

**CHEMISTRY**   
A EUROPEAN JOURNAL

Supporting Information

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# Chemo- and Periselectivity in the Addition of OsO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub> to Ethylene. A Theoretical Study

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A Theoretical Study**

M. Hölscher, W. Leitner, M. C. Holthausen, G. Frenking

Supplementary Material:

Cartesian coordinates (Molden format) of stationary points optimized at B3LYP/I.  
Total Energies in Hartrees obtained from single point calculations at B3LYP/II.

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6
C2H4: -78.6231727698
C 0.00000 0.00000 0.66291
C 0.00000 0.00000 -0.66291
H 0.00000 0.92179 1.23312
H 0.00000 -0.92179 1.23312
H 0.00000 -0.92179 -1.23312
H 0.00000 0.92179 -1.23312
-----
9
1: -319.8172651760
Os 0.02286 -0.04693 0.00000
O 0.75127 -0.64390 -1.47059
O 0.75085 -0.64404 1.47075
C 0.23171 1.83661 0.00013
C -1.84342 -0.20952 -0.00029
H -0.54887 2.58400 0.00104
H 1.25966 2.19316 -0.00056
H -2.39728 -0.33413 -0.92691
H -2.39746 -0.33534 0.92607
-----
9
Ts1? 1a: -319.7509279840
Os -0.09712 -0.04557 -0.03136
O -1.06326 -1.45511 0.17742
O 1.26618 0.31451 1.25224
C 1.59102 -0.15977 -0.89121
C -0.93805 1.62568 -0.19250
H 2.25815 0.67725 -1.06138
H 2.00756 -1.14333 -1.10794
H -2.01913 1.69132 -0.29954
H -0.40646 2.56707 -0.08259
-----
9
1a: -319.8475296870
Os -0.15103 -0.04042 0.00439
O -1.12731 -1.42919 -0.02830
O 1.64068 0.10492 0.76541
C 1.83249 -0.04543 -0.58635
C -0.95176 1.63697 -0.07609
H 2.24196 0.80629 -1.12738
H 2.18774 -1.01917 -0.92716
H -2.02245 1.80537 -0.14843
H -0.32059 2.52465 -0.05265
-----
9
Ts1? 1b: -319.7924631820
Os 0.12361 0.02174 -0.04353
O 1.33090 -1.17288 -0.38220
O 0.52281 1.58493 0.61055
C -1.21846 -0.92770 1.02330
C -1.59234 0.34392 -0.86211
H -1.01655 -1.08202 2.07995
H -2.15960 -1.31955 0.66245
H -1.97453 1.36092 -0.88299
H -2.20862 -0.40560 -1.34502
-----
9
1b: -319.9118615990
Os 0.00003 0.20746 0.00000
O 1.57701 0.86495 0.00000
O -1.57731 0.86427 0.00000
C 0.00003 -1.79520 0.71584
C 0.00003 -1.79520 -0.71584
H 0.91015 -2.01463 -1.26255
H -0.91016 -2.01439 -1.26253
H -0.91016 -2.01439 1.26253
H 0.91015 -2.01463 1.26255
-----
9
Ts1? 1c: -319.6728412100
Os -0.07791 -0.00003 -0.05056
C -1.07514 -1.55694 0.12434
C -1.07198 1.55920 0.12032
H -2.02249 -1.43212 0.65452
H -0.76072 -2.56697 -0.11314
H -2.01907 1.43636 0.65153
H -0.75729 2.56825 -0.12084
O 1.41325 -0.00471 -0.92112
O 1.63214 0.00261 1.08389
-----
9
1c: -319.7117296600
Os 0.10015 -0.00003 -0.00415
C 1.18210 1.50824 -0.01668
C 1.18345 -1.50730 -0.01657
H 2.04159 1.61488 0.64524
H 0.85564 2.41596 -0.52157
H 2.04212 -1.61311 0.64657
H 0.85875 -2.41526 -0.52214
O -1.63627 -0.00047 -0.69689
O -1.81413 -0.00026 0.73023
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9
Ts1a? 1d: -319.7654378340
Os 0.06008 -0.17649 0.00734
O 1.83903 -0.42427 -0.05479
C 1.17326 1.41801 0.00250
```

