Supporting Information:
Origins of Stereoselectivity in the *trans*-Diels-Alder Paradigm

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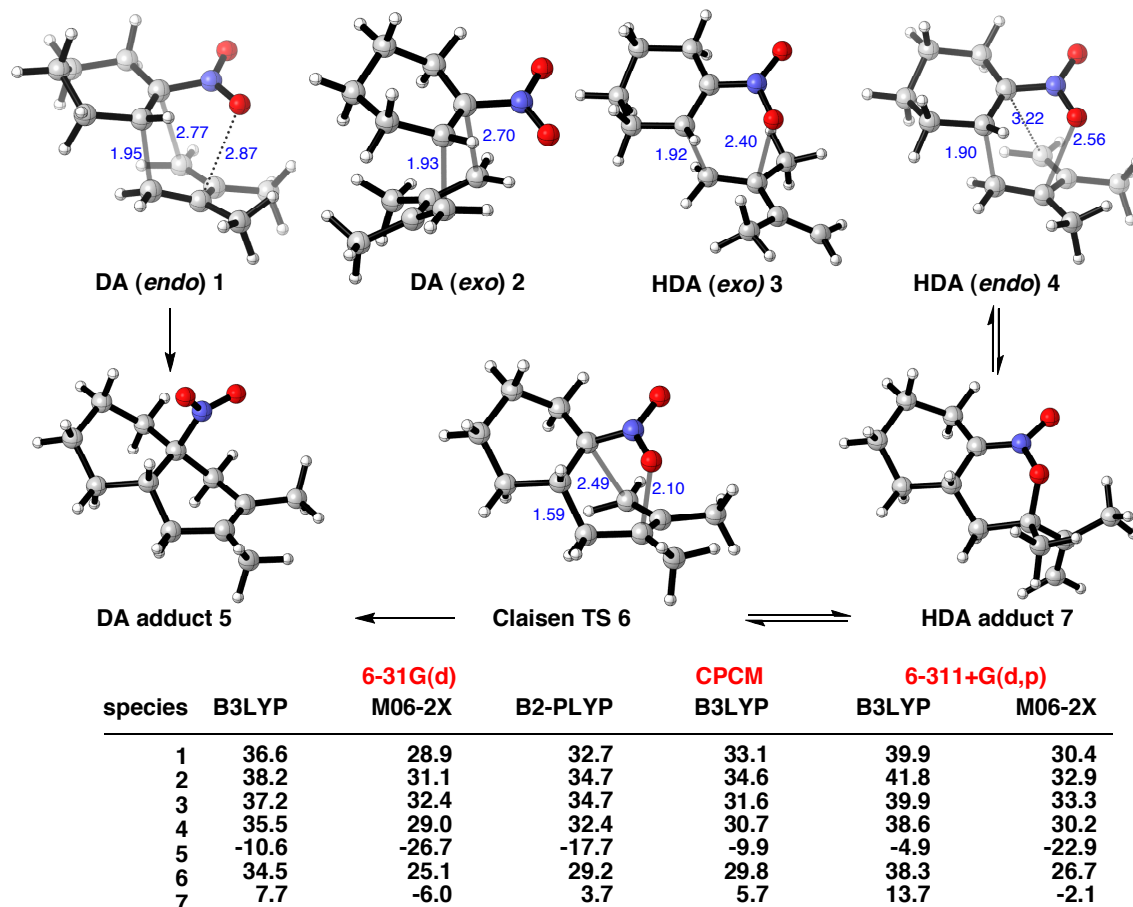
Contents:

Full reference 25:

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Figure S1. Computed free energies for the reaction of nitrocyclohexene and 2,3-dimethylbutadiene. Optimizations performed with B3LYP/6-31G(d), single point energies performed with B3LYP and M06-2X density functionals and the B2-PLYP double-hybrid functional, with 6-31G(d) and 6-311+G(d,p) basis sets and with continuum solvation in trifluoroethanol.

| species | 6-31G(d) | | | CPCM | 6-311+G(d,p) | |
	B3LYP	M06-2X	B2-PLYP	B3LYP	B3LYP	M06-2X
1	36.6	28.9	32.7	33.1	39.9	30.4
2	38.2	31.1	34.7	34.6	41.8	32.9
3	37.2	32.4	34.7	31.6	39.9	33.3
4	35.5	29.0	32.4	30.7	38.6	30.2
5	-10.6	-26.7	-17.7	-9.9	-4.9	-22.9
6	34.5	25.1	29.2	29.8	38.3	26.7
7	7.7	-6.0	3.7	5.7	13.7	-2.1

For all density functionals, basis sets and with and without solvation, the lowest energy transition structure is the hetero-Claisen TS (**TS 6**). Of the cycloaddition TSs, the HDA pathway via **TS 4** is the lowest in energy at all computed levels, bar M06-2X/6-31G(d) where **TS 1** and **TS 4** are separated by 0.1 kcal/mol.

