

Supporting information for the manuscript “Cyclooctyne-based Reagents for Uncatalyzed Click Chemistry: A Computational Survey” by Kimberly Chenoweth, David M. Chenoweth, and William A. Goddard, III

Figure S1. Activation energy dependence on transannular H-H repulsion, alkyne angle, transannular hybridization induced ring strain (THIRS) angle and THIRS distance.

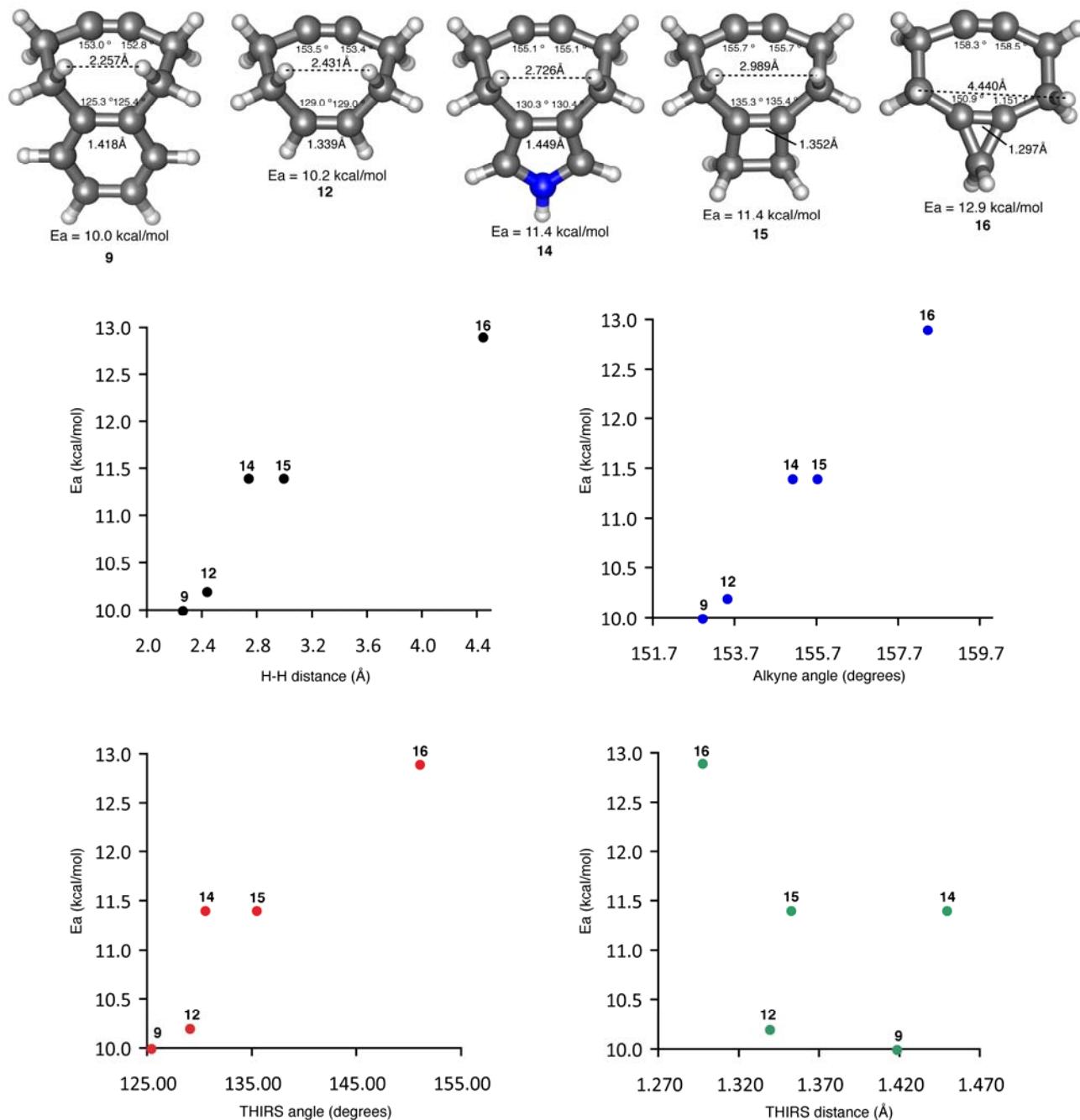


Table 1. Solvation free energies for reported transition states.^a

Structure	ΔG^\ddagger (kcal/mol)
1a-ts1	25.2
1b-ts1	28.1
1b-ts2	27.6
1c-ts1	28.5
1c-ts2	27.3
1d-ts1	26.9
1d-ts2	25.3
1e-ts1	25.8
1e-ts2	25.4
4-ts1	27.3
4-ts2	28.2
7a-ts3	28.2
7b-ts3	27.7
7c-ts3	26.6
7d-ts3	26.9
7e-ts3	28.2
7f-ts3	27.8
7g-ts3	27.5
7h-ts3	26.9
7i-ts3	27.5
9-ts1	27.1
9-ts2	27.4
10-ts1	25.4
10-ts2	25.4
11-ts	24.7
12-ts1	23.0
12-ts2	22.7

^a We considered single-point solvent effects for H₂O (probe radius = 1.40 Å, ϵ = 80.37) using the Jaguar self consistent Poisson-Boltzmann solver.^[1]

[1] (a)Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. *J. Phys. Chem.* 1996, 100, 11775-11788. (b)Tannor, D. J.; Marten, B.; Murphy, R.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Ringnalda, M.; Goddard, W. A., III; Honig, B. *J. Am. Chem. Soc.* 1994, 116, 11875-11882.

Table 2. Absolute energies in hartrees for the structures discussed in the manuscript:

Structure	E, 0K (au)	H, 298K (au)	G, 298K (au)
Methyl Azide	-204.1483611	-204.0928010	-204.1248090
Cyclooctyne-based reagents			
1a(chair)	-312.0842369	-311.8961110	-311.9366560
1a(twist boat)	-312.0791294	-311.8909040	-311.9310190
1a-TS1	-516.2121881	-515.9680420	-516.0218050
2a	-516.3452111	-516.0958350	-516.1443020
1b	-351.4095202	-351.1921000	-351.2359340
1b-TS1	-555.5359947	-555.2624540	-555.3191660
1b-TS2	-555.5362178	-555.2626880	-555.3191790
2b	-555.6700981	-555.3913990	-555.4428700
3b	-555.6699371	-555.3912350	-555.4427080
1c	-450.6763779	-450.4665740	-450.5122060
1c-TS1	-654.8028876	-654.5368670	-654.5954000
1c-TS2	-654.8066775	-654.5405590	-654.5976820
2c	-654.9368248	-654.6657240	-654.7188900
3c	-654.9391145	-654.6679650	-654.7209290
2c-cation	-554.8077383		
3c-cation	-554.7874778		
2c-OH	-630.9134748		
3c-OH	-630.9093730		
1d	-411.3459097	-411.1647520	-411.2073990
1d-TS1	-615.4742510	-615.2369180	-615.2930510
1d-TS2	-615.4775560	-615.2401600	-615.2949600
2d	-615.6117781	-615.3692380	-615.4195370
3d	-615.6062492	-615.3637320	-615.4140800
1e	-510.6201228	-510.4465050	-510.4908400
1e-TS1	-714.7492058	-714.5194760	-714.5764110
1e-TS2	-714.7536736	-714.5237890	-714.5803590
2e	-714.8819432	-714.6471580	-714.6992600
3e	-714.8878955	-714.6530400	-714.7050760
Azacyclooctyne-based reagent			
4	-670.5797997	-670.3215930	-670.378652
4-TS1	-874.7072534	-874.3929740	-874.463613
4-TS2	-874.7100682	-874.3955880	-874.464335
5	-874.8420105	-874.5226710	-874.587940
6	-874.8394445	-874.5201890	-874.585113
Dibenzocyclooctyne-based reagents			
7a	-727.7601922	-727.4844510	-727.5409520
7a-TS3	-931.8891763	-931.5571190	-931.6251700
8a	-932.0138261	-931.6772160	-931.7424240
7b	-846.1195417	-845.8099650	-845.8724730
7b-TS3	-1050.2493899	-1049.8834470	-1049.9575560
8b	-1050.3734484	-1050.0030060	-1050.0742780
7c	-924.7795566	-924.4108590	-924.4805820
7c-TS3	-1128.9093494	-1128.4842890	-1128.5654230
8c	-1129.0333441	-1128.6037830	-1128.6820650
7d	-885.0163936	-884.6227540	-884.6938870
7d-TS3	-1089.1453407	-1088.6954220	-1088.7777520
8d	-1089.2698416	-1088.8154080	-1088.8951550
7e	-617.0126140	-616.7728400	-616.8230870
7e-TS3	-821.1414241	-820.8452620	-820.9072380

