	-0.06772600
O	-3.44747600	-0.76336400	-0.71347000
O	-2.08873300	-0.41128500	1.37136400
O	-1.94925700	1.11377900	-0.57945100
N	2.99579400	-0.42033800	0.19729800
C	3.70672000	-1.36089500	-0.67581600
H	4.75522400	-1.43654200	-0.38587400
H	3.23924500	-2.33276900	-0.52956000
H	-1.15025000	-1.41084500	-1.70946900
C	0.46225700	-2.19477200	1.08639300
H	-0.05475400	-1.69293700	1.90322100
H	0.02856200	-3.18424700	0.93799900
H	1.51585900	-2.29801600	1.34804100
H	0.87446500	-1.91654700	-0.99778700
H	3.62945700	-1.06826600	-1.72538800

HF: -1116.5132594
Sum of electronic and zero-point Energies: -1116.304183
Sum of electronic and thermal Energies: -1116.289358
Sum of electronic and thermal Enthalpies: -1116.288413
Sum of electronic and thermal Free Energies: -1116.345649
Frequencies: -441.6855

X = O, Y = NH

C	0.87741300	-0.00275200	-0.07911500
C	0.81436100	1.22538700	-0.03431900
N	3.31580300	0.74162500	0.17037900
N	2.90533400	1.81407500	0.18881900
C	0.06012300	2.48545500	-0.07450900
H	0.46952700	3.22377400	0.61832100
H	0.12635200	2.91515300	-1.07819700
C	0.32513700	-1.35580600	-0.22711200
C	-1.40303000	2.21342400	0.29654200
H	-1.99847000	3.11839500	0.16834100
H	-1.47470500	1.90710800	1.33946600
S	-2.20338500	-0.38369500	-0.05975500
O	-3.38362200	-0.89620400	-0.71556800
O	-2.06793100	-0.43880800	1.37854300
N	2.97893300	-0.45698100	0.20626100
C	3.67109100	-1.39432800	-0.68686700
H	4.71941000	-1.49030000	-0.40249100
H	3.18938700	-2.36111300	-0.55495500
C	0.40887900	-2.21070100	1.02802100
H	-0.05552400	-1.70825100	1.87438400
H	-0.08735600	-3.16545600	0.85040700
H	1.45979200	-2.39374300	1.25641300
H	0.81766200	-1.86883200	-1.05536700
H	3.59344600	-1.08175900	-1.73062800
N	-2.03683400	1.16611800	-0.50615100
H	-2.17868600	1.33086400	-1.49616700
O	-1.04759400	-1.27807000	-0.73603300

HF: -1116.5143134
Sum of electronic and zero-point Energies: -1116.305755
Sum of electronic and thermal Energies: -1116.290782
Sum of electronic and thermal Enthalpies: -1116.289837
Sum of electronic and thermal Free Energies: -1116.347289
Frequencies: -441.7386

X = O, Y = O

C	0.87022600	-0.01073100	-0.08786800
C	0.79139000	1.21571400	-0.03486500
N	3.28902200	0.75675700	0.21325300
N	2.87204400	1.82549500	0.23984300
C	0.01866100	2.46391900	-0.10553800
H	0.39019000	3.21659000	0.59333900
H	0.09971600	2.88389600	-1.11123800
C	0.32224700	-1.36120800	-0.25606900
C	-1.43709800	2.16709600	0.23089300
H	-2.08387800	3.01189600	0.00307100
H	-1.55126500	1.88101200	1.27520000
S	-2.18289800	-0.37960300	-0.04734100
O	-3.41086400	-0.82350200	-0.64335400
O	-2.01444600	-0.38200200	1.38422400
N	2.97068900	-0.44666000	0.22505500
C	3.67780900	-1.35243800	-0.69026000
H	4.72592100	-1.44148800	-0.40358700
H	3.20786800	-2.32808200	-0.58477600
C	0.40570700	-2.24478300	0.97653400
H	-0.04762100	-1.75833300	1.83824800
H	-0.09713500	-3.19197200	0.77980200
H	1.45693600	-2.43931600	1.19322600
H	0.79405700	-1.85656400	-1.10602100
H	3.59965800	-1.01285700	-1.72525700
O	-1.07007000	-1.26688600	-0.74628900
O	-1.92762200	1.08417900	-0.61190100

HF: -1136.3766548
Sum of electronic and zero-point Energies: -1136.180307
Sum of electronic and thermal Energies: -1136.165688
Sum of electronic and thermal Enthalpies: -1136.164743
Sum of electronic and thermal Free Energies: -1136.221663
Frequencies: -433.4570

X = O, Y = NH_2^+

C	0.89236100	-0.02632400	-0.08321300
C	0.78241300	1.19765500	0.01703400
N	3.26429400	0.77662000	0.24247700
N	2.81293900	1.83020500	0.31206400
C	0.04968500	2.47297200	-0.01930600
H	0.39920100	3.15377500	0.75852700
H	0.23865100	2.96404700	-0.97820300
C	0.38473400	-1.38567600	-0.27738400
C	-1.44589200	2.26476900	0.18608900
H	-2.00851900	3.16155000	-0.06568000
H	-1.67753400	1.97017300	1.20745100
S	-2.14910600	-0.51299300	0.02320900
O	-3.41577200	-0.93315800	-0.47843600
O	-1.86275100	-0.33740300	1.41054300
N	2.96074100	-0.43063000	0.19742000
C	3.68569900	-1.28851500	-0.75181400

