

Supporting Information for Discovery of Conical Intersection Mediated Photochemistry with Growing String Methods

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1 Introduction

This document contains seam maps, reaction paths and Cartesian coordinates x , y , z (in Å) for ethylene (CASSCF(4,4)/6-31G*), stilbene (CASSCF(2,2)/6-31G) and butadiene dimer (CASSCF(8,8)/6-31G*) depicted and/or discussed in the text.

2 SE-GSM for optimizing unique MECI.

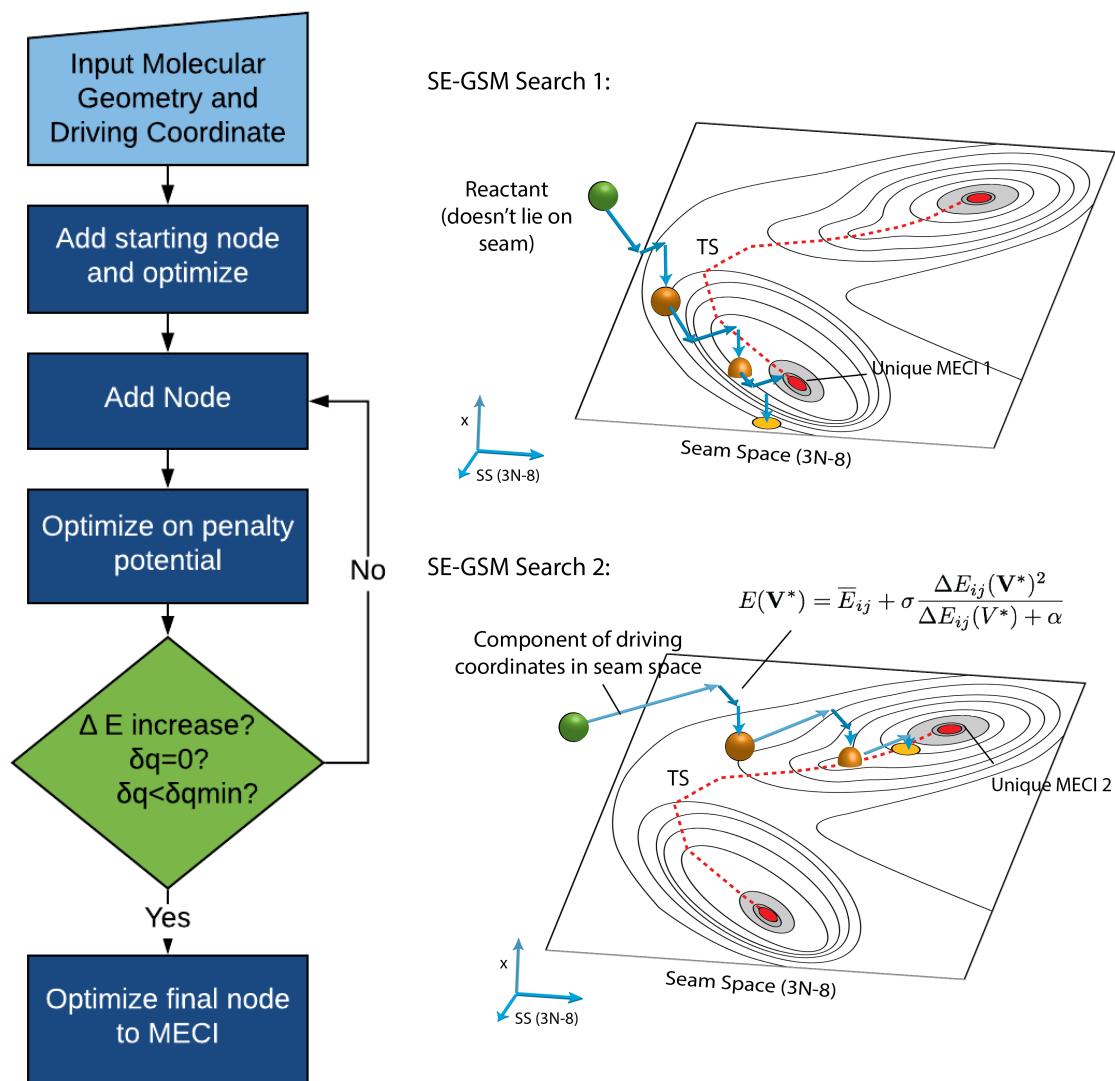


Figure 1: SE-GSM workflow for optimizing unique MECI.

3 Seam Minimum Energy Paths

3.1 Ethylene

Figure 2: DE-GSM seam from 1a to 1b using 11 nodes.

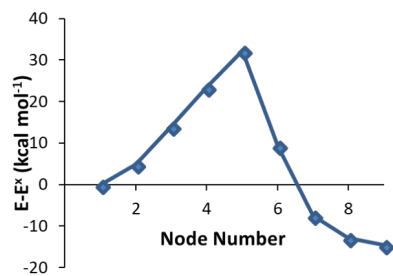


Figure 3: DE-GSM seam from 1a to 1b using 9 nodes.

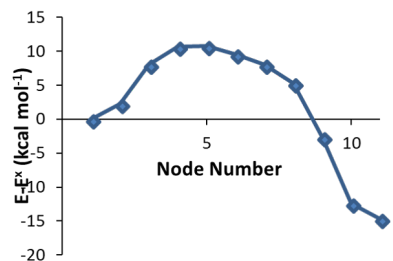
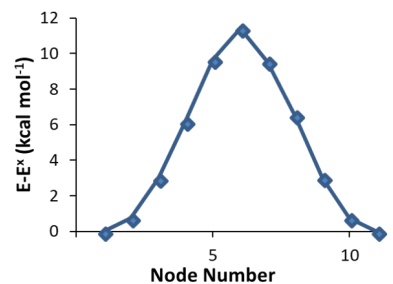


Figure 4: DE-GSM seam from 1a to 1a' (tilt isomer).



3.2 Stilbene

Figure 5: DE-GSM seam from 3a to 3b.

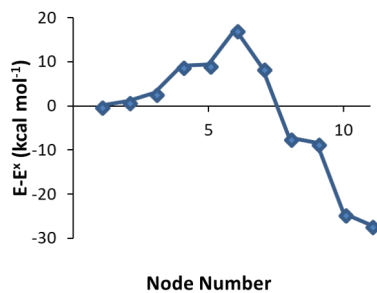


Figure 6: DE-GSM seam from 3a to 3c.

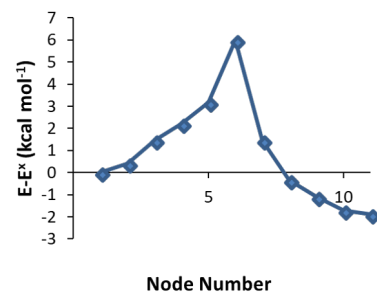
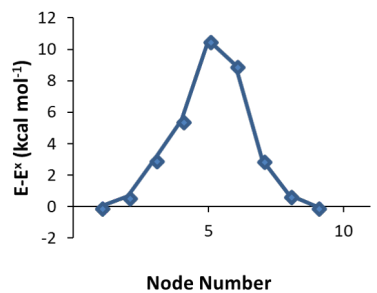


