

SUPPORTING INFORMATION

Stereoelectronic Interactions as a Probe for the Existence of the Intramolecular α -Effect

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1. Computational Details

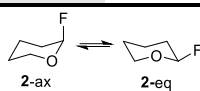
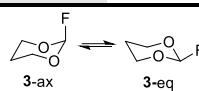
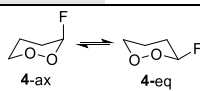
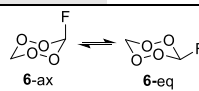
Calculations were carried with the *Gaussian '09* software package,¹ using the (U)M06-2X/6-311++G(d,p)² or the MP2³/6-311+G(d,p) levels of theory. For the relaxed PES scans, we also used the double hybrid B2PLYP functional⁴, with the D3 version of Grimme's dispersion with Becke-Johnson (BJ) damping.⁵ Unless otherwise noted, all calculations were performed at the (U)M06-2X/6-311++G(d,p) level of theory. SMD⁶=solvent was the solvation correction method of choice, for DMSO, water or benzene. Electronic structures and properties were analyzed by the Natural Bond Orbitals (NBO)⁷ method at the M06-2X level of theory. Due to methodology constrictions, NBO deletions were performed at the HF/6-31G(d) level of theory. Chemcraft 1.7⁸ and CYLView⁹ were used to render the orbitals and three-dimensional molecules.

2. NBO deletions for selected systems

Structural effects of hyperconjugation from NBODEL analysis.

In addition to the effects on energies and stabilities, we have briefly explored the effect of donor/acceptor orbital interactions on molecular geometries. The results obtained via deletion of the key NBO interactions followed by re-optimization of the geometries with these interactions "switched off" are collected in Table 3. In all cases, application of NBODEL, "turning off" the hyperconjugative interactions of interest led to the expected structural changes.

Table S1. Comparison of structural parameters in the optimized geometries of **2-4,6-ax** and **2-4,6-eq** (in Å) with the optimized geometries predicted by NBODEL, when "switching off" key NBO interactions. At the HF/6-31G(d) computational level.

Bond	With all interactions		Without $n(\text{O}) \rightarrow \sigma^*(\text{C-F})$		With all interactions		Without $n(\text{O}) \rightarrow \sigma^*(\text{C-F})$	
								
	2-ax	2-eq	2-ax	2-eq	3-ax	3-eq	3-ax	3-eq
C-F _{ax}	1.373	---	1.349	---	1.362	---	1.323	---
C-F _{eq}	---	1.351	---	1.349	---	1.327	---	1.322
C-O	1.368	1.379	1.434	1.403	1.359	1.366	1.411	1.391
								
	4-ax	4-eq	4-ax	4-eq	6-ax	6-eq	6-ax	6-eq
C-F _{ax}	1.355	---	1.337	---	1.328	---	1.303	---

C-F _{eq}	---	1.346	---	1.344	---	1.316	---	1.312
C-O(O)	1.381	1.398	1.440	1.417	1.372	1.383	1.420	1.397
O-O	1.394	1.392	1.392	1.399	1.396	1.395	1.398	1.402

Salient observations are the following,

1. Axial 2-fluoro-oxane, **2-ax**.

Relative to the delocalized system (without NBODEL), “switching off” the anomeric $n_{(O)} \rightarrow \sigma^*_{(C-F)ax}$ interaction in **2-ax** leads to substantial shortening of the C-F_{ax} bond length (1.373 Å versus 1.349 Å, Table 3) and significant bond length lengthening of the O-C bond (1.368 Å versus 1.434 Å).

2. Axial 3-fluoro-1,2-dioxane, **4-ax**.

While similar tendencies of C-F_{ax} bond shortening and O-C bond lengthening are found when “switching off” the $n_{(O-O)} \rightarrow \sigma^*_{(C-F)ax}$ interaction in peroxide **3-ax** [1.355 Å versus 1.337 Å and 1.381 versus 1.440 Å, respectively, Table 3], the magnitude of these structural changes is similar but slightly smaller than the bond changes observed in ether **2-ax**. This observation is not in line with anticipation in terms of the α -effect since one would expect that the increased donor ability in the peroxide would lead to more sizeable structural changes associated with hyperconjugation (or lack of thereof).

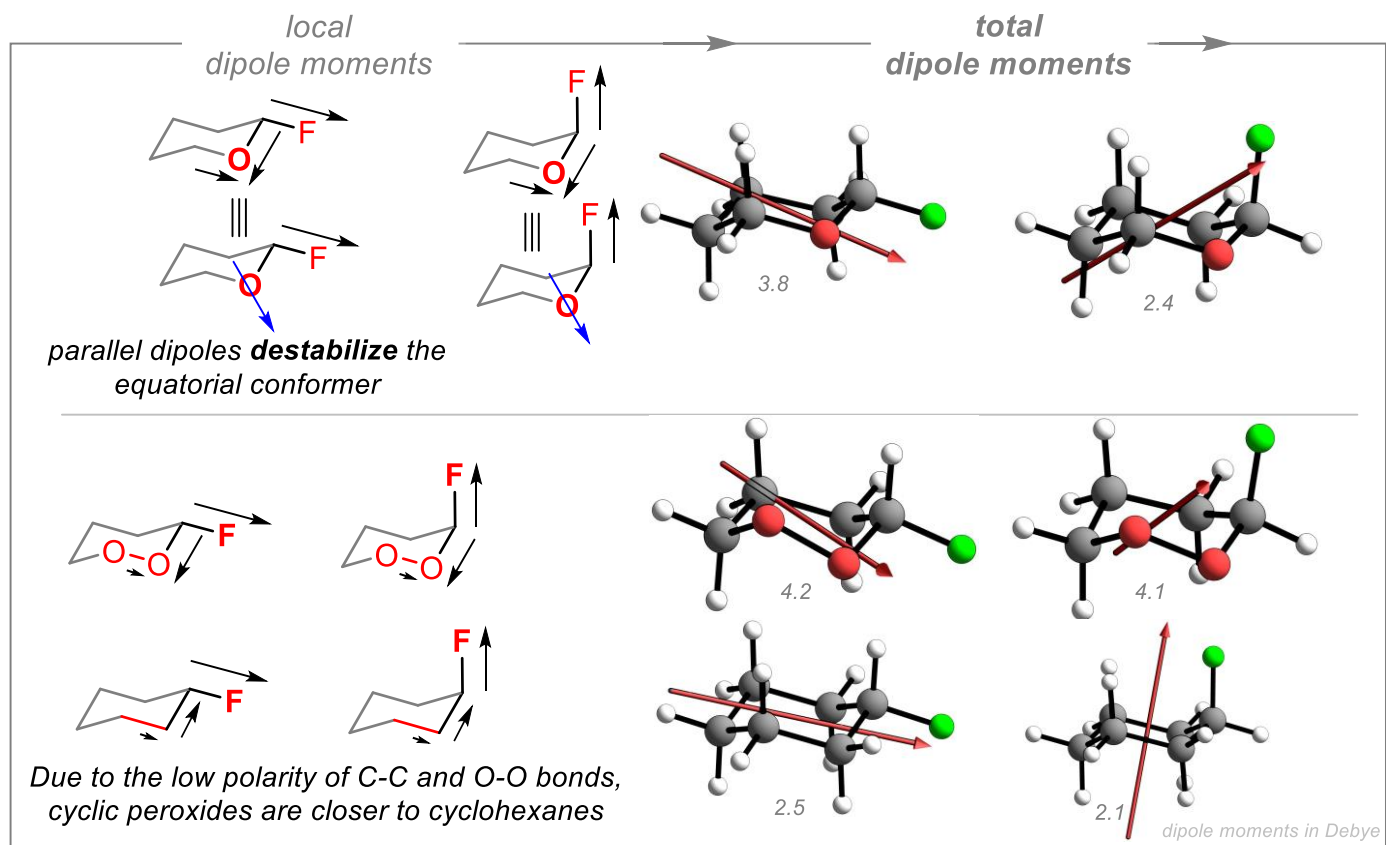
3. Axial 2-fluoro-1,3-dioxane, **3-ax**, versus axial 3-fluoro-1,2,4,5-tetraoxane, **6-ax**.

Both systems exhibit the structural changes anticipated from the double $n_{(O)} \rightarrow \sigma^*_{(C-F)ax}$ interactions in **3-ax** and double $n_{(O-O)} \rightarrow \sigma^*_{(C-F)ax}$ interaction in **6-ax** (that is, shortening of the axial C-F bond and lengthening of the O-C bond when switching off” hyperconjugation). Again, the observed structural changes turn out to be slightly smaller in the bis-peroxide **6-ax** relative to the bis-ether **3-ax**. Again, these structural changes do not suggest the increased donor capacity of the peroxide expected from the α -effect.

4. Ethers **2** and **3** vs. peroxides **4** and **6**.

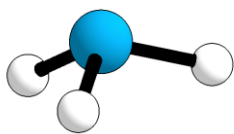
In parallel, one can observe that the C-F bonds are much shorter in peroxides whereas the anomeric C-O bonds are much shorter in ethers. The trend is consistent with the greater importance of the exo-anomeric $n_{(F)} \rightarrow \sigma^*_{(C-O)eq}$ interactions in peroxides.^{22g} However, since this trends gets less pronounced but still persists even after all delocalizing interactions are removed, other factors have to be involved as well.

3. Total Dipole Moments from Scheme 11



4. Geometries

Calculated geometries with their respective energies (in hartree) and number of imaginary frequencies.

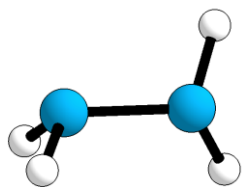


of imaginary frequencies: 0

E = -56.5459687107

symmetry c3v

N	0.000000000	0.000000000	0.109422000
H	0.000000000	0.944874000	-0.255319000
H	-0.818285000	-0.472437000	-0.255319000
H	0.818285000	-0.472437000	-0.255319000

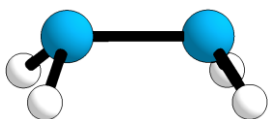


of imaginary frequencies: 0

E = -111.850995355

symmetry c2

N	0.000000000	0.711529000	-0.072104000
H	-0.234621000	1.103710000	0.834039000
H	0.926112000	1.027232000	-0.329308000
N	0.000000000	-0.711529000	-0.072104000
H	0.234621000	-1.103710000	0.834039000
H	-0.926112000	-1.027232000	-0.329308000