H 1.94971 1.61599 0.73055  
H 1.04297 2.18776 -0.76270  
O -1.83842 -0.46149 -0.04821  
C -1.75457 0.89854 0.03050  
H -2.00661 1.45392 -0.87232  
H -2.06929 1.34218 0.97241

9

**1d:** -319.8241782450  
Os 0.00000 -0.20469 0.00021  
O -1.88826 -0.25282 -0.00109  
C -1.59979 1.09191 0.00003  
H -1.81400 1.62528 -0.92457  
H -1.81734 1.62412 0.92446  
O 1.88822 -0.25287 -0.00105  
C 1.59974 1.09188 0.00004  
H 1.81637 1.62404 0.92474  
H 1.81551 1.62564 -0.92395

9

**Tslb? 1e:** -319.6693925080  
Os -0.07212 -0.05235 -0.00002  
O -2.06433 -0.66546 -0.00036  
O -1.24692 1.14997 0.00051  
C 1.94181 0.00894 -0.71107  
C 1.94168 0.00795 0.71106  
H 2.16882 -0.90730 1.25656  
H 2.16611 0.90618 1.27500  
H 2.16593 0.90806 -1.27371  
H 2.16920 -0.90546 -1.25784

9

**1e:** -319.7245426360  
Os 0.03768 -0.00001 -0.03165  
O 1.93105 -0.00032 -0.58012  
O 1.75984 0.00036 0.76726  
C -1.97253 -0.70644 0.05714  
C -1.97255 0.70644 0.05656  
H -2.20451 1.25722 -0.85230  
H -2.15553 1.27276 0.96426  
H -2.15551 -1.27202 0.96530  
H -2.20447 -1.25797 -0.85127

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**Ts1? 2:** -398.3982475720  
Os -0.41902 -0.00940 -0.00718  
O 0.89895 0.13670 -1.26728  
O 0.73986 -0.08228 1.33153  
C -1.45813 1.56311 0.11189  
C -1.62187 -1.44544 -0.06564  
H -2.50101 1.65410 -0.17409  
H -0.95601 2.49459 0.36556  
H -2.14633 -1.57516 -1.01708  
H -1.61589 -2.31334 0.58653  
C 2.74242 -0.06114 0.69130  
C 2.71512 -0.02107 -0.69544  
H 2.93347 0.83595 1.26195  
H 2.87866 -0.99570 1.21475  
H 2.89386 -0.92873 -1.25524  
H 2.98292 0.89431 -1.20323

15

**2:** -398.4565150600  
Os -0.40121 -0.01122 -0.03617  
O 1.11262 -0.34891 -1.27843  
O 0.96184 0.32323 1.29256  
C -1.45933 1.48320 -0.30795  
C -1.46686 -1.40552 0.53332  
H -2.53224 1.33818 -0.44455  
H -1.06997 2.48037 -0.50576  
H -1.13749 -2.29717 1.06235  
C 2.25594 0.47694 0.67083  
C 2.34135 -0.42342 -0.55100  
H 2.39617 1.52768 0.39045  
H 2.99859 0.21893 1.43011  
H 2.53354 -1.46183 -0.25019  
H 3.15192 -0.10526 -1.21339  
H -2.47089 -1.43007 0.09534

15

**Ts1? 3:** -398.4301895640  
C 2.99577 0.46569 0.43195  
C 2.93903 -0.47817 -0.53910  
H 3.22942 0.19537 1.45281  
H 3.11723 1.50999 0.17443  
H 2.94235 -0.21548 -1.58596  
H 3.00684 -1.53285 -0.31126  
Os -0.48481 -0.04348 -0.00149  
O 0.67792 -0.81645 -1.09907  
O -1.48532 -1.11356 0.92432  
C 0.77203 0.83563 1.17113  
C -1.32628 1.36459 -0.90922  
H 0.91979 1.90328 1.24903  
H 1.00227 0.25485 2.05833  
H -0.84514 1.84560 -1.75621  
H -2.35163 1.65731 -0.69816

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**3:** -398.5171199470  
C 2.41059 0.48456 0.52467  
C 2.31394 -0.46188 -0.65733  
H 3.29166 0.27068 1.13846  
H 2.50940 1.51058 0.15862  
H 3.03217 -0.23415 -1.44825  
H 2.46836 -1.50264 -0.34742  
Os -0.45671 -0.03850 -0.00969  
O 1.00314 -0.33192 -1.24392  
O -1.40536 -1.37372 0.47728  
C 1.11747 0.33731 1.33530  
C -1.25009 1.59532 -0.43791  
H 0.92759 1.17364 2.00424  