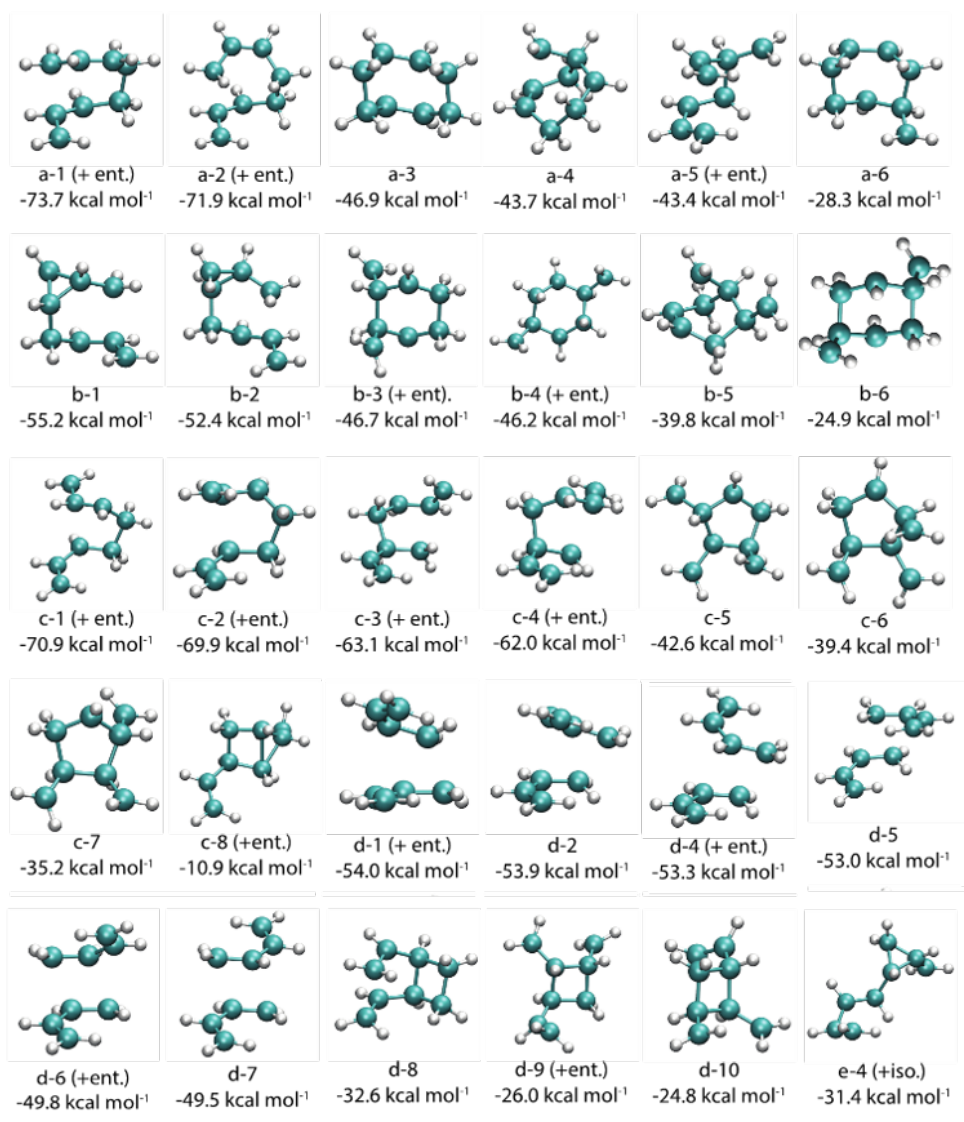
Figure 7: SE-GSM seam.