H	4.73601400	-1.35590100	-0.46887100
H	3.24502100	-2.28022400	-0.67596800
C	0.48616800	-2.30538900	0.92136600
H	0.05433500	-1.84763400	1.80962800
H	-0.01281700	-3.24913000	0.70263300
H	1.54288300	-2.49897800	1.10962200
H	0.82117700	-1.84412000	-1.16479800
H	3.59373300	-0.91493200	-1.77346900
N	-1.97895700	1.16734100	-0.71259300
H	-1.41812100	1.08082600	-1.57137300
O	-1.04881600	-1.29331100	-0.74211400
H	-2.93374900	1.39771800	-1.01300100

HF: -1116.9147269
Sum of electronic and zero-point Energies: -1116.691761
Sum of electronic and thermal Energies: -1116.676781
Sum of electronic and thermal Enthalpies: -1116.675837
Sum of electronic and thermal Free Energies: -1116.733384
Frequencies: -448.4674

X = NH_2^+, Y = NH

C	0.93035600	-0.02005700	-0.10922000
C	0.82611700	1.20764500	-0.08373900
N	3.31968200	0.79541400	0.17420900
N	2.86802200	1.85198000	0.16961700
C	0.06893100	2.46728000	-0.12324100
H	0.51380400	3.21917900	0.53126200
H	0.08870500	2.87000800	-1.13929800
C	0.43351600	-1.39597700	-0.21967100
C	-1.37067200	2.22421200	0.32906200
H	-1.97095800	3.12777000	0.22961200
H	-1.39742800	1.90724000	1.37062900
S	-2.30073400	-0.30854300	-0.00097900
O	-3.43830800	-0.86090000	-0.67731800
O	-2.04484000	-0.46259700	1.39895000
N	3.00795200	-0.41023000	0.21413700
C	3.75279800	-1.35013100	-0.63351400
H	4.79449900	-1.40135800	-0.31619400
H	3.30268600	-2.32991000	-0.48519300
C	0.47824500	-2.18811200	1.08075100
H	-0.03675700	-1.66421100	1.88259600
H	0.04151100	-3.17844900	0.94206800
H	1.52564000	-2.30844600	1.35682200
H	0.98366000	-1.93638200	-0.99469900
H	3.69449600	-1.06889300	-1.68719200
N	-0.97869800	-1.34775100	-0.79558300
H	-0.93062800	-1.03870000	-1.77350400
N	-2.05254700	1.18723100	-0.46565300
H	-2.42550600	1.41812100	-1.38264200
H	-1.37340200	-2.29697100	-0.81131100

HF: -1097.0604246
Sum of electronic and zero-point Energies: -1096.825003
Sum of electronic and thermal Energies: -1096.809711
Sum of electronic and thermal Enthalpies: -1096.808767
Sum of electronic and thermal Free Energies: -1096.866951
Frequencies: -455.7701

X = NH_2^+, Y = O

C	0.91947100	-0.02368100	-0.12503300
C	0.80315100	1.20211400	-0.09658800
N	3.28625900	0.79971700	0.24204300
N	2.83860400	1.85640800	0.23935400
C	0.02954100	2.44924900	-0.18669300
H	0.44153900	3.23158000	0.45448400
H	0.05775800	2.81952800	-1.21416000
C	0.41637900	-1.39162300	-0.28031300
C	-1.40272400	2.20110600	0.24644000
H	-2.05736700	3.04011100	0.02722700
H	-1.47189400	1.92285600	1.29615400
S	-2.26461600	-0.30842400	0.03130800
O	-3.47117500	-0.80810500	-0.53909800
O	-1.94796900	-0.39783300	1.42009900
N	2.98654400	-0.40888900	0.25432600
C	3.74851000	-1.31928100	-0.61249500
H	4.78703100	-1.36899200	-0.28545800
H	3.30573600	-2.30634600	-0.49536500
C	0.45778800	-2.24366500	0.98079600
H	-0.03502900	-1.74950600	1.81460500
H	0.00357500	-3.21919500	0.80166800
H	1.50623400	-2.39476500	1.23700200
H	0.94474700	-1.90379000	-1.08880900
H	3.69762100	-1.00819400	-1.65790600
N	-1.00987400	-1.29652400	-0.84557700
H	-0.96748000	-0.91593500	-1.80105800
H	-1.41600400	-2.23907800	-0.92318300
O	-1.96911100	1.09671400	-0.56273000

HF: -1116.9137543
Sum of electronic and zero-point Energies: -1116.690867
Sum of electronic and thermal Energies: -1116.675833
Sum of electronic and thermal Enthalpies: -1116.674889
Sum of electronic and thermal Free Energies: -1116.732750
Frequencies: -444.9043

X = NH_2^+, Y = NH_2^+

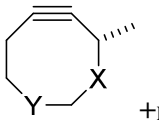
C	0.92885900	-0.04149100	-0.09124400
C	0.78488200	1.18277800	-0.00053900
N	3.25962800	0.83435200	0.20916700
N	2.76271900	1.86955800	0.26600400
C	0.05769600	2.46240400	-0.02087200
H	0.43333500	3.13610100	0.75095400
H	0.23379700	2.95519600	-0.98144400
C	0.48157400	-1.43171600	-0.21870500
C	-1.43135800	2.28444700	0.22124800
H	-1.99348000	3.18446100	-0.02168000
H	-1.65745800	1.98445600	1.24230800
S	-2.21923500	-0.43974800	0.04826200
O	-3.45552800	-0.90369400	-0.46710200
O	-1.83286200	-0.33628000	1.40631200
N	2.97754100	-0.37924800	0.17656300
C	3.73766700	-1.24914800	-0.73380900
H	4.78784400	-1.25994400	-0.44371900
H	3.34153300	-2.25551600	-0.61500900
C	0.56365700	-2.25100200	1.06129000
H	0.05270900	-1.76099600	1.88716500
H	0.16300900	-3.25379100	0.90796100
H	1.61995200	-2.33822500	1.31516700
H	1.00972200	-1.93955200	-1.02935600
H	3.63540900	-0.92241600	-1.77040000
N	-0.96942900	-1.43128800	-0.78108800
H	-0.96468500	-1.20316100	-1.78651200
N	-2.00210600	1.20430600	-0.69433100
H	-1.46332800	1.14897100	-1.57290900
H	-1.35485300	-2.39120000	-0.73161400
H	-2.96494400	1.44999000	-0.97520700