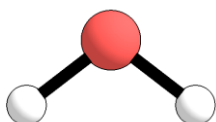


of imaginary frequencies: 0

E = -111.835227608

symmetry c2

N	0.015144000	0.731180000	-0.103788000
H	-0.784781000	1.076651000	0.417781000
H	0.828642000	1.043400000	0.417749000
N	-0.015144000	-0.731180000	-0.103788000
H	0.784781000	-1.076651000	0.417781000
H	-0.828642000	-1.043400000	0.417749000



of imaginary frequencies: 0

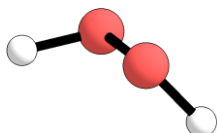
E = -76.4208888612

symmetry c2v

O	0.000000000	0.000000000	0.116598000
---	-------------	-------------	-------------

H	0.000000000	0.761666000	-0.466391000
---	-------------	-------------	--------------

H	0.000000000	-0.761666000	-0.466391000
---	-------------	--------------	--------------



of imaginary frequencies: 0

E = -151.535339287

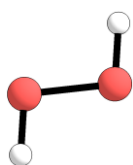
symmetry c2

O	0.000000000	0.711763000	-0.052250000
---	-------------	-------------	--------------

H	0.820154000	0.901002000	0.417997000
---	-------------	-------------	-------------

O	0.000000000	-0.711763000	-0.052250000
---	-------------	--------------	--------------

H	-0.820154000	-0.901002000	0.417997000
---	--------------	--------------	-------------



of imaginary frequencies: 0

E = -151.533984928

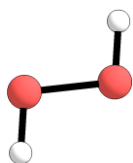
symmetry c2

O	0.002480000	0.716278000	0.000310000
---	-------------	-------------	-------------

H	0.951527000	0.879994000	-0.002530000
---	-------------	-------------	--------------

O	-0.002480000	-0.716278000	0.000310000
---	--------------	--------------	-------------

H	-0.951527000	-0.879994000	-0.002530000
---	--------------	--------------	--------------



of imaginary frequencies: 0

E = -151.533984928

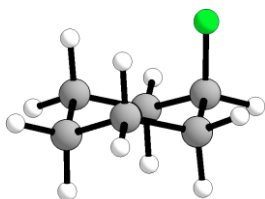
symmetry c2

O	0.002480000	0.716278000	0.000310000
---	-------------	-------------	-------------

H	0.951527000	0.879994000	-0.002530000
---	-------------	-------------	--------------

O	-0.002480000	-0.716278000	0.000310000
---	--------------	--------------	-------------

H	-0.951527000	-0.879994000	-0.002530000
---	--------------	--------------	--------------



of imaginary frequencies: 0

E = -333.151929752

symmetry cs

C	1.452569000	0.153055000	0.000000000
---	-------------	-------------	-------------

C	-0.732999000	0.237884000	-1.260391000
---	--------------	-------------	--------------

C	-0.732999000	0.237884000	1.260391000
---	--------------	-------------	-------------

C	-1.466977000	-0.230128000	0.000000000
---	--------------	--------------	-------------

C	0.716546000	-0.257639000	1.265307000
---	-------------	--------------	-------------

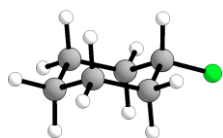
C	0.716546000	-0.257639000	-1.265307000
---	-------------	--------------	--------------

H	-0.738309000	1.333675000	-1.296685000
---	--------------	-------------	--------------

H	-0.738309000	1.333675000	1.296685000
---	--------------	-------------	-------------

S8

H	-1.525964000	-1.328040000	0.000000000
H	0.735549000	-1.354383000	1.323486000
H	0.735549000	-1.354383000	-1.323486000
H	-1.247676000	-0.117488000	-2.160014000
H	-1.247676000	-0.117488000	2.160014000
H	-2.496428000	0.145739000	0.000000000
H	1.260734000	0.126392000	2.134752000
H	1.260734000	0.126392000	-2.134752000
F	1.570993000	1.557634000	0.000000000
H	2.476116000	-0.237142000	0.000000000



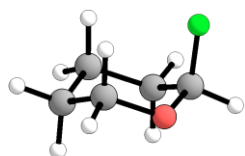
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E = -333.152042038

symmetry cs

C	1.018549000	0.329700000	0.000000000
C	-1.140202000	0.219180000	-1.261244000
C	-1.140202000	0.219180000	1.261244000
C	-1.847926000	-0.286042000	0.000000000
C	0.340570000	-0.181186000	1.257523000
C	0.340570000	-0.181186000	-1.257523000
H	-1.221874000	1.313939000	-1.307318000
H	-1.221874000	1.313939000	1.307318000
H	-1.844905000	-1.384521000	0.000000000

H	0.433054000	-1.274595000	1.277068000
H	0.433054000	-1.274595000	-1.277068000
H	-1.628088000	-0.172844000	-2.160146000
H	-1.628088000	-0.172844000	2.160146000
H	-2.896431000	0.032932000	0.000000000
H	0.858918000	0.211138000	2.138792000
H	0.858918000	0.211138000	-2.138792000
H	1.035682000	1.427506000	0.000000000
F	2.360273000	-0.084839000	0.000000000



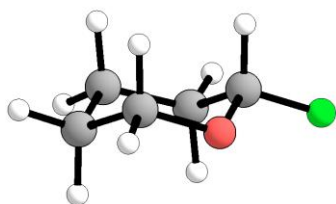
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E = -368.984416654

symmetry c1

H	-1.418138000	2.223585000	0.176886000
C	-0.860293000	1.298208000	0.351051000
C	-0.900759000	-1.193359000	0.226105000
C	1.079871000	-0.089855000	-0.429009000
O	0.251905000	-1.180476000	-0.632010000
C	0.374284000	1.249568000	-0.551432000
C	-1.731982000	0.072070000	0.070388000
H	-0.573078000	-1.311852000	1.265833000
H	0.076851000	1.365715000	-1.600275000

H	-2.123588000	0.119604000	-0.952997000
H	-0.547931000	1.294899000	1.401446000
H	-1.457886000	-2.084048000	-0.069222000
H	1.904442000	-0.201294000	-1.135618000
H	1.086866000	2.043935000	-0.310453000
H	-2.586487000	0.026971000	0.755107000
F	1.640922000	-0.160670000	0.856200000

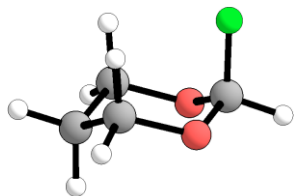


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E = -368.984416654

symmetry c1

H	-1.564025000	2.207290000	-0.194984000
C	-1.109192000	1.300318000	0.214596000
C	-1.077796000	-1.196286000	0.176743000
C	0.957035000	-0.079144000	0.316461000
O	0.288312000	-1.175204000	-0.238769000
C	0.377337000	1.237927000	-0.155639000
C	-1.819760000	0.046523000	-0.301463000
H	-1.126491000	-1.266382000	1.275603000
H	0.506059000	1.280390000	-1.242649000
H	-1.831177000	0.048526000	-1.397349000
H	-1.212641000	1.353493000	1.306792000
H	-1.497997000	-2.110421000	-0.246285000
H	0.941231000	2.061855000	0.292989000
H	-2.858135000	0.008460000	0.047253000
H	0.948096000	-0.155795000	1.415934000
F	2.264145000	-0.191549000	-0.090233000

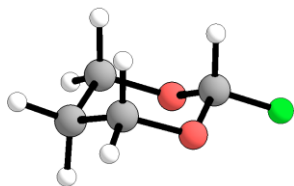


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E = -404.818914214

symmetry cs

O	0.303911000	-0.584530000	1.162875000
C	-1.716647000	0.061359000	0.000000000
O	0.303911000	-0.584530000	-1.162875000
C	-0.849875000	0.269008000	-1.233276000
C	1.020896000	-0.417152000	0.000000000
C	-0.849875000	0.269008000	1.233276000
H	-2.110352000	-0.959444000	0.000000000
H	-0.526375000	1.312823000	-1.314973000
H	-0.526375000	1.312823000	1.314973000
H	-2.556344000	0.764522000	0.000000000
H	-1.362462000	-0.017283000	-2.151867000
H	1.835880000	-1.136816000	0.000000000
H	-1.362462000	-0.017283000	2.151867000
F	1.576167000	0.864494000	0.000000000

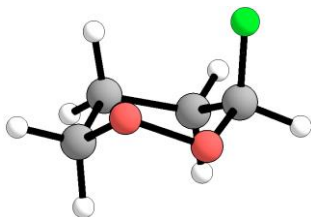


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E = -404.812498394

symmetry cs

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C	-1.796699000	-0.304268000	0.000000000
O	0.322416000	-0.205683000	-1.158141000
C	-1.050853000	0.189564000	-1.232725000
C	0.899388000	0.292492000	0.000000000
C	-1.050853000	0.189564000	1.232725000
H	-1.812301000	-1.397527000	0.000000000
H	-1.113500000	1.286444000	-1.305034000
H	-1.113500000	1.286444000	1.305034000
H	-2.827227000	0.067221000	0.000000000
H	-1.435366000	-0.243220000	-2.156413000
H	-1.435366000	-0.243220000	2.156413000
H	0.870655000	1.395291000	0.000000000
F	2.182791000	-0.115420000	0.000000000



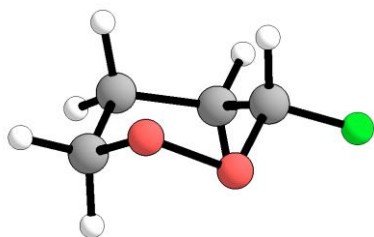
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E = -404.714250652

symmetry c1

H	-1.840440000	-0.153371000	1.194008000
C	-1.072246000	-0.029780000	0.424638000
C	0.953676000	1.246938000	-0.312829000
O	0.787413000	-1.157346000	-0.397182000
C	1.666774000	-0.078897000	-0.089891000
O	-0.269854000	-1.158562000	0.607425000
C	-0.303170000	1.272883000	0.557504000
H	0.684743000	1.328923000	-1.369992000
H	2.023746000	-0.180587000	0.942845000
H	-0.025386000	1.376899000	1.612489000
H	1.612743000	2.083683000	-0.059546000
H	2.501116000	-0.225100000	-0.781828000

H	-0.965354000	2.102180000	0.295489000
F	-1.693759000	-0.071863000	-0.809128000

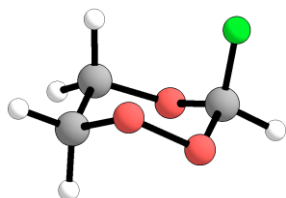


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E = -404.711597653

symmetry c1

C	0.962042000	-0.029761000	0.300035000
C	-1.160189000	1.254128000	0.196091000
O	-1.015093000	-1.154462000	0.332958000
C	-1.757366000	-0.076266000	-0.240268000
O	0.291728000	-1.129249000	-0.305315000
C	0.335990000	1.273527000	-0.141984000
H	-1.302029000	1.366378000	1.276586000
H	-1.760648000	-0.183897000	-1.330680000
H	0.487890000	1.351939000	-1.223682000
H	-1.675666000	2.084119000	-0.298034000
H	-2.769428000	-0.223168000	0.147846000
H	0.845963000	2.111084000	0.343493000
H	0.963147000	-0.169650000	1.385941000
F	2.246659000	-0.125723000	-0.160987000



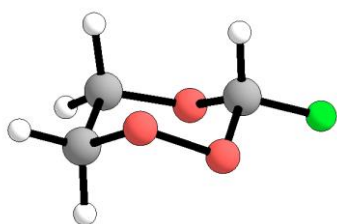
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E = -440.545595793

symmetry c1

O	0.308797000	-1.134597000	-0.592992000
C	-1.645060000	-0.126556000	0.071617000
O	0.258198000	1.189507000	-0.570858000

C	-0.916775000	1.190091000	0.253545000
C	1.013306000	0.053356000	-0.404530000
O	-0.753353000	-1.188839000	0.404101000
H	-1.995649000	-0.248713000	-0.958351000
H	-0.633317000	1.327462000	1.301426000
H	-2.474957000	-0.232093000	0.775424000
H	-1.516470000	2.035945000	-0.084858000
F	1.590042000	0.057463000	0.841121000
H	1.793238000	0.038972000	-1.165644000