H 1.13007 -0.58025 1.93491  
H -0.66089 2.43914 -0.79621  
H -2.32247 1.76203 -0.36341

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**Ts1? 4:** -398.4210578880  
C 3.00642 0.65943 0.11348  
C 3.02674 -0.69250 -0.01337  
H 3.34227 1.29770 -0.69335  
H 2.93524 1.11338 1.09217  
H 2.90684 -1.33772 0.84601  
H 3.34336 -1.16591 -0.93284  
Os -0.51687 0.00303 0.02633

O -0.91871 -0.26020 1.68415  
O -1.74194 0.21114 -1.20389  
C 0.75366 1.44009 -0.18349  
C 0.63357 -1.40278 -0.56899  
H 0.96051 1.78769 -1.19009  
H 0.88404 2.16264 0.61338  
H 0.54099 -2.39417 -0.13626  
H 1.13206 -1.32685 -1.52825

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**4:** -398.5678786230  
C 2.40933 0.70413 -0.29212  
C 2.40927 -0.70415 0.29213  
H 3.26000 0.87573 -0.95922  
H 2.48294 1.43869 0.51550  
H 3.25999 -0.87587 0.95915  
H 2.48269 -1.43872 -0.51550  
Os -0.51385 -0.00001 -0.00001  
O -1.14192 1.23215 1.01396  
O -1.14161 -1.23227 -1.01403  
C 1.08984 0.89041 -1.04222  
C 1.08983 -0.89024 1.04236  
H 1.09085 0.34784 -1.99117  
H 0.83184 1.92952 -1.24523  
H 1.09093 -0.34736 1.99114  
H 0.83185 -1.92928 1.24572

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**Ts1? 5:** -398.4067085070  
C 2.74596 -0.69153 0.35217  
C 3.04533 0.53531 -0.25159  
H 2.93610 -0.79834 1.41084  
H 2.88153 -1.59377 -0.22755  
H 3.30953 0.56792 -1.30141  
H 3.41776 1.35220 0.35665  
Os -0.46750 -0.02371 -0.03947  
O -1.60918 -0.81271 -1.09153  
C -1.37110 0.74121 1.43268  
O 0.95474 -1.02622 0.55335  
C 0.50393 1.39004 -0.67107  
H 1.65207 1.23028 -0.33046  
H 0.39704 2.06268 -1.51713  
H -2.14157 0.11688 1.88286  
H -1.23166 1.72539 1.85814

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**5:** -398.4659854680  
C -2.48401 -0.72711 0.15107  
C -3.18475 0.58974 -0.13667  
H -3.06865 -1.56129 -0.24875  
H -2.37469 -0.87948 1.23097  
H -2.61975 1.43162 0.26772  
H -4.17640 0.59075 0.32307  
Os 0.48174 -0.03115 0.00750  
O 1.82915 -0.88764 -0.71856  
C 0.48490 1.78290 -0.51829  
O -1.21235 -0.82296 -0.47893  
C 0.51909 0.18983 1.73182  
H -3.30378 0.73693 -1.21137  
H 0.89389 0.10271 2.74442  
H 0.48931 2.65341 0.12244  
H 0.60243 1.96562 -1.58595

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**Ts4? 6:** -398.4564027530  
C 1.14570 -0.96359 0.85669  
Os -0.51312 0.00958 -0.01400  
C 0.68681 1.14432 -0.91262  
O -1.21310 -1.07271 -1.17122  
O -1.27889 0.84432 1.29396  
C 2.50484 -0.74149 0.18269  
C 2.71223 0.69150 -0.20032  
H 3.29278 -1.06124 0.87440  
H 2.59284 -1.37417 -0.70466  
H 3.54939 0.90046 -0.86664  
H 2.64625 1.41730 0.60223  
H 1.15021 -0.56035 1.87172  
H 0.89619 -2.02300 0.91595  
H 1.81923 0.78958 -1.18291  
H 0.68853 2.22580 -0.98659

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**6:** -398.4908828690  
C -2.52682 -0.72864 0.15070  
C -3.18881 0.62944 -0.06535  
H -3.22332 -1.51350 -0.16921  
H -2.35223 -0.89885 1.21545  
H -2.57960 1.44332 0.33178  
H -4.15541 0.66702 0.44040  