4 Butadiene Dimerization

4.1 MECI

Figure 8: MECI discovered by ZStruct SE-GSM search



4.2 Reaction paths

Figure 9: 4b to a-1

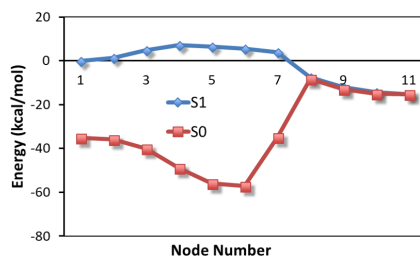


Figure 10: 4d to a-1 partial string

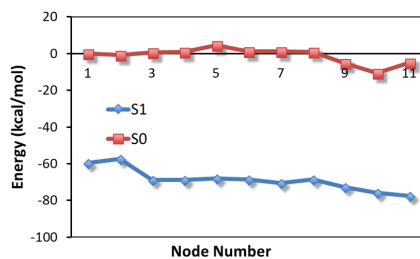


Figure 11: 4e to a-1

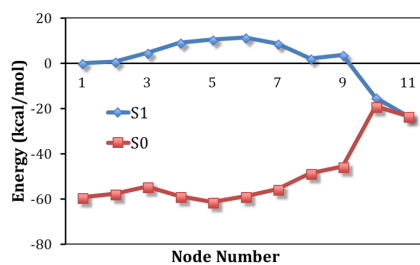


Figure 12: 4a to a-2

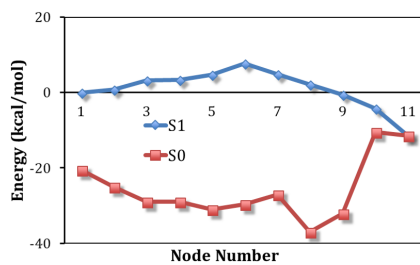


Figure 13: 4a to a-3

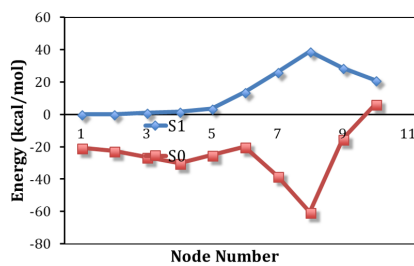


Figure 14: 4b to c-1

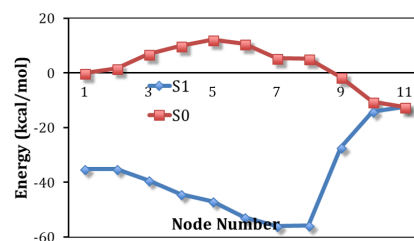


Figure 15: 4c to c-1

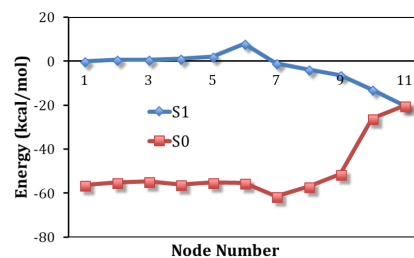


Figure 16: 4a to c-2

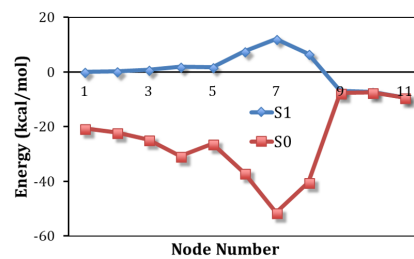


Figure 17: 4a to c-3

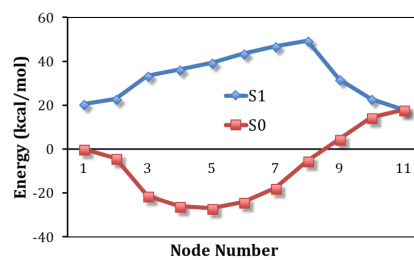


Figure 18: 4c to c-3

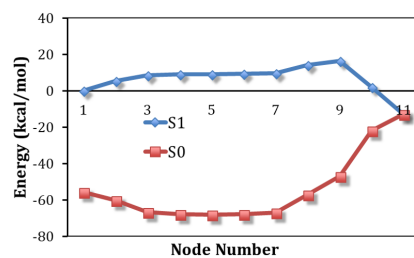


Figure 19: 4c to c-4

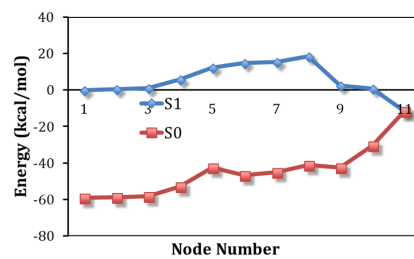


Figure 20: 5a to d-1

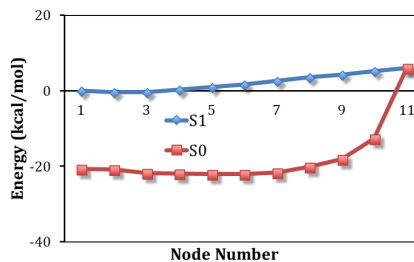


Figure 21: 4d to d-2

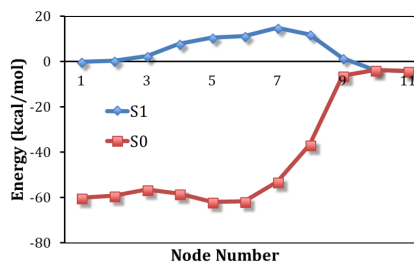


Figure 22: 4e to d-2

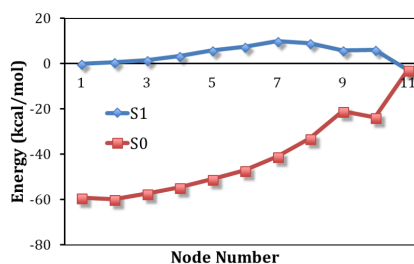


Figure 23: 4e to d-3

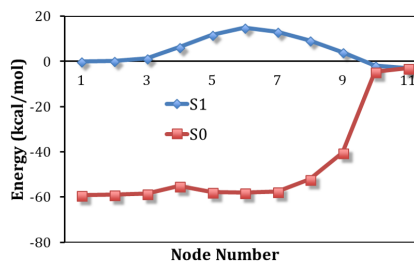
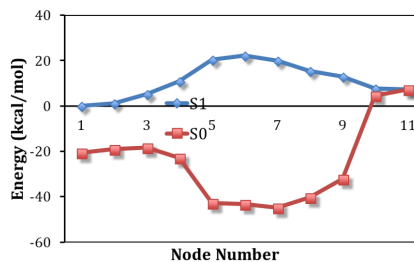


Figure 24: 4e to d-4



All reaction paths to b and e conical intersections involved multiple adiabatic barriers or had too large of reaction barriers and are not reported here.

5 Cartesian Coordinates

6	H -0.735906 1.067876 0.206007
Tw-pyr 1a	H 0.275140 0.974059 -0.920562
C -0.082986 0.760894 -0.369611	C 0.160553 -0.570468 0.019467
H -0.388347 0.745243 0.821728	H 0.749382 -1.308588 0.564650
H 0.822076 1.343303 -0.232077	H -0.563434 -1.047489 -0.645035
C -0.078431 -0.611718 -0.049799	
H 0.539792 -1.072753 0.712982	26
H -0.845366 -1.263038 -0.442630	3a
6	C -5.699148 1.154222 -0.569063
Et 1b	C -5.833133 -0.230975 -0.494420
C -0.307650 0.366051 -0.125929	C -5.432142 -0.897119 0.648328
H -0.830864 0.890128 0.670845	C -4.928483 -0.194746 1.750899
H 0.417053 1.062060 -0.553729	C -4.772086 1.183844 1.644782
C 0.398749 -0.818315 0.348342	C -5.166101 1.860373 0.496220
H 1.201792 -1.483648 0.534360	C -4.718250 -0.848896 3.222491
H -1.063491 0.143941 -0.914061	C -3.421149 -1.137657 2.728489
6	C -2.189526 -0.553095 3.249315
2a	C -0.965705 -0.818989 2.628531
C -0.013251 0.522991 0.093488	C 0.211014 -0.333376 3.166879
H -0.784217 1.189990 0.440730	C 0.168284 0.429902 4.329379
H 0.602873 0.900287 -0.707977	C -1.043603 0.705769 4.952663
C 0.161920 -0.708461 0.693623	C -2.222450 0.222479 4.411175
H 1.019648 -1.316052 0.442114	H -0.944059 -1.407957 1.730641
H -0.799002 -0.742752 -1.054796	H -3.184257 0.413176 4.845706
6	H -1.064159 1.295158 5.849095
2b	H 1.080798 0.811756 4.746676
C -0.013251 0.522991 0.093488	H 1.149428 -0.539713 2.692516
H -0.784217 1.189990 0.440730	H -3.222622 -1.776004 1.862291
H 0.602873 0.900287 -0.707977	H -5.429490 -1.666835 3.259439
C 0.161920 -0.708461 0.693623	H -5.528366 -1.965827 0.706302
H 1.019648 -1.316052 0.442114	H -4.370427 1.716746 2.483126
H -0.799002 -0.742752 -1.054796	H -5.059326 2.925426 0.437271
6	H -6.246813 -0.776180 -1.32158
2c, E=	H -6.006943 1.673336 -1.457448
C 0.400425 0.783333 0.201981	26
	3b
	C -5.314717 1.607943 0.347135
	C -6.159669 0.924905 1.284342

C -5.879635 -0.312718 1.753039
 C -4.704757 -1.028170 1.291906
 C -3.943408 -0.389928 0.232213
 C -4.258423 0.933322 -0.177001
 C -4.055928 -2.102275 1.917744
 C -2.781012 -1.396860 1.786077
 C -2.146007 -0.528045 2.785423
 C -0.809473 -0.168595 2.602034
 C -0.137217 0.564537 3.563559
 C -0.808653 0.957348 4.713136
 C -2.143613 0.615928 4.905150
 C -2.808192 -0.127724 3.948656
 H -0.300397 -0.467547 1.704425
 H -3.835352 -0.394070 4.085171
 H -2.654496 0.927411 5.795008
 H -0.294518 1.530722 5.460323
 H 0.890704 0.831233 3.419541
 H -2.087517 -1.637952 0.99795
 H -4.377312 -2.331133 2.918086
 H -6.520976 -0.797007 2.464152
 H -3.403166 -1.011619 -0.454220
 H -3.665753 1.381497 -0.955630
 H -7.046045 1.426239 1.629642
 H -5.561168 2.601870 0.032732

26

3c
 C -6.665056 0.860163 -0.800327
 C -7.069091 -0.092180 0.128084
 C -6.225743 -0.493392 1.148042
 C -4.937124 0.045627 1.277842
 C -4.543490 1.013034 0.338223
 C -5.398808 1.411787 -0.675933
 C -4.048271 -0.317128 2.377139
 C -2.722116 -0.730197 2.332992
 C -1.714285 -0.437958 3.339020
 C -0.438883 -1.000108 3.229229
 C 0.548156 -0.674435 4.141011
 C 0.259771 0.209983 5.174002
 C -1.007501 0.771080 5.296455
 C -1.996052 0.444197 4.386077
 H -0.226476 -1.683166 2.428178
 H -2.993131 0.832244 4.454422
 H -1.218031 1.448886 6.098848
 H 1.022328 0.459084 5.887063
 H 1.528717 -1.100391 4.052996

H -2.342941 -1.395832 1.548807
 H -4.097271 -1.506294 2.475564
 H -6.563816 -1.221481 1.862606
 H -3.573928 1.468468 0.425804
 H -5.068535 2.155539 -1.376324
 H -8.048087 -0.527572 0.055532
 H -7.322041 1.168920 -1.589390