HF: -1097.4179226
Sum of electronic and zero-point Energies: -1097.168046
Sum of electronic and thermal Energies: -1097.152928
Sum of electronic and thermal Enthalpies: -1097.151984
Sum of electronic and thermal Free Energies: -1097.209351
Frequencies: -465.0242

X = NBoc, Y = O

C	-1.88760400	-0.11294600	0.03072700
C	-2.04165900	0.57627000	1.03857900
N	-4.11438700	-0.93699500	0.99188200
N	-3.97755700	-0.15520100	1.81984800
C	-1.60249600	1.60458600	1.99526600
H	-2.44598900	2.14881600	2.42701100
H	-1.07109100	1.12566800	2.82209900
C	-1.10879800	-0.57987600	-1.13480300
C	-0.69466300	2.61421600	1.30448000
H	-0.25086300	3.30245500	2.02137800
H	-1.23411000	3.17247000	0.54137400
N	0.28177900	-0.03019300	-1.00973000
S	0.48239900	1.63902200	-0.87928500
O	1.79952700	1.98232900	-1.33762600
O	-0.66782400	2.23792200	-1.50838800
O	0.44901200	1.95260200	0.68709400
N	-3.66621400	-1.33358200	-0.10099700
C	-3.55355100	-2.78325900	-0.30686600
H	-4.54245100	-3.23731300	-0.37842300
H	-3.04290300	-2.92257600	-1.25771900
C	-1.75444200	-0.31865300	-2.49261100
H	-1.07307800	-0.63466300	-3.28369100
H	-2.66769900	-0.91158400	-2.55859400
H	-2.00933600	0.72899000	-2.62644500
H	-0.94522900	-1.65370900	-1.04582700
C	1.24396300	-0.92223400	-0.46845700
O	2.24748000	-0.27678000	0.07994600
O	1.09554900	-2.11580700	-0.53275000
C	3.41829800	-0.98750900	0.63123200
C	4.08349500	-1.81330400	-0.46096100
H	5.03113600	-2.19643600	-0.07666600
H	3.46452800	-2.65657800	-0.76269800
H	4.29496800	-1.18832100	-1.33137800
C	4.31567600	0.16105000	1.06674200
H	5.22741600	-0.23883600	1.51337700
H	4.58594600	0.77854100	0.20829000
H	3.80580200	0.78261200	1.80508300
C	2.98346300	-1.82621400	1.82473400
H	2.44954900	-1.20480200	2.54686900
H	2.34588100	-2.65442100	1.51947200
H	3.87388400	-2.23029800	2.31078400
H	-2.98014500	-3.25746800	0.49266200

HF: -1462.2928217
Sum of electronic and zero-point Energies: -1461.957608
Sum of electronic and thermal Energies: -1461.934188
Sum of electronic and thermal Enthalpies: -1461.933243
Sum of electronic and thermal Free Energies: -1462.011031
Frequencies: -441.0202



+methyl azide (*anti*-TSs)

X = CH_2, Y = CH_2

C	0.00455800	0.61937000	-0.17234200
C	0.40329300	-0.54111900	-0.04610600
N	2.57522000	0.82866200	-0.44018700
N	1.89521500	1.74784100	-0.55950500
C	0.21690400	-1.99173400	0.14549400
H	0.96945000	-2.55806600	-0.40828700
H	0.35817900	-2.23155300	1.20566900

C	-1.06659000	1.63939200	-0.22170400
C	-1.18861600	-2.42444400	-0.29824600
H	-1.30235500	-3.48124200	-0.03950300
H	-1.25164800	-2.36066700	-1.38960400
C	-0.74864800	2.89221500	0.59847300
H	0.13034300	3.40783300	0.21388800
H	-1.59788200	3.57910500	0.57042100
H	-0.56123300	2.62248200	1.64132700
H	-1.19083000	1.93642400	-1.27076500
N	2.54983900	-0.41508900	-0.33377900
C	3.44878000	-1.03527800	0.64410400
H	3.14491900	-2.07778200	0.71687100
H	4.48366200	-0.99916400	0.30021700
C	-2.38866300	1.00973700	0.25715500
H	-3.17814800	1.74755300	0.08029600
H	-2.32928900	0.87365000	1.34366700
C	-2.34359600	-1.62242600	0.32386300
H	-3.21189200	-2.28533700	0.35899600
H	-2.10007200	-1.39410900	1.36816900
C	-2.77349300	-0.32374500	-0.40644500
H	-2.39151000	-0.33765300	-1.43365800
H	-3.86259000	-0.34087300	-0.49426600
H	3.36540700	-0.56231700	1.62537900

HF=-555.283997
Sum of electronic and zero-point Energies= -555.022942
Sum of electronic and thermal Energies= -555.009054
Sum of electronic and thermal Enthalpies= -555.008110
Sum of electronic and thermal Free Energies= -555.063793
Frequencies -- -462.8835