8e	-821.2659730	-820.9653330	-821.0246460
7f	-815.5408452	-815.3158180	-815.3703910
7f-TS3	-1019.6703613	-1019.3889400	-1019.4549650
8f	-1019.7947494	-1019.5088560	-1019.5723970
7g	-1536.2558408	-1536.0327740	-1536.0903890
7g-TS3	-1740.3856264	-1740.1061610	-1740.1753810
8g	-1740.5095767	-1740.2266100	-1740.2896230
7h	-1026.1237271	-1025.8738790	-1025.9396460
7h-TS3	-1230.2541634	-1229.9478830	-1230.0244100
8h	-1230.3766352	-1230.0668160	-1230.1371910
7i	-801.5408508	-801.3001790	-801.3596720
7i-TS3	-1005.6711994	-1005.3741260	-1005.4451860
8i	-1005.7939718	-1005.4934000	-1005.5585190
Benzocyclooctyne-based reagents			
9	-464.5469108	-464.3329620	-464.3783940
9-TS1	-668.6750100	-668.4048720	-668.4628350
9-TS2	-668.6760986	-668.4059680	-668.4635140
9-P1	-668.8110984	-668.5361220	-668.5896890
9-P2	-668.8117863	-668.5367780	-668.5904450
10	-464.5381188	-464.3242390	-464.3697710
10-TS1	-668.6689380	-668.3989680	-668.4574510
10-TS2	-668.6683946	-668.3984670	-668.4571470
10-P1	-668.8078110	-668.5328130	-668.5863600
10-P2	-668.8076293	-668.5326490	-668.5860820
11	-464.5415290	-464.3276420	-464.3726070
11-TS	-668.6739234	-668.4039440	-668.4621740
11-P	-668.8034698	-668.5284550	-668.5824210
12	-663.0762414	-662.8769060	-662.9256960
12-TS1	-867.2100983	-866.9546130	-867.0159770
12-TS2	-867.2138419	-866.9582450	-867.0191440
12-P1	-867.3407136	-867.0804250	-867.1375450
12-P2	-867.3400537	-867.0797350	-867.1366450

Cartesian coordinates for the structures discussed in the manuscript:

Methyl Azide

C 0.00028 -0.00010 0.00019
 N -0.00014 -0.00125 1.47353
 N 1.10317 0.00002 2.01502
 N 2.05542 0.00114 2.63362
 H 0.49026 -0.89215 -0.40424
 H 0.48937 0.89299 -0.40293
 H -1.04179 -0.00042 -0.31121

1a(chair)

C -0.03950 0.15245 -0.00472
 H -0.26180 0.32514 1.05313
 C 1.19045 -0.60281 -0.21033
 C 1.92672 -1.41500 -0.70766
 C 2.33295 -2.50908 -1.58147
 C 1.27378 -2.60918 -2.71415
 C -0.20610 -2.57205 -2.25407
 C -0.90398 -1.18152 -2.09677
 C -1.19026 -0.65516 -0.66684
 H 0.04274 1.14032 -0.47316
 H 2.36801 -3.44835 -1.01687
 H 3.32951 -2.36424 -2.01067
 H 1.45342 -3.54150 -3.26106
 H 1.44729 -1.79399 -3.42473
 H -0.31002 -3.14194 -1.32357
 H -0.77489 -3.13032 -3.00431
 H -1.87463 -1.25448 -2.59739
 H -0.34243 -0.42394 -2.65541
 H -2.07842 -0.01402 -0.69425
 H -1.43838 -1.50168 -0.01778

1a(twist boat)

C 0.00112 -0.00006 0.00192
 C 0.00080 -0.00084 1.20696
 C 0.62581 0.00126 2.52775
 C 2.11827 0.36447 2.30034
 C 2.98797 -0.63776 1.50306
 C 2.57172 -1.18011 0.10635
 C 2.18070 -0.17634 -1.01211
 C 0.64942 -0.13622 -1.30147
 H 0.16893 0.72892 3.20630
 H 0.52987 -0.97959 3.00823
 H 2.59833 0.49759 3.27746
 H 2.14086 1.34293 1.81094
 H 3.15609 -1.51873 2.13517
 H 3.97218 -0.16460 1.39917
 H 1.75943 -1.90145 0.23033
 H 3.43020 -1.76435 -0.24264
 H 2.69989 -0.43370 -1.94139
 H 2.50484 0.83453 -0.74511
 H 0.33601 -1.06179 -1.79822
 H 0.40869 0.68489 -1.98374

1a-TS1

C 0.00425 0.00528 0.01911
 N -0.00767 0.00685 2.18858
 C 1.19054 -0.00426 -0.30844
 N 2.22137 0.01732 1.74653
 C -1.42021 -0.00483 -0.34872
 H -2.00172 -0.58759 0.37164
 C 2.29057 0.01418 -1.27542
 C 1.77661 0.45781 -2.66366
 C 0.58623 -0.34114 -3.24171
 C -0.85728 0.13431 -2.90915
 C -1.62669 -0.56947 -1.76869
 H -1.81066 1.01912 -0.29496
 H 2.73774 -0.98524 -1.34809

H 3.08884 0.68864 -0.95164
 H 2.61968 0.38471 -3.36013
 H 1.50814 1.51883 -2.61498
 H 0.69268 -1.40106 -2.97959
 H 0.68620 -0.29878 -4.33105
 H -1.45074 -0.01265 -3.81748
 H -0.85416 1.21755 -2.73469
 H -2.69911 -0.51306 -1.98862
 H -1.37041 -1.63509 -1.76565
 N 1.13945 -0.04101 2.37723
 C 3.44016 -0.50560 2.35751
 H 3.73376 0.07404 3.23869
 H 3.35020 -1.56162 2.63500
 H 4.22882 -0.40848 1.61161

2a

C -0.00370 0.08085 -0.05363
 H -0.03308 0.15717 1.04000
 C 1.42740 0.01531 -0.49934
 C 2.20541 -1.03304 -0.96074
 C 1.93974 -2.47895 -1.25791
 C 1.17099 -2.72922 -2.58036
 C -0.36131 -2.64649 -2.50776
 C -0.98023 -1.32317 -2.02270
 C -0.90737 -1.07914 -0.49326
 H -0.41300 1.02617 -0.42487
 N 2.19461 1.14401 -0.48213
 N 3.39209 0.86541 -0.89654
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 C 4.65334 -1.03628 -1.68857
 H 1.40275 -2.93861 -0.42409
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 H -0.73181 -3.46000 -1.87042
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 H 5.38591 -0.23278 -1.72436
 H 4.51993 -1.45044 -2.69028
 H 5.00963 -1.82007 -1.01639

1b

C 0.02626 0.01895 0.03144
 C -0.00073 -0.01672 1.56672
 C 1.36562 -0.00404 -0.55506
 C 2.24726 -0.29301 -1.32250
 C 2.88499 -0.94496 -2.45972
 C 1.75098 -1.44851 -3.39472
 C 0.58931 -2.19834 -2.69436
 C -0.60459 -1.36290 -2.12788
 C -0.72818 -1.19184 -0.59260
 H -0.47797 0.93732 -0.29701
 H -1.03158 -0.03046 1.93211
 H 0.49936 0.85875 1.98711
 H 0.50801 -0.90883 1.94138
 H 3.49147 -1.79152 -2.11617
 H 3.55884 -0.27982 -3.00906
 H 2.20061 -2.10925 -4.14427
 H 1.34409 -0.59065 -3.94078
 H 0.99664 -2.83928 -1.90385
 H 0.17243 -2.88256 -3.44016
 H -1.52307 -1.85991 -2.45604
 H -0.62022 -0.37607 -2.60471
 H -1.78804 -1.08931 -0.33144

H -0.37463 -2.10495 -0.09926

1b-TS1

C 0.00337 -0.00668 -0.00586
N 0.00724 -0.00708 2.17441
C 1.19394 -0.00629 -0.32682
N 2.22638 -0.02929 1.69885
C -1.42778 0.04000 -0.38128
C -2.28314 -1.02264 0.32832
C 2.30512 0.09302 -1.28119
C 1.89738 0.91272 -2.52443
C 0.64959 0.43068 -3.29206
C -0.74811 0.88687 -2.78826
C -1.56528 -0.09331 -1.91724
H -1.81140 1.02689 -0.08970
H -3.32708 -0.93816 0.01253
H -2.23499 -0.90538 1.41014
H -1.93244 -2.02819 0.07840
H 2.61263 -0.91465 -1.58869
H 3.18086 0.55826 -0.82150
H 2.75239 0.90517 -3.21031
H 1.75232 1.95621 -2.22348
H 0.66997 -0.66317 -3.37596
H 0.75607 0.80344 -4.31603
H -1.35080 1.08939 -3.67928
H -0.65593 1.85032 -2.27282
H -2.62847 0.03406 -2.15204
H -1.31400 -1.12348 -2.19728
N 1.15606 -0.07382 2.35058
C 3.44411 -0.59595 2.27178
H 3.77675 -0.03494 3.15112
H 3.32987 -1.65200 2.53938
H 4.21631 -0.51254 1.50697

1b-TS2

C -0.02701 0.09052 -0.03802
N 0.00245 0.04223 2.28649
C 1.18235 0.09658 -0.27580
N 2.17064 0.03394 1.61175
C -1.45128 0.11266 -0.39732
C -2.24411 -1.07341 0.17526
C 2.28391 0.22006 -1.24750
C 1.91398 1.17842 -2.39695
C 0.66484 0.81956 -3.22834
C -0.73685 1.21905 -2.68707
C -1.56158 0.14211 -1.94524
H -1.89331 1.04033 -0.01016
H -3.29576 -1.00760 -0.11822
H -2.18358 -1.09680 1.26357
H -1.84195 -2.01835 -0.19963
H 2.51409 -0.77278 -1.65403
H 3.19559 0.56929 -0.75576
H 2.77502 1.21917 -3.07426
H 1.79651 2.18890 -1.98920
H 0.67459 -0.25379 -3.45682
H 0.78555 1.32325 -4.19318
H -1.33079 1.52585 -3.55365
H -0.64787 2.11482 -2.06132
H -2.62239 0.28006 -2.18368
H -1.28894 -0.84879 -2.32642
N 1.25583 0.08445 2.33143
C -0.76221 0.57387 3.41328
H -0.53945 1.62895 3.60839
H -1.81534 0.48586 3.14797
H -0.59352 -0.00386 4.32779