26

3d
 C -6.429490 1.372377 -0.388729
 C -6.970385 0.503085 0.551138
 C -6.157417 -0.319333 1.306031
 C -4.757490 -0.299728 1.135766
 C -4.220947 0.590171 0.176746
 C -5.050843 1.408016 -0.564559
 C -3.915036 -1.135743 1.881932
 C -2.562590 -1.622193 2.213034
 C -1.789155 -0.787717 3.231633
 C -0.443288 -0.511868 3.023176
 C 0.286795 0.214185 3.956069
 C -0.326482 0.677308 5.108894
 C -1.671615 0.407459 5.324790
 C -2.397294 -0.318144 4.392081
 H 0.040107 -0.863142 2.130518
 H -3.438884 -0.514615 4.561930
 H -2.154545 0.763781 6.214831
 H 0.233583 1.242099 5.830110
 H 1.325105 0.419528 3.777997
 H -1.975912 -1.690050 1.29763
 H -2.641491 -2.642582 2.583070
 H -6.585216 -0.985316 2.029545
 H -3.158732 0.633632 0.032981
 H -4.620782 2.078078 -1.284516
 H -8.033619 0.468032 0.697095
 H -7.066998 2.009551 -0.969762

26

3e
 C -5.726724 1.799123 1.035769
 C -6.441414 0.583446 0.891326
 C -5.881900 -0.659739 1.022651
 C -4.519846 -0.790395 1.419649
 C -3.733891 0.446415 1.427838
 C -4.376914 1.691682 1.218217
 C -3.971079 -2.028127 1.807723

C -2.668445 -2.097641 2.322440
 C -2.018242 -1.021905 2.892604
 C -0.612422 -0.960197 3.080011
 C 0.026394 0.161006 3.504821
 C -0.785730 1.306655 3.781062
 C -2.130116 1.358334 3.606439
 C -2.857501 0.178774 3.154892
 H -0.048110 -1.850183 2.858846
 H -3.795586 -0.035598 3.648571
 H -2.683566 2.235447 3.878299
 H -0.303270 2.178312 4.189701
 H 1.083467 0.193168 3.665169
 H -2.145392 -3.041178 2.26865
 H -4.522898 -2.924801 1.611051
 H -6.482666 -1.539660 0.906955
 H -2.744172 0.376472 1.010403
 H -3.757160 2.570953 1.216884
 H -7.493115 0.638761 0.675772
 H -6.227536 2.741485 0.954031

26

3f
 C -6.817786 1.075369 -0.570128
 C -6.861279 1.152085 0.812687
 C -5.834707 0.589901 1.562495
 C -4.753191 -0.049348 0.965993
 C -4.730354 -0.106452 -0.434857
 C -5.757698 0.425590 -1.194274
 C -3.674751 -0.562311 1.821326
 C -2.323116 -0.543124 1.975450
 C -1.588952 -0.406049 3.248701
 C -0.197002 -0.480984 3.250238
 C 0.510146 -0.263404 4.417036
 C -0.172020 -0.001679 5.598647
 C -1.562689 0.070705 5.601487
 C -2.269264 -0.129235 4.430942
 H 0.324773 -0.688941 2.334424
 H -3.338886 -0.085262 4.393134
 H -2.083012 0.245756 6.519602
 H 0.364767 0.158856 6.513978
 H 1.581834 -0.325868 4.417986
 H -1.612543 -0.702796 1.147520
 H -3.269220 -1.689632 1.700308
 H -5.856156 0.620360 2.632582
 H -3.934653 -0.630009 -0.93081
 H -5.714889 0.381990 -2.264652

H -7.668581 1.676462 1.294244
 H -7.613095 1.496664 -1.158804

26

tilt CI between 3a and 3c
 C -6.069321 0.931601 -0.835515
 C -6.422022 -0.321947 -0.357152
 C -5.906908 -0.790101 0.843436
 C -5.053168 -0.004413 1.625677
 C -4.718745 1.262846 1.130586
 C -5.211714 1.720444 -0.081010
 C -4.489255 -0.398320 3.038670
 C -3.190347 -0.833964 2.668450
 C -1.978468 -0.455630 3.331194
 C -0.735146 -0.948358 2.902680
 C 0.416453 -0.564685 3.553027
 C 0.316451 0.307145 4.640004
 C -0.907256 0.804227 5.075016
 C -2.063372 0.418448 4.421646
 H -0.690583 -1.618520 2.064388
 H -3.051908 0.734279 4.690917
 H -0.949963 1.475055 5.908599
 H 1.212599 0.599536 5.153730
 H 1.374376 -0.923603 3.236210
 H -2.987877 -1.532821 1.842621
 H -4.818881 -1.510689 2.952707
 H -6.195986 -1.762832 1.195516
 H -4.111557 1.903783 1.740641
 H -4.938161 2.699616 -0.428642
 H -7.096913 -0.939740 -0.920434
 H -6.462556 1.290042 -1.767595

26

H-transfer CI between 3c and 3d
 C -6.685366 1.188188 -0.439462
 C -7.081594 0.121584 0.362895
 C -6.153147 -0.566149 1.116655
 C -4.799160 -0.168396 1.104567
 C -4.410243 0.915017 0.299864
 C -5.348701 1.579383 -0.461454
 C -3.856487 -0.901899 1.858101
 C -2.484074 -1.221878 2.120610
 C -1.681094 -0.680282 3.212280
 C -0.313911 -1.000105 3.293839
 C 0.487687 -0.434498 4.269805
 C -0.048477 0.468219 5.186350

C -1.391468 0.802947 5.112037
 C -2.203778 0.249297 4.130748
 H 0.108392 -1.698244 2.595753
 H -3.240246 0.524339 4.071056
 H -1.808205 1.505236 5.810688
 H 0.576196 0.905009 5.942170
 H 1.529786 -0.691615 4.316100
 H -1.964716 -1.816874 1.386199
 H -3.591927 -1.979581 2.428235
 H -6.453778 -1.356714 1.763247
 H -3.375739 1.225524 0.293755
 H -5.043573 2.404939 -1.074344
 H -8.111811 -0.174393 0.387182
 H -7.408371 1.712974 -1.031846

20

4a

C 0.5497162 0.8993740 1.3066672
 C 0.2326419 1.4302154 0.0339199
 C 0.0259408 0.6419201 -1.1013657
 C 0.2952045 -0.7365562 -1.2358064
 H 0.6044930 1.5651792 2.1470983
 H 0.2685134 -0.1070958 1.5476513
 H 0.1980889 2.4988494 -0.0777508
 H -0.2335842 1.1672355 -2.0065194
 H 0.3755582 -1.3602735 -0.3641462
 H -0.0181827 -1.2391789 -2.1336207
 C 2.5744195 -0.3506832 -1.5296890
 C 2.9991653 0.8690073 -0.9515002
 C 3.1686928 1.0538044 0.4233193
 C 2.7613553 0.1785225 1.4521815
 H 2.5551093 -0.4380824 -2.5995514
 H 2.7375300 -1.2722364 -1.0059398
 H 3.1512497 1.7135697 -1.5989889
 H 3.5202062 2.0244419 0.7346419
 H 2.5789689 -0.8592669 1.2399741
 H 3.0570324 0.3961226 2.4631532

20

4b

C 0.3941324 0.0054487 1.7610230
 C -0.0818073 1.1411981 1.0470535
 C -0.0641480 1.3014698 -0.3417562
 C 0.4346817 0.3574559 -1.2831326
 H 0.2188458 -0.0352153 2.8210463
 H 0.4396261 -0.9490527 1.2737306