X = NH, Y = CH_2

C	0.00271600	0.60592700	-0.16141200
C	0.41422600	-0.54913600	-0.03256700
N	2.56292600	0.84538700	-0.45380500
N	1.88358400	1.76321800	-0.57538800
C	0.22011400	-1.99722200	0.16138000
H	0.96752000	-2.57185900	-0.39050800
H	0.35350800	-2.23829300	1.22205200
C	-1.10266100	1.59859100	-0.21532000
C	-1.19078600	-2.40412000	-0.29073900
H	-1.33184000	-3.45745400	-0.03207500
H	-1.24410800	-2.34053000	-1.38263600
N	-2.38674700	1.01372900	0.18918200
C	-0.83346900	2.82981500	0.64559500
H	0.07397500	3.33703900	0.32221500
H	-1.67596600	3.51950100	0.57469800
H	-0.70862300	2.53538100	1.69152000
H	-1.20623100	1.91964400	-1.25864900
N	2.55474200	-0.39694100	-0.34091000
C	3.45869900	-0.99988800	0.64381800
H	3.16552000	-2.04485100	0.72389200
H	4.49334900	-0.95480000	0.30081300
H	-2.39539900	0.92175600	1.20155100
C	-2.33187800	-1.57341400	0.32050100
H	-3.21567700	-2.21544300	0.35978800
H	-2.09119600	-1.33213400	1.36284600
C	-2.74790700	-0.27290900	-0.42045200
H	-2.35150700	-0.28081400	-1.44051400
H	-3.83706300	-0.28102200	-0.51411600
H	3.36788900	-0.51974000	1.62073900

HF=-571.3210885
Sum of electronic and zero-point Energies= -571.071219
Sum of electronic and thermal Energies= -571.057417
Sum of electronic and thermal Enthalpies= -571.056473
Sum of electronic and thermal Free Energies= -571.111907
Frequencies -- -453.2022

X = NH_2^+, Y = CH_2

C	0.04218900	0.61263200	-0.19922200
C	0.44257500	-0.54499800	-0.05474700
N	2.57187400	0.83701400	-0.44097800
N	1.92515200	1.77325400	-0.57477200
C	0.25054800	-1.99219000	0.15485700
H	1.00450200	-2.56337600	-0.38983800
H	0.38399700	-2.21650300	1.21855500
C	-1.02684700	1.61238600	-0.23255800
C	-1.14896300	-2.42542100	-0.30272500
H	-1.27335500	-3.47640600	-0.03306900
H	-1.20205400	-2.37321200	-1.39424200
N	-2.29915800	0.94039300	0.27093300
C	-0.77603100	2.85262900	0.61451800
H	0.07962800	3.38688600	0.20691400
H	-1.64190400	3.51656500	0.59548300
H	-0.55120800	2.57617900	1.64652300
H	-1.24861100	1.89671400	-1.26422900
N	2.53665100	-0.40259500	-0.32569400
C	3.42478800	-1.03097900	0.66040400
H	3.12777200	-2.07583900	0.71637500
H	4.46094100	-0.98137900	0.32516900
H	-2.18274400	0.75247300	1.27146600
C	-2.31588500	-1.62952000	0.29851500
H	-3.19860800	-2.27048200	0.27904100
H	-2.12728500	-1.42491700	1.35845800
H	-3.06029200	1.62075900	0.20303500
C	-2.71549000	-0.33485600	-0.42995700
H	-2.29863300	-0.28394600	-1.43574700
H	-3.79867000	-0.27229400	-0.50766100
H	3.32357800	-0.56578900	1.64283700

HF=-571.775591
Sum of electronic and zero-point Energies= -571.509891
Sum of electronic and thermal Energies= -571.496168
Sum of electronic and thermal Enthalpies= -571.495224
Sum of electronic and thermal Free Energies= -571.550275
Frequencies -- -440.1775

X = O, Y = CH_2

C	0.00426300	0.60281400	-0.18166700
C	0.41342000	-0.55195200	-0.05385400
N	2.55737000	0.85265900	-0.43969700
N	1.89410600	1.78037100	-0.55897100
C	0.21282800	-1.99783300	0.14636300
H	0.94746700	-2.57904900	-0.41550900
H	0.35912600	-2.23658900	1.20561000
C	-1.11155500	1.57235600	-0.20647700
C	-1.20809700	-2.39191500	-0.28768000
H	-1.35819600	-3.44125800	-0.01950800
H	-1.27095500	-2.33655600	-1.37957300
C	-0.87413500	2.79999800	0.65687400
H	-0.01338300	3.35829100	0.29082600
H	-1.75614500	3.44142700	0.63047600
H	-0.68520000	2.49682000	1.68864300
H	-1.27613900	1.88358100	-1.24806500
N	2.54990100	-0.38973800	-0.34356200
C	3.43923100	-1.00463800	0.64807800
H	3.14829400	-2.05150400	0.70782100
H	4.47876600	-0.95041900	0.32219300
C	-2.33836400	-1.54850300	0.32495100
H	-3.23777100	-2.16971900	0.33806000
H	-2.11357900	-1.31427300	1.37085100
C	-2.70885500	-0.23328200	-0.39445100
H	-2.32113200	-0.23021400	-1.42011500
H	-3.79664300	-0.16098900	-0.45463500
O	-2.30205000	0.95540400	0.27952400
H	3.32983200	-0.53809200	1.62952200

HF=-591.1913715
Sum of electronic and zero-point Energies= -590.953996
Sum of electronic and thermal Energies= -590.940438
Sum of electronic and thermal Enthalpies= -590.939494
Sum of electronic and thermal Free Energies= -590.994349
Frequencies -- -440.9608