2b

C -0.00056 0.00949 0.04482
C 0.04750 -0.17270 1.57370
C 1.39076 0.02622 -0.53017

C 2.11085 -0.90300 -1.26245
C 1.79940 -2.25253 -1.83945
C 0.94627 -2.21319 -3.13199
C -0.57472 -2.11319 -2.94176
C -1.10766 -0.91197 -2.14018
C -0.94330 -1.01869 -0.60261
H -0.41183 1.00800 -0.14980
N 2.18318 1.12028 -0.33096
N 3.33975 0.93245 -0.88794
N 3.31574 -0.28761 -1.46247
C 4.49707 -0.76250 -2.16049
H -0.95254 -0.07974 2.00825
H 0.69304 0.58113 2.02767
H 0.44193 -1.15966 1.83647
H 1.30637 -2.87484 -1.08843
H 2.74314 -2.75738 -2.06335
H 1.15013 -3.12705 -3.70082
H 1.29181 -1.38032 -3.75494
H -0.93661 -3.03665 -2.47120
H -1.02388 -2.09239 -3.94106
H -2.17236 -0.81166 -2.37080
H -0.63736 0.00860 -2.50384
H -1.92154 -0.89624 -0.12761
H -0.61976 -2.02919 -0.32940
H 5.23422 0.03543 -2.10072
H 4.27546 -0.97398 -3.20863
H 4.89845 -1.66093 -1.68606

3b

C 0.04247 -0.01045 0.10491
C 0.13510 -0.31580 1.61478
C 1.40225 0.00099 -0.53781
C 2.11088 -0.91203 -1.30205
C 1.75502 -2.25628 -1.86799
C 0.87486 -2.19798 -3.13854
C -0.63955 -2.04112 -2.93091
C -1.11427 -0.83281 -2.10275
C -0.93618 -0.98928 -0.57216
H -0.38010 0.99730 -0.00609
N 2.26073 1.05901 -0.42442
N 3.41974 0.81495 -1.07163
N 3.32839 -0.36698 -1.59755
H -0.85519 -0.27052 2.07690
H 0.78134 0.39223 2.13823
H 0.54173 -1.31761 1.77681
H 1.29048 -2.89917 -1.11426
H 2.70648 -2.72410 -2.13146
H 1.03470 -3.12125 -3.70628
H 1.24556 -1.38406 -3.77125
H -1.03706 -2.95449 -2.46912
H -1.10133 -1.98468 -3.92306
H -2.17633 -0.67889 -2.31567
H -0.60542 0.07254 -2.45252
H -1.90343 -0.85980 -0.07686
H -0.62694 -2.01235 -0.33764
C 2.07911 2.34005 0.23428
H 1.19427 2.85190 -0.15027
H 1.98522 2.22075 1.31548
H 2.96451 2.93201 0.01212

1c

C 0.03817 -0.01787 0.03310
C -0.00328 -0.01327 1.55508
C 1.37821 -0.01855 -0.54919
C 2.24908 -0.30826 -1.32736
C 2.88079 -0.94419 -2.47498
C 1.74317 -1.43194 -3.41420
C 0.58140 -2.18622 -2.71892
C -0.59882 -1.34767 -2.13168
C -0.71571 -1.21253 -0.59489

F -0.63479 1.16017 -0.39794
H -1.03911 -0.04914 1.89982
H 0.46198 0.89831 1.93342
H 0.53663 -0.87357 1.95650
H 3.48554 -1.79482 -2.13973
H 3.55615 -0.27019 -3.01078
H 2.19115 -2.08389 -4.17201
H 1.33779 -0.56600 -3.94738
H 0.99017 -2.84520 -1.94358
H 0.15472 -2.85441 -3.47337
H -1.52724 -1.81801 -2.46924
H -0.60272 -0.34420 -2.56734
H -1.76821 -1.08289 -0.32131
H -0.36803 -2.13005 -0.10813

1c-TS1

C 0.00306 -0.01033 -0.00572
N 0.00309 0.01190 2.18038
C 1.19381 -0.01407 -0.32650
N 2.21934 0.02422 1.68159
C -1.41907 -0.00181 -0.42152
C -2.31344 -0.92179 0.40064
C 2.31273 0.04475 -1.27429
C 1.89978 0.73221 -2.59280
C 0.67872 0.13931 -3.32378
C -0.73229 0.60771 -2.87727
C -1.53681 -0.30179 -1.92681
F -1.91104 1.32006 -0.23516
H -3.33533 -0.87658 0.01758
H -2.30570 -0.61101 1.44323
H -1.95792 -1.95326 0.34139
H 2.66137 -0.97516 -1.48122
H 3.16117 0.58086 -0.84133
H 2.76603 0.68787 -3.26246
H 1.71689 1.79330 -2.39256
H 0.73187 -0.95674 -3.30028
H 0.78760 0.41286 -4.37799
H -1.33392 0.71405 -3.78475
H -0.67815 1.61003 -2.44189
H -2.60125 -0.20742 -2.16465
H -1.27030 -1.35209 -2.08693
N 1.15340 -0.03638 2.33939
C 3.43482 -0.57951 2.22249
H 3.30594 -1.64073 2.46110
H 4.19942 -0.48447 1.45169
H 3.78493 -0.04852 3.11301

1c-TS2

C -0.00406 -0.01394 -0.02423
N -0.00069 -0.00442 2.21581
C 1.19205 -0.00120 -0.32070
N 2.20241 0.02359 1.63426
C -1.42620 -0.03925 -0.38296
C -2.15953 -1.28044 0.11456
C 2.26554 0.15590 -1.31386
C 1.88410 1.20034 -2.38358
C 0.59791 0.92862 -3.19085
C -0.77474 1.28681 -2.55522
C -1.58401 0.14426 -1.90476
F -2.06296 1.08692 0.23046
H -3.21609 -1.21930 -0.15638
H -2.06725 -1.36312 1.19710
H -1.72904 -2.17839 -0.33363
H 2.44934 -0.81418 -1.79271
H 3.20352 0.44469 -0.83287
H 2.72254 1.26632 -3.08643
H 1.80645 2.18230 -1.90383
H 0.58825 -0.11921 -3.51806
H 0.68554 1.51764 -4.10960
H -1.39944 1.69147 -3.35698

H -0.65887 2.10142 -1.83389
H -2.65261 0.31268 -2.07207
H -1.33613 -0.80796 -2.38521
N 1.24689 0.08890 2.28987
C -0.82211 0.80940 3.11682
H -0.51470 1.85929 3.11529
H -1.83988 0.74906 2.73932
H -0.79466 0.41805 4.13822

2c

C 0.00137 0.02549 -0.01473
C -0.09957 0.31979 1.47988
C 1.44340 -0.04001 -0.44755
C 2.21107 -1.05088 -1.00480
C 1.95537 -2.46803 -1.42688
C 1.12595 -2.63145 -2.72408
C -0.39800 -2.63413 -2.54831
C -1.02823 -1.36729 -1.95077
C -0.84959 -1.17884 -0.42417
F -0.57361 1.14875 -0.67512
N 2.23629 1.05641 -0.26736
N 3.43351 0.79995 -0.68543
N 3.44125 -0.47302 -1.13787
C 4.68096 -1.02908 -1.65315
H -1.14198 0.49684 1.75358
H 0.49061 1.20538 1.71526
H 0.28314 -0.52140 2.06416
H 1.47298 -3.01511 -0.61155
H 2.92199 -2.95643 -1.57119
H 1.41143 -3.58182 -3.18724
H 1.41302 -1.84513 -3.43088
H -0.68569 -3.50141 -1.93949
H -0.83907 -2.80417 -3.53655
H -2.09979 -1.39856 -2.16442
H -0.65443 -0.48058 -2.46965
H -1.82924 -1.02304 0.03455
H -0.44153 -2.08030 0.04336
H 5.41256 -0.22436 -1.63197
H 4.55580 -1.37820 -2.67958
H 5.03246 -1.85232 -1.02742

3c

C 0.04002 -0.03572 0.09107
C 0.11749 -0.26789 1.60070
C 1.40064 0.00831 -0.54846
C 2.10382 -0.90366 -1.31903
C 1.75327 -2.24205 -1.90104
C 0.86539 -2.17771 -3.16564
C -0.64820 -2.05238 -2.93941
C -1.13032 -0.86329 -2.09107
C -0.91830 -1.02872 -0.56784
F -0.54734 1.25801 -0.08935
N 2.27054 1.05303 -0.39688
N 3.42578 0.80331 -1.03951
N 3.33171 -0.37015 -1.58598
H -0.88409 -0.22476 2.03388
H 0.73576 0.48764 2.08647
H 0.55148 -1.24840 1.80834
H 1.29876 -2.89948 -1.15281
H 2.70842 -2.69670 -2.17301
H 1.03942 -3.08798 -3.74951
H 1.21571 -1.34599 -3.78633
H -1.02312 -2.97986 -2.48643
H -1.12404 -1.98995 -3.92428
H -2.20023 -0.73122 -2.27283
H -0.65781 0.06164 -2.43426
H -1.87061 -0.90182 -0.04612
H -0.57956 -2.04139 -0.33256
C 2.11407 2.34099 0.26764
H 1.24671 2.86622 -0.12583