H -0.3935686 1.9907240 1.6311428
 H -0.3631617 2.2627633 -0.7246281
 H 0.4720446 -0.6829823 -1.0245965
 H 0.2865782 0.5593264 -2.3287641
 C 2.7150639 0.1709114 1.8110558
 C 3.2128310 -0.7722894 0.8683033
 C 3.2317378 -0.6095967 -0.5202258
 C 2.7547767 0.5267524 -1.2325747
 H 2.8623667 -0.0332064 2.8563531
 H 2.6795421 1.2118678 1.5546702
 H 3.5105468 -1.7345367 1.2497587
 H 3.5425180 -1.4586633 -1.1055153
 H 2.7075905 1.4802164 -0.7432665
 H 2.9303878 0.5697549 -2.2924582

20

4c

C 0.2598875 0.1268739 0.2006774
 C -0.2676335 -0.4951013 -1.0006104
 C -0.8591102 -1.7435498 -1.0786062
 C -1.0911658 -2.6367185 0.0084073
 H 0.4468186 1.1842943 0.1601307
 H -0.0654963 -0.2323746 1.1600480
 H -0.1388041 0.0493992 -1.9193486
 H -1.1811544 -2.0740961 -2.0513795
 H -0.8064751 -2.3986919 1.0142733
 H -1.5720494 -3.5811388 -0.1568714
 C 2.4262948 -0.4946393 0.3984334
 C 3.0382013 -0.3776024 -0.9130900
 C 3.6493124 0.7517067 -1.4286049
 C 3.8219481 1.9982312 -0.7580969
 H 2.2287885 -1.4881367 0.7571566
 H 2.6936413 0.2112506 1.1636601
 H 2.9619835 -1.2361311 -1.5567338
 H 4.0375116 0.6854727 -2.4306903
 H 3.4711827 2.1626625 0.2416030
 H 4.3254515 2.8115883 -1.2433119

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4d

C 0.3203299 0.6719172 0.0643704
 C -0.1671896 1.8420659 -0.6413292
 C -0.4308678 1.9181885 -1.9963736
 C -0.3173385 0.8487524 -2.9397588
 H 0.2200314 0.6666270 1.1349548
 H 0.2082421 -0.2936912 -0.3917983

H -0.2803585 2.7442260 -0.0649871
H -0.7570896 2.8687366 -2.3824717
H -0.0207848 -0.1396602 -2.6499236
H -0.5481860 1.0118878 -3.9744102
C 2.5574177 0.7043454 0.0139228
C 3.0406136 -0.5940053 0.4449059
C 3.2700487 -1.6844192 -0.3735185
C 3.1186782 -1.7190864 -1.7956417
H 2.6853473 1.5269016 0.6945644
H 2.6459415 0.9737286 -1.0217657
H 3.1799399 -0.7331659 1.5032493
H 3.5976343 -2.5948485 0.0985410
H 2.8172572 -0.8586079 -2.3592291
H 3.3242266 -2.6196115 -2.3408127

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4e
C -0.6362103 2.9423057 1.2139681
C -0.7763547 2.7088043 -0.1902265
C -0.3925700 1.5686626 -0.8714318
C 0.2588447 0.4071894 -0.2947428
H -0.9805459 3.8602018 1.6488352
H -0.2101261 2.2129910 1.8740413
H -1.2266240 3.4985728 -0.7668744
H -0.5434870 1.5581351 -1.9372893
H 0.1885727 0.2469800 0.7653971
H 0.2607544 -0.4967401 -0.8759204
C 2.4746281 0.7340963 -0.3567428
C 3.1255148 -0.4225638 0.2302587
C 3.5108920 -1.5679688 -0.4411326
C 3.3734666 -1.8127131 -1.8437152
H 2.4714732 1.6426647 0.2171453
H 2.5463580 0.8856929 -1.4180767
H 3.2744884 -0.4034669 1.2962397
H 3.9603776 -2.3529640 0.1425444
H 2.9473238 -1.0893762 -2.5102429
H 3.7177932 -2.7344828 -2.2703230

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a-1

C 0.549382 -0.42442 1.498531
C 0.162041 0.91093 1.081917
C 0.234782 1.388326 -0.187371
C 0.760982 0.621607 -1.375041
H 0.475523 -0.648394 2.548588
H 0.288794 -1.249488 0.862266
H -0.114816 1.60228 1.860971

H -0.036111 2.417216 -0.355264
H 0.239782 -0.324183 -1.490056
H 0.578157 1.190088 -2.280855
C 3.266038 0.616369 1.763655
C 2.717573 -0.573379 1.12235
C 2.646598 -0.761438 -0.303522
C 2.315745 0.321454 -1.287001
H 3.360414 0.637715 2.833215
H 3.299222 1.558177 1.252812
H 2.859312 -1.481714 1.684626
H 2.411991 -1.763124 -0.627721
H 2.832623 1.247 -1.053662
H 2.646662 0.014683 -2.275961

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a-2

C 0.78942 0.197651 0.041404
C 0.309467 0.662176 -1.309631
C 0.241877 -0.16545 -2.381875
C 0.52919 -1.591223 -2.308656
H 0.471967 0.880236 0.822578
H 0.359786 -0.769884 0.279612
H 0.134848 1.715893 -1.448652
H 0.041719 0.257368 -3.353075
H 0.125151 -2.129998 -1.471873
H 0.50347 -2.146906 -3.230664
C 2.480014 -2.99436 -0.720314
C 2.639758 -1.858921 -1.619624
C 2.955946 -0.528795 -1.155377
C 2.369469 0.074332 0.091707
H 2.31082 -3.973593 -1.127767
H 2.247614 -2.851118 0.31808
H 3.048367 -2.105658 -2.585833
H 3.266816 0.166998 -1.914786
H 2.633932 -0.500007 0.976224
H 2.787362 1.066777 0.22857

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a-3

C 0.877578 0.550891 1.420274
C 0.79688 1.405481 0.161632
C 0.422689 0.883191 -1.150325
C 0.602922 -0.580287 -1.493327
H 0.423641 1.050842 2.269921
H 0.389267 -0.409495 1.304637
H 0.62262 2.458278 0.299345

H -0.088688 1.53995 -1.831354
H 0.071633 -1.28308 -0.853836
H 0.282004 -0.771065 -2.511178
C 2.168224 -0.695596 -1.361935
C 2.47965 0.759241 -1.031743
C 2.84516 1.226149 0.303348
C 2.447173 0.451148 1.54122
H 2.645326 -1.005324 -2.286989
H 2.48934 -1.376731 -0.58298
H 2.817619 1.380623 -1.84161
H 3.501237 2.074552 0.382356
H 2.804194 -0.575222 1.587907
H 2.804113 0.951875 2.432765

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a-4
C 0.597257 0.999714 0.995008
C 0.472389 1.309714 -0.469474
C 0.246637 0.250607 -1.502615
C 0.919311 -1.092116 -1.336357
H 0.332082 1.865746 1.59469
H -0.075021 0.192606 1.279796
H 0.348194 2.33004 -0.779997
H -0.653435 0.298799 -2.101043
H 0.450515 -1.757195 -0.612184
H 0.933059 -1.614975 -2.288744
C 2.077888 0.584368 1.360958
C 2.588272 -0.57178 0.545108
C 2.38703 -0.659203 -0.945183
C 2.429358 0.672241 -1.671942
H 2.135778 0.343319 2.418035
H 2.703998 1.460703 1.206243
H 2.698926 -1.518884 1.047247
H 3.118242 -1.357707 -1.347086
H 3.002678 1.487448 -1.265256
H 2.474609 0.61429 -2.746844

