Electronic Supporting Information

Stereoelectronic source of the anomalous stability of bis-peroxides

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Contents:

Other information on the differences between peroxides and ketals

On Figure 3 in the main text, we disclosure some of the main discrepancies between peroxides and ketals and tried to address how those structural and electronial (especially stereoelectronical) differences are the source of improved or lack of stability in those systems. Figure 1 illustrats more information on those idiocracies such as hybridizations and *p*-character.

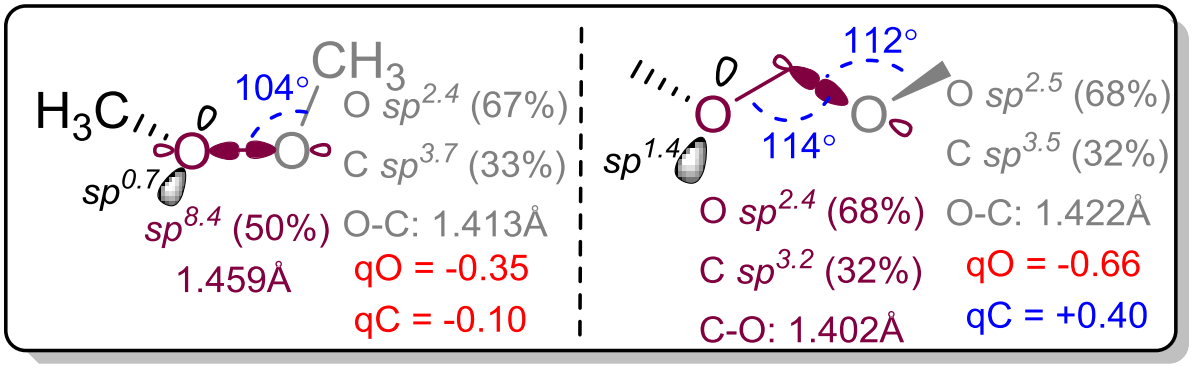
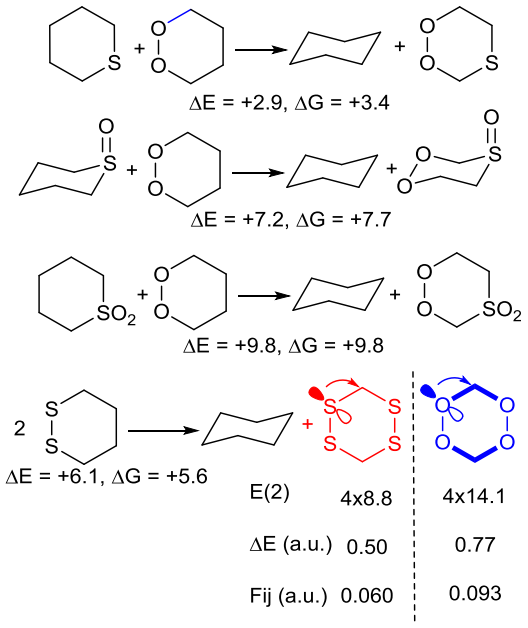


Figure 1: Hybridizations of bonds and lone pairs (polarization in parenthesis), angles, bond lengths and charges of dimetrhylperoxide and dimethoxymethane.

Lack of stabilization in sulfonyl compounds

Although close in the periodic table, oxygen and sulfur are quite different. Bis-disulfides cannot enjoy the anomeric stabilization seen in Schemes 4 and 8 (main paper) therefore bringing two S-S groups together destabilize the molecule. Several stereoelectronic and structural factors are behind this behaviour: C-S bonds are polarized towards the C end and are substantially longer than C-O bonds (23% in this case).
The anomeric $n_S \rightarrow \sigma^*_{C\text{-}S}$ interaction is 5.3 kcal/mol smaller than the $n_O \rightarrow \sigma^*_{C\text{-}O,}$ even though the energy gap between the two interacting orbitals is smaller (0.50 a.u.) but is counterbalanced by the much smaller F_{ij} term, just 0.060 a.u. That can accounted by the longer C-S bond and poor alignment of the orbitals.



Scheme 1: Not every pattern is a stabilizing one: weak anomeric effect in bis-disulfides do not help in its thermodynamic stabilization. ΔE, ΔG and E(2) in kcal/mol

PES relaxed scan for both COCO dihedrals in dimethoxy-methane simultaneously

In the main paper we disclose the best angle for the COCO dihedral that optimizes the anomeric $n_O \rightarrow \sigma^*_{C\text{-}O}$ interaction on dimethoxy-methane (60˚). That was performed taking only with one of the two COCO dihedrals of that molecule. Here we show the same kind of result, but now scanning both symmetrical COCO dihedrals (at the B2PLYPD/6-311++g(d,p) level) in a tridimensional plot.

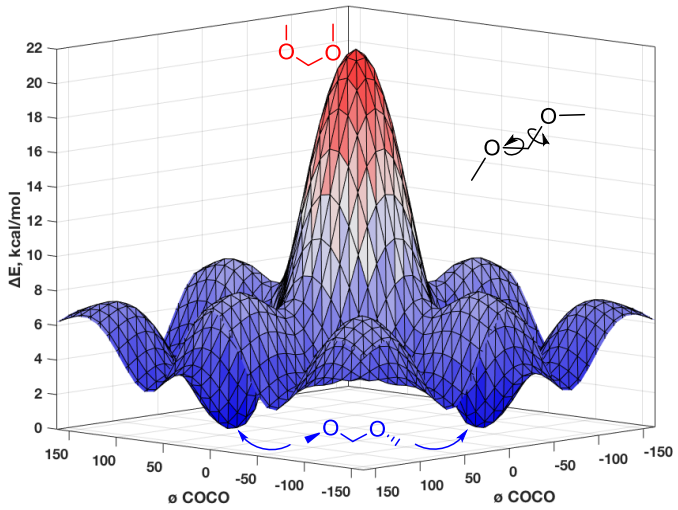


Figure 2: Multidimensional PES for scanning simultaneously both COCO dihedrals of dimethoxy-methane. Two identical global minima (deep blue) and one global maximum (deep red) are located with their designated conformations.

Although the overall result is the same as the two dimensional scan, it helps us to understand the another more intricated result when simulteniously scanning both COOC and OOCF dihedrals of fluoroperoxides.

PES relaxed dihedral scans for fluoroperoxides

Figures 3 and 4 shows the PES in mono- and difluoro-substituted alkyl and dialkyl peroxide.

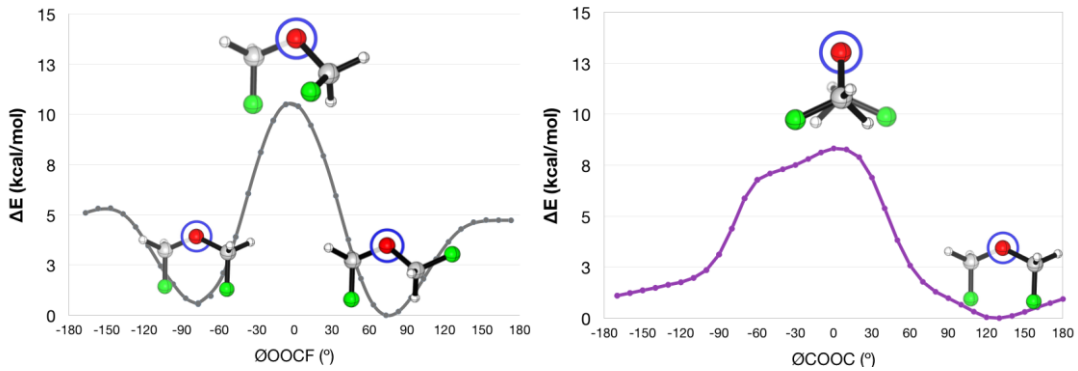


Figure 3: PES scanning both OOCF and COOC dihedrals of 1,4-difluoro-dimethylperoxide

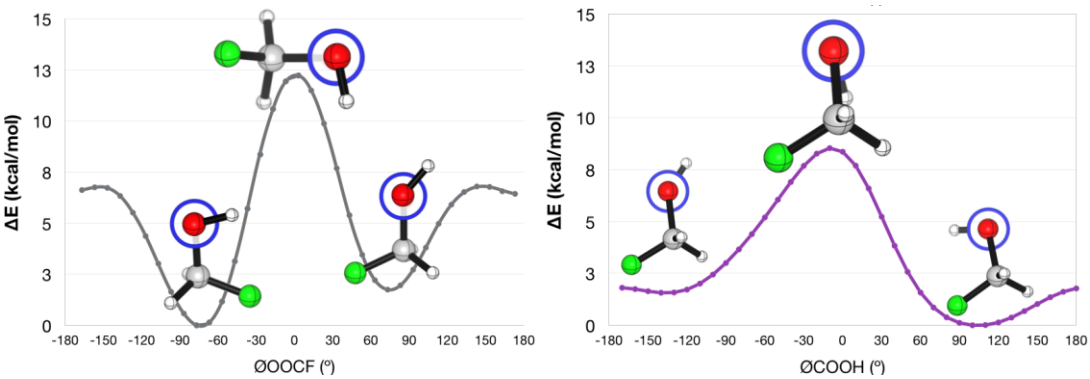


Figure 4: PES scanning both OOCF and COOH dihedrals of fluoro(hydroperoxy)methane

In order to gain more depth on the understating of the structural and stereoelectronic configuration of the those fluoroperoxides, a PES with both COOC and OOCF dihedral scans was perforemed at the B2PLYPD/6-311++G(d,p) level. That was briefly displayed in the main paper and can be seen in more details here:

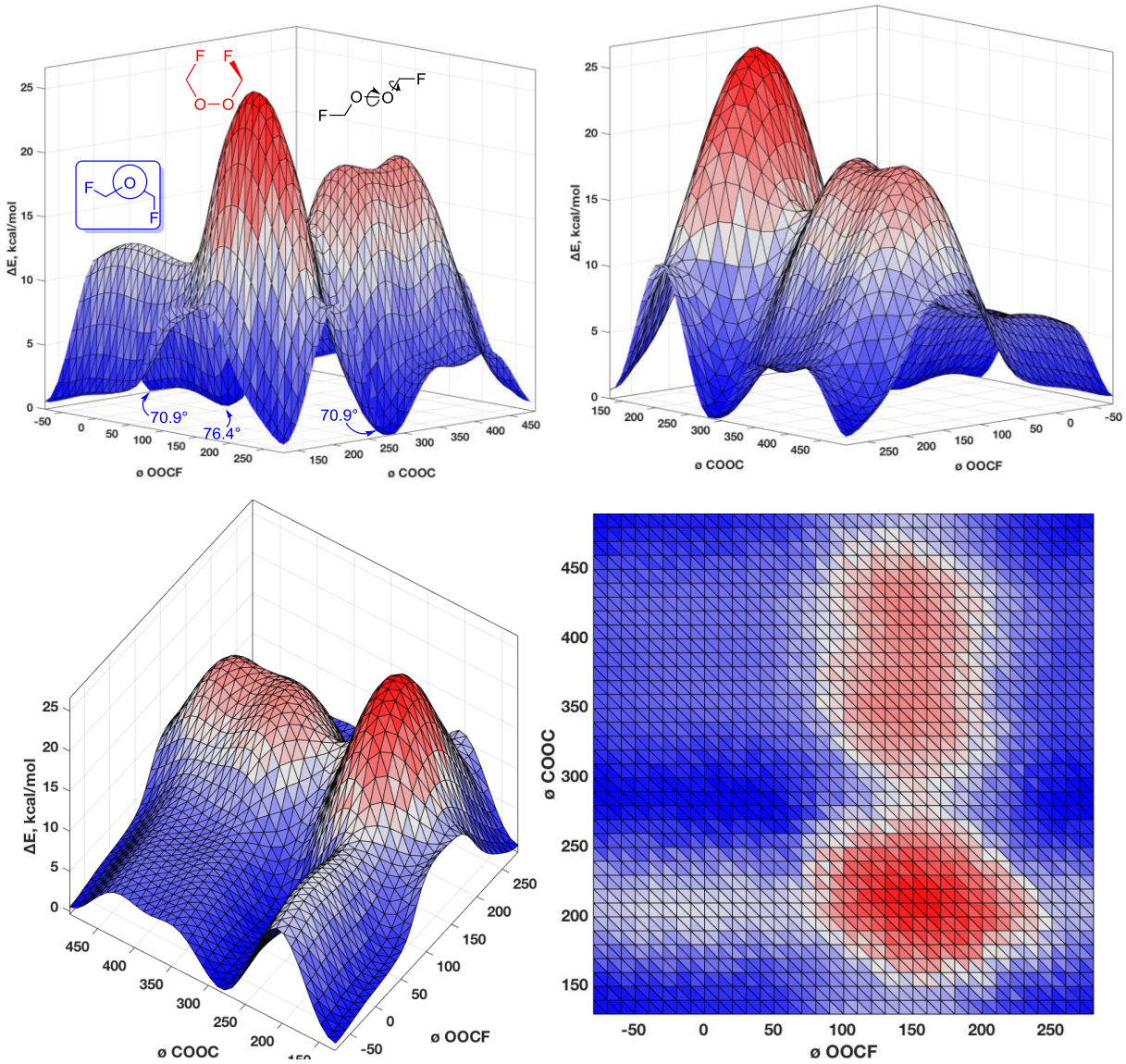


Figure 5: Four different views for the multidimensional PES scanning simultaneously both OOCF and COOC dihedrals of bis(fluoromethyl) peroxide. Three minima (deep blue pointed with arrows, boxed Newman projection conformation) and one global maximum (deep red) are located.