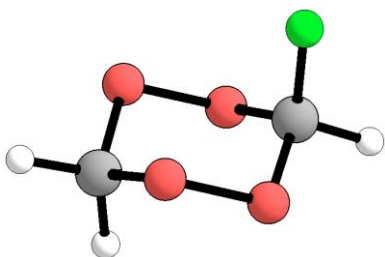


of imaginary frequencies: 0

E = -440.541188750

symmetry c1

O	0.334765000	-1.109879000	-0.289883000
C	-1.726548000	-0.107045000	-0.256713000
O	0.286536000	1.202161000	-0.160402000
C	-1.098983000	1.197228000	0.198132000
C	0.898640000	0.048105000	0.287053000
O	-0.991057000	-1.190663000	0.312320000
H	-1.719916000	-0.193967000	-1.346920000
H	-1.202506000	1.303783000	1.285931000
H	-2.740364000	-0.225693000	0.135529000
H	-1.545219000	2.059505000	-0.298973000
H	0.864953000	-0.037152000	1.379491000
F	2.165702000	0.073615000	-0.152563000

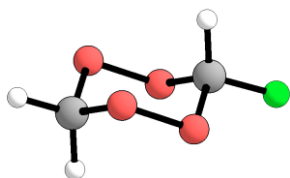


of imaginary frequencies: 0

E = -476.275389183

symmetry cs

O	-0.245312000	0.588893000	-1.162326000
O	-0.245312000	0.588893000	1.162326000
C	1.584567000	-0.085077000	0.000000000
O	0.839736000	-0.386176000	1.154861000
O	0.839736000	-0.386176000	-1.154861000
C	-0.988304000	0.389476000	0.000000000
H	1.871777000	0.969808000	0.000000000
H	2.430928000	-0.773831000	0.000000000
H	-1.747512000	1.174179000	0.000000000
F	-1.559305000	-0.835990000	0.000000000

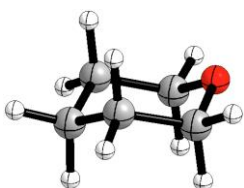


of imaginary frequencies: 0

E = -476.272728776

symmetry cs

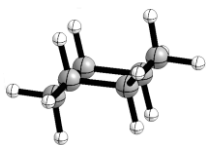
O	-0.287178000	-0.259624000	1.159516000
O	-0.287178000	-0.259624000	-1.159516000
C	1.664372000	-0.214300000	0.000000000
O	1.056783000	0.309725000	-1.156370000
O	1.056783000	0.309725000	1.156370000
C	-0.881095000	0.272774000	0.000000000
H	1.598155000	-1.304309000	0.000000000
H	2.685435000	0.171381000	0.000000000
H	-0.820814000	1.362151000	0.000000000
F	-2.136264000	-0.179900000	0.000000000



of imaginary frequencies: 0

E = -271.7186267

C	1.173518000	-0.767130000	0.201067000
C	-1.172877000	-0.768018000	0.201124000
C	-1.250915000	0.693204000	-0.227356000
C	-0.000594000	1.441382000	0.240617000
C	1.250358000	0.694234000	-0.227298000
H	-2.010712000	-1.345399000	-0.191782000
H	1.194656000	-0.834546000	1.300519000
H	2.011786000	-1.343778000	-0.191999000
H	-1.319821000	0.735112000	-1.319233000
H	-2.158161000	1.147265000	0.180758000
H	-0.001008000	2.469202000	-0.129520000
H	-0.000648000	1.494568000	1.336226000
H	1.319298000	0.736276000	-1.319169000
H	2.157203000	1.149009000	0.180906000
H	-1.193849000	-0.835329000	1.300586000
O	0.000539000	-1.391802000	-0.284527000

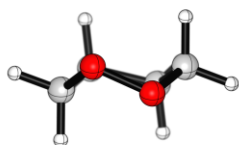


of imaginary frequencies: 0

E = -235.8168138

C	-1.456932000	-0.058872000	-0.233750000
C	-0.677343000	-1.290573000	0.233728000
C	0.779471000	-1.231476000	-0.233499000
C	1.456935000	0.058873000	0.233744000
C	0.677340000	1.290574000	-0.233727000
C	-0.779472000	1.231473000	0.233504000
H	1.330052000	-2.103866000	0.129134000
H	-0.700513000	-1.334099000	1.329763000
H	-1.156487000	-2.203604000	-0.130186000

H	-1.507398000	-0.061151000	-1.329718000
H	-2.487145000	-0.099938000	0.130798000
H	1.507411000	0.061154000	1.329713000
H	2.487144000	0.099940000	-0.130812000
H	1.156483000	2.203605000	0.130189000
H	0.700506000	1.334105000	-1.329762000
H	-0.805721000	1.272989000	1.329596000
H	-1.330052000	2.103865000	-0.129125000
H	0.805721000	-1.272998000	-1.329593000

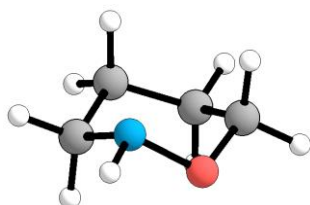


of imaginary frequencies: 0

E = -307.5428347

C	-0.739398000	1.213029000	0.200483000
C	0.738143000	1.213714000	-0.200556000
C	1.375235000	-0.104743000	0.220847000
C	-1.375242000	-0.106114000	-0.220665000
H	2.378849000	-0.227783000	-0.190438000
H	0.828705000	1.314150000	-1.286586000
H	1.269400000	2.051155000	0.258378000
H	-0.830028000	1.313605000	1.286493000
H	-1.271497000	2.049856000	-0.258599000
H	-1.417196000	-0.204036000	-1.310923000

H	-2.378572000	-0.230237000	0.190977000
H	1.416932000	-0.202599000	1.311132000
O	-0.638464000	-1.197857000	0.312511000
O	0.639836000	-1.197072000	-0.312648000

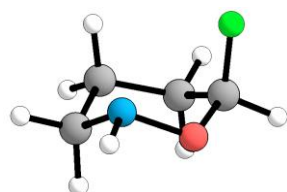


of imaginary frequencies: 0

E = -287.709678888

symmetry c1

C	1.141640000	0.861759000	-0.206058000
C	-1.325015000	0.446605000	-0.221327000
C	1.263029000	-0.600537000	0.211690000
H	-2.296086000	0.749297000	0.178055000
H	1.243820000	0.921519000	-1.294466000
H	1.952082000	1.446458000	0.237131000
H	2.156444000	-1.067173000	-0.205747000
C	-0.224759000	1.412159000	0.214658000
H	-0.263307000	1.510447000	1.303926000
H	-0.394259000	2.401034000	-0.217851000
H	-1.385741000	0.408857000	-1.317849000
N	-1.012531000	-0.869574000	0.340952000
H	-1.706133000	-1.547582000	0.040011000
O	0.171690000	-1.344856000	-0.300931000
H	1.278006000	-0.696912000	1.303793000



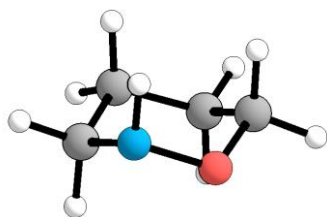
of imaginary frequencies: 0

E = -386.961204080

S19

symmetry c1

C	-0.283086000	1.279034000	0.504619000
C	1.684714000	-0.142295000	-0.031672000
C	-1.102121000	0.001032000	0.408871000
H	2.549256000	-0.295828000	-0.681246000
H	-0.021733000	1.416053000	1.558464000
H	-0.907531000	2.120712000	0.200357000
H	-1.891592000	-0.050375000	1.160764000
F	-1.708433000	-0.053204000	-0.830778000
C	0.989266000	1.179650000	-0.338901000
H	0.733486000	1.199452000	-1.400864000
H	1.649465000	2.023451000	-0.129154000
H	2.014038000	-0.170994000	1.016838000
N	0.731109000	-1.207216000	-0.335383000
H	1.129100000	-2.114974000	-0.117374000
O	-0.341125000	-1.137834000	0.619925000



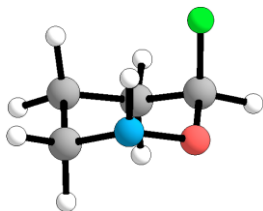
of imaginary frequencies: 0

E = -287.707233835

symmetry c1

C	0.680446000	1.252277000	-0.211241000
C	-1.391786000	-0.130078000	-0.227161000
C	1.381335000	-0.030682000	0.212342000
H	-2.394312000	-0.275619000	0.182747000
H	0.739237000	1.340331000	-1.300742000
H	1.192133000	2.116295000	0.221047000
H	2.398653000	-0.088804000	-0.177267000
C	-0.782949000	1.196492000	0.227731000
H	-0.841534000	1.265541000	1.320926000
H	-1.349517000	2.036929000	-0.181481000

H	-1.469968000	-0.157883000	-1.317702000
N	-0.605835000	-1.298388000	0.167419000
H	-0.542388000	-1.342375000	1.186722000
O	0.720172000	-1.179106000	-0.303320000
H	1.424882000	-0.100902000	1.310356000

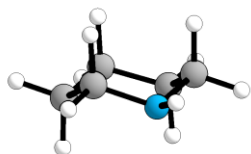


of imaginary frequencies: 0

E = -386.963576533

symmetry c1

C	0.224122000	1.294637000	-0.527425000
C	-1.653826000	-0.224988000	0.045625000
C	1.094254000	0.058734000	-0.411936000
H	-2.479496000	-0.444420000	0.726394000
H	-0.056111000	1.398788000	-1.579943000
H	0.811200000	2.170289000	-0.244521000
H	1.943558000	0.057812000	-1.095708000
F	1.605303000	0.006875000	0.883776000
C	-1.023856000	1.135181000	0.340525000
H	-0.746181000	1.188784000	1.397733000
H	-1.734580000	1.941082000	0.144619000
H	-2.044953000	-0.255340000	-0.975455000
N	-0.711361000	-1.333812000	0.174969000
H	-0.332488000	-1.360961000	1.121629000
O	0.415836000	-1.125325000	-0.669280000



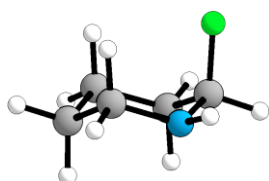
of imaginary frequencies: 0

E = -251.850617416

symmetry cs

S21

C	0.015314000	0.749280000	1.257860000
C	0.015314000	0.749280000	-1.257860000
C	0.015314000	-0.776348000	-1.209366000
C	0.015314000	-0.776348000	1.209366000
H	-0.506041000	1.092292000	-2.155644000
H	1.051963000	1.095257000	1.319553000
H	-0.506041000	1.092292000	2.155644000
H	-1.030294000	-1.132415000	-1.244785000
H	0.535585000	-1.185975000	-2.078035000
H	0.535585000	-1.185975000	2.078035000
C	-0.643628000	1.320781000	0.000000000
H	-1.707638000	1.053037000	0.000000000
H	-0.590285000	2.412441000	0.000000000
H	1.051963000	1.095257000	-1.319553000
N	0.700124000	-1.224346000	0.000000000
H	0.788869000	-2.233248000	0.000000000
H	-1.030294000	-1.132415000	1.244785000