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a-5
C 0.61426 -0.156138 -0.211037
C 0.090208 1.206025 0.222811
C -0.398898 2.189293 -0.668455
C 0.008555 2.2586 -2.010364
H 0.196425 -0.977066 0.36273
H 0.405203 -0.355318 -1.256184
H -0.181203 1.303746 1.261108

H -0.807837 3.082018 -0.2242
H 0.174902 1.36295 -2.578362
H -0.249587 3.122956 -2.596573
C 2.270075 2.245805 -1.376265
C 2.219863 1.57984 -0.08336
C 2.150728 0.057977 0.034345
C 3.116457 -0.655998 -0.852418
H 2.469952 3.301558 -1.389105
H 2.590859 1.714764 -2.25134
H 2.629622 2.122511 0.752147
H 2.361198 -0.203125 1.066702
H 3.048613 -0.563717 -1.919973
H 3.811516 -1.378105 -0.46801

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a-6
C 0.876965 -0.195113 1.300882
C 0.792758 0.665595 0.030842
C 0.847148 0.012399 -1.358415
C 0.236323 -1.323629 -1.560117
H 0.328791 0.294326 2.099229
H 0.471737 -1.195026 1.196342
H 0.116144 1.503264 0.099972
H 0.417656 0.708789 -2.069908
H 0.23425 -2.057104 -0.774924
H 0.246878 -1.723554 -2.559794
C 2.430388 0.114095 -1.557996
C 2.710383 1.299661 -0.683649
C 2.715692 1.208586 0.879738
C 2.400055 -0.103925 1.573693
H 2.713282 0.281375 -2.58988
H 2.923801 -0.787639 -1.217544
H 2.379389 2.248786 -1.071822
H 2.344937 2.088751 1.379405
H 2.942378 -0.930675 1.126313
H 2.657107 -0.079666 2.626472

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b-1
C -0.065674 0.31691 0.75803
C 0.990848 0.02304 -0.248806
C 0.086361 -1.103387 0.203202
C 0.529079 -2.210653 1.108123
H -0.905886 0.924274 0.468763
H 0.240591 0.4562 1.781517
H 0.781123 0.385162 -1.242299

H -0.645792 -1.40396 -0.529211
H 0.360063 -2.079388 2.163363
H 0.324721 -3.210021 0.764256
C 2.507248 0.080549 0.095131
C 2.880828 -0.775376 1.267792
C 2.781499 -2.198961 1.181914
C 3.018764 -2.987063 -0.017694
H 2.776881 1.116956 0.274533
H 3.059232 -0.234179 -0.785504
H 2.807162 -0.342134 2.250465
H 2.902221 -2.736917 2.107379
H 2.929819 -2.553685 -0.994951
H 2.971705 -4.057851 0.044933

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b-2
C 0.106506 2.020423 0.417016
C -0.258012 0.593502 0.174769
C 0.806316 -0.442467 -0.090772
C 0.076746 -0.495248 1.20871
H -0.532811 2.759599 -0.03311
H 0.432831 2.281387 1.407909
H -1.176465 0.454322 -0.372289
H 0.545823 -1.195273 -0.81628
H 0.603139 -0.18443 2.096116
H -0.642626 -1.278869 1.371382
C 2.285671 0.026705 -0.200767
C 2.3385 1.178426 -1.167328
C 2.051667 2.5045 -0.70014
C 2.756317 3.139174 0.409818
H 2.899236 -0.805677 -0.53183
H 2.653131 0.324717 0.775099
H 2.018353 0.947259 -2.170772
H 1.665623 3.193277 -1.434595
H 3.373473 2.562979 1.073059
H 2.441361 4.107342 0.752063

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b-3
C 0.313776 -1.392889 1.519919
C 0.644994 0.050811 1.252441
C 0.149875 0.502665 -0.089338
C 0.706296 -0.204104 -1.287248
H 0.802456 -1.901836 2.331866
H -0.63968 -1.785147 1.211643
H 0.216773 0.676963 2.033177

H -0.104245 1.543776 -0.197256
H 0.404409 -1.246933 -1.288912
H 0.348891 0.240797 -2.210296
C 2.655991 1.665958 1.400544
C 2.249624 0.218873 1.308721
C 2.803585 -0.505526 0.10945
C 2.29409 -0.159627 -1.25493
H 3.300437 2.004143 2.190314
H 2.473502 2.344536 0.588086
H 2.592133 -0.281227 2.209134
H 3.667605 -1.134156 0.218691
H 2.598816 0.84719 -1.541229
H 2.699877 -0.834719 -2.002911

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b-4
C -0.260812 0.464624 2.20746
C 0.626176 0.761598 1.033661
C 0.116206 0.14175 -0.247136
C 0.90987 -0.931406 -0.930625
H -0.301218 1.147024 3.037814
H -0.558238 -0.550074 2.403793
H 0.661116 1.841807 0.90348
H -0.92332 0.270132 -0.492756
H 0.948929 -1.834254 -0.321964
H 0.449486 -1.21629 -1.871474
C 3.291419 -1.601653 -1.560665
C 2.394363 -0.449982 -1.20264
C 2.88997 0.331451 -0.012484
C 2.1265 0.288705 1.273767
H 3.18646 -2.069512 -2.524835
H 3.719864 -2.203837 -0.778069
H 2.350055 0.217653 -2.062229
H 3.871951 0.765873 -0.052152
H 2.102487 -0.723996 1.676304
H 2.585745 0.9158 2.030132

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b-5
C 0.885433 1.145234 0.919512
C 0.285408 1.410499 -0.420987
C 0.044904 0.239604 -1.331408
C 0.864464 -0.988414 -1.015264
H 1.120425 2.065589 1.440331
H 0.193787 0.588729 1.548369
H 0.068639 2.403557 -0.762253

H -0.852454 0.17843 -1.925374
H 0.484419 -1.609632 -0.203187
H 0.962699 -1.623386 -1.891853
C 3.469251 1.006035 1.071078
C 2.223493 0.250114 0.741891
C 2.221898 -0.282404 -0.695815
C 2.080055 0.867139 -1.675318
H 3.62569 1.389067 2.063368
H 4.280356 1.08857 0.372077
H 2.135089 -0.593902 1.423977
H 3.098275 -0.900398 -0.871692
H 2.570825 1.804887 -1.472
H 2.098843 0.607112 -2.721674

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b-6
C 0.262999 0.732547 2.05633
C 0.830738 1.204424 0.738377
C 0.455839 0.34378 -0.506171
C 0.843901 -1.128663 -0.608379
H 0.52798 1.254434 2.956753
H -0.577756 0.067953 2.096026
H 0.475886 2.21994 0.567136
H 0.666677 0.884816 -1.418759
H 0.50281 -1.679121 0.260396
H 0.361248 -1.584448 -1.466421
C 2.365853 1.123938 0.672633
C 2.650959 -0.369423 0.554506
C 2.397256 -1.196351 -0.719857
C 2.839918 -0.833084 -2.094956
H 2.849997 1.540566 1.554771
H 2.737683 1.676624 -0.184319
H 2.259936 -0.9035 1.407017
H 2.755388 -2.210528 -0.539765
H 3.109551 0.175457 -2.359573
H 2.422953 -1.420665 -2.89405

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c-1
C 0.793357 -0.21967 0.840579
C 0.521383 -0.029356 -0.638297
C -0.215821 -0.989835 -1.43661
C -0.487492 -2.286155 -1.134981
H 0.152131 0.427582 1.433837
H 0.588581 -1.239392 1.143824
H 0.367522 0.993459 -0.934426