More details on the Cambridge structural database search for the peroxide motifs

Histograms and heat plots

Histograms and heat plots were prepared with the implemented tool on Mercury 3.5 or with MATLAB R2015a using the data acquired from the CSD using ConQuest 1.17 on August 11, 2015. Queries with only accurate structures (errors excluded), T < 140K and R-factor < 5% were performed for the C(sp^3)-OO-C(sp^3) motif, varying to include only cyclic, acyclic or both kind of structures. We also performed a similar query with the OOCX motif (X = O, N, Halogens) in order to gauge that dihedral with an acceptor group next to the peroxide moiety. For dimethylperoxide, calculated COOC dihedral lies around 150^o (149.3^o from MP2=full/6-311++g(d,p) optimization) and C-O bond length is 1.413A.

1. Acyclic:

Restraining the search for only acyclic crystal structures around the COOC motif. Histograms and heat plot for those occurrences are presented below. Data is in good agreement with computations.

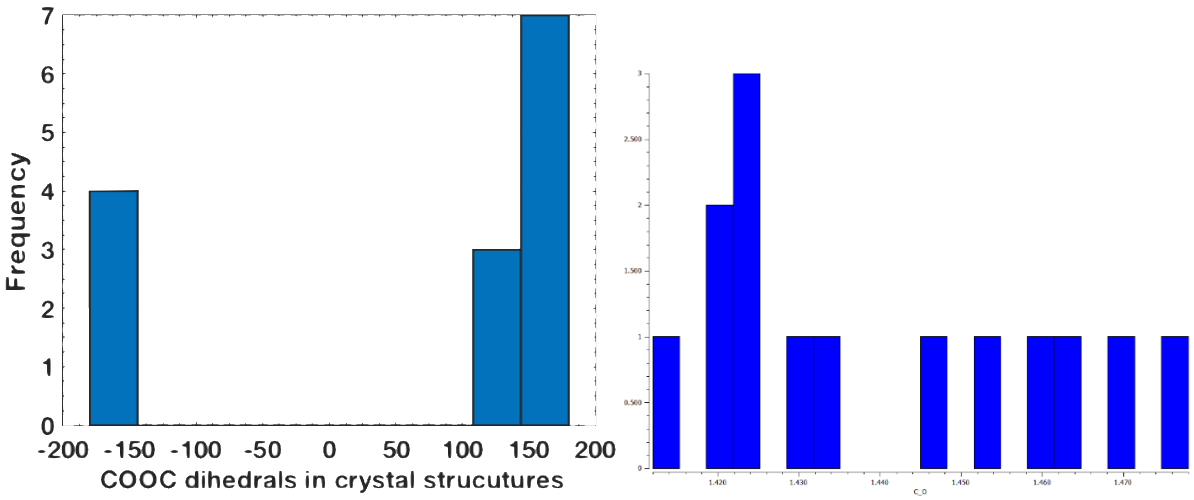


Figure 6: Left: COOC dihedrals. Right: C-O bond lengths

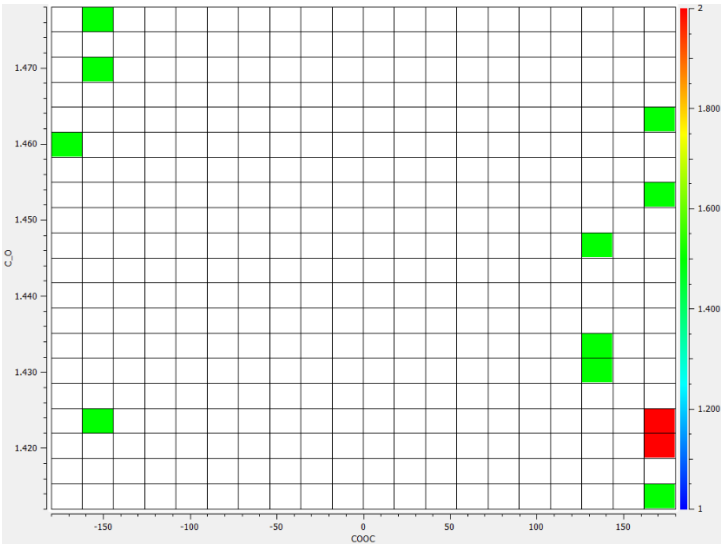


Figure 7: Heat plot of COOC dihedral vs. C-O bond lengths

2. Cyclic:

Restraining the search for only cyclic crystal structures around the COOC motif. Histograms and heat plot for those occurrences are presented below.

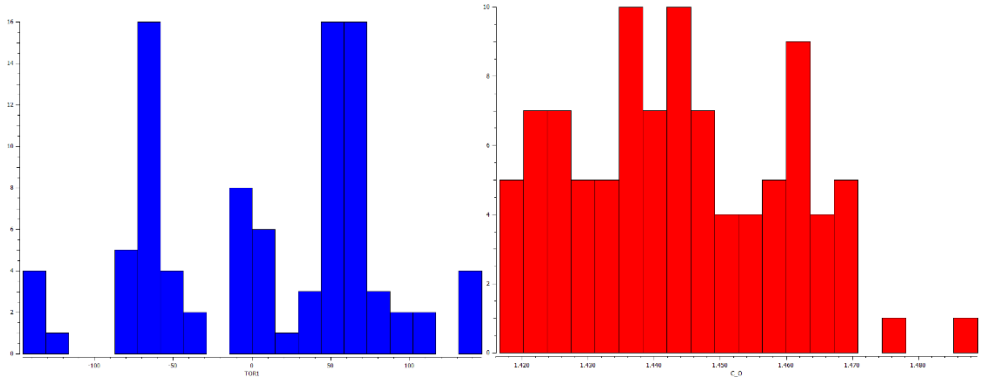


Figure 8: Left: COOC dihedrals. Right: C-O bond lengths

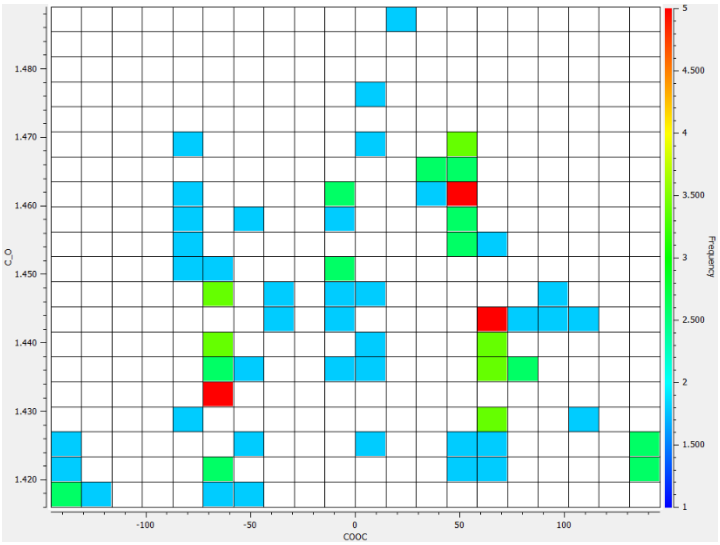


Figure 9: Heat plot of COOC dihedral vs. C-O bond lengths

3. No restrains on cyclicity:

No restrains on the cyclicity around the COOC motif of the crystal structures. Histograms and heat plot for those occurrences are presented below.

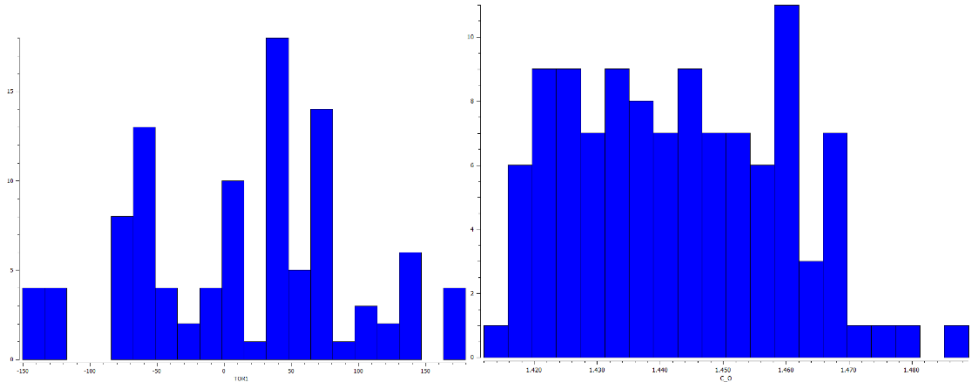


Figure 10: Left: COOC dihedrals. Right: C-O bond lengths

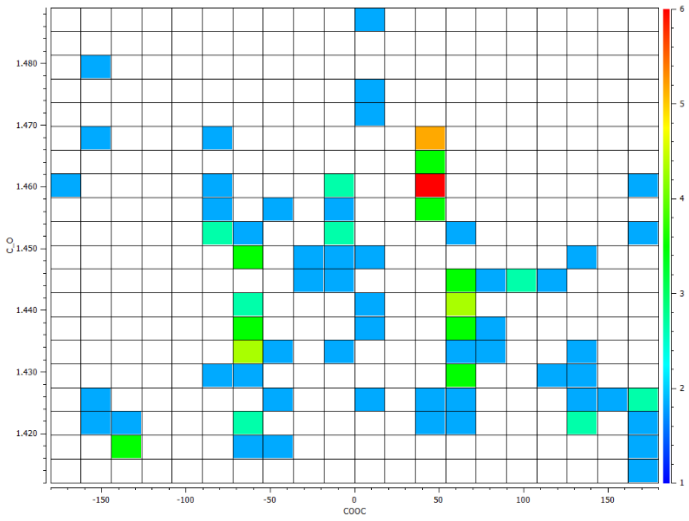


Figure 11: Heat plot of COOC dihedral vs. C-O bond lengths

4. OOCX dihedral:

An additional search selecting only interesting OOCX motifs of the crystal structures was performed. Histogram for this occurrence is presented below.

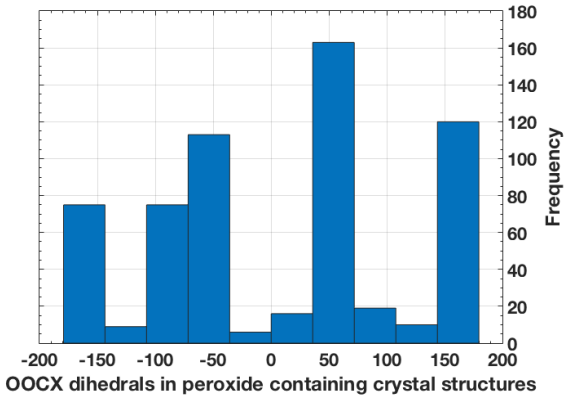


Figure 12: OOCX dihedrals histogram

Computational Details

1. General Information

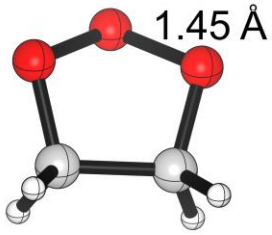
All calculations were performed using the software package Gaussian ’09 and NBO 3.0 included in this same package. The methods used were mainly M06-2X, with also B2PLYPD and MP2 for PES scans, all with the 6-311++G(d,p) basis set.