H 1.99732 2.21208 1.34484
H 3.02586 2.89914 0.06661

2c-cation

C 0.19328 -0.28029 0.10771
C -0.36580 0.82642 0.92051
C 1.51015 -0.23105 -0.31342
C 2.30201 -1.14617 -1.08394
C 1.98054 -2.43746 -1.75569
C 0.99046 -2.30355 -2.94988
C -0.49928 -2.47151 -2.62208
C -1.16469 -1.40472 -1.74418
C -0.72409 -1.40588 -0.23813
N 2.33814 0.84464 0.02282
N 3.48904 0.66616 -0.43968
N 3.49101 -0.56995 -1.13718
C 4.74009 -0.99802 -1.76810
H -1.28480 1.18957 0.44319
H 0.32985 1.64456 1.08050
H -0.68814 0.41589 1.88713
H 1.57841 -3.13446 -1.01300
H 2.91209 -2.87956 -2.11019
H 1.25955 -3.08493 -3.66404
H 1.16214 -1.35242 -3.46430
H -0.65760 -3.45682 -2.16796
H -1.03790 -2.49286 -3.57391
H -2.24132 -1.58425 -1.75351
H -1.02205 -0.41032 -2.17902
H -1.60776 -1.33206 0.39523
H -0.24684 -2.36217 -0.00261
H 5.44485 -0.17837 -1.64930
H 4.57893 -1.19438 -2.82770
H 5.12651 -1.88825 -1.27097

3c-cation

C 0.16266 -0.19563 0.04105
C -0.56898 0.94974 0.64780
C 1.50730 -0.18162 -0.28225
C 2.29074 -1.12911 -1.03311
C 1.94056 -2.38994 -1.74940
C 0.94264 -2.23858 -2.93075
C -0.54271 -2.45214 -2.60961
C -1.22049 -1.41730 -1.70643
C -0.67321 -1.40054 -0.22974
N 2.45840 0.81287 0.02572
N 3.62309 0.47809 -0.44385
N 3.53649 -0.66856 -1.11134
H -1.58038 0.98913 0.23407
H -0.09607 1.91850 0.53155
H -0.69918 0.74753 1.72101
H 1.57260 -3.13801 -1.03751
H 2.89124 -2.76587 -2.12889
H 1.22719 -2.98883 -3.67149
H 1.09475 -1.26909 -3.41630
H -0.67632 -3.44756 -2.17026
H -1.09043 -2.46739 -3.55649
H -2.28622 -1.64553 -1.64830
H -1.14620 -0.41929 -2.15041
H -1.51800 -1.38061 0.46033
H -0.11660 -2.31813 -0.03905
C 2.38738 2.03958 0.83260
H 1.93676 1.82700 1.80058
H 3.41458 2.36940 0.96702
H 1.82528 2.80845 0.30294

2c-OH

C -0.01658 0.03223 0.02590
C -0.04722 0.09939 1.56417
C 1.41853 -0.04131 -0.45137
C 2.21818 -1.06867 -0.91485

C 1.98009 -2.51796 -1.21169
C 1.22930 -2.77050 -2.54341
C -0.30298 -2.66870 -2.49194
C -0.91361 -1.34124 -2.00719
C -0.89224 -1.12487 -0.47562
O -0.60355 1.22859 -0.50594
N 2.15119 1.10729 -0.45201
N 3.35052 0.86591 -0.88586
N 3.41000 -0.44906 -1.17367
C 4.65569 -1.00888 -1.67022
H -1.07763 0.22631 1.90475
H 0.54145 0.95216 1.90897
H 0.36795 -0.80718 2.01487
H 1.43600 -2.98130 -0.38451
H 2.94611 -3.02860 -1.25196
H 1.48539 -3.77779 -2.88956
H 1.61587 -2.07821 -3.29997
H -0.69163 -3.48441 -1.86813
H -0.66959 -2.87000 -3.50468
H -1.95399 -1.31876 -2.34222
H -0.43153 -0.49303 -2.50207
H -1.90252 -0.89547 -0.12646
H -0.59871 -2.04442 0.04025
H 0.08703 1.90458 -0.48620
H 5.35512 -0.18073 -1.76136
H 4.51224 -1.47259 -2.64791
H 5.05716 -1.74656 -0.97221

3c-OH

C 0.00767 0.02204 0.01778
C -0.02488 0.02658 1.55169
C 1.43689 0.01469 -0.49428
C 2.22903 -0.96264 -1.08329
C 1.99562 -2.39388 -1.47972
C 1.19115 -2.60413 -2.78230
C -0.33807 -2.56429 -2.65986
C -0.93455 -1.28476 -2.05111
C -0.79966 -1.17810 -0.51137
O -0.65737 1.24311 -0.37370
N 2.27013 1.10038 -0.41747
N 3.48081 0.81225 -0.92606
N 3.45914 -0.42213 -1.32600
H -1.06131 0.05821 1.89469
H 0.49111 0.89972 1.95275
H 0.45591 -0.87034 1.94697
H 1.54295 -2.96505 -0.66279
H 2.99541 -2.80831 -1.62682
H 1.46606 -3.58002 -3.19670
H 1.52146 -1.85899 -3.51454
H -0.67952 -3.42461 -2.06996
H -0.75722 -2.70332 -3.66247
H -1.99512 -1.24108 -2.31336
H -0.47117 -0.42036 -2.54475
H -1.79264 -1.08079 -0.06531
H -0.37291 -2.09834 -0.10551
H -0.73302 1.24183 -1.33448
C 2.07508 2.41913 0.17455
H 1.04966 2.74081 0.01816
H 2.29309 2.39250 1.24506
H 2.77629 3.09365 -0.31306

1d

C -0.14252 0.08244 0.02776
H -0.41480 0.28236 1.06764
C 1.09168 -0.67497 -0.11865
C 1.82940 -1.49428 -0.60107
C 2.26767 -2.56558 -1.48394
C 1.27087 -2.61561 -2.67491
C -0.23119 -2.57542 -2.29431
C -0.91559 -1.18213 -2.11805

C -1.25809 -0.69967 -0.68793
F -0.01029 1.34332 -0.59195
H 2.25912 -3.51834 -0.94199
H 3.28945 -2.41983 -1.84726
H 1.47195 -3.53194 -3.24017
H 1.49128 -1.77981 -3.34679
H -0.39512 -3.18559 -1.39802
H -0.76377 -3.09148 -3.09887
H -1.86285 -1.21809 -2.66370
H -0.32184 -0.40646 -2.61134
H -2.12829 -0.03619 -0.72366
H -1.53165 -1.55142 -0.05545

1d-TS1

C 0.01359 -0.00027 0.01418
N -0.00347 0.01976 2.18730
C 1.19856 -0.00093 -0.31621
N 2.22523 -0.06095 1.73758
C -1.40221 -0.06561 -0.37851
H -2.03628 -0.38782 0.44996
C 2.29118 -0.09238 -1.28397
C 1.73264 0.00672 -2.72143
C 0.61628 -1.00181 -3.08220
C -0.86020 -0.56230 -2.87963
C -1.60203 -0.97665 -1.59218
F -1.84772 1.23036 -0.72622
H 2.81445 -1.04606 -1.14903
H 3.03387 0.69520 -1.12058
H 2.57531 -0.13456 -3.40696
H 1.36641 1.02527 -2.88677
H 0.79669 -1.95236 -2.56516
H 0.73048 -1.22323 -4.14782
H -1.43391 -0.98892 -3.70799
H -0.94369 0.52307 -2.99180
H -2.67779 -0.98427 -1.79817
H -1.32907 -1.99713 -1.30068
N 1.14450 0.03262 2.36401
C 3.45363 0.45819 2.33404
H 3.75365 -0.12429 3.21073
H 4.23279 0.35648 1.57903
H 3.36931 1.51378 2.61248

1d-TS2

C -0.00018 0.00863 0.02374
N 0.00759 0.00051 2.24162
C 1.19029 0.00230 -0.29035
N 2.22175 0.03472 1.69754
C -1.42442 0.00755 -0.29676
H -1.95668 -0.78360 0.23810
C 2.25461 0.07667 -1.29967
C 1.79198 0.86369 -2.54380
C 0.51399 0.35428 -3.24502
C -0.86631 0.83180 -2.71043
C -1.66349 -0.12847 -1.80227
F -2.00838 1.22604 0.14519
H 2.53798 -0.94342 -1.58800
H 3.15525 0.53518 -0.88193
H 2.61594 0.84338 -3.26603
H 1.65371 1.91403 -2.26466
H 0.53383 -0.74211 -3.28856
H 0.58155 0.68684 -4.28562
H -1.49686 1.02603 -3.58290
H -0.76207 1.79595 -2.20267
H -2.73619 0.02743 -1.95572
H -1.45507 -1.16837 -2.07807
N 1.25339 0.09648 2.33197
C -0.83598 0.80592 3.12781
H -0.83543 0.40593 4.14618
H -0.53160 1.85668 3.14223
H -1.84550 0.74650 2.72640