H -0.542348 -0.629971 -2.398885
H -0.19681 -2.744438 -0.208313
H -1.019682 -2.90965 -1.830366
C 2.316692 0.084054 1.141571
C 3.047128 -0.564998 0.003886
C 2.653168 -0.095538 -1.295176
C 2.820357 1.307993 -1.709822
H 2.604367 -0.303771 2.111833
H 2.47084 1.158739 1.156616
H 3.225242 -1.623868 0.099561
H 2.709961 -0.805519 -2.106389
H 3.151773 2.056964 -1.018177
H 2.417417 1.638629 -2.647152

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c-2
C 0.281074 1.173759 2.479564
C 0.308761 1.546642 1.171722
C 0.76531 0.761138 0.048529
C 0.93168 -0.75054 0.117384
H -0.047306 1.857721 3.240126
H 0.569783 0.192389 2.808418
H 0.015995 2.557882 0.939606
H 0.448232 1.139706 -0.908613
H 0.456381 -1.166523 0.998441
H 0.447943 -1.201937 -0.74368
C 2.46834 -1.149334 0.088042
C 3.117352 -0.088825 -0.746463
C 2.923528 1.245979 -0.266931
C 3.376221 1.670929 1.072057
H 2.598892 -2.146281 -0.317357
H 2.855587 -1.153812 1.10208
H 3.083326 -0.232423 -1.814838
H 2.950386 2.032861 -1.004317
H 3.570505 0.95329 1.845013
H 3.237655 2.691089 1.37499

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c-3
C -0.450063 -0.826151 2.601373
C 0.212568 0.222907 2.097088
C 0.812116 0.36444 0.717491
C 0.743954 -0.857901 -0.175546
H -0.834102 -0.803483 3.606501
H -0.635853 -1.723223 2.039435
H 0.340082 1.091216 2.726195

H 0.284312 1.1745 0.21757
H 0.824943 -1.827342 0.280842
H 0.074068 -0.827343 -1.016723
C 3.41639 -1.818115 -0.485289
C 2.805489 -0.653221 -1.129491
C 2.857701 0.676897 -0.595609
C 2.333094 0.834733 0.799067
H 3.225536 -2.797412 -0.882296
H 3.793689 -1.760874 0.517525
H 2.687884 -0.745761 -2.198221
H 2.6389 1.480139 -1.280275
H 2.860432 0.202494 1.506351
H 2.396739 1.855748 1.160103

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c-4
C 0.581867 -0.805837 0.863236
C -0.057365 0.456941 0.374068
C 0.290128 0.834493 -0.964539
C 0.10555 -0.03011 -2.130909
H 0.293263 -1.066548 1.87595
H 0.344874 -1.649617 0.22379
H -0.13078 1.258663 1.08969
H 0.295816 1.889296 -1.188725
H -0.170052 -1.061369 -2.021638
H 0.480831 0.281081 -3.086887
C 2.735438 1.45774 2.280365
C 2.629447 0.142574 2.049205
C 2.161631 -0.532974 0.776979
C 2.437141 0.234438 -0.500621
H 3.036742 1.826979 3.244467
H 2.521166 2.199357 1.53259
H 2.832694 -0.532711 2.864972
H 2.652203 -1.501381 0.721161
H 2.937295 1.182621 -0.434984
H 2.714371 -0.344646 -1.363189

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c-5
C -0.152325 -0.634642 1.544077
C 0.796338 0.105771 0.652758
C 0.574924 -0.070319 -0.865087
C 0.290342 -1.486448 -1.274069
H -0.012253 -0.582252 2.610013
H -1.138312 -0.884191 1.198178
H 0.720531 1.1731 0.863518

H -0.239128 0.5639 -1.205473
H 0.847472 -2.297217 -0.837808
H -0.150136 -1.673738 -2.23748
C 2.953307 0.405017 2.057142
C 2.323688 -0.294491 0.888174
C 2.964553 0.01762 -0.444542
C 1.942482 0.455595 -1.461002
H 2.852554 -0.004145 3.046585
H 3.174251 1.455632 1.983988
H 2.365069 -1.367213 1.077889
H 3.870359 -0.481877 -0.737404
H 1.898662 1.542352 -1.525904
H 2.135267 0.082786 -2.461183

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c-6
C 0.03741 0.711542 1.783972
C 0.552751 0.996659 0.398507
C -0.005995 0.023925 -0.612144
C 0.94401 -1.120131 -0.850582
H -0.105865 1.506482 2.491838
H -0.0039 -0.296175 2.150579
H 0.3046 2.022632 0.143455
H -0.723598 0.325924 -1.351831
H 0.541742 -2.056894 -0.472
H 1.141927 -1.274903 -1.908551
C 2.468061 -1.614124 1.144998
C 2.26859 -0.739291 -0.060616
C 2.107939 0.774208 0.242692
C 2.909727 1.324325 1.38516
H 2.299184 -2.671892 1.045758
H 3.13577 -1.311557 1.930007
H 3.121875 -0.869251 -0.726017
H 2.395444 1.298989 -0.671868
H 3.94031 1.035596 1.49938
H 2.656172 2.299942 1.765974

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c-7
C 0.549151 0.301573 1.083287
C -0.076428 0.33421 -0.280565
C 0.818136 -0.434533 -1.212603
C 0.514224 -1.915566 -1.13029
H 0.258432 1.131678 1.715288
H 0.264608 -0.614863 1.598083
H -0.626716 1.192378 -0.62301

H 0.694311 -0.114336 -2.242927
H -0.191618 -2.284359 -0.409345
H 0.681498 -2.532941 -1.995229
C 2.768248 1.550285 1.267625
C 2.118416 0.27515 0.809408
C 2.293322 -0.072285 -0.706894
C 2.907418 0.996948 -1.562052
H 2.544931 1.893811 2.263556
H 3.725062 1.844186 0.875254
H 2.543047 -0.539736 1.394237
H 2.906781 -0.963512 -0.802185
H 2.790454 2.03902 -1.331184
H 3.111963 0.757852 -2.590839

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d-1
C 0.350448 -2.309985 0.747267
C 0.447894 -0.988177 1.058507
C 0.32628 0.083935 0.116478
C -0.01972 -0.029723 -1.275141
H 0.475388 -3.062797 1.502486
H 0.099356 -2.653088 -0.237378
H 0.706162 -0.70698 2.063451
H 0.250696 1.069504 0.539295
H -0.148886 -0.995238 -1.723014
H -0.514828 0.795448 -1.751128
C 2.006883 0.50459 -1.181036
C 2.756174 0.212748 0.033589
C 3.416127 -1.021432 0.24529
C 3.312317 -2.155883 -0.51775
H 1.856151 1.543471 -1.413583
H 2.225421 -0.089512 -2.048363
H 2.909535 1.016082 0.729254
H 4.0229 -1.082449 1.135426
H 2.726948 -2.193003 -1.418297
H 3.867625 -3.040046 -0.268302

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d-2
C -0.370588 2.754702 1.162351
C -0.364419 2.485408 -0.165008
C 0.109467 1.286751 -0.818411
C 0.42633 0.048728 -0.127644
H -0.748364 3.690156 1.531992
H -0.017032 2.057347 1.900516
H -0.72186 3.25602 -0.829038