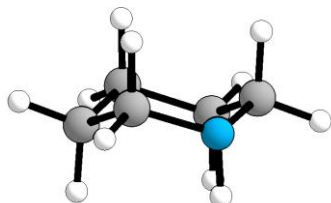
of imaginary frequencies: 0

E = -351.107960573

symmetry c1

C	0.313503000	1.266825000	-0.571841000
C	-1.733657000	-0.043807000	0.042255000
C	-0.849393000	-1.270138000	0.237277000
C	1.121908000	-0.010371000	-0.424512000
H	-2.599306000	-0.105735000	0.706173000
H	0.024760000	1.357587000	-1.623035000
H	0.953132000	2.114973000	-0.320706000
H	-0.564803000	-1.350451000	1.295433000
H	-1.388297000	-2.178577000	-0.037446000
H	1.980246000	-0.034221000	-1.097807000

F	1.680394000	0.001701000	0.883792000
C	-0.930363000	1.228388000	0.317247000
H	-0.621332000	1.243698000	1.367250000
H	-1.540047000	2.118210000	0.145080000
H	-2.102262000	-0.032752000	-0.988763000
N	0.329400000	-1.166934000	-0.630102000
H	0.896576000	-2.004897000	-0.592154000

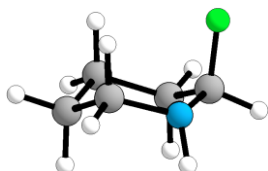


of imaginary frequencies: 0

E = -251.849674048

symmetry c1

C	1.256827000	0.707595000	-0.233368000
C	-1.256652000	0.707892000	-0.233364000
C	-1.210471000	-0.753169000	0.226705000
C	1.210282000	-0.753468000	0.226710000
H	-2.157739000	1.194533000	0.151650000
H	1.316734000	0.736071000	-1.328452000
H	2.158039000	1.194010000	0.151637000
H	-1.252413000	-0.786756000	1.322536000
H	-2.077944000	-1.306039000	-0.141461000
H	2.077623000	-1.306547000	-0.141456000
C	0.000181000	1.451182000	0.226022000
H	0.000196000	1.511638000	1.321522000
H	0.000297000	2.478176000	-0.148020000
H	-1.316563000	0.736390000	-1.328448000
N	-0.000179000	-1.463239000	-0.181180000
H	-0.000189000	-1.581917000	-1.190025000
H	1.252207000	-0.787077000	1.322541000

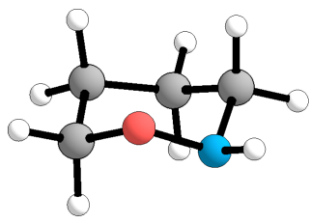


of imaginary frequencies: 0

E = -351.100099111

symmetry c1

C	-0.351713000	1.246457000	0.572008000
C	1.739721000	0.006452000	-0.038372000
C	0.886749000	-1.241531000	-0.270007000
C	-1.132582000	-0.053675000	0.409410000
H	2.619360000	-0.017017000	-0.687451000
H	-0.065210000	1.329874000	1.626706000
H	-1.009599000	2.087422000	0.340331000
H	0.610936000	-1.298532000	-1.327611000
H	1.438407000	-2.152971000	-0.033587000
H	-1.952803000	-0.115647000	1.128657000
F	-1.707648000	-0.029853000	-0.862395000
C	0.899931000	1.257555000	-0.306154000
H	0.601013000	1.274398000	-1.359361000
H	1.478897000	2.165075000	-0.120286000
H	2.098599000	0.018128000	0.998278000
N	-0.356652000	-1.257477000	0.503281000
H	-0.206832000	-1.511260000	1.471605000



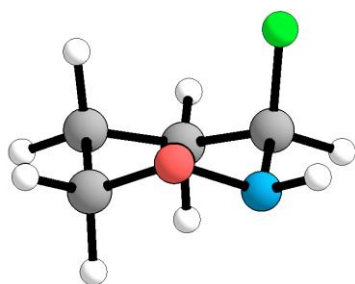
of imaginary frequencies: 0

E = -287.709678862

symmetry c1

C	-0.224781000	1.412188000	0.214625000
C	1.263048000	-0.600567000	0.211656000
C	-1.325013000	0.446590000	-0.221300000
H	2.156453000	-1.067163000	-0.205846000
H	-0.263331000	1.510609000	1.303883000

H	-0.394239000	2.401008000	-0.218015000
H	-2.296082000	0.749281000	0.178087000
C	1.141629000	0.861782000	-0.206031000
H	1.243900000	0.921617000	-1.294430000
H	1.952019000	1.446471000	0.237265000
H	1.278122000	-0.696962000	1.303761000
N	-1.012534000	-0.869615000	0.341008000
H	-1.706116000	-1.547465000	0.039658000
O	0.171681000	-1.344854000	-0.300913000
H	-1.385733000	0.408786000	-1.317819000

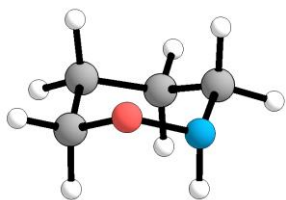


of imaginary frequencies: 0

E = -386.960927169

symmetry c1

C	-0.221944000	1.281303000	0.547638000
C	1.665739000	-0.227982000	-0.054753000
C	-1.099650000	0.048418000	0.411666000
H	2.494797000	-0.427659000	-0.734194000
H	0.050364000	1.376028000	1.602549000
H	-0.802865000	2.160545000	0.265194000
H	-1.921566000	0.039646000	1.131671000
F	-1.682467000	0.056333000	-0.860286000
C	1.035418000	1.135191000	-0.312801000
H	0.767958000	1.201253000	-1.370310000
H	1.746787000	1.934173000	-0.091870000
H	2.012896000	-0.316759000	0.982095000
N	-0.331393000	-1.137083000	0.640501000
H	-0.894373000	-1.963288000	0.461295000
O	0.716322000	-1.246617000	-0.317234000

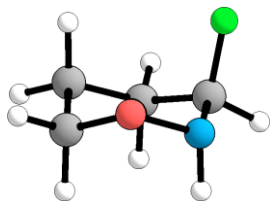


of imaginary frequencies: 0

E = -287.707233723

symmetry c1

C	-0.782825000	1.196561000	0.227742000
C	1.381335000	-0.030803000	0.212343000
C	-1.391790000	-0.129943000	-0.227166000
H	2.398656000	-0.089031000	-0.177236000
H	-0.841380000	1.265597000	1.320938000
H	-1.349328000	2.037057000	-0.181443000
H	-2.394339000	-0.275386000	0.182716000
C	0.680557000	1.252215000	-0.211253000
H	0.739349000	1.340265000	-1.300753000
H	1.192315000	2.116191000	0.221029000
H	1.424833000	-0.101015000	1.310358000
N	-0.605965000	-1.298327000	0.167417000
H	-0.542525000	-1.342363000	1.186717000
O	0.720057000	-1.179184000	-0.303318000
H	-1.469942000	-0.157732000	-1.317708000



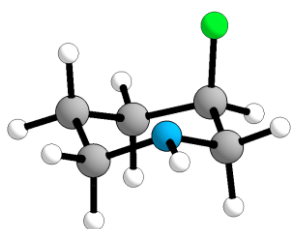
of imaginary frequencies: 0

E = -386.953615924

symmetry c1

C	-0.292477000	1.250284000	0.562598000
C	1.671220000	-0.122327000	-0.055959000
C	-1.098087000	-0.033078000	0.405842000
H	2.533357000	-0.257755000	-0.709481000

H	-0.007997000	1.341855000	1.616760000
H	-0.928525000	2.101720000	0.313839000
H	-1.867280000	-0.127678000	1.177645000
C	0.959010000	1.195946000	-0.310986000
H	0.681248000	1.246872000	-1.366624000
H	1.621411000	2.036618000	-0.092111000
H	2.007738000	-0.189978000	0.990182000
N	-0.333783000	-1.255753000	0.460241000
H	-0.033980000	-1.433550000	1.419409000
O	0.813072000	-1.218433000	-0.349875000
F	-1.734674000	0.008298000	-0.820143000



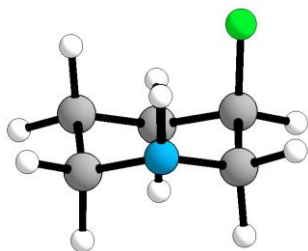
of imaginary frequencies: 0

E = -351.094377877

symmetry c1

C	-0.343066000	1.249953000	0.588631000
C	1.712441000	-0.020185000	-0.066446000
C	-1.146240000	-0.026969000	0.399436000
H	2.582135000	-0.044725000	-0.725754000
H	-0.046770000	1.308765000	1.642448000
H	-0.984194000	2.109119000	0.378930000
H	-1.971143000	-0.081642000	1.115929000
F	-1.723270000	-0.004323000	-0.868808000
C	0.901241000	1.251197000	-0.300935000
H	0.599818000	1.284801000	-1.350833000
H	1.511335000	2.133441000	-0.092825000
H	2.079413000	-0.027129000	0.976567000
N	0.872008000	-1.175696000	-0.360287000
H	1.406927000	-2.034300000	-0.339061000
C	-0.276353000	-1.267456000	0.526661000

H	-0.868334000	-2.145343000	0.260261000
H	0.008039000	-1.353446000	1.591544000

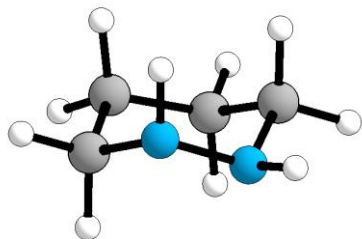


of imaginary frequencies: 0

E = -351.097058565

symmetry c1

C	-0.282642000	1.278964000	0.585631000
C	1.699034000	-0.123321000	-0.066439000
C	-1.146861000	0.041259000	0.407721000
H	2.561192000	-0.210999000	-0.730852000
H	0.008859000	1.336714000	1.640877000
H	-0.874392000	2.169228000	0.360142000
H	-2.011937000	0.054619000	1.076721000
F	-1.655286000	0.049967000	-0.899571000
C	0.965600000	1.200713000	-0.298119000
H	0.667498000	1.267512000	-1.349242000
H	1.627904000	2.045812000	-0.091910000
H	2.081592000	-0.155949000	0.961504000
N	0.849406000	-1.298787000	-0.252341000
H	0.572161000	-1.368943000	-1.226734000
C	-0.344923000	-1.242694000	0.578449000
H	-0.979757000	-2.101217000	0.349130000
H	-0.042633000	-1.324498000	1.629440000