2d

C 0.01239 0.44398 -0.84280
H -0.12268 1.35849 -0.26207
C 1.45311 0.07903 -0.66758
C 2.29119 -0.84228 -1.27448
C 2.14835 -1.82368 -2.39627
C 0.71386 -2.06097 -2.88196
C -0.24481 -2.65325 -1.81830
C -1.37764 -1.71793 -1.36340
C -1.02159 -0.59098 -0.38253
F -0.25605 0.79369 -2.19185
N 2.16255 0.73663 0.29754
N 3.37575 0.28575 0.33116
N 3.47382 -0.67022 -0.61919
C 4.74612 -1.33425 -0.83855
H 2.58500 -2.78165 -2.08515
H 2.75608 -1.47836 -3.24281
H 0.77457 -2.74176 -3.73552
H 0.31091 -1.12258 -3.26489
H 0.32367 -2.99358 -0.94379
H -0.71150 -3.55099 -2.23441
H -2.14964 -2.32365 -0.87648
H -1.84953 -1.27759 -2.24741
H -1.94595 -0.05171 -0.15115
H -0.66244 -1.00938 0.56433
H 5.43758 -0.94288 -0.09550
H 5.12717 -1.12144 -1.83991
H 4.64679 -2.41437 -0.71231

3d

C 0.02097 0.53066 -0.92214
H -0.14159 1.47910 -0.40347
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C 2.29244 -0.82673 -1.24521
C 2.13301 -1.80624 -2.36901
C 0.70276 -2.09191 -2.83812
C -0.26085 -2.61162 -1.74143
C -1.39149 -1.64214 -1.35769
C -1.04493 -0.46269 -0.43572
F -0.19405 0.81913 -2.28745
N 2.20367 0.71407 0.27719
N 3.42867 0.16331 0.32931
N 3.48473 -0.75633 -0.58497
H 2.61615 -2.73615 -2.05024
H 2.72052 -1.44591 -3.22175
H 0.76943 -2.83301 -3.63973
H 0.28794 -1.19146 -3.29430
H 0.30275 -2.89721 -0.84510
H -0.73365 -3.53129 -2.09836
H -2.17852 -2.20674 -0.84594
H -1.84698 -1.24866 -2.27199
H -1.96618 0.10384 -0.26366
H -0.71972 -0.83446 0.54289
C 1.87389 1.77921 1.20939
H 1.06299 1.48315 1.87851
H 2.77228 1.96308 1.79488
H 1.59633 2.69237 0.67871

4

C -0.24034 0.13883 0.02800
O -0.70348 0.10380 1.36913
C 0.96945 -0.66247 -0.11872
C 1.74038 -1.44893 -0.60421
C 2.19989 -2.45830 -1.54839
C 1.31665 -2.28469 -2.81705
N -0.11765 -2.17223 -2.53449
C -0.78963 -0.87422 -2.37527
C -1.29123 -0.49580 -0.94512
H -0.03613 1.17938 -0.26581

H 2.05927 -3.46163 -1.13671
H 3.25422 -2.35650 -1.82228
H 1.45494 -3.14712 -3.47017
H 1.62778 -1.38239 -3.34760
H -1.68819 -0.87712 -3.00062
H -0.12097 -0.10998 -2.77432
O -2.47746 0.29632 -1.02552
H -1.61871 -1.41043 -0.44673
C -2.39167 1.53183 -1.72248
C -1.47635 1.22257 1.78228
H -3.38370 1.97992 -1.66562
H -1.67245 2.22415 -1.26863
H -2.13346 1.40032 -2.77967
H -1.60870 1.12029 2.85962
H -0.94712 2.16539 1.58306
H -2.45606 1.24555 1.29705
C -0.85483 -3.32298 -2.51570
H -1.93565 -3.13020 -2.38041
O -0.40208 -4.44322 -2.64192

4-TS1

C 0.01154 -0.00702 0.00973
O 0.01501 -0.02218 1.43151
C 1.39414 -0.00777 -0.50438
N 2.28986 1.67978 0.55904
C 2.29780 -0.44652 -1.21868
N 4.04461 0.79394 -0.58283
C 2.82362 -1.37552 -2.22459
C 1.65743 -1.88695 -3.09807
N 0.54459 -2.44746 -2.33226
C -0.63204 -1.65031 -1.97311
C -0.76536 -1.26202 -0.47571
H -0.48893 0.90027 -0.35360
H 3.30907 -2.22448 -1.73416
H 3.56846 -0.90915 -2.87647
H 2.02911 -2.67090 -3.75996
H 1.27043 -1.06588 -3.70582
H -1.52739 -2.23502 -2.20699
H -0.64430 -0.77028 -2.61882
O -2.14227 -1.17557 -0.09795
H -0.38268 -2.09015 0.12400
C -2.96011 -0.26212 -0.81382
C -0.84976 0.91174 2.05513
H -3.94892 -0.32228 -0.35845
H -2.60812 0.77420 -0.73800
H -3.05438 -0.52283 -1.87509
H -0.67863 0.81846 3.12811
H -0.61351 1.93974 1.75156
H -1.90333 0.69375 1.84582
C 0.58505 -3.77844 -2.02832
N 3.36295 1.57125 0.12687
H -0.33389 -4.12461 -1.51964
O 1.51004 -4.52314 -2.28688
C 5.21810 1.30198 -1.28878
H 5.58622 0.48481 -1.90864
H 4.98505 2.15767 -1.93197
H 6.01467 1.57985 -0.59175

4-TS2

C -0.00262 -0.00049 -0.00546
O 0.00004 0.00285 1.42022
C 1.38141 0.00066 -0.49719
N 2.31685 1.74501 0.59353
C 2.30743 -0.37060 -1.22147
N 3.97688 0.89888 -0.71198
C 2.85029 -1.26298 -2.25610
C 1.71220 -1.77185 -3.16080
N 0.59729 -2.37019 -2.42428
C -0.58592 -1.59497 -2.04778
C -0.74523 -1.26368 -0.53742

H -0.50850 0.90597 -0.36948
H 3.34300 -2.11581 -1.77904
H 3.60546 -0.76089 -2.86711
H 2.10513 -2.53397 -3.83559
H 1.31883 -0.94448 -3.75634
H -1.47566 -2.17507 -2.31266
H -0.59686 -0.69006 -2.65799
O -2.13240 -1.23203 -0.18337
H -0.34805 -2.10181 0.03863
C -2.96275 -0.30739 -0.87285
C -1.14885 0.55440 2.04950
H -3.95990 -0.42206 -0.44727
H -2.64483 0.73296 -0.73554
H -3.02171 -0.51695 -1.94719
H -0.89639 0.66231 3.10548
H -1.38750 1.54771 1.64204
H -2.02195 -0.09424 1.95126
C 0.63629 -3.71276 -2.17477
N 3.45049 1.53579 0.10597
C 2.21814 2.19858 1.98211
H 2.77181 3.13009 2.13055
H 1.16558 2.38319 2.18015
H 2.57831 1.44020 2.68396
H -0.28788 -4.07851 -1.68859
O 1.56201 -4.44817 -2.45387

5

C -0.07983 0.09578 0.04419
O -0.14173 -0.13673 1.44884
C 1.26672 0.60741 -0.39302
N 1.51791 1.94938 -0.35464
C 2.41606 -0.03772 -0.82208
N 3.29970 0.98163 -1.01684
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C 2.17484 -1.91464 -2.53481
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C -0.49142 -1.23860 -0.60211
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H 2.36780 -2.13107 -0.38156
H 3.81870 -1.59156 -1.18921
H 2.70315 -2.80959 -2.86294
H 2.34742 -1.12408 -3.27506
H -1.20054 -1.62602 -2.59563
H 0.00011 -0.33848 -2.56764
O -1.81527 -1.63820 -0.26343
H 0.11939 -2.01242 -0.13436
C -2.85827 -0.71114 -0.51086
C -0.20024 1.03815 2.24574
H -3.79018 -1.25668 -0.35998
H -2.83431 0.13318 0.18720
H -2.84746 -0.32273 -1.53907
H -0.29562 0.70285 3.27872
H 0.69802 1.65471 2.14054
H -1.07359 1.65167 1.98465
C 0.40990 -3.55784 -2.86645
N 2.74028 2.17550 -0.72299
H -0.68554 -3.70007 -2.84319
O 1.17895 -4.44858 -3.16379
C 4.68317 0.94022 -1.46267
H 5.29189 0.34167 -0.78226
H 4.75701 0.53323 -2.47291
H 5.04112 1.96737 -1.45949

6

C -0.18687 0.21607 -0.00280
O -0.63641 -0.01320 1.33545
C 1.25807 -0.18907 -0.02375
C 1.95975 -1.31371 -0.42670
C 1.54361 -2.58999 -1.09462

C 1.23291 -2.47359 -2.59893
N -0.09173 -1.94043 -2.90664
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H 1.26085 -3.46201 -3.05614
H 1.99672 -1.85242 -3.08097
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H -2.23520 1.43348 -2.53196
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7a

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C 1.47598 -3.09970 -2.38522
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7a-TS3

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7b-TS3

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8b

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7c-TS3

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H 5.17571 -6.18996 -4.17431
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7d-TS3

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7e-TS3

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7f-TS3

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7g-TS3

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7h

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7h-TS3

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8h

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H -0.17514 0.77079 -3.66205
H 1.42812 0.77830 -2.95875
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C 3.35287 -4.36752 -2.35495
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7i