X = CH_2, Y = O

C	-0.01983600	0.60204500	-0.16852700
C	0.42124400	-0.54084800	-0.03651800
N	2.54960900	0.87414500	-0.45479300
N	1.86225100	1.78564500	-0.57444200
C	0.22739100	-1.98637500	0.17006400
H	0.93937100	-2.58280400	-0.40653300
H	0.37376700	-2.23358700	1.22614100
C	-1.12950000	1.57984400	-0.21777800
C	-1.19825800	-2.35783200	-0.25943600
H	-1.40282400	-3.39460500	0.01959100
H	-1.28248700	-2.27379500	-1.34791900
O	-2.17325700	-1.54822500	0.37014900
C	-0.86305000	2.83893300	0.61029200
H	0.00455700	3.38139000	0.23621700
H	-1.73239000	3.49977400	0.57471200
H	-0.67901900	2.57105800	1.65408700
H	-1.25998600	1.87811800	-1.26541500
N	2.56017900	-0.36845800	-0.34698700
C	3.46084300	-0.95837700	0.64918100
H	3.18039400	-2.00707900	0.72708000
H	4.49851600	-0.89982400	0.31786400
C	-2.43016800	0.89738500	0.25122000
H	-3.26322000	1.57454200	0.03598500
H	-2.39635200	0.76808600	1.33834100
C	-2.72994600	-0.46454800	-0.37516300
H	-2.37108200	-0.49762800	-1.40983300
H	-3.81232400	-0.62020500	-0.39228800
H	3.35254600	-0.47833200	1.62432700

HF=-591.1910657
Sum of electronic and zero-point Energies= -590.953702
Sum of electronic and thermal Energies= -590.940150
Sum of electronic and thermal Enthalpies= -590.939206
Sum of electronic and thermal Free Energies= -590.994042
Frequencies -- -452.0594

X = CH_2, Y = NH

C	-0.00450700	0.60873200	-0.16142000
C	0.41729900	-0.54070400	-0.02088000
N	2.56370700	0.84777900	-0.46624500
N	1.88036500	1.76264400	-0.58970500
C	0.21473700	-1.98391000	0.18700600
H	0.95268700	-2.57988000	-0.35661900
H	0.33372800	-2.22153800	1.25007800
C	-1.09708800	1.60366500	-0.21212800
C	-1.20018800	-2.38483100	-0.28022900
H	-1.34037400	-3.44325100	-0.03714800
H	-1.24758400	-2.30063800	-1.36899600
C	-0.80893200	2.85760200	0.61712800
H	0.06969400	3.38384700	0.24559700
H	-1.66547100	3.53479400	0.57962400
H	-0.63229100	2.58607000	1.66132400
H	-1.22370000	1.90512100	-1.25945100
N	2.55971900	-0.39401300	-0.34475700
C	3.46528400	-0.98462900	0.64602000
H	3.17043300	-2.02800300	0.74140200
H	4.49924800	-0.94583600	0.30028200
C	-2.40718800	0.94177100	0.25655800

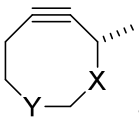
H	-3.21914600	1.65396700	0.07544800
H	-2.35743000	0.79988800	1.34329900
N	-2.30983700	-1.62098000	0.27126900
H	-2.19533100	-1.46904400	1.26691900
C	-2.76777300	-0.39951200	-0.40575300
H	-2.39030400	-0.41585400	-1.43313900
H	-3.85959900	-0.44569700	-0.47704300
H	3.37787900	-0.49105600	1.61666800

HF=-571.3206962
Sum of electronic and zero-point Energies= -571.071204
Sum of electronic and thermal Energies= -571.057298
Sum of electronic and thermal Enthalpies= -571.056354
Sum of electronic and thermal Free Energies= -571.112077
Frequencies -- -457.0268

X = CH_2, Y = NH_2^+

C	0.00126100	0.61935400	-0.15479500
C	0.44906500	-0.52682300	-0.05302700
N	2.54100500	0.89273700	-0.44405600
N	1.83603900	1.79410300	-0.54450100
C	0.29716100	-1.98300200	0.13223200
H	0.99792500	-2.54350600	-0.48917200
H	0.50870800	-2.24941400	1.17275700
C	-1.07813700	1.63081900	-0.22113500
C	-1.11252400	-2.43392300	-0.24400600
H	-1.30038900	-3.44281900	0.11827400
H	-1.26829600	-2.40897300	-1.32035800
C	-0.82638200	2.84514700	0.67567500
H	0.06943200	3.38211200	0.36848500
H	-1.67861100	3.52628200	0.62364900
H	-0.70310100	2.52720800	1.71388500
H	-1.13640500	1.97236400	-1.26098500
N	2.54787900	-0.35152200	-0.34921600
C	3.47075800	-0.96294100	0.61442600
H	3.20562300	-2.01708200	0.66422900
H	4.49992400	-0.88146300	0.26340400
C	-2.42961300	0.98509900	0.14437200
H	-3.23053000	1.65444300	-0.17761600
H	-2.51828600	0.91167500	1.23444300
N	-2.16056700	-1.53283300	0.36851200
H	-2.95887200	-2.11023200	0.63613800
H	-1.79282800	-1.15632100	1.24741200
C	-2.68243900	-0.38075700	-0.48530300
H	-2.20608000	-0.46654900	-1.46074900
H	-3.74806900	-0.56092800	-0.60383100
H	3.37446700	-0.51202900	1.60423800

HF=-571.7747783
Sum of electronic and zero-point Energies= -571.508657
Sum of electronic and thermal Energies= -571.494993
Sum of electronic and thermal Enthalpies= -571.494049
Sum of electronic and thermal Free Energies= -571.548881
Frequencies -- -463.2412



+methyl azide (*syn*-TSs)