Os 0.52225 0.02450 0.01935  
O 0.77531 -0.44413 1.68287  
O 1.74486 -0.31802 -1.18115  
C -1.23696 -0.96496 -0.63306  
C -0.00383 1.67668 -0.08742  
H -1.34843 -0.69095 -1.68388  
H -0.93103 -2.01313 -0.57889  
H -3.36109 0.82221 -1.12729  
H -0.16243 2.74406 -0.10210

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**Ts1a? 7:** -398.3765671210  
C 2.09752 -0.98209 -0.09710  
C 2.59841 0.31495 0.05128  
H 2.06498 -1.44060 -1.07721  
H 2.07800 -1.66072 0.74425  
H 2.96392 0.63782 1.01842  
H 3.05850 0.81356 -0.79203  
Os -0.35780 -0.07264 -0.02908  
O 1.03169 1.28408 -0.00606  
O -0.80183 -1.06790 -1.35996  
C -0.66268 -0.69172 1.70522  
C -0.92107 1.77828 -0.13893  
H -0.38273 -0.06976 2.55346  
H -1.09227 -1.66324 1.93346  
H -1.12763 2.38163 0.73491  
H -0.88209 2.27628 -1.09986

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**Ts7? 2:** -398.3842053630  
Os -0.26476 0.00814 -0.00591  
O 1.13445 -1.39000 -0.37370  
C 2.23272 -0.62059 0.04663  
H 3.10666 -0.78596 -0.59983  
H 2.52309 -0.85852 1.07699

C 1.83010 0.88136 -0.07912  
H 2.28967 1.56069 0.62433  
H 1.85157 1.25154 -1.09945  
O 0.09306 1.78943 0.41634  
C -1.54152 -0.08305 -1.35713  
H -1.24305 0.07773 -2.39608  
H -2.61605 -0.12868 -1.18012  
C -1.26663 -0.70975 1.38516  
H -0.78306 -1.07979 2.29197  
H -2.35522 -0.65886 1.41693

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**Ts7? 3:** -398.4198397740

Os 0.30886 -0.02166 -0.06803  
O 1.58380 0.03842 -1.24973  
C -1.66668 1.07226 -0.13512  
H -2.09168 1.77121 0.57649  
H -1.60970 1.52162 -1.12632  
C -2.32330 -0.33109 -0.11273  
H -2.78604 -0.49802 0.86620  
H -3.09780 -0.43749 -0.88364  
O -1.26567 -1.24298 -0.31269  
C 0.22684 1.65414 0.89236  
H 0.47527 2.57125 0.36192  
H -0.08371 1.78316 1.92227  
C 0.68280 -1.13101 1.41233  
H 0.17201 -2.08826 1.49622  
H 1.48552 -0.92671 2.11540

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**7:** -398.4330212100

C 1.58812 -1.12772 0.02456  
C 2.43518 0.11772 0.08205  
H 1.61811 -1.66799 -0.91989  
H 1.60605 -1.80028 0.87720  
H 2.84676 0.29287 1.08425  
H 3.26095 0.13505 -0.63883  
Os -0.28980 -0.03072 -0.06078  
O 1.45801 1.09361 -0.23320  
O -1.19133 -1.07879 -1.12341  
C -0.76717 -0.45245 1.72045  
C -0.84182 1.78231 -0.02141  
H -1.25321 0.21244 2.42140  
H -0.64325 -1.48328 2.04821  
H -0.14410 2.61201 0.02319  
H -1.88569 1.99611 -0.25687

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**Ts1a? 8:** -398.3878390770

C -2.83551 0.11508 0.08741  
C -1.17684 1.29837 -0.02225  
H -3.33062 0.46151 -0.81132  
H -3.25584 0.48099 1.01638  
H -1.36660 1.88571 0.86275  
H -1.40245 1.74249 -0.97903  
Os 0.42767 -0.03996 -0.04419  
C 0.83268 -0.57996 1.70293  
O 0.68639 -1.13857 -1.34522  
C -2.20561 -1.11165 0.07527  
O 0.70918 1.75013 -0.20375  
H -2.02365 -1.64619 -0.84736  
H -1.99350 -1.64392 0.99161

H 0.96766 0.14721 2.49879  
H 1.04890 -1.61452 1.95831

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**8:** -398.4615423010