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C 2.34873 -1.37133 -0.51549
C 2.69827 -2.41110 -1.41340
C 1.59286 -2.93333 -2.14570
C 0.17877 -2.46707 -1.84929
C -0.14270 -0.94806 -2.13310
C -0.54382 -0.09942 -0.93986
H -0.03707 -2.68125 -0.79857
H -0.51042 -3.07924 -2.43395
H -0.94608 -0.89884 -2.87047
H 0.73137 -0.48590 -2.60096
C 3.99437 -2.89197 -1.63553
C 4.22216 -3.87565 -2.58453
C 3.14763 -4.38563 -3.32595
C 1.84547 -3.91085 -3.10033
C 3.37385 -5.39818 -4.31023
H 1.02725 -4.32637 -3.67665
H 4.81789 -2.48302 -1.06386
H 5.22244 -4.24985 -2.76099
C 0.03301 0.98316 1.18726
C -1.21554 1.58261 1.23105
C -2.13757 1.33973 0.20385
C -1.79425 0.50260 -0.86995
H 0.75002 1.15529 1.98004
H -2.51768 0.33694 -1.65951
C -3.42939 1.95203 0.24225
H -1.48601 2.23290 2.05306
N 3.55627 -6.21625 -5.10546
N -4.47309 2.44659 0.27258

7i-TS3

C -0.00201 0.01361 -0.03023
N 0.00722 0.01195 2.15062
C 1.20755 0.02541 -0.33175
N 2.22752 -0.05956 1.65018
C -1.37574 -0.05350 -0.45375
C 2.26014 0.01548 -1.30249
C 1.95300 -0.52839 -2.57867
C 0.56177 -1.03829 -2.86169
C -0.52307 0.09972 -2.85625
C -1.63879 -0.06519 -1.85186
H 0.29431 -1.79337 -2.11774
H 0.55191 -1.53786 -3.83215
H -0.95903 0.17725 -3.85401
H -0.02674 1.05547 -2.66487
N 1.15304 -0.09756 2.29272

C 3.30943 -0.96183 2.06590
H 3.77071 -0.61352 2.99415
H 2.96093 -1.99087 2.19178
H 4.05940 -0.93556 1.27787
C -2.44778 -0.14173 0.44867
C -3.75342 -0.25694 0.00086
C -4.01539 -0.29047 -1.37425
C -2.95406 -0.19376 -2.28498
C 3.53408 0.55563 -1.06780
C 4.50613 0.54380 -2.05446
C 4.21811 -0.01796 -3.30571
C 2.94100 -0.54080 -3.55649
H 3.73947 1.00521 -0.10552
H 5.48476 0.96770 -1.86762
C 5.21863 -0.05175 -4.32660
H 2.72435 -0.95819 -4.53286
H -3.16927 -0.20832 -3.34698
H -4.57124 -0.32461 0.70713
C -5.35762 -0.41672 -1.85142
H -2.24182 -0.12450 1.50843
N 6.02857 -0.08131 -5.15030
N -6.44172 -0.52055 -2.23763

8i

C 0.00805 -0.01936 0.01714
N 0.00403 -0.00132 1.38364
C 1.33081 -0.00910 -0.40596
N 2.04701 -0.00631 0.75492
C -1.24823 0.14105 -0.74240
C 1.91070 -0.00038 -1.75309
C 1.52791 -1.00129 -2.66625
C 0.56209 -2.08913 -2.26045
C -0.91740 -1.77012 -2.53689
C -1.61097 -0.56055 -1.91201
H 0.70080 -2.33577 -1.20668
H 0.79822 -2.99582 -2.82493
H -1.49580 -2.65327 -2.23846
H -1.04562 -1.68909 -3.62081
N 1.22370 -0.00905 1.82245
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H 3.92001 0.96274 0.84877
H 3.65267 -0.37852 1.98388
H 3.95547 -0.71734 0.25881
C -2.13135 1.10688 -0.22114
C -3.32739 1.42171 -0.83578
C -3.67055 0.76460 -2.02407
C -2.81503 -0.21144 -2.53614
C 2.82026 0.99232 -2.14400
C 3.35232 1.00779 -3.42341
C 2.97532 0.01473 -4.33730
C 2.06889 -0.97952 -3.95056
H 3.09320 1.77381 -1.44513
H 4.04790 1.78117 -3.72293
C 3.52128 0.01009 -5.66016
H 1.79623 -1.74974 -4.66275
H -3.10709 -0.73098 -3.44157
H -3.98524 2.17250 -0.41721
C -4.88865 1.07861 -2.70574
H -1.84657 1.61195 0.69248
N -5.87280 1.33039 -3.25599
N 3.96510 0.00434 -6.72654

9

C 0.25640 0.69713 -0.15266
C 0.40027 1.05197 1.21971
C 0.91654 1.03972 2.31157
C 1.95418 0.76897 3.29837
C 2.77958 -0.45526 2.79324
C 2.99064 -0.52391 1.25882
C 1.84284 -1.22122 0.44806

C 1.05291 -0.40617 -0.56315
C 1.03014 -0.76062 -1.91183
C -0.53518 1.38444 -1.07857
C -0.54208 1.00238 -2.41600
C 0.24572 -0.06673 -2.83363
H 1.55838 0.57319 4.29957
H 2.60591 1.64630 3.38711
H 2.28109 -1.37371 3.12001
H 3.75136 -0.43506 3.29684
H 3.17753 0.47904 0.86465
H 3.90890 -1.09116 1.08163
H -1.13472 2.22157 -0.74095
H -1.15589 1.54039 -3.12934
H 0.24851 -0.36571 -3.87581
H 1.63172 -1.59934 -2.24732
H 1.12559 -1.63808 1.16491
H 2.26631 -2.07713 -0.08410

9-TS1

C 0.00800 0.00066 -0.03426
N 0.01440 0.10326 2.18021
C 1.20733 -0.02797 -0.33789
N 2.22634 0.00874 1.66193
C 2.32202 -0.00395 -1.29519
C -1.37314 -0.01343 -0.44798
C 1.93224 -0.64792 -2.64941
C 0.50691 -0.32240 -3.14037
C -0.60759 -1.24448 -2.54907
C -1.67779 -0.57861 -1.71247
C -3.00185 -0.54487 -2.15333
C -2.39815 0.54786 0.32520
C -3.70771 0.57311 -0.14019
C -4.01227 0.02775 -1.38401
H 3.20820 -0.50371 -0.89539
H 2.60660 1.04301 -1.46133
H 2.03823 -1.73522 -2.57167
H 2.66538 -0.31933 -3.39336
H 0.27430 0.72719 -2.93537
H 0.49144 -0.42583 -4.22894
H -2.15172 0.95892 1.29454
H -4.48791 1.01450 0.46956
H -5.03171 0.04123 -1.75311
H -3.24488 -0.97909 -3.11788
H -0.12910 -2.01803 -1.93801
H -1.10221 -1.77033 -3.36966
N 1.16666 0.12993 2.32028
C 3.45826 0.61387 2.16343
H 3.80650 0.11847 3.07492
H 4.21321 0.46792 1.39146
H 3.35133 1.68743 2.35245

9-TS2

C 0.01142 -0.00634 -0.00798
N -0.00132 0.00376 2.29123
C 1.22396 -0.01298 -0.24778
N 2.19854 -0.00386 1.69301
C 2.32171 0.00171 -1.22910
C -1.36042 -0.02896 -0.42495
C 1.97211 -0.82663 -2.48748
C 0.55171 -0.59963 -3.04836
C -0.57345 -1.46073 -2.38441
C -1.65365 -0.71262 -1.63242
C -2.96974 -0.69634 -2.09761
C -2.38103 0.64225 0.26208
C -3.68186 0.64752 -0.22755
C -3.97897 -0.02534 -1.41003
H 3.25600 -0.35604 -0.78890
H 2.49977 1.04492 -1.51963
H 2.09951 -1.89141 -2.26293
H 2.71232 -0.58517 -3.25762

H 0.29567 0.46272 -2.98417
H 0.56963 -0.83884 -4.11539
H -2.12973 1.17105 1.17309
H -4.45970 1.17724 0.31071
H -4.99152 -0.02837 -1.79736
H -3.20706 -1.22063 -3.01776
H -0.10395 -2.17267 -1.69645
H -1.05959 -2.06098 -3.15771
N 1.24776 -0.07030 2.35606
C -0.80153 -0.77374 3.23843
H -1.83280 -0.71197 2.89364
H -0.50244 -1.82638 3.26919
H -0.74920 -0.35129 4.24676

9-P1

C -0.01480 0.23250 0.02304
C -0.40868 0.09364 1.43257
C 0.29865 0.45850 2.56635
C 1.63154 1.11498 2.74070
C 2.85077 0.17451 2.62398
C 3.24118 -0.23795 1.19958
C 2.18720 -1.04606 0.39904
C 1.22177 -0.24546 -0.45509
C 1.53764 -0.03041 -1.80298
C -0.90726 0.85544 -0.86159
C -0.57731 1.04889 -2.19599
C 0.66034 0.61491 -2.66673
H 1.65863 1.60788 3.71684
H 1.72334 1.91105 1.99405
H 2.67340 -0.72273 3.22869
H 3.70964 0.68416 3.07390
H 3.52459 0.65164 0.62546
H 4.14659 -0.84880 1.27941
H -1.86533 1.18627 -0.47891
H -1.27928 1.53463 -2.86419
H 0.93284 0.76050 -3.70614
H 2.48315 -0.40290 -2.18491
H 1.62748 -1.68961 1.08496
H 2.72705 -1.71723 -0.27449
N -0.54954 0.14997 3.58601
N -1.71011 -0.36007 3.11204
N -1.62801 -0.38878 1.81780
C -0.37980 0.31769 5.01839
H -1.28005 -0.07401 5.48711
H 0.48885 -0.23874 5.37596
H -0.26728 1.37286 5.27750