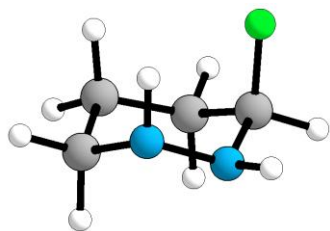


of imaginary frequencies: 0

E = -267.860656614

symmetry c1

C	-1.151836000	0.860003000	0.211408000
C	1.327505000	0.470710000	0.216158000
C	-1.288100000	-0.600509000	-0.231108000
H	2.291685000	0.805042000	-0.174247000
H	-1.242356000	0.906945000	1.304082000
H	-1.964090000	1.463324000	-0.203463000
H	-2.198066000	-1.049647000	0.174159000
C	0.209998000	1.422696000	-0.208310000
H	0.244458000	1.525573000	-1.297220000
H	0.369534000	2.412725000	0.226804000
H	1.394575000	0.446152000	1.318671000
N	-0.153548000	-1.418356000	0.197227000
H	-0.115147000	-1.387241000	1.220961000
N	1.035860000	-0.848351000	-0.337818000
H	1.790204000	-1.507047000	-0.193160000
H	-1.332386000	-0.666277000	-1.321342000



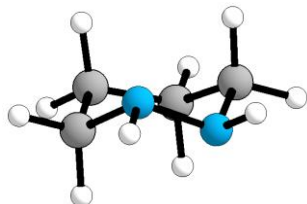
of imaginary frequencies: 0

E = -367.117228317

symmetry c1

C	0.222252000	1.294153000	-0.545192000
C	-1.686627000	-0.226163000	0.048980000
C	1.107460000	0.065135000	-0.420800000
H	-2.522131000	-0.400041000	0.730496000
H	-0.044112000	1.395525000	-1.601086000
H	0.793700000	2.176897000	-0.252777000
H	1.961615000	0.092311000	-1.099475000
F	1.651442000	0.059882000	0.888281000
C	-1.041481000	1.139016000	0.306618000

H	-0.773638000	1.211479000	1.365796000
H	-1.744610000	1.947579000	0.092213000
H	-2.062954000	-0.289133000	-0.975714000
N	0.359417000	-1.116853000	-0.666299000
H	0.926340000	-1.954407000	-0.693868000
N	-0.734306000	-1.321149000	0.225993000
H	-0.382586000	-1.285978000	1.184391000

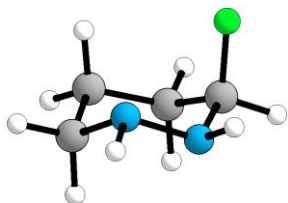


of imaginary frequencies: 0

E = -267.857361403

symmetry c2

C	0.591614000	-0.484827000	1.242688000
C	-0.591614000	1.294360000	-0.050012000
C	0.591614000	-1.294360000	-0.050012000
H	-1.477854000	1.929698000	-0.111616000
H	1.528786000	0.077637000	1.303863000
H	0.546309000	-1.155508000	2.104331000
H	1.477854000	-1.929698000	-0.111616000
C	-0.591614000	0.484827000	1.242688000
H	-1.528786000	-0.077637000	1.303863000
H	-0.546309000	1.155508000	2.104331000
H	0.305387000	1.930686000	-0.081741000
N	0.626531000	-0.374996000	-1.190921000
H	0.589169000	-0.940128000	-2.034443000
N	-0.626531000	0.374996000	-1.190921000
H	-0.589169000	0.940128000	-2.034443000
H	-0.305387000	-1.930686000	-0.081741000

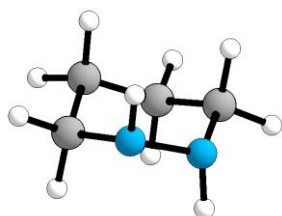


of imaginary frequencies: 0

E = -367.109539202

symmetry c1

C	-0.302169000	1.264771000	0.564252000
C	1.696585000	-0.081203000	-0.047348000
C	-1.107931000	-0.013277000	0.416842000
H	2.565663000	-0.174243000	-0.701192000
H	-0.012615000	1.357936000	1.614913000
H	-0.942769000	2.110942000	0.310670000
H	-1.932745000	-0.067132000	1.130371000
F	-1.702622000	-0.000669000	-0.857228000
C	0.940459000	1.212363000	-0.324143000
H	0.643633000	1.230285000	-1.375704000
H	1.580164000	2.076759000	-0.134005000
H	2.035732000	-0.093098000	1.000077000
N	-0.297926000	-1.174108000	0.611624000
H	-0.869670000	-1.987104000	0.399478000
N	0.809973000	-1.209306000	-0.338350000
H	1.310202000	-2.060353000	-0.100090000



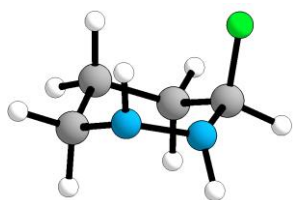
of imaginary frequencies: 0

E = -267.860328705

symmetry c2

C	0.609432000	-0.461261000	1.239085000
C	-0.609432000	1.286510000	-0.048064000
C	0.609432000	-1.286510000	-0.048064000
H	-1.509449000	1.900991000	-0.129225000
H	1.524582000	0.141549000	1.285697000
H	0.608325000	-1.120390000	2.111611000

H	1.509449000	-1.900991000	-0.129225000
C	-0.609432000	0.461261000	1.239085000
H	-1.524582000	-0.141549000	1.285697000
H	-0.608325000	1.120390000	2.111611000
H	0.248387000	1.970072000	-0.036976000
N	0.513086000	-0.489930000	-1.272154000
H	1.386208000	-0.014193000	-1.472161000
N	-0.513086000	0.489930000	-1.272154000
H	-1.386208000	0.014193000	-1.472161000
H	-0.248387000	-1.970072000	-0.036976000

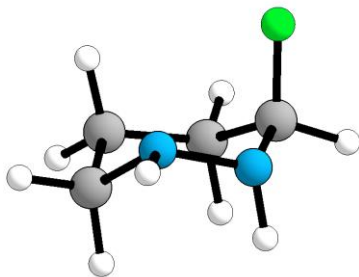


of imaginary frequencies: 0

E = -367.111930071

symmetry c1

C	-0.315779000	1.244644000	0.580020000
C	1.702819000	-0.061603000	-0.045683000
C	-1.108123000	-0.045140000	0.411927000
H	2.567976000	-0.151312000	-0.706035000
H	-0.015011000	1.319122000	1.630969000
H	-0.964993000	2.093671000	0.356612000
H	-1.905805000	-0.133719000	1.153149000
F	-1.718815000	0.016287000	-0.843936000
C	0.922586000	1.224606000	-0.313784000
H	0.618410000	1.257060000	-1.364607000
H	1.547242000	2.100676000	-0.122179000
H	2.077067000	-0.058504000	0.985049000
N	-0.342927000	-1.255441000	0.458021000
H	-0.243108000	-1.631476000	1.391112000
N	0.897378000	-1.270475000	-0.218669000
H	0.697377000	-1.435727000	-1.198989000

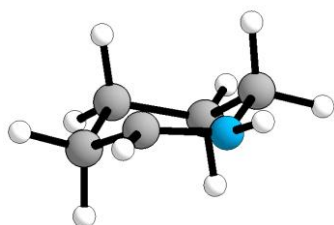


of imaginary frequencies: 0

E = -367.106781671

symmetry c1

C	-0.312994000	1.263918000	0.524257000
C	1.705063000	-0.095291000	-0.048620000
C	-1.122533000	-0.025311000	0.399545000
H	2.576030000	-0.189852000	-0.700273000
H	-0.055114000	1.382619000	1.583214000
H	-0.944121000	2.110194000	0.244611000
H	-1.899898000	-0.076791000	1.167200000
C	0.967669000	1.215862000	-0.312696000
H	0.715923000	1.258319000	-1.374925000
H	1.602163000	2.073404000	-0.077064000
H	2.052467000	-0.128975000	0.999959000
N	-0.334489000	-1.231333000	0.518835000
H	-0.033822000	-1.300541000	1.495612000
N	0.779609000	-1.176564000	-0.357013000
H	1.205499000	-2.092234000	-0.385725000
F	-1.750911000	-0.037326000	-0.828920000



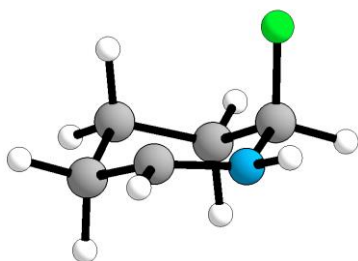
of imaginary frequencies: 0

E = -251.196830168

symmetry c1

C	-0.085293000	-1.388416000	-0.286426000
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C	1.303244000	0.691978000	-0.157044000
C	0.043680000	1.437306000	0.157193000
C	-1.298785000	-0.597826000	0.191323000
H	2.150616000	1.180854000	0.328861000
H	-0.055036000	-1.367743000	-1.381109000
H	-0.188516000	-2.431135000	0.024116000
H	0.030759000	2.517874000	0.078054000
H	-2.213770000	-0.981009000	-0.264730000
C	1.198758000	-0.774741000	0.273821000
H	1.176099000	-0.828752000	1.368025000
H	2.073223000	-1.335787000	-0.064892000
H	1.499650000	0.719916000	-1.242425000
N	-1.154284000	0.808872000	-0.175912000
H	-1.974974000	1.360950000	0.028989000
H	-1.387688000	-0.707082000	1.283289000



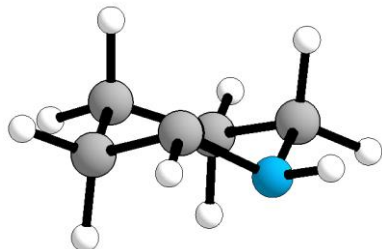
of imaginary frequencies: 0

E = -350.45072897

symmetry c1

C	-0.267749000	-1.190033000	-0.634063000
C	1.763012000	0.065054000	0.108408000
C	0.900701000	1.279943000	0.210927000
C	-1.110407000	0.052079000	-0.412080000
H	2.571077000	0.126801000	0.840154000
H	0.071664000	-1.188296000	-1.674471000
H	-0.905332000	-2.063477000	-0.486677000
H	1.345126000	2.263817000	0.285130000
H	-1.930431000	0.132385000	-1.127157000
F	-1.733120000	-0.080546000	0.849204000
C	0.930248000	-1.204373000	0.314701000

H	0.571196000	-1.243557000	1.346563000
H	1.536370000	-2.095337000	0.138062000
H	2.237528000	0.013651000	-0.886629000
N	-0.330308000	1.239998000	-0.460532000
H	-0.881795000	2.082912000	-0.381441000

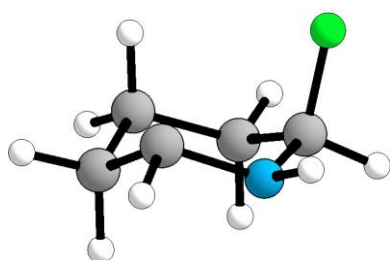


of imaginary frequencies: 0

E = -251.180067630

symmetry c1

C	0.023157000	-1.412521000	-0.225534000
C	1.200416000	0.806663000	-0.193290000
C	-0.069223000	1.435766000	0.333379000
C	-1.246441000	-0.669456000	0.201150000
H	2.076535000	1.350490000	0.177238000
H	0.026160000	-1.479864000	-1.320061000
H	0.006608000	-2.435031000	0.172938000
H	-0.138804000	2.476348000	-0.006374000
H	-2.127454000	-1.178833000	-0.212295000
C	1.283954000	-0.666803000	0.232204000
H	1.347590000	-0.704144000	1.325297000
H	2.176224000	-1.156545000	-0.183446000
H	1.252616000	0.811677000	-1.312584000
N	-1.200970000	0.698524000	-0.289417000
H	-2.059745000	1.156529000	-0.009323000
H	-1.304116000	-0.692188000	1.307066000