C 2.48987 0.00005 0.06419  
C 1.53505 -1.13563 -0.24164  
H 3.40057 0.00005 -0.54192  
H 2.77683 0.00009 1.11766  
H 1.51690 -1.99760 0.42280  
H 1.53282 -1.45552 -1.28100  
Os -0.34179 -0.00001 -0.00837  
C -0.41242 -0.00009 1.86377  
O -1.00805 1.45018 -0.73361  
C 1.53499 1.13566 -0.24171  
O -1.00800 -1.45009 -0.73386  
H 1.53274 1.45547 -1.28110  
H 1.51679 1.99768 0.42266  
H -0.52849 -0.92371 2.42457  
H -0.52848 0.92350 2.42462

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**Ts8? 4:** -398.4230960530

C 2.31121 -0.14208 0.37158  
C 1.15750 -0.12285 1.43101  
H 2.60749 -1.17974 0.22351  
H 3.15874 0.43727 0.74853  
H 1.18434 0.76516 2.05740  
H 1.09382 -1.02536 2.03358  
Os -0.34276 -0.06904 -0.00992  
C -0.17640 1.83516 -0.34719  
O 0.01749 -1.55542 -0.88209  
C 1.80079 0.43436 -0.93628  
H 1.78759 -0.21023 -1.80637  
H 2.12807 1.44444 -1.14685  
H -0.55532 2.55129 0.39186  
H 0.13649 2.29115 -1.27660  
O -2.02371 0.07362 0.43387

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**Ts1b? 9:** -398.4335594220

Os -0.28381 -0.00012 -0.00015  
O 0.95668 1.28280 -0.00003  
O 0.95707 -1.28253 -0.00007  
C -2.33099 0.00038 -0.70919  
C -2.33042 0.00010 0.71011  
H -2.54876 0.90761 1.26459  
H -2.54917 -0.90764 1.26407  
H -2.55019 -0.90708 -1.26340  
H -2.54975 0.90817 -1.26304  
C 2.70783 -0.70749 0.00015  
C 2.70792 0.70785 0.00035  
H 2.98302 1.22373 -0.90997  
H 2.98254 1.22345 0.91099  
H 2.98282 -1.22331 0.91055  
H 2.98311 -1.22306 -0.91032

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**Ts2? 9:** -398.4221831530

Os 0.33674 -0.15867 -0.08236  
O -1.34176 -1.19785 -0.14466  
O -0.85056 1.35343 0.07773

C 1.80657 -0.24993 1.14150  
C 1.85017 0.90631 -0.69703  
H 1.77476 0.09428 2.17533  
H 2.75036 -0.73455 0.87636  
H 1.74542 1.97908 -0.88315  
C -2.16360 0.94558 0.50736  
C -2.50113 -0.36542 -0.18306  
H -2.16350 0.81922 1.59698  
H -2.84739 1.76018 0.25134  
H -2.79634 -0.18500 -1.22497  
H -3.32397 -0.88723 0.31653  
H 2.85491 0.54936 -0.92630

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**9:** -398.4584477340  
Os -0.28355 -0.00059 -0.00010  
O 1.15181 1.23986 0.19170  
O 1.15389 -1.23938 -0.19150  
C -2.31954 0.08135 -0.70527  
C -2.31954 -0.07898 0.70574  
H -2.55588 0.75292 1.36161  
H -2.52372 -1.04937 1.14959  
H -2.55705 -0.75047 -1.36087  
H -2.52236 1.05185 -1.14947  
C 2.45694 -0.73676 0.17436  
C 2.45582 0.73925 -0.17409  
H 2.61073 0.88179 -1.24784  
H 3.19803 1.32517 0.37340  
H 2.61215 -0.87904 1.24811  
H 3.20024 -1.32142 -0.37304

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**Ts1b? 10:** -398.4480993290  
Os 0.10545 -0.15696 -0.06084  
O 0.15666 -1.20407 1.38999  
O -1.08147 -0.60032 -1.29490  
C 2.20118 0.13481 -0.27916  
C 1.59719 1.38555 0.05828  
H 1.69987 1.79410 1.05691  
H 1.45226 2.13160 -0.71707  
H 2.51450 -0.04405 -1.30248  
H 2.74006 -0.42967 0.47410  
C -2.47893 0.42268 0.09853  