X = CH_2, Y = CH_2

C	-0.28622400	0.09818900	-0.07235100
C	0.08536200	-1.07421200	-0.00080400
N	-2.48792900	-1.28721700	0.13274900
N	-1.80305500	-2.21188800	0.13757800
C	1.12502400	-2.11813900	0.00225200
H	0.86381100	-2.93040000	0.68505500
H	1.17755000	-2.55922100	-0.99940400
C	-0.08903600	1.55530200	-0.18922600
C	2.49088700	-1.52358400	0.37670900
H	3.23972500	-2.31229300	0.25805800
H	2.48405500	-1.25518800	1.43838400
N	-2.46621200	-0.04307900	0.20917100
C	-3.40711400	0.72490000	-0.60788300
H	-4.43583500	0.55275200	-0.28708600
H	-3.16717200	1.77435000	-0.44599000
C	-0.38154800	2.26799700	1.13578900
H	0.29436700	1.92303200	1.92150500
H	-0.25368500	3.34639500	1.01720300
H	-1.40450500	2.06818600	1.46009700
H	-0.77796400	1.95254400	-0.94254500
C	1.34732700	1.81670900	-0.69328000
H	1.40351100	1.53670700	-1.75005100
H	1.51115200	2.89832100	-0.64842000
C	2.47159200	1.09558100	0.07494400
H	2.20233700	1.01258800	1.13346300
H	3.34807200	1.74761700	0.04642500
C	2.90584500	-0.29642900	-0.45519700
H	3.99710500	-0.30076000	-0.51487200
H	2.54997600	-0.42533300	-1.48411600
H	-3.30481400	0.48810900	-1.66990800

HF=-555.2850031
Sum of electronic and zero-point Energies= -555.024229
Sum of electronic and thermal Energies= -555.011078
Sum of electronic and thermal Enthalpies= -555.010134
Sum of electronic and thermal Free Energies= -555.063620
Frequencies -- -455.0757

X = NH, Y = CH_2

C	0.27910900	-0.08524400	-0.04513000
C	-0.08907000	1.08790600	0.02626400
N	2.48629400	1.27196900	0.14722100
N	1.81715600	2.20662200	0.16679700
C	-1.13612800	2.12265500	0.01787600
H	-0.90250900	2.92809500	0.71833200
H	-1.17176800	2.57580100	-0.97896000
C	0.04691200	-1.54439900	-0.17802900
C	-2.49863100	1.49740600	0.35378600
H	-3.26439500	2.26710500	0.22100400
H	-2.51174400	1.22295300	1.41392300
N	2.45898500	0.02744800	0.21266400
C	3.36189000	-0.73288100	-0.65544000
H	4.40433900	-0.55022500	-0.39073000
H	3.14098700	-1.78451800	-0.48255500
C	0.35456300	-2.27870400	1.12822300
H	-0.30047200	-1.93547900	1.93156700
H	0.20876000	-3.35089800	0.98928100
H	1.38560800	-2.09010600	1.43177600
H	0.71042500	-1.94296100	-0.95149100
H	-1.37714800	-1.63410900	-1.63274700
C	-2.41811300	-1.12542000	0.04799900
H	-2.15919300	-1.04267900	1.10704700
H	-3.28468800	-1.78969400	-0.00030200
C	-2.85870800	0.26323400	-0.49347000
H	-2.47097600	0.39281900	-1.51090200
H	-3.94716900	0.23759000	-0.58971100
N	-1.32102900	-1.82559400	-0.63791900
H	3.19915200	-0.49412600	-1.70934400

HF=-571.3212893
Sum of electronic and zero-point Energies= -571.071338
Sum of electronic and thermal Energies= -571.057556
Sum of electronic and thermal Enthalpies= -571.056612
Sum of electronic and thermal Free Energies= -571.111697

X = NH_2^+, Y = CH_2

C	0.33872300	-0.07336700	-0.07519800
C	-0.07448600	1.08598600	-0.03126200
N	2.47007200	1.28520300	0.20340800
N	1.78694400	2.20796700	0.21072000
C	-1.11696900	2.12442700	-0.06816800
H	-0.85214700	2.96392900	0.57717100
H	-1.17098800	2.51681400	-1.08895400
C	0.13184700	-1.52017800	-0.18887700
C	-2.47832500	1.54743300	0.34459400
H	-3.23306200	2.31919700	0.17831800
H	-2.47302600	1.34135700	1.41894600
N	2.46004000	0.03923600	0.23855500
C	3.37316400	-0.68306400	-0.65642500
H	4.41004500	-0.48717600	-0.38261200
H	3.17413500	-1.74323100	-0.51276400
C	0.39017600	-2.29027500	1.09921700
H	-0.20327900	-1.90203600	1.92705400
H	0.18038200	-3.35202700	0.96278500
H	1.44216900	-2.17332900	1.35829900
H	0.73515300	-1.94289600	-0.99565600
H	-1.37482000	-1.39708700	-1.62003200
H	-1.48365100	-2.73154000	-0.68865700
C	-2.39591400	-1.05700900	0.16363900
H	-2.00803400	-0.94075700	1.17402300
H	-3.20672900	-1.78118800	0.19436400
C	-2.90094900	0.27885100	-0.41108600
H	-2.62962900	0.36396500	-1.46936700
H	-3.99032000	0.22479500	-0.39165600
N	-1.30608800	-1.72430700	-0.65253900
H	3.20342400	-0.41230900	-1.70088100

HF=-571.7740241
Sum of electronic and zero-point Energies= -571.508550
Sum of electronic and thermal Energies= -571.494726
Sum of electronic and thermal Enthalpies= -571.493782
Sum of electronic and thermal Free Energies= -571.548976
Frequencies -- -450.8004