Figure S2. Regioisomeric hetero-Diels Alder transition structures for the cycloaddition of 2,3-dimethylbutadiene and nitrocyclohexene. Selected distances shown in Å, B3LYP/6-31G(d) activation free energies, shown in kcal/mol.

regioisomeric HDA (*endo*) regioisomeric HDA (*exo*)
47.3 **47.2**
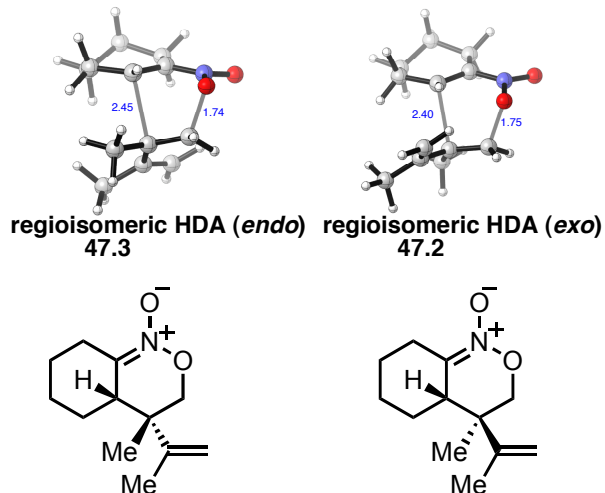
These structures lie around 10 kcal/mol higher in energy than the other transition structures considered, so can be regarded as uncompetitive.

Figure S3. *Exo* Diels-Alder and hetero-Diels Alder transition structures for the cycloaddition of 2-methylbutadiene and nitrocyclohexene. Selected distances shown in Å, B3LYP/6-31G(d) activation free energies, with M06-2X/6-31G(d) values in parentheses, shown in kcal/mol.
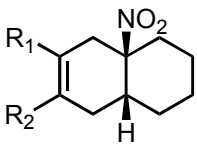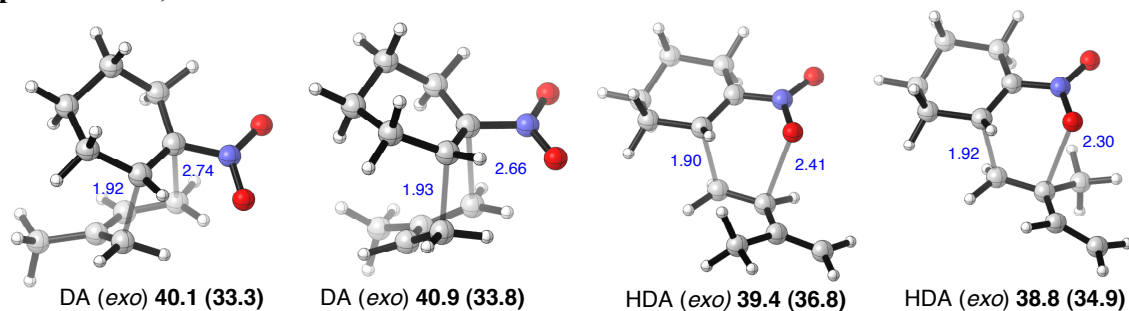