H -3.07486 0.71033 -0.75524  
H -2.82055 -0.41672 0.68734  
C -1.41457 1.24796 0.56790  
H -1.29490 2.22073 0.10178  
H -1.26151 1.25200 1.64467

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**Ts7? 10:** -398.4196039480  
C 1.58831 0.81089 0.77027  
C 2.40935 0.15383 -0.33046  
H 1.70776 0.38515 1.76638  
H 1.59628 1.89272 0.79405  
H 2.91058 0.86744 -0.98991  
H 3.14747 -0.56355 0.04071  
Os -0.20307 -0.12976 0.01014  
O 1.37942 -0.53361 -1.05633  
O -0.71984 -1.36284 1.11172  
C -0.94327 1.67241 0.37406  
C -1.78472 0.26730 -1.02884

H -1.45859 2.34101 -0.29868  
H -0.76987 2.08861 1.36368  
H -2.07231 1.12986 -1.60696  
H -2.52260 -0.53421 -0.99309

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**10:** -398.5317613120  
Os 0.17358 -0.21523 -0.02246  
O 0.70063 -1.83158 -0.10928  
O -1.27238 0.54865 -1.08709  
C 1.46117 1.36024 -0.58859  
C 1.44305 1.22703 0.84948  
H 2.29282 0.75759 1.33672  
H 0.93449 1.95386 1.47430  
H 0.93884 2.17344 -1.08031  
H 2.32025 0.98334 -1.13559  
C -2.33885 0.51210 -0.11657  
H -2.80623 1.50030 -0.06445  
H -3.09718 -0.21908 -0.41128  
C -1.55063 0.12821 1.13361  
H -1.44671 0.91327 1.88027  
H -1.84281 -0.80743 1.61084

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**T1b? 11:** -398.5288940620  
Os -0.09950 0.00242 -0.11361  
C -1.81599 -0.00852 1.18820  
H -1.85408 0.90042 1.77609  
H -1.84300 -0.92306 1.76805  
C -2.25192 -0.00554 -0.17024  
H -2.62722 0.91082 -0.60904  
H -2.62022 -0.91907 -0.62020  
O 0.15541 -1.68361 -0.42208  
O 0.15926 1.68711 -0.42394  
C 2.54364 -0.02027 -0.22328  
H 2.72551 0.89212 -0.77636  
H 2.70437 -0.95686 -0.74073  
C 2.23212 0.00830 1.08897  
H 2.16440 0.94131 1.63319  
H 2.14804 -0.90124 1.66948

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**11:** -398.5299445650  
Os 0.00000 0.00010 -0.11450  
C -1.88198 -0.00025 1.15850  
H -1.87440 0.91533 1.73552  
H -1.87404 -0.91578 1.73558  
C -2.28007 -0.00050 -0.17774  
H -2.58991 0.92130 -0.65230  
H -2.58937 -0.92244 -0.65234  
O 0.00027 -1.70312 -0.46273  
O -0.00012 1.70338 -0.46251  
C 2.28014 -0.00036 -0.17758  
H 2.59018 0.92144 -0.65203  
H 2.58941 -0.92229 -0.65220  
C 1.88174 -0.00010 1.15855  
H 1.87415 0.91545 1.73562  
H 1.87355 -0.91565 1.73556

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**Ts7? 12:** -398.4075420260  
Os -0.31803 -0.01239 -0.07081

O -1.60759 -0.56083 -1.10068  
C -0.71972 -0.41373 1.73544  
H -0.59235 -1.42864 2.10828  
H -1.19720 0.27722 2.42338  
C -0.01768 1.87351 0.32632  
H 0.68504 2.24202 1.06289  
H -0.50083 2.64229 -0.27906  
O 1.56769 0.85132 -0.54444  
C 2.33750 -0.23018 0.04798  
H 2.62115 0.02271 1.07434  
H 3.24827 -0.37255 -0.54322  
C 1.32839 -1.36477 0.01567  
H 1.32610 -2.03695 0.86829  
H 1.32808 -1.91718 -0.92513

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**12:** -398.4937349730

C 1.13673 0.55860 1.23971  
C 2.42533 0.51081 0.41971  
H 1.14157 -0.22809 2.00119  
H 0.98250 1.51407 1.73991  