Full reference for Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.;

Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

2. M06-2X (MP2, B2PLYPD when denoted) with 6-311++G(d,p) basis set geometries and total energies (in hartree) in gas phase

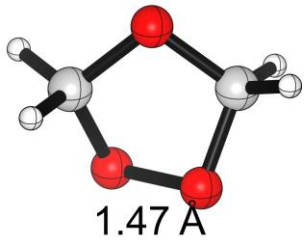
1. 1, 2, 3-trioxolane:



Total Energy = -304.0566399

C	-0.776424000	0.904040000	0.068059000
H	-1.174061000	1.180007000	1.046712000
H	-1.214728000	1.518513000	-0.716481000
C	0.773750000	0.906220000	0.068293000
H	1.210647000	1.522324000	-0.715741000
H	1.170273000	1.182750000	1.047242000
O	-1.095362000	-0.443368000	-0.241592000
O	1.096512000	-0.440150000	-0.241893000
O	0.001839000	-1.149626000	0.298504000

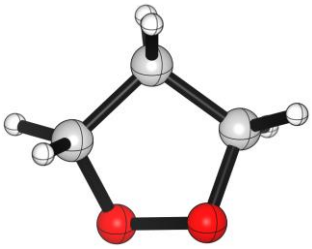
2. 1, 2, 4-trioxolane:



Total Energy = -304.1402012

C	0.000000000	1.120943000	0.319795000
H	-1.000447000	1.562178000	0.286404000
H	0.765269000	1.838725000	0.614802000
O	0.364232000	0.614078000	-0.942059000
O	-0.364232000	-0.614078000	-0.942059000
O	0.000000000	0.000000000	1.179124000
C	0.000000000	-1.120943000	0.319795000
H	-0.765269000	-1.838725000	0.614802000
H	1.000447000	-1.562178000	0.286404000

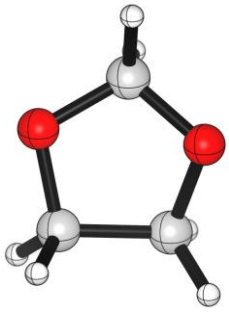
3. 1, 2-dioxolane:



Total Energy = -268.2316312

C	1.178419000	0.265118000	-0.126765000
H	1.528475000	0.189841000	-1.159775000
H	2.012814000	0.482521000	0.538983000
C	0.000407000	1.246794000	0.000002000
H	0.082847000	1.880683000	0.882114000
H	-0.081602000	1.880757000	-0.882090000
O	0.650648000	-0.986107000	0.290250000
C	-1.178276000	0.265819000	0.126768000
H	-2.012496000	0.483670000	-0.539008000
H	-1.528383000	0.190717000	1.159754000
O	-0.651267000	-0.985714000	-0.290250000

4. 1, 3-dioxolane:

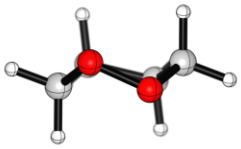


Total Energy = -268.3133747

C	0.840271000	0.849953000	0.148643000
H	0.943814000	1.130501000	1.203945000
H	1.501761000	1.463199000	-0.460015000
C	1.031863000	-0.663633000	-0.047296000
H	1.513647000	-0.898392000	-0.998278000
H	1.594710000	-1.120907000	0.769583000
O	-0.493109000	1.058117000	-0.280997000
O	-0.297295000	-1.174648000	-0.076069000
C	-1.166052000	-0.088368000	0.155149000
H	-2.076556000	-0.217280000	-0.427913000

H	-1.390639000	-0.012578000	1.230225000

5. 1, 2-dioxane:



Total Energy = -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

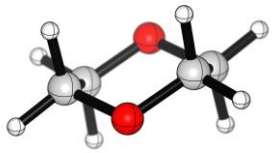
6. 1, 3-dioxane:

Total Energy = -307.6265926

C	0.621209000	-1.238390000	0.208496000
C	-1.343110000	0.001460000	0.172145000
C	0.624044000	1.236972000	0.208498000
C	1.404360000	-0.001606000	-0.220002000
H	-2.349625000	0.002660000	-0.239663000
H	0.604905000	-1.314773000	1.306542000
H	1.048426000	-2.155840000	-0.194853000
H	1.053393000	2.153439000	-0.194832000
H	0.607950000	1.313383000	1.306550000
H	1.512211000	-0.001728000	-1.307220000
H	2.400621000	-0.002755000	0.229908000
H	-1.370291000	0.001530000	1.276027000
O	-0.707802000	1.164637000	-0.274821000

O	-0.710524000	-1.162953000	-0.274840000

7. 1, 4-dioxane:



Total Energy = -307.6178304

C	0.000000000	0.759641000	-1.163886000
C	0.000000000	0.759641000	1.163886000
C	0.000000000	-0.759641000	-1.163886000
H	0.551601000	1.151197000	2.019800000
H	-1.034994000	1.126937000	-1.203910000
H	0.551601000	1.151197000	-2.019800000
H	1.034994000	-1.126937000	-1.203910000
H	-0.551601000	-1.151197000	-2.019800000
H	-1.034994000	1.126937000	1.203910000
O	-0.637891000	-1.252696000	0.000000000
O	0.637891000	1.252696000	0.000000000
C	0.000000000	-0.759641000	1.163886000
H	-0.551601000	-1.151197000	2.019800000
H	1.034994000	-1.126937000	1.203910000

8. dimethyl-peroxide PES dihedral scan:

PES relaxed scan for the COOC dihedral was performed at MP2=full/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken. Final and initial geometries are the same:

Total Energy = -228.893444

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.412605000
H	1.021515000	0.000000000	-0.391185000
H	-0.553820000	0.858245000	-0.391459000
H	-0.505521000	-0.928002000	-0.273217000
O	0.680741000	1.243568000	1.767056000
C	0.680742000	1.243561000	3.179690000
H	1.187470000	2.170871000	3.452928000
H	1.233234000	0.384367000	3.570958000
H	-0.340742000	1.244834000	3.570994000

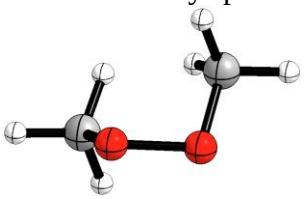
9. dimethoxy-methane PES dihedral scan:

PES relaxed scan for the COCO dihedral was performed at MP2=full/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken. Final and initial geometries are the same:

Total Energy = -268.0232567

C	-0.235153000	-0.181140000	0.123600000
O	0.919054000	0.489583000	0.586814000
H	-1.045996000	0.525095000	-0.100019000
H	-0.594355000	-0.913998000	0.858537000
H	0.047747000	-0.701227000	-0.790466000
C	0.643048000	1.184621000	1.760766000
H	0.304225000	0.488320000	2.552450000
H	-0.150620000	1.937304000	1.587648000
O	1.830472000	1.806784000	2.135381000
C	1.650322000	2.544182000	3.327210000
H	1.347905000	1.893536000	4.158732000
H	2.609886000	3.002170000	3.562896000
H	0.896442000	3.332667000	3.200074000

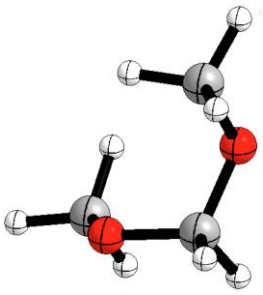
10. dimethyl-peroxide *gauche*:



Total Energy = -228.8662355

O	-0.258089000	0.682194000	-0.678724000
C	0.258089000	1.252590000	0.507065000
H	-0.131502000	0.741203000	1.392149000
H	1.351554000	1.224220000	0.508888000
H	-0.086837000	2.288122000	0.486369000
O	0.258089000	-0.682194000	-0.678724000
C	-0.258089000	-1.252590000	0.507065000
H	-1.351554000	-1.224220000	0.508888000
H	0.131502000	-0.741203000	1.392149000
H	0.086837000	-2.288122000	0.486369000

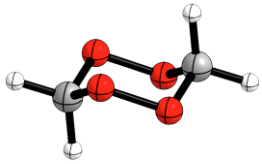
11. dimethoxy-methane *gauche,gauche*:



Total Energy = -268.0314026

O	-0.966283000	0.164666000	-0.665224000
C	-1.782875000	-0.566151000	0.240621000
H	-2.292891000	0.113051000	0.936623000
H	-1.194931000	-1.288816000	0.815076000
H	-2.524503000	-1.091379000	-0.361334000
C	1.782878000	-0.566150000	-0.240623000
H	2.293189000	0.113081000	-0.936377000
H	2.524271000	-1.091673000	0.361362000
H	1.194866000	-1.288557000	-0.815336000
C	0.000004000	0.931580000	0.000004000
H	0.461517000	1.552008000	-0.777826000
H	-0.461516000	1.551989000	0.777846000
O	0.966277000	0.164662000	0.665218000

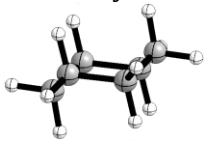
12. 1, 2, 4, 5-tetraoxane:



Total Energy = -379.2750587

C	-1.284835000	-0.000254000	-0.222050000
C	1.284794000	0.000128000	0.222115000
H	-1.248015000	-0.000410000	-1.313688000
H	-2.298197000	-0.000428000	0.177638000
H	1.247816000	-0.000012000	1.313749000
H	2.298215000	0.000326000	-0.177426000
O	0.657105000	-1.151309000	-0.280192000
O	-0.656658000	-1.151586000	0.280140000
O	-0.657218000	1.151422000	0.279871000
O	0.656825000	1.151632000	-0.279901000

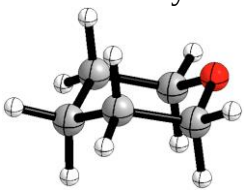
13. cyclohexane:



Total Energy = -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

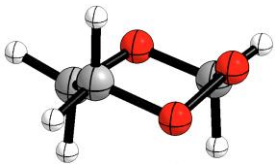
14. tetrahydro-*2H*-pyran:



Total Energy = -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

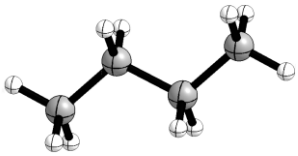
15. 1, 2, 4-trioxane:



Total Energy = -343.4482703

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

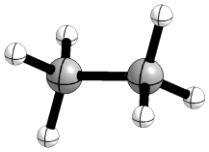
16. butane:



Total Energy = -158.4041757

C	-0.423403000	-1.905506000	0.000000000
H	-1.067734000	-1.942108000	0.882419000
C	0.423403000	1.905506000	0.000000000
H	1.067734000	1.942108000	-0.882419000
H	1.067734000	1.942108000	0.882419000
H	-0.196892000	2.804012000	0.000000000
H	-1.067734000	-1.942108000	-0.882419000
H	0.196892000	-2.804012000	0.000000000
C	-0.423403000	0.635576000	0.000000000
H	-1.080628000	0.628215000	0.876470000
H	-1.080628000	0.628215000	-0.876470000
C	0.423403000	-0.635576000	0.000000000
H	1.080628000	-0.628215000	0.876470000
H	1.080628000	-0.628215000	-0.876470000

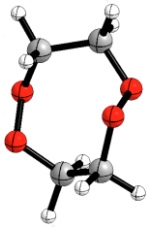
17. ethane:



Total Energy = -79.7971011

C	0.000000000	0.000000000	0.763440000
H	0.506277000	0.882722000	1.158962000
H	0.511321000	-0.879810000	1.158962000
H	-1.017598000	-0.002912000	1.158962000
C	0.000000000	0.000000000	-0.763440000
H	1.017598000	-0.002912000	-1.158962000
H	-0.511321000	-0.879810000	-1.158962000
H	-0.506277000	0.882722000	-1.158962000

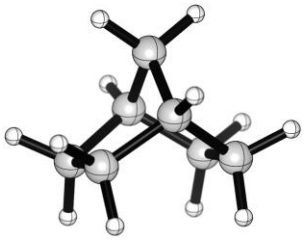
18. 1,2,5,6-tetraoxacyclooctane:



Total Energy = -457.8723064

C	-1.485045000	-0.612245000	0.463462000
C	1.642642000	0.742583000	0.211561000
C	1.484698000	-0.612598000	-0.463970000
H	-1.078314000	-0.513819000	1.469643000
H	2.169662000	0.645289000	1.163460000
H	-2.465096000	-1.094207000	0.522946000
H	2.208343000	1.412428000	-0.447522000
H	2.464354000	-1.095231000	-0.524424000
H	1.077239000	-0.513459000	-1.469784000
C	-1.642124000	0.743395000	-0.211594000
H	-2.207458000	1.412973000	0.448092000
H	-2.169503000	0.646859000	-1.163385000
O	-0.412582000	1.337180000	-0.581549000
O	0.413128000	1.336112000	0.581884000
O	0.653516000	-1.490642000	0.280076000
O	-0.654092000	-1.491104000	-0.279885000

19. norborane:

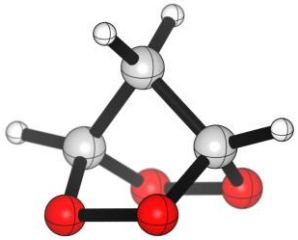


Total Energy = -273.9055542

C	-1.247709000	-0.779558000	-0.492466000
C	-0.000077000	-1.129588000	0.341067000
C	0.000076000	1.129588000	0.341067000

C	-1.247569000	0.779709000	-0.492521000
H	-1.192938000	-1.200338000	-1.498824000
H	-2.151801000	-1.170473000	-0.020215000
H	-1.192649000	1.200404000	-1.498907000
H	-2.151628000	1.170819000	-0.020372000
C	0.000000000	0.000000000	1.384566000
H	0.892077000	-0.000057000	2.016525000
H	-0.892076000	0.000057000	2.016526000
C	1.247569000	-0.779709000	-0.492522000
H	2.151628000	-1.170819000	-0.020372000
H	1.192649000	-1.200405000	-1.498908000
C	1.247709000	0.779559000	-0.492466000
H	2.151801000	1.170473000	-0.020216000
H	1.192938000	1.200339000	-1.498824000
H	-0.000128000	-2.147273000	0.731616000
H	0.000129000	2.147274000	0.731615000

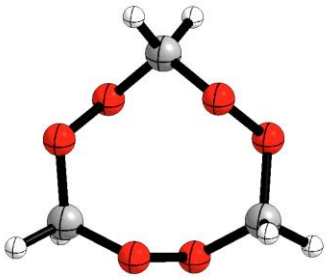
20. (1s,4s)-2,3,5,6-tetraoxabicyclo[2.2.1]heptane:



Total Energy = -417.3695135

C	0.000999000	-1.046611000	0.251701000
C	-0.000926000	1.046613000	0.251700000
C	0.000046000	0.000002000	1.352005000
H	0.909382000	0.000821000	1.945802000
H	-0.909272000	-0.000817000	1.945826000
H	0.001790000	-2.109712000	0.475800000
H	-0.001686000	2.109714000	0.475796000
O	-1.147610000	-0.732041000	-0.499259000
O	-1.148714000	0.730361000	-0.499155000
O	1.148655000	-0.730367000	-0.499217000
O	1.147553000	0.732044000	-0.499326000

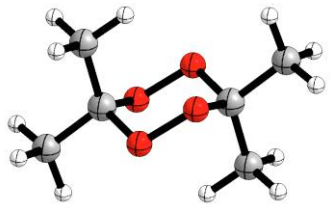
21. 1,2,4,5,7,8-hexaoxonane:



Total Energy = -568.9317805

C	0.008031000	1.865729000	0.000384000
C	-1.661382000	-0.928846000	-0.003054000
C	1.652797000	-0.942764000	0.003121000
H	0.501748000	2.470237000	-0.763522000
H	-1.743678000	-1.136313000	-1.071501000
H	-0.482193000	2.471967000	0.765214000
H	-2.488250000	-1.351881000	0.569438000
H	2.475643000	-1.373854000	-0.569160000
H	1.733465000	-1.150159000	1.071745000
O	-0.917025000	1.105921000	-0.715045000
O	-1.748566000	0.445025000	0.237532000
O	-0.509789000	-1.531168000	0.509544000
O	0.496184000	-1.536169000	-0.508679000
O	1.751457000	0.430183000	-0.238719000
O	0.928563000	1.099369000	0.714752000

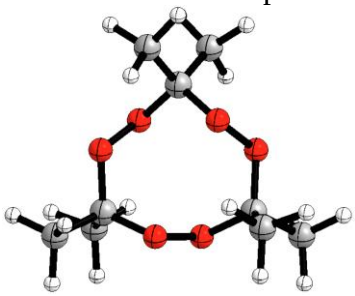
22. diacetone-diperoxide (DADP):



Total Energy = -536.523878

C	-1.357713000	0.036874000	0.000001000
C	1.357695000	-0.036868000	-0.000015000
O	0.616714000	0.357173000	-1.149508000
O	-0.616756000	-0.357198000	-1.149502000
O	-0.616771000	-0.357204000	1.149510000
O	0.616733000	0.357108000	1.149526000
C	-1.668381000	1.521790000	0.000005000
H	-2.249939000	1.764403000	-0.890162000
H	-2.249797000	1.764426000	0.890258000
H	-0.756550000	2.113662000	-0.000079000
C	-2.584356000	-0.848123000	-0.000008000
H	-3.178658000	-0.639448000	0.889678000
H	-3.178662000	-0.639429000	-0.889688000
H	-2.284647000	-1.896084000	-0.000018000
C	2.584289000	0.848201000	0.000011000
H	3.178497000	0.639644000	0.889786000
H	3.178705000	0.639437000	-0.889580000
H	2.284535000	1.896148000	-0.000143000
C	1.668525000	-1.521774000	-0.000031000
H	2.250177000	-1.764278000	0.890104000
H	0.756745000	-2.113735000	0.000172000
H	2.249895000	-1.764390000	-0.890312000

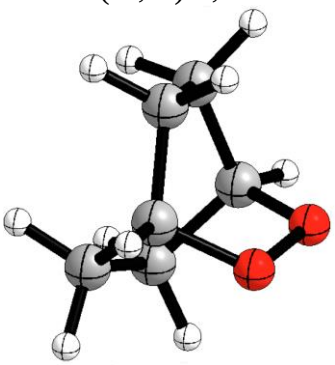
23. triacetone-triperoxide (TATP):



Total Energy = -804.7952355

C	0.000000000	0.000000000	1.919611000
C	0.000000000	1.710608000	-0.954297000
C	0.000000000	-1.710608000	-0.954297000
O	0.714197000	0.919866000	1.117097000
O	-0.218001000	1.761544000	0.446052000
O	-0.499722000	0.509094000	-1.512812000
O	0.499722000	-0.509094000	-1.512812000
O	0.218001000	-1.761544000	0.446052000
O	-0.714197000	-0.919866000	1.117097000
C	0.949357000	-2.773101000	-1.487529000
H	0.711115000	-3.733795000	-1.032430000
H	0.840636000	-2.840718000	-2.569340000
H	1.978138000	-2.504779000	-1.244888000
C	-1.451727000	-1.968746000	-1.313490000
H	-2.102918000	-1.233925000	-0.848742000
H	-1.568772000	-1.916719000	-2.396547000
H	-1.724080000	-2.965648000	-0.965203000
C	1.451727000	1.968746000	-1.313490000
H	1.568772000	1.916719000	-2.396547000
H	1.724080000	2.965648000	-0.965203000
H	2.102918000	1.233925000	-0.848742000
C	-0.949357000	2.773101000	-1.487529000
H	-0.711115000	3.733795000	-1.032430000
H	-0.840636000	2.840718000	-2.569340000
H	-1.978138000	2.504779000	-1.244888000
C	-1.079102000	0.666087000	2.757001000
H	-1.461252000	-0.046337000	3.488169000
H	-0.644385000	1.522059000	3.273924000
H	-1.895022000	1.008224000	2.123415000
C	1.079102000	-0.666087000	2.757001000
H	1.895022000	-1.008224000	2.123415000
H	1.461252000	0.046337000	3.488169000
H	0.644385000	-1.522059000	3.273924000

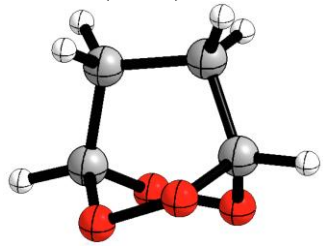
24. (1s,4s)-2,3-dioxabicyclo[2.2.2]octane:



Total Energy = -384.9455798

C	0.179411000	-1.228032000	0.055266000
C	-0.179454000	1.228032000	0.055292000
H	-0.336558000	2.295518000	0.216754000
H	0.336442000	-2.295533000	0.216720000
O	0.268945000	-0.671372000	1.372733000
O	-0.269106000	0.671325000	1.372754000
C	-1.278442000	0.587825000	-0.795573000
H	-1.108488000	0.819605000	-1.851101000
H	-2.256347000	0.982943000	-0.518558000
C	-1.200514000	-0.931652000	-0.525961000
H	-1.356331000	-1.513770000	-1.436292000
H	-1.953580000	-1.234050000	0.203568000
C	1.200565000	0.931696000	-0.525820000
H	1.953567000	1.234119000	0.203753000
H	1.356414000	1.513822000	-1.436132000
C	1.278581000	-0.587830000	-0.795442000
H	2.256422000	-0.982910000	-0.518183000
H	1.108858000	-0.819602000	-1.850994000

25. (1s,4s)-2,3,5,6-tetraoxabicyclo[2.2.2]octane:

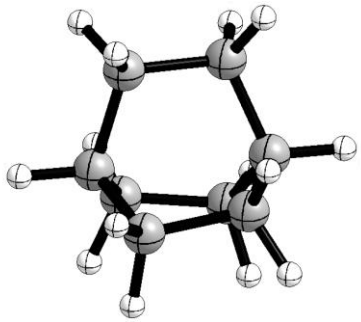


Total Energy = -456.6751607

C	1.193586000	-0.065990000	0.041493000
C	-1.193799000	-0.062396000	-0.041499000
H	-2.269347000	-0.223777000	-0.107279000
H	2.268631000	-0.230725000	0.107281000
O	0.647325000	-0.566478000	1.261180000
O	-0.746917000	-0.858413000	1.021698000

O	0.744288000	-0.860698000	-1.021649000
O	-0.649081000	-0.564633000	-1.261144000
C	-0.757572000	1.383503000	0.129922000
H	-0.997037000	1.706608000	1.143755000
H	-1.289730000	2.015944000	-0.579712000
C	0.761846000	1.381233000	-0.130005000
H	1.295867000	2.012073000	0.579653000
H	1.002336000	1.703548000	-1.143845000

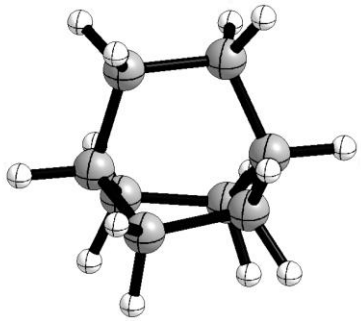
26. bicyclo[2.2.2]octane:



Total Energy = -313.2180474

C	1.295712000	-0.001881000	0.008136000
C	-1.295742000	0.002497000	-0.008075000
H	-2.388511000	0.004431000	-0.015136000
H	2.388473000	-0.003604000	0.015165000
C	-0.763004000	1.441257000	0.066956000
H	-0.994864000	1.860619000	1.051183000
H	-1.264355000	2.070612000	-0.672897000
C	0.768507000	1.429761000	-0.171776000
H	1.271657000	2.109752000	0.520518000
H	1.002028000	1.775342000	-1.183876000
C	-0.774177000	-0.780562000	1.206509000
H	-1.003016000	-1.843010000	1.075539000
H	-1.285240000	-0.454862000	2.116232000
C	0.755767000	-0.564461000	1.331676000
H	1.259169000	-1.502812000	1.578453000
H	0.978904000	0.138805000	2.140310000
C	0.771283000	-0.868913000	-1.146477000
H	0.996549000	-1.919811000	-0.939027000
H	1.282837000	-0.611606000	-2.077539000
C	-0.758201000	-0.657502000	-1.286967000
H	-1.264588000	-1.609948000	-1.463708000
H	-0.979908000	-0.015082000	-2.145104000

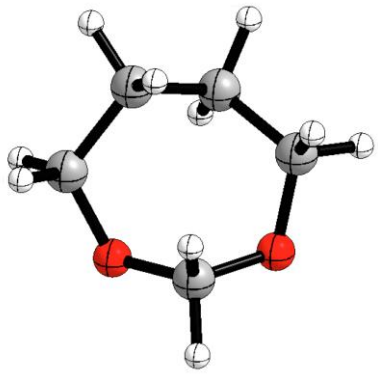
27. bicyclo[2.2.2]octane:



Total Energy = -313.2180474

C	1.295712000	-0.001881000	0.008136000
C	-1.295742000	0.002497000	-0.008075000
H	-2.388511000	0.004431000	-0.015136000
H	2.388473000	-0.003604000	0.015165000
C	-0.763004000	1.441257000	0.066956000
H	-0.994864000	1.860619000	1.051183000
H	-1.264355000	2.070612000	-0.672897000
C	0.768507000	1.429761000	-0.171776000
H	1.271657000	2.109752000	0.520518000
H	1.002028000	1.775342000	-1.183876000
C	-0.774177000	-0.780562000	1.206509000
H	-1.003016000	-1.843010000	1.075539000
H	-1.285240000	-0.454862000	2.116232000
C	0.755767000	-0.564461000	1.331676000
H	1.259169000	-1.502812000	1.578453000
H	0.978904000	0.138805000	2.140310000
C	0.771283000	-0.868913000	-1.146477000
H	0.996549000	-1.919811000	-0.939027000
H	1.282837000	-0.611606000	-2.077539000
C	-0.758201000	-0.657502000	-1.286967000
H	-1.264588000	-1.609948000	-1.463708000
H	-0.979908000	-0.015082000	-2.145104000