9-P2

C 0.04958 0.43698 0.00115
C -0.29179 0.49939 1.42891
C 0.50141 0.74614 2.53672
C 1.96866 1.02780 2.61793
C 2.87255 -0.21973 2.53787
C 3.06037 -0.84327 1.14792
C 1.78814 -1.40415 0.45460
C 1.05677 -0.43860 -0.45654
C 1.37395 -0.42299 -1.82063
C -0.60319 1.28152 -0.91038
C -0.27448 1.27536 -2.25950
C 0.72409 0.41851 -2.71629
H 2.13969 1.52418 3.57617
H 2.25655 1.73627 1.83276
H 2.48658 -0.97690 3.22985
H 3.86447 0.05880 2.91036
H 3.54039 -0.11853 0.48013
H 3.77016 -1.66991 1.25760
H -1.35832 1.96836 -0.54521
H -0.78655 1.93910 -2.94640
H 0.99211 0.40184 -3.76664
H 2.14055 -1.09890 -2.18578

H 1.10587 -1.79435 1.21553
H 2.08844 -2.25897 -0.15756
N -0.28982 0.71310 3.64515
N -1.51662 0.45819 3.29562
N -1.54161 0.32857 1.95393
C -2.79825 0.02329 1.29005
H -3.23640 0.91734 0.84149
H -2.63771 -0.72586 0.51454
H -3.47348 -0.36493 2.04977

10

C 0.14610 -0.89680 -0.11342
C 1.33640 -0.77711 -0.24655
C 2.54179 -0.60098 -1.05220
C -1.25725 -0.90326 -0.51113
C 2.06317 -0.05625 -2.43143
C 0.75684 -0.71915 -2.97801
C -0.53536 0.08711 -2.81321
C -1.44685 0.00859 -1.73210
C -2.59663 0.80503 -1.75054
C -0.84219 0.97303 -3.85620
C -2.87701 1.67582 -2.79749
C -1.98623 1.76345 -3.86007
H -1.56345 -1.92981 -0.75389
H -1.92325 -0.56925 0.28899
H 3.05415 -1.56162 -1.17847
H 3.26649 0.08535 -0.60480
H 2.87114 -0.19701 -3.15650
H 1.90243 1.02112 -2.34262
H 0.64828 -1.71782 -2.55066
H 0.88888 -0.86537 -4.05356
H -3.28671 0.74149 -0.91526
H -2.17910 2.43512 -4.68906
H -3.77675 2.28016 -2.77698
H -0.15722 1.03659 -4.69627

10-TS1

C 0.02418 0.10049 -0.10076
N 0.11095 -0.08435 2.10315
C 1.19836 0.09696 -0.46431
N 2.31529 -0.18750 1.52755
C 2.21242 0.02684 -1.52097
C -1.41218 0.14589 -0.42285
C 1.56677 0.42218 -2.87403
C 0.14448 -0.17023 -3.11881
C -1.00522 0.80572 -2.89301
C -1.70672 0.96384 -1.67814
C -2.73775 1.90642 -1.60642
C -1.38203 1.60499 -3.98030
C -3.09397 2.69300 -2.69685
C -2.40751 2.54100 -3.89602
H -1.76470 -0.88608 -0.55888
H -1.98911 0.54885 0.41198
H 2.60105 -0.99694 -1.57453
H 3.07162 0.67375 -1.31915
H 2.23864 0.09984 -3.67601
H 1.50903 1.51211 -2.93295
H 0.01362 -1.07255 -2.51696
H 0.08799 -0.49197 -4.16229
H -3.27019 2.02582 -0.66824
H -2.66825 3.14081 -4.76098
H -3.89705 3.41600 -2.60712
H -0.85546 1.48174 -4.92201
N 1.26584 -0.10750 2.20687
C 3.56104 0.34411 2.07699
H 3.47733 1.39935 2.35877
H 3.89969 -0.23467 2.94210
H 4.31173 0.24888 1.29314

10-TS2

C -0.01522 0.05436 -0.04823
N -0.01675 -0.00933 2.27281
C 1.19290 0.04068 -0.27598
N 2.17995 0.03244 1.66798
C 2.27558 -0.06475 -1.26702
C -1.42669 -0.00113 -0.45017
C 1.71792 0.17935 -2.68851
C 0.35621 -0.52480 -2.97946
C -0.85874 0.39511 -2.95010
C -1.65956 0.64875 -1.81519
C -2.73909 1.53169 -1.92788
C -1.19243 1.04255 -4.14744
C -3.05087 2.16570 -3.12547
C -2.26759 1.91860 -4.24688
H -1.74084 -1.05376 -0.47734
H -2.07539 0.48649 0.28040
H 2.71484 -1.06715 -1.20022
H 3.08727 0.63530 -1.04995
H 2.46534 -0.15996 -3.41286
H 1.59924 1.25503 -2.84315
H 0.22467 -1.36525 -2.29381
H 0.40328 -0.95738 -3.98244
H -3.34783 1.72631 -1.05057
H -2.49103 2.39924 -5.19268
H -3.89418 2.84493 -3.17813
H -0.58810 0.84605 -5.02773
C -0.82525 0.56006 3.34855
H -1.86687 0.44868 3.04815
H -0.68604 0.01800 4.28930
H -0.61785 1.62335 3.51069
N 1.23157 0.06761 2.33774

10-P1

C -0.06552 -0.11831 0.28632
N -0.35780 0.65885 1.36436
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N 1.76867 0.61821 1.14841
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C 1.97501 -0.50879 -2.34469
C 0.65841 -1.00368 -3.00044
C -0.52593 -0.05533 -2.95590
C -1.38021 0.05703 -1.84240
C -2.45507 0.94917 -1.89314
C -0.78770 0.73479 -4.08159
C -2.69826 1.73095 -3.01787
C -1.85688 1.62413 -4.12033
H -0.88165 -1.76875 -0.80072
H -2.05391 -0.75282 0.02711
H 2.03603 -1.95362 -0.74254
H 3.22817 -0.68584 -0.60443
H 2.80762 -0.96280 -2.89228
H 2.06771 0.57314 -2.47819
H 0.38907 -1.97364 -2.56782
H 0.87367 -1.20147 -4.05389
H -3.10502 1.03475 -1.02884
H -2.03417 2.22151 -5.00762
H -3.53894 2.41539 -3.03168
H -0.14131 0.64211 -4.94909
N 0.74719 1.10156 1.88862
C 3.13196 0.94835 1.52458
H 3.06515 1.60176 2.39184
H 3.69338 0.05003 1.79053
H 3.64420 1.47192 0.71474

10-P2

C 0.05164 -0.31039 0.23804
N -0.19563 0.38178 1.38376
C 1.42031 -0.20888 0.07666
N 1.92068 0.52005 1.11392

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C -0.99216 -0.94467 -0.63257
C 2.03629 -0.24341 -2.42896
C 0.74979 -0.77102 -3.11954
C -0.52164 0.04092 -2.94373
C -1.36148 -0.06495 -1.81774
C -2.54101 0.68326 -1.76700
C -0.89784 0.91755 -3.96837
C -2.89734 1.55111 -2.79459
C -2.06378 1.67400 -3.90063
H -0.61158 -1.90991 -0.97973
H -1.89043 -1.16056 -0.04905
H 2.25342 -1.85323 -1.00706
H 3.32785 -0.49762 -0.71785
H 2.88608 -0.55658 -3.04438
H 2.03652 0.85073 -2.43412
H 0.58190 -1.80834 -2.80758
H 0.94814 -0.81829 -4.19359
H -3.19546 0.57875 -0.90728
H -2.32392 2.34302 -4.71307
H -3.81780 2.12023 -2.73187
H -0.26248 0.99917 -4.84463
C -1.45243 0.64212 2.06217
H -1.96821 -0.29155 2.29614
H -1.20639 1.15991 2.98681
H -2.09990 1.27523 1.45205
N 0.95066 0.87467 1.90336

11

C -0.20322 -0.01461 0.15232
H -0.34375 0.23603 1.20863
C 1.15469 -0.46800 -0.14358
C 1.95075 -1.25060 -0.59621
C 2.30828 -2.49386 -1.27743
C 0.96941 -3.28056 -1.43279
C -0.09319 -2.53803 -2.23701
C -1.02872 -1.61434 -1.70553
C -1.13186 -1.20609 -0.23918
H -0.46291 0.87679 -0.42848
H 3.02918 -3.09260 -0.71173
H 2.75090 -2.29840 -2.25982
H 0.60387 -3.51452 -0.42975
H 1.17744 -4.23486 -1.92681
H -2.16909 -0.92824 -0.02676
H -0.88750 -2.04662 0.41534
C -1.93672 -1.00918 -2.58443
C -1.94559 -1.27383 -3.94951
C -1.02939 -2.17960 -4.46994
C -0.12599 -2.79840 -3.61310
H -2.66163 -0.30987 -2.17870
H -2.66662 -0.78375 -4.59417
H -1.02101 -2.41121 -5.52913
H 0.58050 -3.51491 -4.02094