H 2.57302 1.45409 -0.12855  
H 3.30720 0.33765 1.03857  
Os -0.47127 -0.03496 0.00964  
O 2.34870 -0.57194 -0.50074  
O -1.25416 -1.42955 0.59997  
C -1.36343 1.49389 -0.57493  
H -0.78165 2.30600 -1.01770  
H -2.43494 1.66451 -0.51026  
C 1.14732 -0.46257 -1.23678  
H 1.00611 -1.37856 -1.80734  
H 1.19085 0.39506 -1.92826

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**Ts4? 13:** -398.4538258390

Os -0.32472 -0.08818 0.00456  
O -1.87003 0.37850 -0.63630  
O -0.26389 -0.90017 1.56652  
C 2.06385 -0.60556 -0.19218  
C 1.10806 -1.28717 -1.02023  
H 1.11852 -1.03408 -2.07716  
H 0.88265 -2.33049 -0.82815  
C 0.50789 1.81562 -0.40932  
C 1.37720 1.36805 0.67924  
H 2.41495 -1.07666 0.71649  
H 2.77049 0.03929 -0.69068  
H 1.02204 1.49170 1.69574  
H 2.44945 1.49146 0.61496  
H -0.22126 2.58806 -0.18120  
H 0.97144 1.96049 -1.38355

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**Ts11? 13:** -398.4832638720

Os -0.01115 -0.16694 -0.07509  
O -0.10383 -1.00922 1.55619  
O 0.01876 -1.25644 -1.41293  
C -1.31332 1.57844 -0.12177  
C -2.02229 0.44741 0.35868  
H -2.21024 0.30041 1.41378  
H -2.67346 -0.10105 -0.31447  
C 1.96015 0.37740 0.62754  
C 1.56197 1.35614 -0.31204

H -1.46395 1.93081 -1.13702  
H -0.99528 2.34655 0.57326  
H 1.93170 1.30503 -1.33189  
H 1.28701 2.34816 0.01786  
H 2.61233 -0.43664 0.33175  
H 1.92046 0.56290 1.69270

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**13:** -398.4922744930

Os 0.03221 -0.19665 -0.00083  
O -0.13308 -1.20150 -1.44387  
O -0.11969 -1.20094 1.44476  
C 1.17739 1.65764 -0.00017  
C 2.04239 0.52673 -0.00169  
H 2.53332 0.21549 -0.91692  
H 2.53497 0.21363 0.91194  
C -1.63081 0.98775 -0.71185  
C -1.63256 0.97698 0.72012  
H 1.03206 2.22158 0.91351  
H 1.03352 2.22644 -0.91099  
H -2.29062 0.30398 1.25719  
H -1.36201 1.87302 1.26634  
H -2.28653 0.32318 -1.26217  
H -1.35888 1.89322 -1.24143

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**Ts4? 14:** -398.4937526280

Os 0.57170 -0.04951 -0.02673  
O 2.00259 0.63659 0.58520  
O -0.15850 -1.52081 -0.67849  
C -1.62968 -1.20619 0.61698  
H -1.32899 -1.04859 1.64632  
H -1.82675 -2.24747 0.40253  
C -2.58305 -0.21039 0.02696  
H -3.54986 -0.37227 0.52636  
H -2.74137 -0.43762 -1.03053  
C -2.11579 1.23429 0.20327  
H -2.01106 1.45221 1.26999  
H -2.87559 1.92072 -0.18718  
C -0.77934 1.46370 -0.51685  
H -0.31619 2.40883 -0.22895  
H -0.90481 1.47253 -1.60280

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**14:** -398.5267891040

Os 0.66375 -0.13487 -0.03744  
O -0.81718 -1.23569 -0.13023  
O 2.17705 0.51696 0.35053  
C -2.18896 -1.19540 0.23636  
H -2.26128 -1.36030 1.31540  
H -2.70667 -2.01051 -0.27349  
C -0.55944 1.54702 -0.30320  
H -0.03620 2.38235 0.16158  
C -2.76073 0.16543 -0.16383  
H -3.78117 0.22404 0.22809  
H -0.65208 1.74177 -1.37455  
H -2.83478 0.21204 -1.25455  
C -1.94095 1.35730 0.34775  
H -1.83710 1.29517 1.43445  
H -2.51456 2.26951 0.14328