28. 1,3-dioxepane:

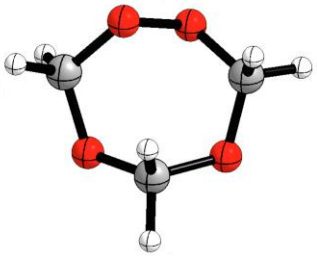


Total Energy = -346.925912

C	1.504294000	0.644312000	0.119773000

C	-1.689502000	-0.110945000	-0.043760000
C	0.308754000	-1.398583000	0.329279000
H	1.608794000	0.793227000	1.205646000
H	-2.300805000	0.094062000	-0.924534000
H	2.423026000	0.988787000	-0.356637000
H	-2.357631000	-0.462502000	0.752554000
H	0.529320000	-2.462037000	0.252821000
H	0.126491000	-1.123499000	1.380614000
O	1.439570000	-0.740684000	-0.160081000
O	-0.828798000	-1.165195000	-0.447961000
C	0.310793000	1.453395000	-0.383795000
H	0.163873000	1.258873000	-1.450240000
H	0.569565000	2.510887000	-0.274959000
C	-0.973430000	1.167401000	0.399741000
H	-0.732726000	1.123016000	1.467144000
H	-1.681534000	1.992743000	0.284502000

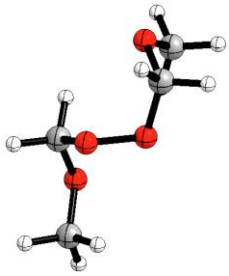
29. 1,2,4,6-tetraoxepane:



Total Energy = -418.668966

C	-1.489649000	-0.461660000	0.077856000
C	1.564892000	-0.308300000	-0.090507000
C	-0.058860000	1.393052000	0.333926000
H	-1.602504000	-0.619278000	1.156750000
H	1.932084000	-0.724039000	-1.029994000
H	-2.382983000	-0.756768000	-0.470116000
H	2.356874000	-0.262462000	0.664496000
H	-0.110365000	2.471256000	0.211494000
H	0.021549000	1.119058000	1.393768000
O	-0.473885000	-1.317348000	-0.391367000
O	0.621262000	-1.152752000	0.507080000
O	-1.250090000	0.878977000	-0.210379000
O	1.063594000	0.970333000	-0.387090000

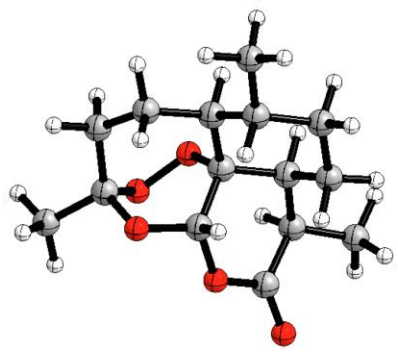
30. methoxy((methoxymethyl)peroxy)methane *gauche,gauche*:



Total Energy = -459.1607853

C	-1.000901000	0.188797000	0.924341000
O	-0.525153000	-1.062194000	0.467044000
H	-0.174705000	0.826537000	1.236599000
H	-1.623688000	-0.108354000	1.779466000
O	0.312848000	-0.855236000	-0.664180000
C	1.650137000	-0.963051000	-0.244532000
H	2.196986000	-1.071348000	-1.190328000
H	1.773373000	-1.835934000	0.396721000
O	-1.719420000	0.887096000	-0.025808000
O	2.089047000	0.137716000	0.477318000
C	-2.831164000	0.171684000	-0.534379000
H	-3.479515000	-0.168484000	0.282309000
H	-3.382950000	0.860126000	-1.171293000
H	-2.505616000	-0.692392000	-1.117884000
C	2.109533000	1.333944000	-0.284708000
H	1.105288000	1.601985000	-0.627319000
H	2.497568000	2.115192000	0.366078000
H	2.769050000	1.225363000	-1.153666000

31. artemisin:

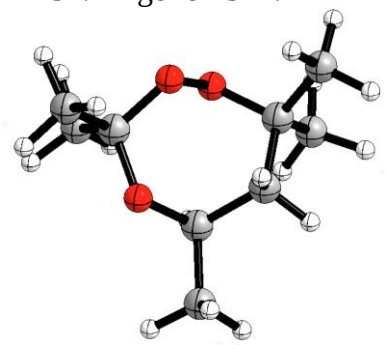


Total Energy = -960.7803291

C	0.072630000	-0.550194000	-0.953831000
H	0.026520000	0.169139000	-1.774326000
C	1.877225000	-1.679050000	0.074643000
C	2.858775000	-0.584701000	0.531571000
H	3.850246000	-0.845798000	0.153640000
H	2.904623000	-0.613751000	1.622695000

C	2.509075000	0.817579000	0.020348000
H	2.616798000	0.819150000	-1.069431000
H	3.253719000	1.516264000	0.407845000
C	1.106253000	1.339761000	0.376912000
H	1.119128000	1.691026000	1.417997000
C	0.050643000	0.215073000	0.375292000
C	-1.357248000	0.732382000	0.673390000
H	-1.321579000	1.140259000	1.691994000
C	-1.743240000	1.870820000	-0.273004000
H	-1.825797000	1.501017000	-1.303805000
H	-2.732367000	2.245326000	-0.000723000
C	-0.718852000	3.001252000	-0.194341000
H	-0.732151000	3.424699000	0.818710000
H	-0.995388000	3.810381000	-0.876214000
C	0.703132000	2.532874000	-0.511614000
H	0.725404000	2.202677000	-1.559321000
C	-2.329576000	-0.452073000	0.685335000
H	-1.978566000	-1.129576000	1.473127000
C	-2.243128000	-1.290342000	-0.576387000
C	2.519236000	-3.024568000	-0.166218000
H	3.116745000	-3.311724000	0.699880000
H	3.159502000	-2.955301000	-1.046035000
H	1.744405000	-3.769588000	-0.346647000
C	1.690052000	3.691931000	-0.368152000
H	1.349940000	4.556533000	-0.942818000
H	2.687522000	3.429029000	-0.723070000
H	1.770062000	3.996308000	0.680469000
C	-3.775706000	-0.065473000	0.974664000
H	-4.216611000	0.483713000	0.141099000
H	-3.823705000	0.556838000	1.871666000
H	-4.381033000	-0.957015000	1.131948000
O	-1.022943000	-1.442482000	-1.149418000
O	1.240035000	-1.280855000	-1.139501000
O	0.873612000	-1.907890000	1.039402000
O	0.377691000	-0.650582000	1.483102000
O	-3.172525000	-1.879594000	-1.043627000

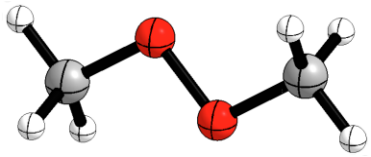
32. Trigonox 311:



Total Energy = -579.3033909

C	-1.541740000	-0.533346000	0.021229000
C	1.661624000	-0.346504000	-0.034564000
C	-0.155577000	1.472456000	0.131917000
H	-0.031330000	1.311618000	1.210024000
O	-0.420873000	-1.333557000	-0.352212000
O	0.629118000	-1.131266000	0.585359000
C	1.067055000	0.942594000	-0.623091000
H	0.758988000	0.779479000	-1.659935000
H	1.853120000	1.704317000	-0.633502000
O	-1.343356000	0.819981000	-0.316781000
C	-2.651888000	-1.028756000	-0.887649000
H	-2.892512000	-2.066700000	-0.658031000
H	-3.534088000	-0.405814000	-0.740420000
H	-2.330789000	-0.948576000	-1.926454000
C	-1.881727000	-0.709784000	1.495273000
H	-2.813806000	-0.182905000	1.704039000
H	-2.010308000	-1.770644000	1.714373000
H	-1.097922000	-0.322095000	2.142712000
C	2.361236000	-1.171097000	-1.106375000
H	3.121373000	-0.569055000	-1.610790000
H	2.841544000	-2.044835000	-0.661252000
H	1.634030000	-1.506751000	-1.847271000
C	2.591992000	-0.048719000	1.135647000
H	2.876320000	-0.976940000	1.634546000
H	3.495842000	0.442789000	0.770531000
H	2.107544000	0.603508000	1.865876000
C	-0.380947000	2.950318000	-0.135401000
H	-1.292541000	3.287851000	0.358843000
H	0.461655000	3.538724000	0.233165000
H	-0.486415000	3.121794000	-1.209294000

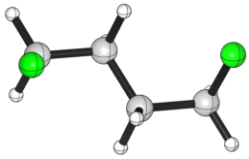
33. Dimethyl peroxide *anti*:



Total Energy = -230.1245089

C	0.691699000	1.593110000	0.000403000
H	0.198653000	1.980342000	-0.895088000
C	-0.691699000	-1.593110000	0.000403000
H	-0.198795000	-1.979135000	0.896492000
H	-0.198653000	-1.980342000	-0.895088000
O	0.691699000	0.185407000	-0.000539000
O	-0.691699000	-0.185407000	-0.000539000
H	-1.744155000	-1.876950000	0.000493000
H	0.198795000	1.979135000	0.896492000
H	1.744155000	1.876950000	0.000493000

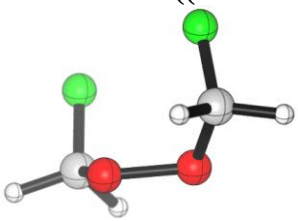
34. 1,4-difluorobutane (*gauche,gauche*):



Total Energy = -356.883619

C	-1.910267000	0.376674000	0.313527000
H	-2.191521000	1.232705000	-0.306791000
H	-2.518583000	0.372478000	1.220204000
C	1.910385000	0.377162000	-0.312867000
H	2.191860000	1.231977000	0.309037000
H	2.518721000	0.374423000	-1.219544000
F	2.228397000	-0.771813000	0.404132000
F	-2.228704000	-0.770934000	-0.405472000
C	-0.431191000	0.381927000	0.630364000
H	-0.214630000	1.269525000	1.236054000
H	-0.190346000	-0.493308000	1.239081000
C	0.431364000	0.383378000	-0.629715000
H	0.215076000	1.272461000	-1.233332000
H	0.190443000	-0.490382000	-1.240504000

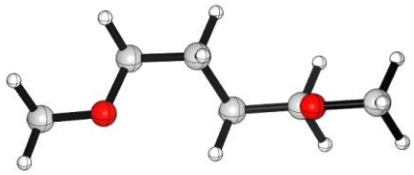
35. fluoro((fluoromethyl)peroxy)methane (*gauche,gauche*):



Total Energy = -428.6223534

C	1.643303000	-0.288067000	0.027055000
O	0.498389000	-0.837957000	-0.513304000
H	2.434075000	-0.543333000	-0.679647000
H	1.824256000	-0.677228000	1.030082000
O	-0.498448000	-0.837987000	0.513276000
C	-1.643334000	-0.288014000	-0.027038000
H	-2.434089000	-0.543205000	0.679707000
H	-1.824354000	-0.677176000	-1.030054000
F	-1.547178000	1.072519000	-0.111684000
F	1.547264000	1.072479000	0.111687000

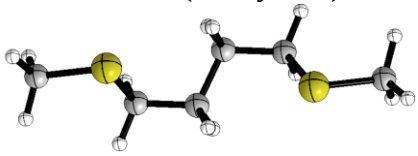
36. 1,4-dimethoxybutane:



Total Energy = -387.4162228

C	-1.852670000	0.582585000	0.575013000
H	-2.170441000	1.490247000	0.036703000
H	-2.310265000	0.611269000	1.574881000
C	1.852671000	0.582593000	-0.575006000
H	2.170449000	1.490248000	-0.036687000
H	2.310265000	0.611284000	-1.574875000
C	-0.340940000	0.534393000	0.682640000
H	-0.009407000	1.402798000	1.263881000
H	-0.046482000	-0.359367000	1.237495000
C	0.340942000	0.534410000	-0.682630000
H	0.009413000	1.402833000	-1.263847000
H	0.046477000	-0.359334000	-1.237510000
O	2.298362000	-0.559714000	0.121862000
O	-2.298364000	-0.559713000	-0.121868000
C	-3.695337000	-0.590711000	-0.261942000
H	-3.951548000	-1.495104000	-0.812408000
H	-4.192648000	-0.613353000	0.716836000
H	-4.058094000	0.283526000	-0.818743000
C	3.695335000	-0.590716000	0.261932000
H	3.951546000	-1.495110000	0.812397000
H	4.192643000	-0.613359000	-0.716847000
H	4.058097000	0.283519000	0.818733000