11-TS

C -0.00285 -0.00439 -0.01844
N 0.01376 -0.00254 2.20511
C 1.17891 -0.00250 -0.35268
N 2.24472 0.07549 1.71630
C -1.41490 -0.03091 -0.42933
H -1.88119 -0.96871 -0.10870
C 2.22059 0.01125 -1.38431
C 1.52897 0.14445 -2.77055
C 0.57001 -0.99242 -3.09075
C -0.79757 -1.00743 -2.73066
C -1.49919 0.10936 -1.97277
H -1.97888 0.77591 0.04925
H 2.81390 -0.90936 -1.35169
H 2.91495 0.84481 -1.23773
H 2.30493 0.17683 -3.54185

H 1.01352 1.10766 -2.80025
H -1.08817 1.08396 -2.24874
H -2.55444 0.11923 -2.26368
N 1.16489 -0.02041 2.34094
C 3.45207 -0.51808 2.28800
H 3.75743 -0.00642 3.20596
H 3.33504 -1.58760 2.49303
H 4.24216 -0.38736 1.54948
C 1.09290 -2.09593 -3.77711
C 0.31680 -3.20232 -4.10354
C -1.02759 -3.21757 -3.74931
C -1.56602 -2.12638 -3.07687
H 2.13962 -2.07989 -4.06575
H 0.75670 -4.03761 -4.63669
H -1.65506 -4.06521 -4.00083
H -2.61893 -2.13494 -2.81183

11-P

C -0.05272 -0.04005 0.03623
H 0.04941 0.11843 1.11707
C 1.29217 -0.01313 -0.62514
C 2.14691 -1.05916 -0.91575
C 2.01096 -2.52385 -0.65223
C 1.07556 -3.30101 -1.63144
C -0.05719 -2.55444 -2.32432
C -0.97297 -1.70768 -1.66785
C -0.85726 -1.34279 -0.20202
H -0.61864 0.81347 -0.34700
N 1.85538 1.14196 -1.07711
N 3.00459 0.87674 -1.62545
N 3.19700 -0.45764 -1.53987
C 4.40686 -1.04042 -2.08956
H 1.65232 -2.64624 0.37156
H 2.99448 -3.00137 -0.67372
H 0.66070 -4.15362 -1.08004
H 1.69570 -3.73682 -2.41846
H -1.86015 -1.19772 0.20954
H -0.41907 -2.16499 0.36707
H 5.00317 -0.21638 -2.47541
H 4.17337 -1.73078 -2.90301
H 4.97262 -1.56588 -1.31704
C -2.01433 -1.13522 -2.40714
C -2.16845 -1.37304 -3.76801
C -1.26151 -2.20108 -4.41992
C -0.22274 -2.77748 -3.69747
H -2.71910 -0.48590 -1.89667
H -2.98641 -0.91426 -4.31175
H -1.35810 -2.39708 -5.48172
H 0.48116 -3.42489 -4.21076

12

C -0.21045 -0.01614 0.13075
H -0.33124 0.23747 1.18767
C 1.13575 -0.48130 -0.17592
C 1.98042 -1.22713 -0.60176
C 2.27013 -2.49457 -1.27106
C 0.94733 -3.26843 -1.43309
C -0.10712 -2.53135 -2.24548
C -1.05174 -1.61870 -1.71435
C -1.14735 -1.20810 -0.24973
H -0.46352 0.87476 -0.45132
F 3.14912 -3.27221 -0.55333
F 2.85399 -2.29846 -2.50015
H 0.60188 -3.49812 -0.42366
H 1.19721 -4.21494 -1.91927
H -2.17906 -0.91874 -0.03058
H -0.90609 -2.04586 0.40964
C -1.96341 -1.02115 -2.59389
C -1.95944 -1.28261 -3.95932
C -1.02569 -2.17032 -4.47914

C -0.11889 -2.78286 -3.62267
H -2.69812 -0.33138 -2.19025
H -2.68221 -0.79973 -4.60678
H -1.00280 -2.39014 -5.54012
H 0.61035 -3.47513 -4.02813

12-TS1

C -0.00833 -0.00792 0.00949
N -0.00395 0.00152 2.24401
C 1.17226 -0.00987 -0.33321
N 2.21767 0.06908 1.68868
C -1.39413 -0.02200 -0.47272
F -2.03062 -1.18016 -0.08493
C 2.22300 0.00993 -1.35517
C 1.55676 0.15889 -2.75221
C 0.60978 -0.97767 -3.10076
C -0.75798 -1.00550 -2.74871
C -1.46409 0.10991 -2.00090
F -2.12101 1.01098 0.07680
H 2.81183 -0.91291 -1.31655
H 2.91531 0.83980 -1.18270
H 2.34936 0.20261 -3.50504
H 1.04180 1.12252 -2.78175
H -1.05783 1.09226 -2.24750
H -2.52558 0.12075 -2.26060
N 1.14788 -0.02665 2.33248
C 3.39656 -0.65440 2.16949
H 3.77149 -0.22576 3.10401
H 3.20179 -1.72278 2.31140
H 4.16718 -0.53213 1.40920
C 1.14225 -2.07153 -3.79440
C 0.37180 -3.17949 -4.12837
C -0.97169 -3.20922 -3.77073
C -1.52040 -2.12823 -3.09160
H 2.18926 -2.04757 -4.08083
H 0.81681 -4.00821 -4.66733
H -1.59070 -4.06304 -4.02133
H -2.56735 -2.14996 -2.81066

12-TS2

C 0.00406 0.00193 -0.00162
N -0.00331 -0.00602 2.22685
C 1.18512 0.00206 -0.33839
N 2.22796 0.09283 1.71191
C -1.39012 -0.02167 -0.43789
F -2.02719 -1.17059 -0.02764
C 2.21157 -0.00188 -1.38601
C 1.52749 0.16132 -2.77168
C 0.56411 -0.96395 -3.11242
C -0.79729 -0.99273 -2.73368
C -1.49108 0.11719 -1.96306
F -2.11029 1.01798 0.13609
H 2.77827 -0.93802 -1.34756
H 2.93241 0.80530 -1.22378
H 2.30695 0.20083 -3.53852
H 1.02154 1.13045 -2.78899
H -1.08967 1.10097 -2.21214
H -2.55734 0.12812 -2.20254
N 1.23396 0.12779 2.29985
C 1.07681 -2.05112 -3.83136
C 0.29537 -3.15053 -4.16728
C -1.04115 -3.17984 -3.78522
C -1.57108 -2.10698 -3.07885
H 2.11850 -2.02826 -4.13615
H 0.72682 -3.97274 -4.72677
H -1.66922 -4.02622 -4.03821
H -2.61325 -2.12806 -2.78040
C -0.87673 0.79182 3.09156
H -1.88849 0.62714 2.72925
H -0.81218 0.45534 4.12989

H -0.64726 1.86003 3.03271

12-P1

C -0.02790 -0.02997 0.03073
H 0.10144 0.13228 1.10744
C 1.31129 -0.04157 -0.64076
C 2.19391 -1.05294 -0.97341
C 2.04089 -2.52207 -0.73373
C 1.04678 -3.27877 -1.63415
C -0.09238 -2.53148 -2.31056
C -1.00365 -1.68580 -1.64661
C -0.86255 -1.31724 -0.18570
H -0.60023 0.82362 -0.34624
N 1.94134 1.07408 -1.09468
N 3.12734 0.76502 -1.67196
N 3.27549 -0.52046 -1.59933
F 1.67221 -2.70826 0.60180
F 3.25647 -3.13610 -0.85537
H 0.66201 -4.10865 -1.03156
H 1.66362 -3.72132 -2.41716
H -1.85412 -1.13841 0.23834
H -0.42272 -2.13245 0.38501
C -2.05849 -1.12327 -2.37450
C -2.22817 -1.36936 -3.73213
C -1.32264 -2.19326 -4.39153
C -0.27151 -2.76116 -3.68073
H -2.76553 -0.48229 -1.85632
H -3.05895 -0.92355 -4.26699
H -1.43162 -2.39577 -5.45069
H 0.43089 -3.40531 -4.19882
C 1.51635 2.46226 -1.03908
H 0.57016 2.59738 -1.56697
H 1.40871 2.79490 -0.00482
H 2.29160 3.04586 -1.53064

12-P2

C -0.06900 -0.06029 0.05625
H 0.06856 0.05119 1.13761
C 1.26453 -0.03432 -0.62794
C 2.13821 -1.05642 -0.94916
C 2.00041 -2.52561 -0.70451
C 0.98223 -3.29912 -1.56840
C -0.10645 -2.53799 -2.30666
C -1.02368 -1.67586 -1.67447
C -0.92237 -1.32542 -0.20682
H -0.60919 0.82725 -0.28295
N 1.81540 1.13247 -1.05810
N 2.96352 0.89046 -1.61888
N 3.18316 -0.43514 -1.56685
C 4.41976 -0.95833 -2.13699
F 1.68654 -2.70568 0.63370
F 3.23198 -3.13816 -0.86449
H 0.54971 -4.05912 -0.90957
H 1.58012 -3.83441 -2.30752
H -1.92410 -1.14002 0.18976
H -0.51812 -2.16208 0.36297
H 4.94922 -0.10017 -2.54435
H 4.20446 -1.67341 -2.93119
H 5.01869 -1.44424 -1.36864
C -2.03238 -1.08620 -2.44301
C -2.14950 -1.32675 -3.80753
C -1.24014 -2.17274 -4.43295
C -0.23207 -2.76735 -3.68193
H -2.74080 -0.42465 -1.95442
H -2.94415 -0.85707 -4.37581
H -1.31377 -2.37172 -5.49583
H 0.47147 -3.43321 -4.17120