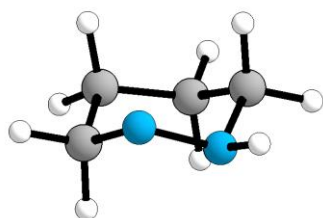


of imaginary frequencies: 0

E = -350.437875807

symmetry c1

C	-0.278182000	-1.221382000	-0.555623000
C	1.760925000	0.084684000	0.054338000
C	0.907642000	1.284686000	0.405064000
C	-1.079720000	0.069233000	-0.440299000
H	2.679955000	0.095901000	0.649826000
H	0.021970000	-1.321125000	-1.604324000
H	-0.937285000	-2.060236000	-0.310648000
H	1.442431000	2.191057000	0.086968000
H	-1.881176000	0.107745000	-1.187192000
F	-1.831162000	-0.039611000	0.803235000
C	0.973092000	-1.203400000	0.327506000
H	0.675937000	-1.209521000	1.380528000
H	1.568648000	-2.104303000	0.125602000
H	2.066778000	0.037603000	-1.025895000
N	-0.284455000	1.214800000	-0.526453000
H	-0.868162000	2.032856000	-0.404731000



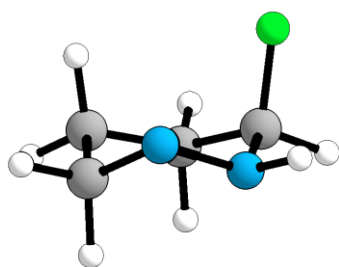
of imaginary frequencies: 0

E = -267.224097083

symmetry c1

C	-0.112721000	1.405234000	0.215781000
C	1.201543000	-0.735765000	0.188058000
C	-1.289437000	0.526612000	-0.216866000
H	2.109765000	-1.212845000	-0.205285000
H	-0.135052000	1.476597000	1.310623000
H	-0.220084000	2.419487000	-0.187935000

H	-2.231652000	0.933088000	0.181157000
C	1.211786000	0.763607000	-0.213131000
H	1.309516000	0.821939000	-1.303994000
H	2.060162000	1.299053000	0.242103000
H	1.276416000	-0.746160000	1.310576000
N	-1.075009000	-0.817943000	0.311812000
H	-1.869345000	-1.393122000	0.055152000
N	0.070992000	-1.449350000	-0.300840000
H	-1.338632000	0.514889000	-1.322245000

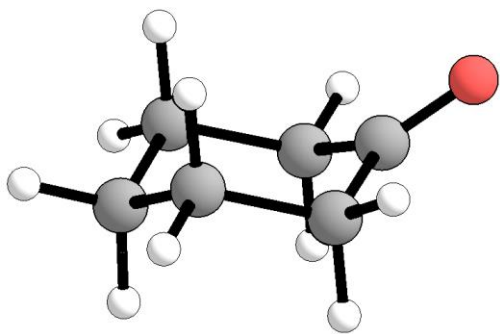


of imaginary frequencies: 0

E = -366.483878844

symmetry c1

C	-0.227771000	1.242692000	0.539156000
C	1.700307000	-0.231648000	-0.068587000
C	-1.066814000	-0.026217000	0.437035000
H	2.590192000	-0.318808000	-0.706097000
H	0.056913000	1.345684000	1.592361000
H	-0.849237000	2.102973000	0.271781000
H	-1.868238000	-0.043914000	1.186256000
F	-1.798563000	0.064239000	-0.813953000
C	1.039179000	1.149125000	-0.315816000
H	0.773559000	1.211179000	-1.375727000
H	1.712777000	1.984773000	-0.070848000
H	2.055689000	-0.211424000	1.002349000
N	-0.276056000	-1.177149000	0.565541000
H	-0.846318000	-2.010835000	0.497564000
N	0.832102000	-1.314493000	-0.368796000

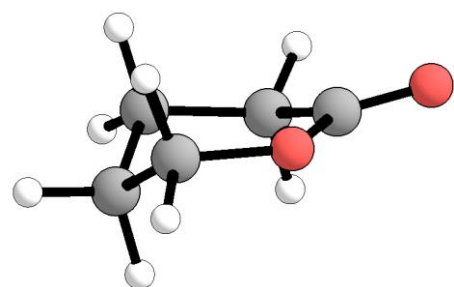


of imaginary frequencies: 0

E = -309.834249776

symmetry cs

C	-0.169882000	0.513430000	1.279348000
C	-0.850260000	-1.561153000	0.000000000
H	-0.830073000	-2.653761000	0.000000000
H	-1.205424000	0.869842000	1.344919000
H	0.386126000	0.916608000	2.126078000
C	-0.169882000	-1.023704000	1.259691000
H	0.865142000	-1.381431000	1.292046000
H	-0.664057000	-1.401899000	2.157486000
H	-1.905394000	-1.261387000	0.000000000
C	0.426878000	1.067631000	0.000000000
O	1.323668000	1.874166000	0.000000000
C	-0.169882000	0.513430000	-1.279348000
H	0.386126000	0.916608000	-2.126078000
H	-1.205424000	0.869842000	-1.344919000
C	-0.169882000	-1.023704000	-1.259691000
H	-0.664057000	-1.401899000	-2.157486000
H	0.865142000	-1.381431000	-1.292046000

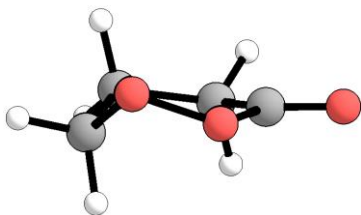


of imaginary frequencies: 0

E = -345.755662678

symmetry c1

C	0.343934000	1.280071000	-0.124014000
C	-1.723839000	-0.065616000	-0.318212000
H	-2.774516000	-0.184552000	-0.043498000
H	0.408066000	1.556400000	-1.182778000
H	0.902269000	2.033813000	0.430423000
C	-1.120055000	1.190757000	0.296246000
H	-1.196518000	1.134608000	1.387238000
H	-1.654749000	2.089028000	-0.017698000
H	-1.669088000	-0.015210000	-1.410687000
O	0.458999000	-1.186204000	-0.061683000
C	-0.952310000	-1.270359000	0.182486000
H	-1.267318000	-2.190993000	-0.307478000
H	-1.096479000	-1.388275000	1.261879000
C	1.130565000	-0.015490000	-0.014370000
O	2.325821000	-0.032671000	0.030406000



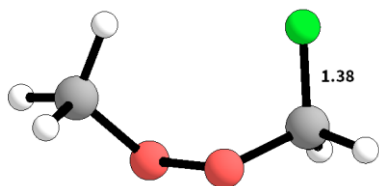
of imaginary frequencies: 0

E = -381.570729193

symmetry c1

C	-0.262838000	1.292137000	0.036678000
C	1.642216000	-0.255585000	0.325884000
H	2.669811000	-0.515348000	0.067526000
H	-0.454830000	1.683809000	1.041422000
H	-0.711024000	2.000910000	-0.659377000
C	1.240177000	1.112634000	-0.183511000
H	1.477240000	1.162363000	-1.248210000
H	1.795658000	1.904884000	0.322267000
H	1.500607000	-0.367723000	1.406194000
O	-0.483725000	-1.182353000	0.117187000

O	0.860854000	-1.224344000	-0.357972000
C	-1.106102000	0.033087000	-0.009526000
O	-2.296902000	0.036380000	-0.002586000

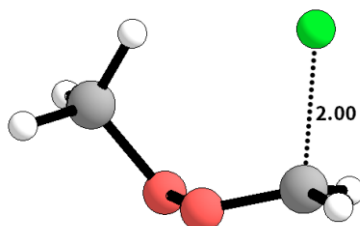


of imaginary frequencies: 0

E = -328.936971610

symmetry c1

C	1.278636000	0.407685000	0.091444000
H	2.043239000	0.897032000	-0.513206000
F	1.453258000	-0.956308000	-0.006795000
C	-1.780873000	-0.526482000	-0.136334000
H	-1.214733000	-1.438922000	-0.330413000
H	-2.574523000	-0.717351000	0.587518000
H	-2.208159000	-0.134350000	-1.061332000
O	0.079425000	0.805205000	-0.460492000
H	1.334353000	0.667744000	1.148388000
O	-0.967853000	0.454451000	0.497928000



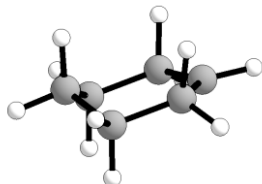
of imaginary frequencies: 0

E = -328.870939813

symmetry c1

C	1.220876000	0.526770000	0.087819000
H	2.069755000	0.798149000	-0.524764000
F	1.426502000	-1.455021000	-0.086032000
C	-1.747357000	-0.529370000	-0.129833000
H	-1.113957000	-1.407455000	-0.255059000

H	-2.533746000	-0.710283000	0.603833000
H	-2.181155000	-0.200705000	-1.074869000
O	0.089008000	0.814524000	-0.475716000
H	1.269580000	0.473046000	1.165599000
O	-0.991689000	0.532214000	0.468545000

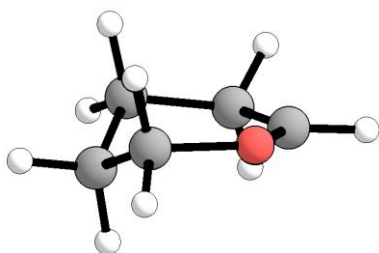


of imaginary frequencies: 0

E = -234.889842117

symmetry c1

C	1.272398000	0.767917000	0.027400000
C	-0.000179000	-1.386000000	0.342820000
C	0.000323000	1.442058000	-0.012224000
H	-0.000385000	-2.452732000	0.118250000
H	1.548225000	0.996102000	1.090287000
H	2.031900000	1.348915000	-0.512085000
H	0.000548000	2.533165000	0.028548000
C	1.259704000	-0.738699000	-0.234007000
H	1.306487000	-0.904307000	-1.313813000
H	2.160713000	-1.179816000	0.191970000
H	-0.000007000	-1.296888000	1.435439000
C	-1.260021000	-0.738275000	-0.233701000
H	-2.161038000	-1.178908000	0.192768000
H	-1.307324000	-0.904245000	-1.313434000
C	-1.272177000	0.768420000	0.027192000
H	-1.548010000	0.996881000	1.089902000
H	-2.031398000	1.349302000	-0.512715000