X = O, Y = CH_2

C	0.27935800	-0.07451600	-0.05825100
C	-0.11307800	1.08972800	0.01062500
N	2.45515600	1.28714900	0.19913000
N	1.78475200	2.21906500	0.22536400
C	-1.17366400	2.11010300	-0.02613600
H	-0.95735000	2.93286300	0.65901600
H	-1.20448800	2.53954300	-1.03330500
C	0.05355800	-1.52534600	-0.22191000
C	-2.53212500	1.47415300	0.31105600
H	-3.30816200	2.22260200	0.12879200
H	-2.56247800	1.24875900	1.38226700
N	2.44205300	0.04142200	0.23397800
C	3.34057200	-0.68107600	-0.67283100
H	4.38371100	-0.50340900	-0.40852300
H	3.12546200	-1.73951500	-0.53957700
C	0.39001900	-2.32448800	1.03525000
H	-0.19751500	-1.98418300	1.88968800
H	0.18474500	-3.38133800	0.85875800
H	1.44554600	-2.20131900	1.28233100
H	0.66534800	-1.89800600	-1.04840300
C	-2.32640900	-1.13249600	0.10355800
H	-2.00584600	-0.98856000	1.14016800
H	-3.13436200	-1.86627200	0.11187900

C	-2.85706700	0.19604700	-0.48133700
H	-2.49579000	0.28680800	-1.51089100
H	-3.94500700	0.11217900	-0.54417700
O	-1.28767100	-1.75075200	-0.65788800
H	3.16683900	-0.40025200	-1.71436500

HF=-591.1900279
Sum of electronic and zero-point Energies= -590.952916
Sum of electronic and thermal Energies= -590.939264
Sum of electronic and thermal Enthalpies= -590.938320
Sum of electronic and thermal Free Energies= -590.993295
Frequencies -- -443.2803

X = CH_2, Y = O

C	-0.26867400	0.09036400	-0.08961400
C	0.07167600	-1.09069300	-0.01939400
N	-2.50198900	-1.24009200	0.16123000
N	-1.85600600	-2.19040400	0.16580600
C	1.12742100	-2.11549000	-0.03744700
H	0.92355000	-2.93164900	0.66074100
H	1.18972900	-2.55530800	-1.03736000
C	-0.02319500	1.54072400	-0.21095600
C	2.46494800	-1.45660000	0.32573600
H	3.27685600	-2.17263200	0.17464900
H	2.45424800	-1.16966900	1.38246900
N	-2.45237400	0.00262600	0.22329200
C	-3.38262600	0.78136700	-0.59683200
H	-4.40493600	0.68175400	-0.22864500
H	-3.08010500	1.82211300	-0.49502800
C	-0.30568300	2.27023800	1.10729000
H	0.35236000	1.90955200	1.90147800
H	-0.14342400	3.34318700	0.98396300
H	-1.33653900	2.10341300	1.42410000
H	-0.68676300	1.95689600	-0.97616600
C	1.43016500	1.75227200	-0.69273900
H	1.51042200	1.48191100	-1.74928100
H	1.65781100	2.82054300	-0.61716200
C	2.50361500	0.96845900	0.06726200
H	2.24669600	0.87975400	1.12813000
H	3.45023900	1.51217100	0.00107700
O	2.73649400	-0.32756600	-0.48455600
H	-3.33539700	0.48972900	-1.64864700

HF=-591.1919896
Sum of electronic and zero-point Energies= -590.954597
Sum of electronic and thermal Energies= -590.941095
Sum of electronic and thermal Enthalpies= -590.940151
Sum of electronic and thermal Free Energies= -590.994476
Frequencies -- -442.3930

X = CH_2, Y = NH

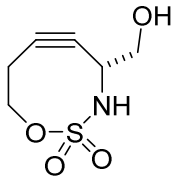
C	-0.27780900	0.09093400	-0.08802800
C	0.06580800	-1.08958200	-0.02187400
N	-2.50951200	-1.24663900	0.15072300
N	-1.85520300	-2.19205300	0.14964500
C	1.11416400	-2.12055100	-0.02970700
H	0.88214300	-2.94415800	0.65105400
H	1.18410000	-2.55394700	-1.03339900
C	-0.03974600	1.54138700	-0.20520900
C	2.46849600	-1.49320900	0.36023600
H	3.23505100	-2.26909800	0.26101300
H	2.43714600	-1.21116000	1.41590200
N	-2.46200500	-0.00372500	0.22047600
C	-3.39937200	0.77828100	-0.58779200
H	-4.41937000	0.67269800	-0.21506500
H	-3.09964800	1.81928600	-0.47975500
C	-0.31549500	2.26557900	1.11710300
H	0.34610300	1.90158600	1.90656800
H	-0.15415500	3.33916100	0.99726000
H	-1.34508700	2.09767700	1.43775200
H	-0.71210800	1.95746700	-0.96321000
C	1.40614300	1.76173900	-0.70163700
H	1.46882700	1.47378300	-1.75656200
H	1.60707300	2.83746700	-0.66184400
N	2.87690200	-0.32017200	-0.40139800
H	2.67027100	-0.43128400	-1.38756200
C	2.51700600	1.02388800	0.07083300
H	2.25701000	0.95219900	1.13122100
H	3.41381300	1.65027600	0.01931100
H	-3.35760900	0.49537600	-1.64235700

HF=-571.3216952
Sum of electronic and zero-point Energies= -571.072113
Sum of electronic and thermal Energies= -571.058224
Sum of electronic and thermal Enthalpies= -571.057280
Sum of electronic and thermal Free Energies= -571.112548
Frequencies -- -447.8901