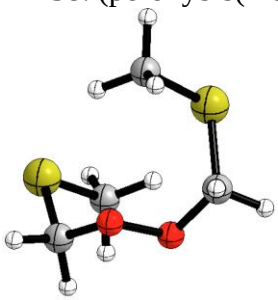
37. 1,4-bis(methylthio)butane:



Total Energy = -1033.3739718

C	-1.851737000	0.767980000	0.621573000
H	-2.134907000	1.682338000	0.091053000
H	-2.272431000	0.808300000	1.629044000
C	1.851735000	0.767984000	-0.621572000
H	2.134906000	1.682337000	-0.091044000
H	2.272431000	0.808310000	-1.629041000
C	-0.333127000	0.642481000	0.688137000
H	0.053221000	1.485812000	1.271972000
H	-0.065555000	-0.264600000	1.237433000
C	0.333126000	0.642484000	-0.688137000
H	-0.053223000	1.485817000	-1.271968000
H	0.065555000	-0.264594000	-1.237437000
C	-4.330454000	-0.209555000	-0.057055000
H	-4.919530000	-0.983588000	-0.547226000
H	-4.608093000	-0.166740000	0.996941000
H	-4.537059000	0.748667000	-0.535328000
C	4.330454000	-0.209552000	0.057060000
H	4.919531000	-0.983583000	0.547234000
H	4.608100000	-0.166733000	-0.996933000
H	4.537052000	0.748671000	0.535337000
S	-2.585102000	-0.657227000	-0.246162000
S	2.585103000	-0.657232000	0.246157000

38. (peroxybis(methylene))bis(methylsulfane):

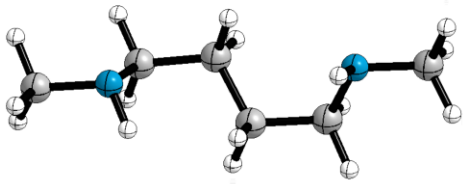


Total Energy = -1105.1058928

C	1.568879000	1.014050000	0.678800000
C	-1.568796000	1.014039000	-0.678871000
H	2.109491000	1.601401000	-0.068132000
H	1.918817000	1.270690000	1.679185000
H	-1.918725000	1.270613000	-1.679276000
H	-2.109434000	1.601417000	0.068026000
O	0.212778000	1.385179000	0.682556000
O	-0.212715000	1.385209000	-0.682634000
C	1.810671000	-0.885679000	-1.364895000
H	2.354219000	-0.064070000	-1.831913000
H	2.291045000	-1.826502000	-1.631641000
H	0.773790000	-0.891082000	-1.692163000

C	-1.810997000	-0.885489000	1.364972000
H	-2.355061000	-0.064085000	1.831748000
H	-2.291002000	-1.826514000	1.631679000
H	-0.774207000	-0.890387000	1.692536000
S	-1.911304000	-0.746447000	-0.443424000
S	1.911431000	-0.746434000	0.443458000

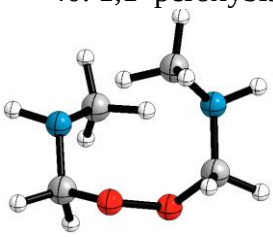
39. N^1,N^4-dimethylbutane-1,4-diamine:



Total Energy = -347.68027

C	1.862659000	0.653303000	-0.483908000
H	2.136940000	1.529733000	0.131591000
H	2.295077000	0.819733000	-1.475965000
C	-1.867344000	0.478449000	0.656215000
H	-2.125573000	1.480453000	0.292772000
H	-2.304681000	0.383923000	1.665077000
C	0.346234000	0.565561000	-0.602752000
H	-0.025840000	1.497188000	-1.043393000
H	0.080595000	-0.239722000	-1.290342000
C	-0.350790000	0.346110000	0.740173000
H	0.023070000	1.070686000	1.473617000
H	-0.110024000	-0.650641000	1.130544000
C	3.893518000	-0.522073000	0.107720000
H	4.278987000	-1.437549000	0.558964000
H	4.297604000	-0.454257000	-0.905457000
H	4.273761000	0.339158000	0.679589000
C	-3.884668000	-0.434014000	-0.324368000
H	-4.261493000	-1.207816000	-0.994588000
H	-4.363024000	-0.557098000	0.660202000
H	-4.194586000	0.533883000	-0.726796000
N	2.441050000	-0.578215000	0.039251000
H	2.069779000	-0.759393000	0.965036000
N	-2.432548000	-0.486401000	-0.276383000
H	-2.127768000	-1.419981000	-0.019404000

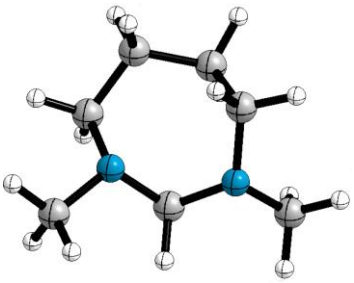
40. 1,1'-peroxybis(*N*-methylmethanamine):



Total Energy = -419.4179282

C	1.620404000	-0.773331000	-0.486909000
C	-1.620727000	-0.773098000	0.486943000
H	2.049341000	-1.271892000	0.394075000
H	2.128270000	-1.119395000	-1.389307000
H	-2.128596000	-1.118869000	1.389463000
H	-2.050030000	-1.271551000	-0.393910000
O	0.303555000	-1.264344000	-0.649348000
O	-0.303988000	-1.264817000	0.649113000
C	1.662864000	1.228639000	0.932326000
H	2.419119000	0.791434000	1.600191000
H	1.836663000	2.303593000	0.865687000
H	0.674568000	1.070552000	1.362849000
C	-1.662610000	1.229028000	-0.932240000
H	-2.418997000	0.791981000	-1.600057000
H	-1.836394000	2.303967000	-0.865350000
H	-0.674390000	1.071042000	-1.362994000
N	1.695048000	0.657362000	-0.410385000
H	2.475780000	1.004986000	-0.949048000
N	-1.694650000	0.657497000	0.410319000
H	-2.474241000	1.006006000	0.950012000

41. 1,3-dimethyl-1,3-diazepane:

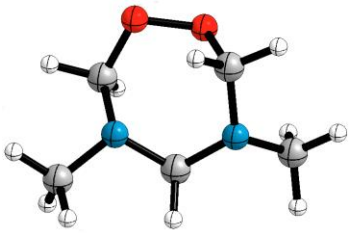


Total Energy = -385.7735739

C	1.545913000	0.776929000	0.449398000
C	-1.322715000	0.622851000	-0.824948000
C	0.011768000	-1.092018000	0.320680000
H	1.526136000	0.623220000	1.543690000
H	-0.739862000	0.734866000	-1.743518000
H	2.575705000	1.029706000	0.184586000
H	-2.369795000	0.791098000	-1.087767000
H	0.127390000	-2.179129000	0.280869000
H	-0.078438000	-0.822710000	1.396535000
N	-1.222591000	-0.769055000	-0.388512000
N	1.193537000	-0.463000000	-0.242784000
C	-2.356193000	-1.194021000	0.411588000
H	-2.252451000	-2.255074000	0.654462000
H	-2.451024000	-0.641848000	1.363806000
H	-3.279601000	-1.068269000	-0.155873000

C	2.321412000	-1.382753000	-0.288447000
H	2.652128000	-1.704531000	0.714014000
H	2.049360000	-2.267924000	-0.864814000
H	3.164519000	-0.901878000	-0.787110000
C	-0.852310000	1.685468000	0.184192000
H	-1.121920000	1.388571000	1.205003000
H	-1.384875000	2.619790000	-0.014533000
C	0.650478000	1.955544000	0.076978000
H	0.925929000	2.804814000	0.710278000
H	0.870057000	2.241681000	-0.957193000

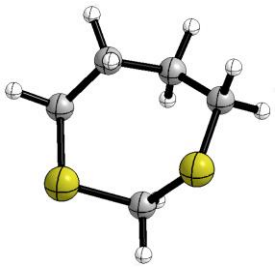
42. 4,6-dimethyl-1,2,4,6-dioxadiazepane:



Total Energy = -457.5126286

C	1.307316000	0.837016000	0.535555000
C	-1.243652000	0.637594000	-0.798521000
C	0.064949000	-1.201775000	0.158125000
H	1.045249000	0.672779000	1.593055000
H	-0.591775000	0.814561000	-1.652133000
H	2.324997000	1.222941000	0.458195000
H	-2.274540000	0.899843000	-1.042067000
H	0.235958000	-2.226227000	-0.183805000
H	-0.011738000	-1.230960000	1.265197000
O	0.518896000	1.886876000	0.032269000
O	-0.851027000	1.562537000	0.229811000
N	-1.207139000	-0.734635000	-0.400575000
N	1.197498000	-0.386811000	-0.239216000
C	-2.316428000	-1.138642000	0.450725000
H	-2.288080000	-2.221664000	0.592148000
H	-2.287384000	-0.660306000	1.441194000
H	-3.260648000	-0.890582000	-0.035726000
C	2.441035000	-1.147877000	-0.232383000
H	2.708061000	-1.530391000	0.766117000
H	2.349516000	-1.996078000	-0.911336000
H	3.255601000	-0.516985000	-0.589949000

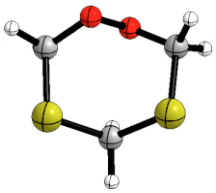
43. 1,3-dithiepane:



Total Energy = -992.8700383

C	1.596437000	1.061373000	0.037462000
C	-1.940651000	0.527887000	0.095058000
C	0.168730000	-1.305651000	0.642486000
H	1.762457000	1.352748000	1.078179000
H	-2.485186000	0.864559000	-0.789854000
H	2.453134000	1.416960000	-0.538810000
H	-2.662374000	0.420470000	0.906435000
H	0.298777000	-2.377763000	0.788994000
H	0.021203000	-0.858672000	1.626107000
C	0.307226000	1.701796000	-0.483821000
H	0.059037000	1.289748000	-1.465877000
H	0.518309000	2.765262000	-0.628225000
C	-0.883171000	1.560188000	0.480808000
H	-0.511933000	1.342702000	1.486743000
H	-1.404810000	2.518321000	0.565978000
S	1.728578000	-0.746516000	-0.103227000
S	-1.324831000	-1.128977000	-0.375625000

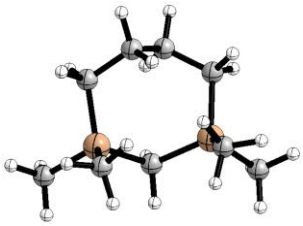
44. 1,2,4,6-dioxadithiepane:



Total Energy = -1064.5974598

C	1.531934000	0.999378000	0.032988000
C	-1.733510000	0.771459000	0.043135000
C	0.072513000	-1.275035000	0.655642000
H	1.635769000	1.288684000	1.079958000
H	-2.109267000	1.231336000	-0.872491000
H	2.349993000	1.415208000	-0.555599000
H	-2.466397000	0.861825000	0.845354000
H	0.132596000	-2.351174000	0.812232000
H	-0.015158000	-0.789553000	1.627189000
O	0.355912000	1.575275000	-0.485158000
O	-0.626141000	1.460673000	0.542409000
S	1.636246000	-0.803740000	-0.151594000
S	-1.423204000	-1.003680000	-0.334984000

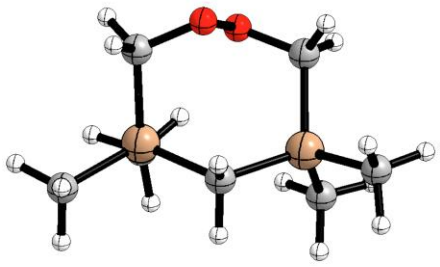
45. 1,1,3,3-tetramethyl-1,3-disilepane:



Total Energy = -935.16304

C	-1.761968000	1.472692000	0.138095000
C	1.881053000	1.452480000	-0.171434000
C	-0.001319000	-0.888186000	-0.921969000
H	-2.079202000	1.962595000	-0.789897000
H	2.352959000	1.784156000	0.761535000
H	-2.580443000	1.627355000	0.852009000
H	2.612778000	1.650680000	-0.963073000
H	-0.015223000	-1.981062000	-1.030272000
H	0.028426000	-0.487965000	-1.943908000
C	-0.480439000	2.152874000	0.652156000
H	-0.083687000	1.600560000	1.513553000
H	-0.732047000	3.145329000	1.035997000
C	0.616863000	2.288307000	-0.429501000
H	0.194111000	2.005557000	-1.400026000
H	0.900237000	3.340305000	-0.526280000
Si	-1.639699000	-0.394550000	-0.136596000
Si	1.618520000	-0.425441000	-0.081166000
C	-3.052861000	-0.935668000	-1.256938000
H	-3.067059000	-2.022195000	-1.377290000
H	-4.019397000	-0.631646000	-0.845441000
H	-2.956842000	-0.490729000	-2.251053000
C	-1.837296000	-1.255916000	1.527898000
H	-2.868190000	-1.159726000	1.880097000
H	-1.609320000	-2.322834000	1.452298000
H	-1.183891000	-0.831219000	2.292831000
C	1.658477000	-1.003620000	1.714165000
H	1.055384000	-0.369968000	2.368075000
H	1.297019000	-2.030683000	1.814527000
H	2.687076000	-0.973436000	2.085417000
C	3.037672000	-1.277904000	-0.981434000
H	3.037350000	-1.023677000	-2.044874000
H	4.003060000	-0.976413000	-0.565045000
H	2.962321000	-2.365452000	-0.896746000