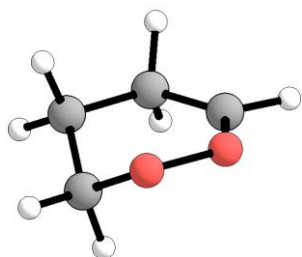


of imaginary frequencies: 0

E = -270.834197883

symmetry c1

C	-1.440687000	-0.217389000	-0.051832000
C	0.898045000	-1.019795000	-0.354348000
C	-0.834844000	1.120721000	-0.072815000
H	1.636427000	-1.786229000	-0.111988000
H	-1.895309000	-0.324913000	-1.051465000
H	-2.304598000	-0.164542000	0.622938000
H	-1.449051000	2.015027000	-0.199232000
C	-0.458249000	-1.341228000	0.273269000
H	-0.356114000	-1.439956000	1.356947000
H	-0.848323000	-2.286590000	-0.100752000
H	0.821534000	-0.978400000	-1.445155000
O	0.381725000	1.368400000	0.028850000
C	1.411850000	0.295516000	0.175733000
H	2.259830000	0.705182000	-0.367322000
H	1.625114000	0.286275000	1.245184000



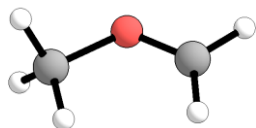
of imaginary frequencies: 0

E = -306.631353549

symmetry c1

C	-0.201204000	1.417673000	0.018390000
C	1.161081000	-0.603570000	0.352867000
C	-1.285569000	0.433367000	0.081562000
H	2.044954000	-1.187486000	0.092643000
H	-0.272944000	1.972240000	0.967648000
H	-0.502049000	2.154826000	-0.739532000
H	-2.328789000	0.712957000	0.246803000

C	1.173101000	0.798208000	-0.224531000
H	1.388360000	0.748566000	-1.292267000
H	1.947293000	1.399795000	0.250702000
H	1.012361000	-0.628572000	1.436970000
O	-1.166241000	-0.807509000	-0.017659000
O	0.119535000	-1.373290000	-0.273929000

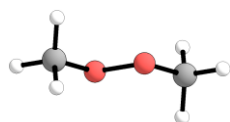


of imaginary frequencies: 0

E = -154.077041357

symmetry c1

C	1.185758000	0.197988000	0.000005000
H	2.122457000	-0.359287000	0.000030000
H	1.155122000	1.291202000	-0.000016000
O	0.150444000	-0.467039000	-0.000016000
C	-1.192684000	0.143583000	0.000001000
H	-1.090906000	1.227493000	-0.000415000
H	-1.674514000	-0.236589000	-0.897294000
H	-1.674156000	-0.235931000	0.897788000



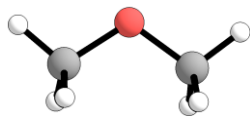
of imaginary frequencies: 0

E = -230.124516650

symmetry c1

C	1.733935000	-0.105766000	0.000239000
H	2.463521000	0.704154000	0.000173000
C	-1.733943000	0.105754000	0.000238000
H	-1.855431000	0.720745000	-0.895465000
H	-2.463495000	-0.704195000	0.000210000
H	-1.854885000	0.720202000	0.896389000
O	0.478980000	0.532069000	-0.000321000
H	1.855371000	-0.720794000	-0.895450000

O	-0.478965000	-0.532050000	-0.000321000
H	1.854849000	-0.720191000	0.896409000

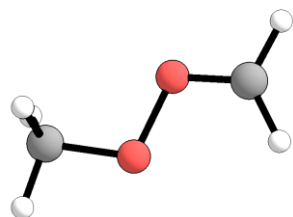


of imaginary frequencies: 0

E = -154.994930691

symmetry c1

C	-1.163742000	0.195540000	-0.000003000
H	-2.018099000	-0.479834000	0.000026000
H	-1.210366000	0.834868000	0.891626000
H	-1.210340000	0.834850000	-0.891645000
O	-0.000015000	-0.590773000	-0.000003000
C	1.163756000	0.195535000	0.000003000
H	1.210321000	0.834901000	0.891637000
H	2.018111000	-0.479856000	0.000081000
H	1.210410000	0.834801000	-0.891698000

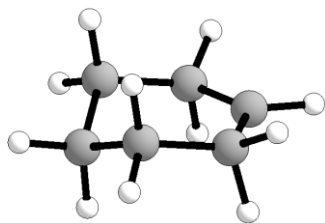


of imaginary frequencies: 0

E = -229.195973751

symmetry c1

C	1.730545000	0.071102000	-0.000136000
H	2.554783000	-0.642101000	-0.000114000
C	-1.692337000	-0.163118000	-0.000133000
H	-1.790526000	-0.753562000	0.908887000
H	-2.400160000	0.667270000	-0.000550000
H	-1.789879000	-0.753866000	-0.909029000
O	0.603861000	-0.433480000	0.000158000
H	1.838187000	1.157978000	-0.000393000
O	-0.434067000	0.543027000	0.000194000

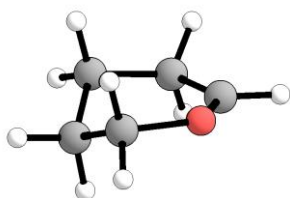


of imaginary frequencies: 0

E = -234.889839181

symmetry cs

C	0.104762000	0.760999000	1.272494000
C	-0.575775000	-1.305962000	0.000000000
C	0.256677000	1.419074000	0.000000000
H	-0.539865000	-2.395401000	0.000000000
H	-0.902109000	1.168126000	1.552268000
H	0.738731000	1.241122000	2.029734000
H	0.400978000	2.501373000	0.000000000
C	0.104762000	-0.767934000	1.259338000
H	1.140397000	-1.115686000	1.304100000
H	-0.389247000	-1.130082000	2.160823000
H	-1.636348000	-1.028377000	0.000000000
C	0.104762000	-0.767934000	-1.259338000
H	-0.389247000	-1.130082000	-2.160823000
H	1.140397000	-1.115686000	-1.304100000
C	0.104762000	0.760999000	-1.272494000
H	-0.902109000	1.168126000	-1.552268000
H	0.738731000	1.241122000	-2.029734000



of imaginary frequencies: 0

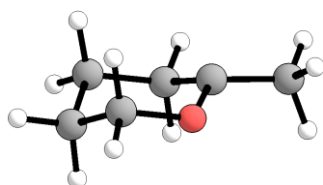
E = -270.834197884

symmetry c1

C	1.440687000	0.217391000	-0.051832000
C	-0.898046000	1.019794000	-0.354348000

S45

C	0.834845000	-1.120720000	-0.072815000
H	-1.636429000	1.786227000	-0.111988000
H	1.895309000	0.324915000	-1.051465000
H	2.304598000	0.164544000	0.622938000
H	1.449053000	-2.015025000	-0.199232000
C	0.458248000	1.341229000	0.273269000
H	0.356113000	1.439956000	1.356947000
H	0.848321000	2.286591000	-0.100752000
H	-0.821535000	0.978399000	-1.445155000
O	-0.381724000	-1.368400000	0.028850000
C	-1.411850000	-0.295517000	0.175733000
H	-2.259829000	-0.705184000	-0.367322000
H	-1.625114000	-0.286277000	1.245184000



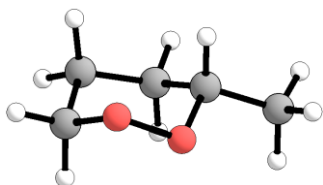
of imaginary frequencies: 0

E = -310.370362985

symmetry c1

C	-0.223736000	1.285973000	0.138496000
C	1.823925000	-0.123877000	0.289940000
C	-0.977344000	0.029240000	-0.185604000
H	2.860586000	-0.266855000	-0.026438000
H	-0.293144000	1.472609000	1.225127000
H	-0.707318000	2.132052000	-0.355852000
C	1.252351000	1.185328000	-0.251704000
H	1.340595000	1.193999000	-1.343547000
H	1.809398000	2.044136000	0.129445000
H	1.807833000	-0.113859000	1.384977000
O	-0.385295000	-1.156828000	0.161048000
C	-2.454698000	-0.012468000	-0.006447000
H	-2.870820000	-0.914699000	-0.457829000
H	-2.725269000	-0.018733000	1.060361000

H	-2.921094000	0.861621000	-0.464350000
C	0.983884000	-1.288547000	-0.209687000
H	1.312243000	-2.237722000	0.213872000
H	1.043061000	-1.351827000	-1.304106000

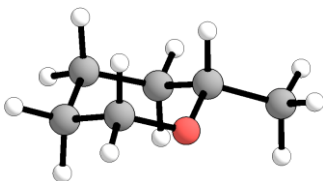


of imaginary frequencies: 0

E = -346.853074836

symmetry c1

C	-0.202033000	1.275285000	0.129197000
C	1.771379000	-0.231269000	0.294757000
C	-0.946401000	0.030343000	-0.345819000
H	2.787575000	-0.447638000	-0.040604000
H	-0.363682000	1.377614000	1.208419000
H	-0.618401000	2.162854000	-0.354985000
C	1.292771000	1.139266000	-0.164884000
H	1.471386000	1.229641000	-1.240771000
H	1.863943000	1.925525000	0.335271000
H	1.720725000	-0.331813000	1.384659000
O	-0.337197000	-1.128892000	0.226345000
O	0.979187000	-1.248273000	-0.300572000
C	-2.393185000	-0.011378000	0.102328000
H	-2.879574000	-0.921195000	-0.250651000
H	-2.450618000	0.016555000	1.192653000
H	-2.927874000	0.852861000	-0.296856000
H	-0.874588000	-0.060568000	-1.436794000

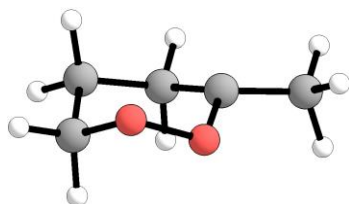


of imaginary frequencies: 0

E = -311.028586226

symmetry c1

C	0.237434000	1.269539000	-0.153237000
C	-1.843607000	-0.110277000	-0.302779000
C	0.966621000	0.015361000	0.325547000
H	-2.877216000	-0.231161000	0.033140000
H	0.354832000	1.338045000	-1.241108000
H	0.707327000	2.153772000	0.287229000
C	-1.248061000	1.203050000	0.206651000
H	-1.358281000	1.250592000	1.296937000
H	-1.784558000	2.060658000	-0.206180000
H	-1.845268000	-0.116367000	-1.397527000
O	0.350152000	-1.151928000	-0.201125000
C	2.419528000	-0.020371000	-0.102616000
H	2.896498000	-0.935536000	0.250600000
H	2.484237000	0.004886000	-1.192776000
H	2.958846000	0.838900000	0.301685000
C	-1.003019000	-1.281505000	0.190856000
H	-1.351742000	-2.227962000	-0.224585000
H	-1.061944000	-1.346218000	1.288896000
H	0.902677000	-0.028972000	1.426151000



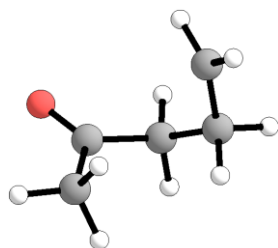
of imaginary frequencies: 0

E = -346.190568228

symmetry c1

C	-0.179126000	1.292769000	0.135552000
C	1.759139000	-0.252643000	0.257800000
C	-0.954858000	0.049117000	-0.181987000
H	2.767104000	-0.494039000	-0.084865000
H	-0.276809000	1.500756000	1.214923000
H	-0.614796000	2.143308000	-0.392879000
C	1.301326000	1.119671000	-0.212446000