DA (*exo*) **40.1 (33.3)** DA (*exo*) **40.9 (33.8)** HDA (*exo*) **39.4 (36.8)** HDA (*exo*) **38.8 (34.9)**
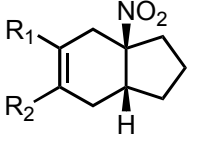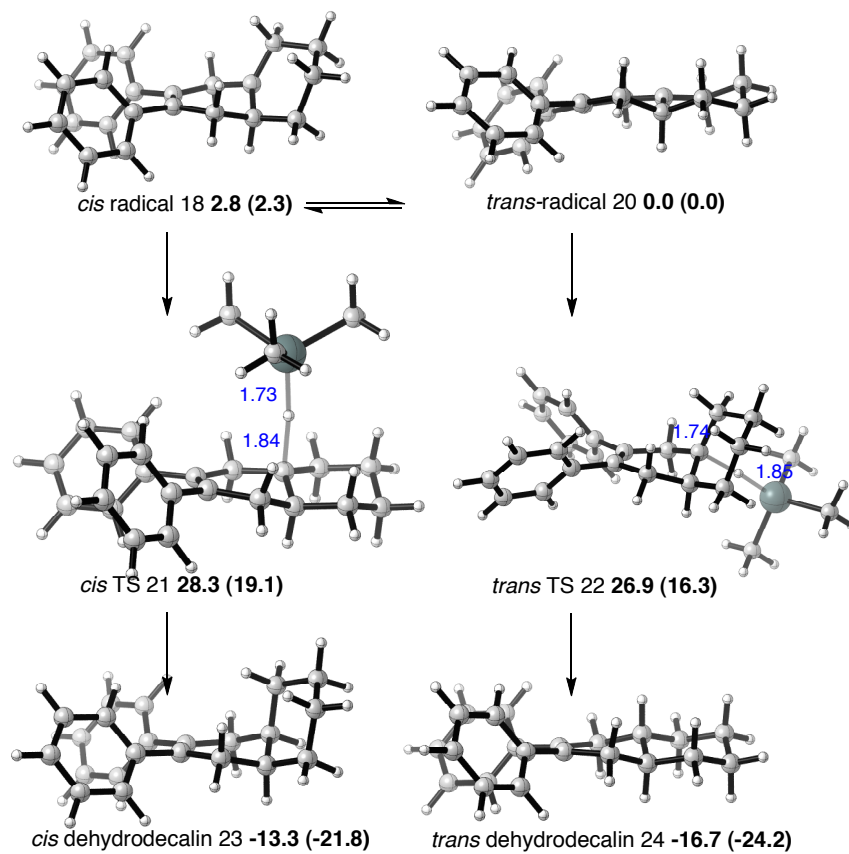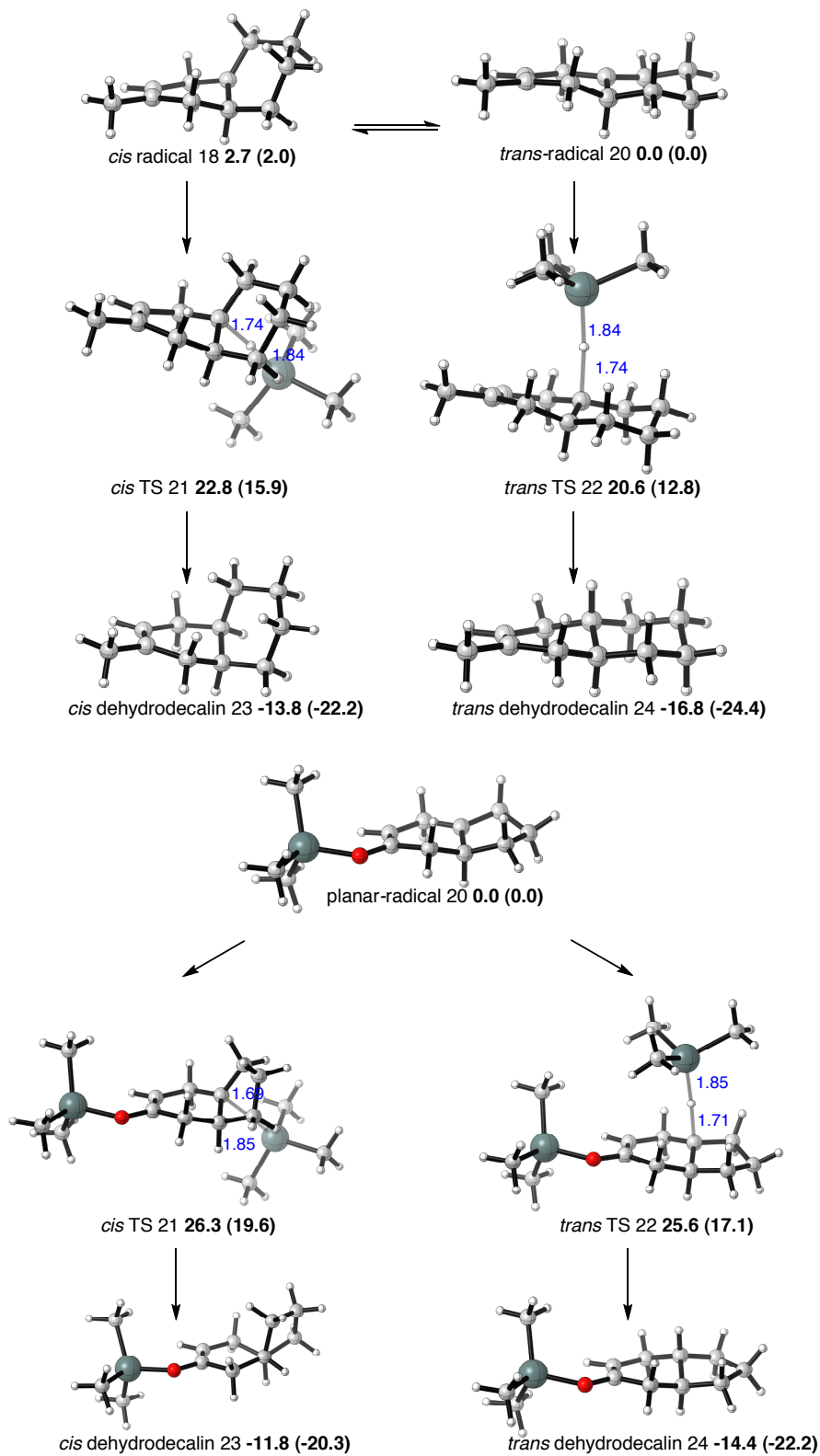
Figure S4. Computed radical hydrodenitation of three 6,6-bicyclic cycloadducts and two 5,6-bicyclic cycloadduct. UB3LYP/6-31G(d) relative free energies in kcal/mol tabulated.