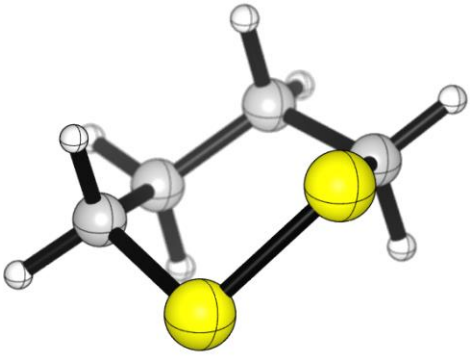
46. 4,4,6,6-tetramethyl-1,2,4,6-dioxadisilepane:



Total Energy = -1006.8850332

C	-1.506590000	1.446642000	0.488593000
C	1.761641000	1.469444000	-0.341137000
C	-0.021217000	-0.877745000	-0.959986000
H	-1.904881000	2.180168000	-0.221201000
H	2.390049000	1.949169000	0.420144000
H	-2.068644000	1.564694000	1.421472000
H	2.203250000	1.688990000	-1.318949000
H	-0.055128000	-1.965882000	-1.095222000
H	0.020005000	-0.439438000	-1.964710000
O	-0.171519000	1.827192000	0.837834000
O	0.492420000	2.117794000	-0.395874000
Si	-1.631990000	-0.355651000	-0.146090000
Si	1.584733000	-0.417025000	-0.097942000
C	3.048744000	-1.252480000	-0.935143000
H	3.996944000	-0.890427000	-0.527678000
H	3.017274000	-2.334736000	-0.783759000
H	3.050676000	-1.064743000	-2.011809000
C	1.593233000	-0.859245000	1.727084000
H	1.348185000	-1.912558000	1.889305000
H	2.584397000	-0.680297000	2.153454000
H	0.877520000	-0.243085000	2.274898000
C	-3.062794000	-0.451970000	-1.361416000
H	-3.216594000	-1.478425000	-1.704151000
H	-3.996223000	-0.110586000	-0.905173000
H	-2.871101000	0.170267000	-2.239416000
C	-1.991146000	-1.479280000	1.319139000
H	-2.961145000	-1.238653000	1.762978000
H	-2.019185000	-2.527685000	1.009223000
H	-1.232240000	-1.381403000	2.098566000

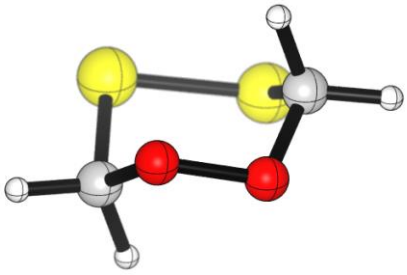
47. 1,2-dithiane:



Total Energy = -953.5815096

C	-1.271647000	0.910805000	0.458065000
C	1.271647000	-0.910805000	0.458065000
H	-1.773384000	1.877706000	0.539111000
H	2.032130000	-0.130642000	0.377389000
H	1.773384000	-1.877706000	0.539111000
H	-2.032130000	0.130642000	0.377389000
S	0.356982000	-0.977664000	-1.117648000
S	-0.356982000	0.977664000	-1.117648000
C	-0.356982000	0.678124000	1.658419000
H	-0.960598000	0.751746000	2.568723000
H	0.384510000	1.482693000	1.698238000
C	0.356982000	-0.678124000	1.658419000
H	0.960598000	-0.751746000	2.568723000
H	-0.384510000	-1.482693000	1.698238000

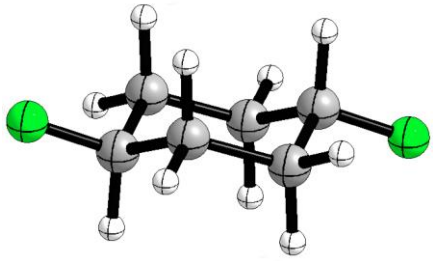
48. 1,2,4,5-dioxadithiane:



Total Energy = -1025.2992221

C	0.556924000	1.375497000	0.421883000
C	0.556937000	-1.375490000	-0.421883000
H	0.761491000	2.429361000	0.232556000
H	0.562928000	-1.149959000	-1.489203000
H	0.761515000	-2.429353000	-0.232555000
H	0.562917000	1.149964000	1.489203000
O	1.588443000	-0.673812000	0.227720000
O	1.588435000	0.673829000	-0.227721000
S	-1.085838000	-1.006838000	0.281311000
S	-1.085852000	1.006826000	-0.281311000

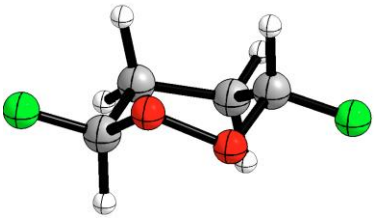
49. (1r,4r)-1,4-difluorocyclohexane (*both F equatorial*):



Total Energy = -434.3089678

C	-0.743430000	-1.257163000	0.183912000
C	-1.415987000	0.000000000	-0.338590000
C	-0.743431000	1.257164000	0.183911000
C	0.743431000	1.257164000	-0.183911000
C	1.415987000	0.000000000	0.338590000
C	0.743430000	-1.257163000	-0.183913000
H	-1.242742000	2.139565000	-0.220599000
H	-1.421242000	-0.000001000	-1.434883000
H	-0.867175000	-1.280764000	1.272401000
H	-1.242740000	-2.139564000	-0.220597000
H	0.867179000	1.280766000	-1.272399000
H	1.242742000	2.139565000	0.220599000
H	1.421242000	-0.000001000	1.434883000
H	0.867175000	-1.280763000	-1.272401000
H	1.242740000	-2.139564000	0.220596000
H	-0.867179000	1.280767000	1.272399000
F	-2.749379000	-0.000001000	0.065338000
F	2.749379000	-0.000001000	-0.065338000

50. (3S,6S)-3,6-difluoro-1,2-dioxane:

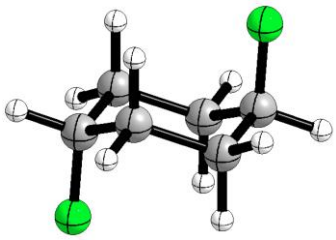


Total Energy = -506.0351444

C	1.340014000	-0.046402000	0.344749000
C	-1.339979000	-0.046402000	-0.344755000
H	1.306499000	-0.190144000	1.428341000
O	-0.650773000	-1.123184000	0.279684000
O	0.650767000	-1.123230000	-0.279579000
F	-2.621816000	-0.179261000	0.082835000
H	-1.306365000	-0.190158000	-1.428344000
C	0.756673000	1.268991000	-0.121793000
H	0.981493000	1.355928000	-1.188596000
H	1.239435000	2.097689000	0.398576000

C	-0.756697000	1.268977000	0.121844000
H	-0.981510000	1.355874000	1.188654000
H	-1.239444000	2.097714000	-0.398476000
F	2.621802000	-0.179247000	-0.082976000

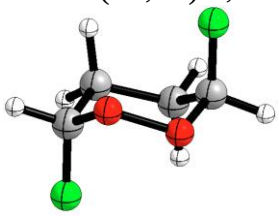
51. (1r,4r)-1,4-difluorocyclohexane (*both F axial*):



Total Energy = -434.3115382

C	1.354555000	0.000000000	0.552513000
C	0.510173000	1.262686000	0.570680000
C	-0.510168000	1.262688000	-0.570668000
C	-1.354549000	0.000001000	-0.552515000
C	-0.510163000	-1.262683000	-0.570674000
C	0.510167000	-1.262682000	0.570684000
H	-1.162924000	2.135560000	-0.502042000
H	-0.009504000	1.311981000	1.532091000
H	1.162932000	2.135555000	0.502059000
H	2.075448000	0.000000000	1.374013000
H	-2.075426000	0.000002000	-1.374028000
H	-1.162922000	-2.135554000	-0.502060000
H	0.009526000	-1.311978000	-1.532078000
H	-0.009523000	-1.311968000	1.532087000
H	1.162918000	-2.135560000	0.502076000
H	0.009516000	1.311995000	-1.532074000
F	-2.110181000	-0.000005000	0.630502000
F	2.110166000	-0.000006000	-0.630520000

52. (3*R*,6*R*)-3,6-difluoro-1,2-dioxane:

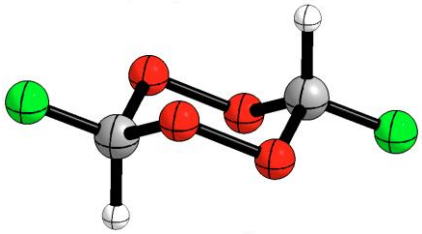


Total Energy = -506.0447263

C	-1.285172000	-0.062161000	0.530622000
C	1.285189000	-0.062075000	-0.530596000
H	-1.924481000	-0.212822000	1.403072000
O	0.445574000	-1.170738000	-0.559407000
O	-0.445575000	-1.170739000	0.559506000
C	-0.518074000	1.244107000	0.560262000

H	-0.026601000	1.319627000	1.532597000
H	-1.217206000	2.074563000	0.458658000
C	0.517962000	1.244141000	-0.560139000
H	0.026353000	1.319624000	-1.532405000
H	1.216990000	2.074691000	-0.458603000
H	1.924340000	-0.212657000	-1.403170000
F	2.075835000	-0.100837000	0.595443000
F	-2.075703000	-0.100861000	-0.595647000

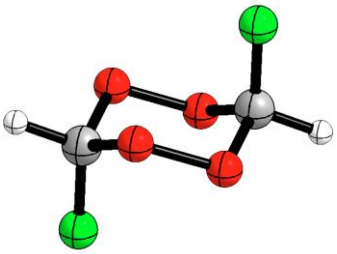
53. (3*r*,6*r*)-3,6-difluoro-1,2,4,5-tetraoxane (*both F equatorial*):



Total Energy = -577.762214

C	-0.719448000	1.086076000	0.000000000
C	0.719446000	-1.086077000	0.000000000
H	-1.718256000	0.646665000	0.000000000
O	0.000001000	-0.710513000	1.146518000
O	0.000001000	0.710514000	1.146514000
O	0.000001000	0.710514000	-1.146514000
O	0.000001000	-0.710513000	-1.146518000
F	0.735895000	-2.410836000	0.000000000
H	1.718252000	-0.646668000	0.000000000
F	-0.735899000	2.410836000	0.000000000

54. (3*r*,6*r*)-3,6-difluoro-1,2,4,5-tetraoxane (*both F axial*):

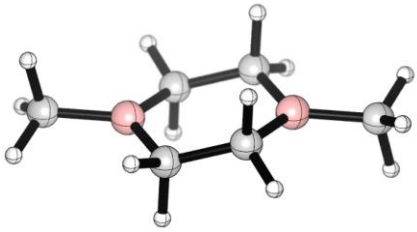


Total Energy = -577.771407

C	-0.645358000	1.149330000	0.000000000
C	0.645264000	-1.149252000	0.000000000
H	-0.574247000	2.237028000	0.000000000
H	0.573723000	-2.236926000	0.000000000
O	0.000011000	-0.713286000	1.147508000
O	0.000011000	0.713508000	1.147508000
O	0.000011000	0.713508000	-1.147508000
O	0.000011000	-0.713286000	-1.147508000
F	1.928988000	-0.741974000	0.000000000

F	-1.928905000	0.741516000	0.000000000

55. 1,4-dimethyl-1,4-diborinane:



Total Energy = -286.7237353

B	-1.526993000	-0.000037000	-0.046537000
B	1.527006000	-0.000033000	0.046513000
C	-0.747110000	1.357888000	-0.187680000
H	-1.286064000	2.193678000	0.271593000
H	-0.842010000	1.548863000	-1.272344000
C	0.747108000	1.357860000	0.187809000
H	0.841942000	1.548553000	1.272533000
H	1.286067000	2.193756000	-0.271255000
C	-3.091737000	-0.000051000	0.096736000
H	-3.301770000	0.000716000	1.176637000
H	-3.575738000	0.892340000	-0.308057000
H	-3.575610000	-0.893102000	-0.306759000
C	3.091743000	-0.000028000	-0.096969000
H	3.575690000	0.892756000	0.307014000
H	3.575703000	-0.892707000	0.307244000
H	3.301759000	-0.000168000	-1.176870000
C	-0.747048000	-1.357839000	-0.187903000
H	-0.841517000	-1.548166000	-1.272737000
H	-1.286025000	-2.193958000	0.270721000
C	0.747041000	-1.357836000	0.188045000
H	0.841539000	-1.548249000	1.272848000
H	1.285986000	-2.193929000	-0.270669000

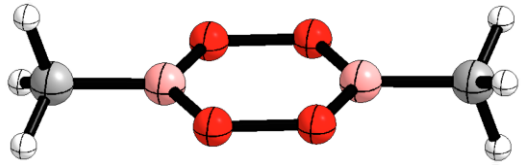
56. 3,6-dimethyl-1,2,3,6-dioxadiborinane:

Total Energy = -358.5728001

O	0.710675000	-1.183973000	-0.106744000
O	-0.710580000	-1.184067000	0.106268000
B	1.417772000	-0.028805000	0.087697000
B	-1.417782000	-0.028918000	-0.087778000
C	0.670059000	1.318209000	0.379008000
H	1.295032000	2.179040000	0.129429000

H	0.484504000	1.382234000	1.460043000
C	-0.670255000	1.318057000	-0.379311000
H	-0.484555000	1.381731000	-1.460342000
H	-1.295299000	2.178928000	-0.130052000
C	2.966614000	-0.201349000	-0.076768000
H	3.485193000	0.221954000	0.789089000
H	3.276106000	-1.239067000	-0.202636000
H	3.307773000	0.372031000	-0.945082000
C	-2.966538000	-0.201407000	0.077421000
H	-3.485736000	0.223154000	-0.787440000
H	-3.276213000	-1.239174000	0.202377000
H	-3.306789000	0.371038000	0.946733000

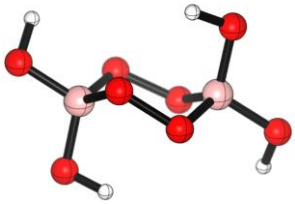
57. 3,6-dimethyl-1,2,4,5,3,6-tetraoxadiborinane:



Total Energy = -430.397247

O	0.713670000	-1.207814000	-0.015386000
O	-0.713647000	-1.207819000	0.015138000
O	-0.713695000	1.207842000	0.014685000
O	0.713657000	1.207838000	-0.014922000
B	-1.355433000	-0.000003000	0.013426000
B	1.355418000	-0.000006000	-0.013477000
C	-2.913383000	0.000030000	-0.003301000
H	-3.314935000	-0.887683000	0.486658000
H	-3.314913000	0.893305000	0.476432000
H	-3.264557000	-0.006098000	-1.038924000
C	2.913407000	-0.000038000	0.003701000
H	3.315098000	-0.892288000	-0.477801000
H	3.315187000	0.888747000	-0.484116000
H	3.264171000	0.003734000	1.039487000

58. borax anion:

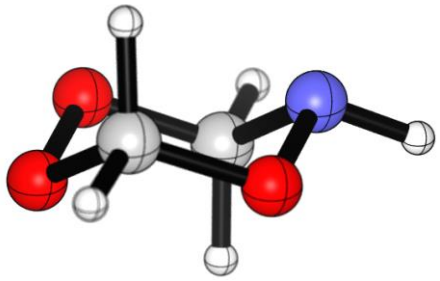


Total Energy = -654.015302

B	-1.410313000	-0.068196000	-0.000115000
O	-1.706306000	-1.490570000	0.110121000
H	-0.879617000	-1.851730000	0.446485000
O	-2.641476000	0.723360000	-0.058304000

H	-2.373652000	1.538947000	-0.486021000
O	-0.611837000	0.391304000	1.186614000
O	-0.652110000	0.307292000	-1.233438000
O	0.611751000	-0.391132000	1.186693000
O	0.652106000	-0.307360000	-1.233445000
B	1.410333000	0.068224000	-0.000113000
O	1.706429000	1.490542000	0.109964000
H	0.879909000	1.851733000	0.446697000
O	2.641399000	-0.723441000	-0.058215000
H	2.373607000	-1.539041000	-0.485935000

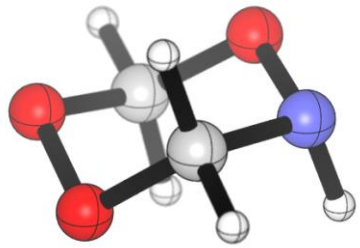
59. 1,2,4,5-trioxazinane (*equatorial*):



Total Energy = -359.4389949

C	-1.276355000	-0.286080000	-0.214076000
C	1.282309000	0.241472000	0.210350000
H	-1.255909000	-0.319314000	-1.309358000
H	-2.263905000	-0.520636000	0.185018000
H	1.267213000	0.225463000	1.303475000
H	2.272798000	0.414902000	-0.206712000
O	0.441468000	1.251175000	-0.266536000
N	-0.842529000	0.999469000	0.317207000
H	-1.416994000	1.746228000	-0.065023000
O	0.872785000	-1.010703000	-0.286638000
O	-0.406906000	-1.274882000	0.289988000

60. 1,2,4,5-trioxazinane (*axial*):

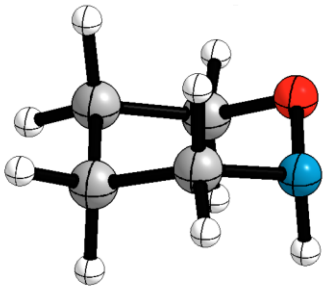


Total Energy = -359.442052

C	-1.309031000	-0.028579000	-0.233057000
C	1.294818000	-0.011457000	0.206222000
H	-1.315131000	-0.103101000	-1.321359000
H	-2.318692000	-0.052318000	0.178020000

H	1.282277000	-0.026631000	1.303072000
H	2.305796000	-0.032951000	-0.198032000
O	0.681198000	1.158795000	-0.272260000
N	-0.672549000	1.208984000	0.139674000
H	-0.663232000	1.305552000	1.156350000
O	0.653866000	-1.159416000	-0.279188000
O	-0.647301000	-1.163532000	0.309604000

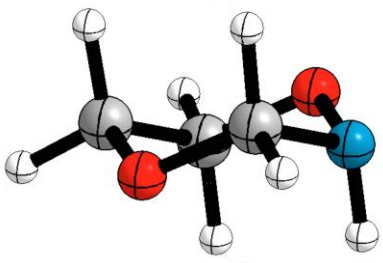
61. 1,2-oxazinane:



Total Energy = -287.7072343

C	1.391878000	-0.130621000	-0.227069000
C	-1.381348000	-0.030291000	0.212322000
H	1.470197000	-0.158535000	-1.317551000
H	2.394241000	-0.276527000	0.183020000
H	-1.425019000	-0.100616000	1.310263000
H	-2.398619000	-0.088133000	-0.177348000
O	-0.720616000	-1.178740000	-0.303415000
N	0.605347000	-1.298689000	0.167481000
H	0.541668000	-1.342153000	1.186749000
C	0.783459000	1.196283000	0.227562000
H	1.350088000	2.036445000	-0.182055000
H	0.842232000	1.265614000	1.320669000
C	-0.680127000	1.252518000	-0.211098000
H	-1.191411000	2.116603000	0.221442000
H	-0.739052000	1.340708000	-1.300533000

62. 1,4,2-dioxazinane:

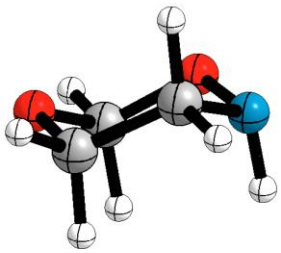


Total Energy = -323.6134411

C	-1.309184000	0.279575000	0.206419000
C	1.312661000	-0.344401000	-0.203233000

H	-1.343602000	0.322532000	1.301075000
H	-2.297455000	0.468386000	-0.211903000
H	1.368389000	-0.436531000	-1.296243000
H	2.282272000	-0.592860000	0.230767000
O	0.396313000	-1.306198000	0.308726000
N	-0.914301000	-1.056777000	-0.160009000
H	-0.880376000	-1.140924000	-1.177368000
C	0.871902000	1.057514000	0.179516000
H	1.513236000	1.812141000	-0.277120000
H	0.904793000	1.169794000	1.271829000
O	-0.446241000	1.286044000	-0.285874000

63. 1,5,2-dioxazinane:

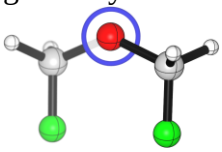


Total Energy = -323.6137029

C	1.306390000	-0.412971000	-0.223942000
C	-1.277099000	0.344641000	0.182341000
H	1.390722000	-0.466729000	-1.311184000
H	2.254488000	-0.729091000	0.217657000
H	-1.296124000	0.327417000	1.286014000
H	-2.254586000	0.598227000	-0.222940000
O	-0.974043000	-0.942273000	-0.292733000
N	0.287956000	-1.384378000	0.175631000
H	0.215266000	-1.417403000	1.195109000
O	-0.367587000	1.308169000	-0.256457000
C	0.940810000	1.003388000	0.198661000
H	1.610256000	1.744579000	-0.238176000
H	0.976717000	1.096121000	1.295260000

64. 1,4-difluoro-dimethyl-peroxide PES dihedral scan:

PES relaxed scan for the COOC and OOCF dihedral (not simultaneously) were performed at M062X/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken. Initial geometry:



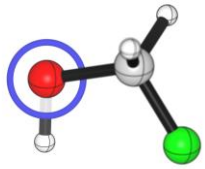
Total Energy = -428.6223534

C	1.510073000	0.171061000	0.471465000
O	0.236438000	-0.145065000	0.900338000
H	2.146460000	-0.009085000	1.338868000

H	1.555010000	1.200828000	0.114115000
O	-0.683960000	0.382905000	-0.059921000
C	-1.533644000	-0.641513000	-0.426395000
H	-2.367261000	-0.145622000	-0.925173000
H	-1.840099000	-1.221467000	0.445126000
F	-0.931470000	-1.491838000	-1.310900000
F	1.908337000	-0.648172000	-0.547444000

65. fluoromethyl-hydroperoxide PES dihedral scan:

PES relaxed scan for the COOH and OOCF dihedral (not simultaneously) were performed at M062X/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken. Initial geometry:



Total Energy = -290.0808917

O	0.361661000	-1.331463000	0.227693000
O	-0.234624000	-0.064231000	0.468612000
C	-1.524428000	-0.109186000	-0.008022000
H	-2.020260000	0.766980000	0.410680000
H	-2.008851000	-1.051064000	0.251439000
F	-1.530961000	0.000817000	-1.381151000
H	0.879098000	-1.161643000	-0.570703000

66. dimethoxy-methane PES dihedral scan:

PES relaxed scan for both COCO dihedrals was performed at B2PLYPD/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken. Final and initial geometries are the same:

Total Energy = -269.08787189

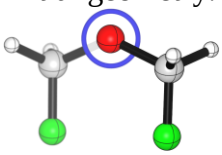
C	-0.235153000	-0.181140000	0.123600000
O	0.919054000	0.489583000	0.586814000
H	-1.045996000	0.525095000	-0.100019000
H	-0.594355000	-0.913998000	0.858537000
H	0.047747000	-0.701227000	-0.790466000
C	0.643048000	1.184621000	1.760766000
H	0.304225000	0.488320000	2.552450000
H	-0.150620000	1.937304000	1.587648000
O	1.830472000	1.806784000	2.135381000
C	1.650322000	2.544182000	3.327210000
H	1.347905000	1.893536000	4.158732000
H	2.609886000	3.002170000	3.562896000

H	0.896442000	3.332667000	3.200074000

67. 1,4-difluoro-dimethyl-peroxide PES dihedral scan:

PES relaxed scan for the COOC and OOCF dihedrals simultaneously was performed at B2PLYPD/6-311++G(d,p) level using fopt=modredundant. 36 steps of 10º each were taken.

Initial geometry:



Total Energy = -428.08499245

C	1.510073000	0.171061000	0.471465000
O	0.236438000	-0.145065000	0.900338000
H	2.146460000	-0.009085000	1.338868000
H	1.555010000	1.200828000	0.114115000
O	-0.683960000	0.382905000	-0.059921000
C	-1.533644000	-0.641513000	-0.426395000
H	-2.367261000	-0.145622000	-0.925173000
H	-1.840099000	-1.221467000	0.445126000
F	-0.931470000	-1.491838000	-1.310900000
F	1.908337000	-0.648172000	-0.547444000