H	1.438555000	1.179521000	-1.295146000
H	1.905737000	1.901885000	0.252852000
H	1.717421000	-0.344503000	1.349392000
O	-0.375813000	-1.127938000	0.219541000
O	0.946336000	-1.258000000	-0.326404000
C	-2.434121000	-0.002442000	-0.033807000
H	-2.833556000	-0.909704000	-0.489409000
H	-2.735174000	0.004793000	1.023801000
H	-2.886825000	0.866653000	-0.514436000

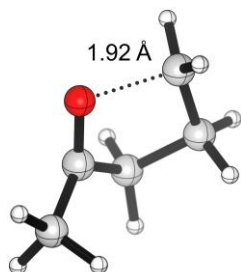


of imaginary frequencies: 0

E = -271.057109306

symmetry c1

C	0.954603000	-0.178793000	-0.041424000
O	1.673813000	-0.929870000	0.569029000
C	1.211317000	1.312138000	-0.074122000
H	2.210677000	1.517331000	0.304138000
H	1.094818000	1.710763000	-1.084743000
H	0.475460000	1.810530000	0.564442000
C	-0.252324000	-0.689284000	-0.809854000
H	-0.376858000	-1.744737000	-0.560089000
H	-0.021237000	-0.620339000	-1.878787000
C	-1.532220000	0.099895000	-0.504344000
H	-1.443232000	1.127627000	-0.873345000
H	-2.355887000	-0.344961000	-1.081587000
C	-1.859303000	0.103241000	0.949743000
H	-2.552911000	0.824545000	1.360350000
H	-1.553769000	-0.724984000	1.577394000

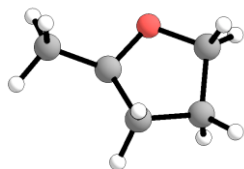


of imaginary frequencies: 1

E = -271.020911444

symmetry c1

C	0.770376000	-0.076917000	-0.308644000
O	0.155754000	-1.173420000	-0.421104000
C	2.086226000	0.021373000	0.404103000
H	2.530155000	-0.967831000	0.505574000
H	2.775723000	0.675453000	-0.134361000
H	1.945625000	0.452283000	1.405368000
C	-0.114449000	1.103872000	-0.504988000
H	-0.461171000	1.165664000	-1.539790000
H	0.335085000	2.056201000	-0.219504000
C	-1.349944000	0.720074000	0.402465000
H	-1.116076000	0.958376000	1.442219000
H	-2.211185000	1.319764000	0.103994000
C	-1.595139000	-0.739560000	0.228250000
H	-1.640744000	-1.381576000	1.097794000
H	-2.185860000	-1.064032000	-0.619581000



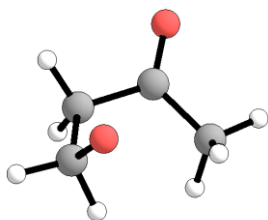
of imaginary frequencies: 0

E = -271.061468512

symmetry c1

C	0.734422000	0.062450000	-0.239595000
O	0.047635000	-1.119219000	-0.083942000
C	2.192305000	-0.018382000	0.029936000

H	2.635330000	-0.865931000	-0.496600000
H	2.690708000	0.894909000	-0.299511000
H	2.398071000	-0.149440000	1.103466000
C	-0.149321000	1.209110000	0.143574000
H	0.078284000	2.121689000	-0.409521000
H	-0.059066000	1.439105000	1.218423000
C	-1.535581000	0.633212000	-0.169012000
H	-2.340727000	1.084607000	0.410557000
H	-1.756988000	0.753272000	-1.231313000
C	-1.334578000	-0.845813000	0.167062000
H	-1.534546000	-1.045338000	1.224746000
H	-1.935635000	-1.522578000	-0.440501000

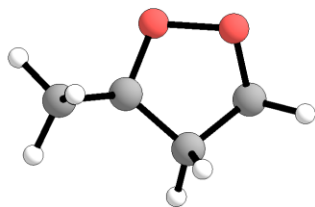


of imaginary frequencies: 0

E = -306.962126194

symmetry c1

C	0.959913000	-0.160975000	0.020776000
O	1.838098000	-0.755097000	-0.549508000
C	1.045382000	1.323521000	0.291727000
H	2.047476000	1.676445000	0.057991000
H	0.320492000	1.845824000	-0.339141000
H	0.800363000	1.544857000	1.334320000
C	-0.274175000	-0.897313000	0.524024000
H	-0.113402000	-1.118836000	1.586186000
H	-0.330571000	-1.848732000	-0.006783000
C	-1.572746000	-0.111973000	0.367863000
H	-2.443787000	-0.694185000	0.703557000
H	-1.579331000	0.788338000	1.010665000
O	-1.794534000	0.365938000	-0.897133000

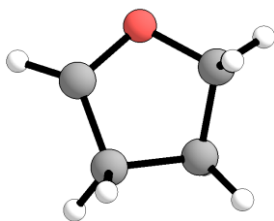


of imaginary frequencies: 0

E = -306.882546415

symmetry c1

C	0.720045000	0.087167000	-0.293502000
O	0.051829000	-1.109672000	-0.230723000
C	2.147762000	0.036413000	0.124839000
H	2.660087000	-0.805651000	-0.342856000
H	2.657764000	0.955945000	-0.166004000
H	2.235172000	-0.077133000	1.215065000
C	-0.226364000	1.200347000	0.039375000
H	-0.140917000	2.052242000	-0.637670000
H	-0.071060000	1.556036000	1.067070000
C	-1.554319000	0.466002000	-0.097927000
H	-2.340843000	0.826352000	0.564341000
H	-1.899705000	0.454604000	-1.136571000
O	-1.254735000	-0.853073000	0.330713000



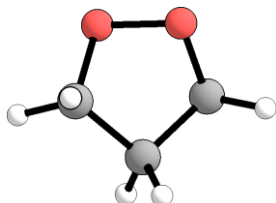
of imaginary frequencies: 0

E = -231.749755563

symmetry c1

C	1.258106000	0.155689000	0.137760000
C	0.174176000	1.190955000	-0.220353000
C	0.493964000	-1.135131000	0.047975000
H	0.294214000	2.143448000	0.295269000
H	2.114661000	0.190603000	-0.539775000
H	1.640134000	0.328737000	1.151047000

H	0.167116000	1.372773000	-1.296989000
O	-0.842004000	-0.911378000	-0.130600000
C	-1.101592000	0.457394000	0.185616000
H	-1.993185000	0.761064000	-0.360638000
H	-1.285515000	0.545164000	1.262564000
H	0.850680000	-2.064214000	-0.372668000

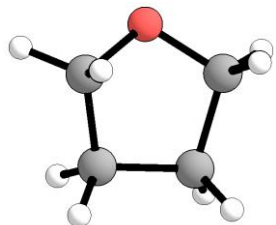


of imaginary frequencies: 0

E = -268.231630760

symmetry c1

C	-0.002479000	1.246848000	0.000312000
C	-1.178618000	0.263329000	-0.127116000
C	1.177770000	0.267459000	0.126717000
H	-2.014191000	0.479595000	0.537550000
H	0.078260000	1.880802000	-0.881972000
H	-0.085675000	1.880454000	0.882585000
H	-1.527244000	0.186688000	-1.160545000
O	0.652484000	-0.984619000	-0.290612000
H	1.527887000	0.192349000	1.159732000
H	2.011628000	0.486563000	-0.539117000
O	-0.648822000	-0.986915000	0.290898000



of imaginary frequencies: 0

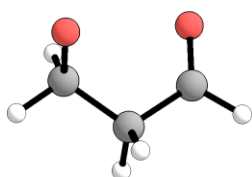
E = -232.406364368

symmetry c1

C	0.823206000	0.962845000	-0.108970000
C	-0.716025000	1.055868000	0.006662000

S53

C	1.094786000	-0.512123000	0.199713000
H	-1.025952000	1.622105000	0.885661000
H	1.145756000	1.192723000	-1.125211000
H	1.343042000	1.634607000	0.574461000
H	-1.148167000	1.538443000	-0.869724000
O	-0.041728000	-1.195172000	-0.292355000
C	-1.156886000	-0.420949000	0.113423000
H	-1.996097000	-0.678719000	-0.531560000
H	-1.419062000	-0.670635000	1.150091000
H	1.187155000	-0.672068000	1.284003000
H	1.976662000	-0.918930000	-0.293856000

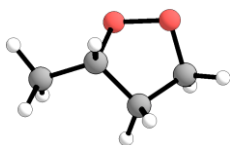


of imaginary frequencies: 0

E = -267.648115575

symmetry c1

C	-0.052725000	1.027895000	0.087351000
C	1.112113000	0.201155000	-0.436367000
C	-1.321298000	0.214207000	0.190157000
H	0.868548000	-0.284344000	-1.392644000
H	0.179915000	1.433933000	1.077322000
H	-0.262491000	1.887497000	-0.561096000
H	1.985693000	0.841735000	-0.646993000
O	-1.428310000	-0.907845000	-0.220463000
H	-2.181245000	0.722686000	0.668627000
O	1.550941000	-0.749786000	0.446456000

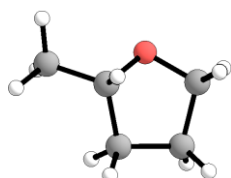


of imaginary frequencies: 0

E = -307.541559147

symmetry c1

C	0.181806000	1.205709000	-0.103950000
C	1.508537000	0.518698000	0.257358000
C	-0.714290000	-0.007589000	-0.413471000
H	2.374605000	0.904835000	-0.279379000
H	-0.207726000	1.782247000	0.736532000
H	0.271140000	1.862943000	-0.968601000
H	1.692865000	0.543416000	1.334697000
O	-0.009960000	-1.105079000	0.165658000
H	-0.765450000	-0.170197000	-1.495554000
O	1.345914000	-0.829837000	-0.167670000
C	-2.097110000	0.024557000	0.199317000
H	-2.669679000	0.852900000	-0.222286000
H	-2.631117000	-0.904231000	-0.005298000
H	-2.025930000	0.159160000	1.280456000



of imaginary frequencies: 0

E = -271.716563291

symmetry c1

C	-0.104630000	1.221472000	0.004883000
C	-1.542456000	0.671517000	-0.127206000
C	0.724180000	-0.017523000	0.379141000
H	-2.220334000	1.087669000	0.618739000
H	0.248480000	1.617945000	-0.949936000
H	-0.014768000	2.010974000	0.752082000
H	-1.954849000	0.891861000	-1.111951000
O	0.010326000	-1.102675000	-0.194588000
C	-1.356244000	-0.847099000	0.066772000
H	-1.951108000	-1.456604000	-0.612578000
H	-1.594737000	-1.135332000	1.099788000
H	0.720987000	-0.139084000	1.474150000
C	2.144247000	-0.025079000	-0.139624000

H	2.704817000	0.814047000	0.278273000
H	2.649698000	-0.952602000	0.132636000
H	2.138622000	0.062790000	-1.228301000

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- ⁹ CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (<http://www.cylview.org>).