H -0.014093 1.225832 -1.883721
H 0.178578 -0.044217 0.913191
H 0.377832 -0.864884 -0.687501
C 2.309625 1.095968 -0.551691
C 2.570637 -0.136183 0.165463
C 3.068644 -1.350223 -0.450328
C 3.175136 -1.625752 -1.771288
H 2.346707 2.021256 -0.012041
H 2.545045 1.162637 -1.597071
H 2.676871 -0.053681 1.2322
H 3.344929 -2.129333 0.242197
H 2.910245 -0.919555 -2.538873
H 3.546438 -2.576795 -2.107087

20

d-3
C 0.275947 -1.760775 2.335833
C -0.064246 -0.469345 2.090019
C 0.129146 0.27967 0.877295
C 0.543278 -0.310054 -0.386616
H 0.073543 -2.212045 3.289573
H 0.740878 -2.391813 1.598096
H -0.51517 0.0834 2.89994
H -0.228224 1.290189 0.846807
H 0.474513 -1.376392 -0.494482
H 0.295131 0.234408 -1.276985
C 2.79952 2.778531 -0.360034
C 2.486681 1.894494 0.612741
C 2.391977 0.451131 0.443708
C 2.608151 -0.253531 -0.791581
H 2.850532 3.831945 -0.149527
H 3.015087 2.477496 -1.368408
H 2.281003 2.257986 1.603076
H 2.499867 -0.12494 1.341411
H 2.73506 0.282872 -1.711415
H 3.00743 -1.248995 -0.751354

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d-4
C 0.449452 0.236315 0.139822
C 0.305718 1.542778 -0.477328
C -0.073465 1.761806 -1.856966
C -0.084772 0.863985 -2.870528
H 0.251604 0.142603 1.190775
H 0.23455 -0.638569 -0.442274
H 0.200059 2.378867 0.190738

H -0.355908 2.775653 -2.090406
H 0.210737 -0.162055 -2.742797
H -0.391495 1.155757 -3.857852
C 2.449361 1.028727 -0.307421
C 2.571571 -0.270671 0.326914
C 2.881785 -1.49055 -0.390853
C 2.894593 -1.678689 -1.732002
H 2.678375 1.915898 0.250514
H 2.607072 1.10611 -1.366091
H 2.739857 -0.274876 1.388147
H 3.093761 -2.343816 0.232807
H 2.68662 -0.889589 -2.432766
H 3.136408 -2.639083 -2.149316

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d-5
C -0.059827 -1.394861 1.959542
C 0.390808 -0.247756 1.415276
C 0.527465 0.006125 -0.020617
C 0.150399 -0.949228 -1.034722
H -0.131944 -1.503764 3.026853
H -0.3688 -2.235157 1.369218
H 0.689432 0.558815 2.061017
H 0.445362 1.039393 -0.301326
H -0.056672 -1.967785 -0.779335
H -0.227346 -0.589457 -1.973559
C 3.338016 -2.77716 -0.234179
C 2.678875 -2.065083 -1.16948
C 2.34966 -0.641326 -1.075882
C 2.714932 0.204858 0.034524
H 3.549125 -3.819805 -0.388245
H 3.682843 -2.346124 0.685377
H 2.351574 -2.557896 -2.068042
H 2.241203 -0.149051 -2.023901
H 3.119057 -0.229692 0.927777
H 2.98907 1.223856 -0.172791

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d-6
C 0.267969 2.186153 1.819303
C 0.586555 1.937186 0.534078
C 0.596801 0.613526 -0.095031
C 0.267912 -0.612694 0.589516
H 0.277828 3.189612 2.202537
H -0.01302 1.411195 2.504817
H 0.859862 2.757227 -0.107427

H 0.388524 0.621202 -1.147594
H 0.214399 -0.642244 1.660654
H -0.265118 -1.372696 0.051051
C 2.743143 0.609187 -0.617852
C 2.424864 -0.602321 0.097772
C 2.459975 -1.944948 -0.489585
C 2.800719 -2.22898 -1.761738
H 3.289085 1.376291 -0.103177
H 2.804177 0.603345 -1.689259
H 2.618362 -0.573489 1.153538
H 2.187263 -2.748236 0.172661
H 3.08185 -1.470562 -2.467577
H 2.8096 -3.24524 -2.114227

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d-7

C 1.056001 2.164844 1.526574
C 0.579196 1.877705 0.173265
C 0.986415 0.598022 -0.526493
C 0.946234 -0.706113 0.301784
H 0.842198 3.150893 1.895866
H 0.971903 1.40126 2.280124
H 0.251588 2.706915 -0.426358
H 0.560153 0.529109 -1.5191
H 0.341206 -0.665805 1.199659
H 0.650383 -1.578705 -0.269675
C 2.510964 -0.613738 0.51973
C 2.570911 0.630704 -0.397948
C 2.742542 2.010156 0.202751
C 3.111985 2.29376 1.576538
H 3.055509 -1.460512 0.120408
H 2.823812 -0.46848 1.545232
H 3.184977 0.499895 -1.284273
H 2.837481 2.801393 -0.517868
H 3.518227 1.501558 2.179481
H 3.487431 3.278551 1.798921

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d-8

C 0.950099 -0.330873 0.863332
C 0.867645 0.015961 -0.641285
C 0.082207 -0.862719 -1.562113
C 0.229831 -2.324755 -1.601034
H 0.322916 0.258313 1.522423
H 0.790926 -1.383034 1.071378
H 0.546894 1.045449 -0.769733
H -0.636383 -0.408602 -2.224042

H -0.251826 -2.963168 -0.881699
H 0.840909 -2.806369 -2.344731
C 2.810965 1.364573 1.465205
C 2.493086 0.042935 0.859637
C 2.453589 -0.040328 -0.70933
C 3.158104 0.971611 -1.545847
H 3.630586 1.486446 2.145967
H 2.255707 2.244314 1.196341
H 3.122818 -0.7202 1.302595
H 2.754579 -1.038059 -1.012677
H 2.939743 2.01758 -1.432118
H 4.040115 0.715371 -2.10243

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d-9

C 0.011767 0.951104 1.571169
C 0.696131 0.663893 0.280274
C 0.732709 -0.799241 -0.264732
C 0.120984 -1.891114 0.541796
H -0.421932 1.919841 1.744466
H 0.244044 0.369442 2.445055
H 0.316774 1.337584 -0.479957
H 0.345231 -0.839435 -1.282198
H -0.456293 -1.704237 1.424251
H 0.282651 -2.91407 0.25569
C 2.284446 0.682235 0.301732
C 2.331153 -0.752543 -0.29568
C 2.976589 -0.912702 -1.634342
C 2.505823 -0.194205 -2.831364
H 2.70301 0.746148 1.300539
H 2.734881 1.458102 -0.30716
H 2.767473 -1.462633 0.397576
H 3.934477 -1.406947 -1.685169
H 2.819475 0.817096 -3.028855
H 2.097831 -0.734068 -3.668168

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d-10

C -0.20024 0.807195 2.352505
C -0.004701 1.452936 1.042362
C 0.718051 0.829992 -0.119836
C 0.719039 -0.71376 -0.202655
H 0.438268 1.050816 3.184968
H -1.1303 0.320193 2.59028
H -0.250019 2.500429 0.959686
H 0.378785 1.314034 -1.030402

H 0.071543 -1.223772 0.497794
H 0.515646 -1.084079 -1.201033
C 2.611722 -1.300756 1.506182
C 2.27271 -0.754205 0.158696
C 2.315624 0.791963 -0.019953
C 2.953753 1.644535 1.029857
H 2.799675 -2.355122 1.608214
H 2.305509 -0.78028 2.394589
H 2.855158 -1.277496 -0.592772
H 2.739093 1.032768 -0.994692
H 3.859999 1.319054 1.507959
H 2.768706 2.703523 1.017074