X = CH_2, Y = NH_2^+

C	-0.31178600	0.10167500	-0.05406700
C	0.07366500	-1.06596700	0.04504400
N	-2.46854300	-1.29940000	0.13243000
N	-1.78500100	-2.22275200	0.17139800
C	1.11447800	-2.10710600	0.07055900
H	0.92021800	-2.85312300	0.84339600
H	1.11862200	-2.64109400	-0.88417700
C	-0.12590500	1.56415400	-0.16249200
C	2.48863800	-1.49559900	0.33793200
H	3.28102100	-2.20569900	0.10924200
H	2.59010700	-1.17181100	1.37170000
N	-2.45070500	-0.05507500	0.18006500
C	-3.37038100	0.69963100	-0.67541300
H	-4.40626900	0.49162000	-0.40536100
H	-3.17047300	1.75303500	-0.48908100
C	-0.43675800	2.25735100	1.16925500
H	0.23986300	1.91619300	1.95657400
H	-0.32972000	3.33848200	1.06227800
H	-1.45651100	2.03175900	1.48435200
H	-0.80422400	1.96150400	-0.92288600
C	1.31153500	1.85323600	-0.64442400
H	1.39411500	1.65705200	-1.71756800
H	1.51041100	2.91952200	-0.51437300
N	2.71605900	-0.27168400	-0.52344500
H	2.17549300	-0.37469200	-1.38795700
H	3.69426600	-0.26590200	-0.81542200
C	2.40475200	1.08698100	0.09748700
H	2.13886000	0.90216000	1.13687400
H	3.33955400	1.64173200	0.07816900
H	-3.20742800	0.47550800	-1.73218200

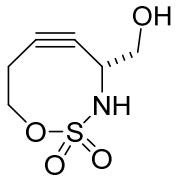
HF=-571.7760822
Sum of electronic and zero-point Energies= -571.510050
Sum of electronic and thermal Energies= -571.496380
Sum of electronic and thermal Enthalpies= -571.495436
Sum of electronic and thermal Free Energies= -571.550177
Frequencies -- -457.5580



+methyl azide (*anti*-TSs)

C	-0.67697000	0.38840600	0.46144400
C	-0.99238900	-0.78057100	0.23074200
C	-3.87229200	-1.57442500	-0.71502300
N	-3.26337900	0.40234000	0.37239700
N	-2.72418900	1.39661800	0.56364700
C	-0.66174000	-2.18351000	-0.06887800
H	-1.21676700	-2.87264900	0.57269900
H	-0.91624700	-2.41970400	-1.10591400
C	0.36037600	1.43611800	0.60650200
C	0.82834300	-2.39232500	0.16524600
H	1.14859300	-3.38124100	-0.15850100
H	1.08805700	-2.24483500	1.21307600
N	1.53751300	1.14746300	-0.24091000
S	2.39982400	-0.22470400	-0.02258500
O	3.56273900	-0.11854700	-0.86802700
O	2.52275800	-0.43135300	1.40242700
O	1.58064600	-1.45720200	-0.65036600
C	-0.11677100	2.83326900	0.21215500
H	-0.90391500	3.14637600	0.90031600
H	0.72015800	3.52777800	0.28304000
H	0.70403000	1.46702500	1.64336800
H	1.37080500	1.34148800	-1.22732900
O	-0.55899200	2.85615100	-1.13114100
H	-1.39319600	2.37345100	-1.17410500
N	-3.10804700	-0.82640700	0.28989400
H	-3.73285700	-1.15608700	-1.71367600
H	-3.49650200	-2.59462000	-0.68707700
H	-4.93116700	-1.58597200	-0.45600400

HF=-1191.7371488
Sum of electronic and zero-point Energies= -1191.522659
Sum of electronic and thermal Energies= -1191.506869
Sum of electronic and thermal Enthalpies= -1191.505925
Sum of electronic and thermal Free Energies= -1191.566011
Frequencies -- -433.9149



+methyl azide (*syn*-TSs)

C	0.79565800	0.09273800	-0.02886000
C	0.65442000	1.25561600	-0.41069800
C	3.45025500	-0.60186800	1.56004500
N	3.16919200	1.07423600	-0.01348100
N	2.69289900	2.03059900	-0.43138300
C	-0.19237000	2.40105800	-0.77871100
H	0.24478200	3.34767400	-0.45258700
H	-0.30499600	2.44890900	-1.86482900
C	0.26856900	-1.25766800	0.27065800
C	-1.55488400	2.24005900	-0.11768700
H	-2.24363900	3.02437100	-0.42772500
H	-1.46753800	2.23231800	0.96847100
N	-1.14653000	-1.38038000	-0.13692400
S	-2.27085100	-0.30444300	0.37451200
O	-3.55658600	-0.86478700	0.03979000

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 O                 -1.94075300    0.05438100    1.73428600
 O                 -2.17458000    1.00337500   -0.55432700
 C                  1.01039300   -2.36223700   -0.49017700
 H                  2.04566300   -2.40642500   -0.15021100
 H                  0.52534800   -3.31710400   -0.28813900
 H                  0.32848700   -1.46180900    1.34264000
 H                 -1.24876600   -1.58365700   -1.13070200
 O                  0.93410600   -2.15046100   -1.88540900
 H                  1.44576500   -1.36022800   -2.09733600
 N                  2.94303600   -0.12072700    0.26487400
 H                  3.14628100    0.05714700    2.37562200
 H                  3.02550500   -1.59137300    1.71459600
 H                  4.53679100   -0.69107500    1.53425600
HF=-1191.7359903
Sum of electronic and zero-point Energies=          -1191.521560
Sum of electronic and thermal Energies=             -1191.505748
Sum of electronic and thermal Enthalpies=           -1191.504804
Sum of electronic and thermal Free Energies=        -1191.564819
Frequencies --   -444.9963
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