system			cis : trans	computed $\Delta\Delta G^{\ddagger}$
	$R_1 = R_2 = Me$		1 : 8	2.5
	$R_1 = R_2 = Ph$		1 : 7	1.4
	$R_1 = H, R_2 = Me$		1 : 8	2.0
	$R_1 = R_2 = Me$		1 : 1.3	0.0
	$R_1 = H, R_2 = OTBS$		1 : 1.4	0.7

cis radical 18 **2.8 (2.3)** ⟺ *trans*-radical 20 **0.0 (0.0)**

1.73
1.84

1.74
1.85

cis TS 21 **28.3 (19.1)**　　　*trans* TS 22 **26.9 (16.3)**

cis dehydrodecalin 23 **-13.3 (-21.8)**　　　*trans* dehydrodecalin 24 **-16.7 (-24.2)**

cis radical 18 **2.7 (2.0)**

trans-radical 20 **0.0 (0.0)**

cis TS 21 **22.8 (15.9)**

trans TS 22 **20.6 (12.8)**

cis dehydrodecalin 23 **-13.8 (-22.2)**

trans dehydrodecalin 24 **-16.8 (-24.4)**

planar-radical 20 **0.0 (0.0)**

cis TS 21 **26.3 (19.6)**

trans TS 22 **25.6 (17.1)**

cis dehydrodecalin 23 **-11.8 (-20.3)**

trans dehydrodecalin 24 **-14.4 (-22.2)**

Bicyclic radicals and hydrogen transfer TSs and bicyclic products in the cycloaddition of a) 2,3-diphenyl-1,3-butadiene and 1-nitrocyclohexene; b) 2-methyl-1,3-butadiene and 1-nitrocyclohexene; c) 2-OTBS-1,3-butadiene and 1-

nitrocyclopentene. Selected distances shown in Å, UB3LYP/LANL2DZ relative free energies, UM06-2X/LANL2DZ in parentheses, in kcal/mol.

Cartesian Coordinates of B3LYP/6-31G(d) stationary points. B3LYP/6-31G(d) and M06-2X/6-31G(d) energetics.

1:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.743019	-673.43242	-673.490675	-673.430579

C -0.866089 -0.852788 -0.627996
C -0.866948 0.522392 -0.2858
C 1.962218 0.020926 0.997319
C 0.97224 0.542493 1.781521
H 1.080057 1.53043 2.219898
C 1.741689 -1.193342 0.263032
C 0.496174 -1.846274 0.347312
H 0.41904 -2.815744 -0.142351
H -0.401217 -1.03725 -1.591865
O 0.990365 0.755563 -1.605852
O 0.00117 2.570283 -0.857193
N 0.08456 1.332762 -0.954117
H -0.022636 -1.821517 1.300437
H 0.106322 -0.019844 2.1041
C -1.982387 1.253203 0.416405
H -1.598215 1.908828 1.204591
H -2.448601 1.930936 -0.314083
C -2.146922 -1.662831 -0.356878
H -2.005618 -2.324906 0.506773
H -2.330162 -2.322847 -1.212959
C -3.376908 -0.782803 -0.084462
H -3.703671 -0.293297 -1.012322
H -4.208749 -1.41385 0.251494
C -3.042799 0.28637 0.960917
H -2.681565 -0.202372 1.877845
H -3.93816 0.852296 1.242864
C 3.223477 0.819778 0.752128
H 3.242653 1.192954 -0.278224
H 3.281216 1.678926 1.425918
H 4.12296 0.211637 0.905424
C 2.782482 -1.692274 -0.704694
H 3.075945 -0.917991 -1.420352
H 3.691524 -2.004362 -0.171273
H 2.41732 -2.557223 -1.265564

2:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.740598	-673.430028	-673.488132	-673.427201

```
C  0.946925 -0.513323 -1.668467
C -0.532439  0.607443 -1.141897
C -1.208715  0.097399 -0.00261
C  0.411964 -1.945086  0.696856
H  0.106409 -2.3524    1.657004
H  1.261566 -0.035963 -2.5955
H -1.048907  0.364672 -2.068114
C -0.026721  2.051745 -1.0868
H  0.868444  2.168812 -1.707486
H -0.800714  2.680106 -1.552361
C -1.278287  0.804592  1.333953
H -0.549467  0.381514  2.035851
C  0.222813  2.570185  0.333347
C -1.009356  2.31328   1.205653
H  0.461972  3.640014  0.295714
H  1.095059  2.066242  0.773841
H -1.87929   2.811425  0.755281
H -0.879086  2.745112  2.205103
N -2.156458 -0.9483   -0.2452
O -2.110868 -1.540043 -1.349111
O -2.963596 -1.257473  0.646248
H -2.263267  0.615288  1.767603
C  1.593852 -1.259277  0.577952
C  1.90879  -0.579529 -0.641521
H -0.16959  -2.271154 -0.153797
H  0.302209 -1.372418 -1.837721
C  2.506692 -1.108311  1.778122
H  3.508701 -1.503058  1.567592
H  2.636253 -0.058517  2.071688
H  2.112681 -1.65242   2.640839
C  3.185724  0.216279 -0.749827
H  3.272873  0.981356  0.033254
H  4.062162 -0.436864 -0.638107
H  3.265454  0.714101 -1.719935
```

3:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.741938	-673.4318	-673.489742	-673.424741

```
C -0.527806 -1.159938  0.743701
C  0.815244 -0.779207 -0.57126
```

C 1.260349 0.556228 -0.428773
C -1.603622 -0.238483 0.736342
H 0.098812 -1.135147 1.634165
H -0.753004 -2.171415 0.4154
H 0.137046 -0.928572 -1.406242
C 1.867575 -1.872014 -0.40692
H 1.392722 -2.818216 -0.122623
H 2.317049 -2.04397 -1.39606
C 2.543796 0.977704 0.227669
H 2.345939 1.29366 1.265985
C 2.976043 -1.497731 0.586181
C 3.59399 -0.144632 0.212862
H 3.741603 -2.282865 0.595476
H 2.566447 -1.449211 1.605842
H 4.032491 -0.2201 -0.791812
H 4.41331 0.109097 0.895374
N 0.331667 1.546698 -0.699544
O -0.833107 1.159924 -1.0544
O 0.607578 2.752814 -0.514673
H 2.918012 1.876305 -0.273158
C -2.850528 -0.527115 0.0198
C -4.008367 0.064642 0.375614
H -4.936129 -0.171583 -0.137135
H -4.076605 0.785981 1.18228
C -1.535432 0.921006 1.6943
H -2.094387 1.786847 1.33673
H -1.929349 0.628365 2.678689
H -0.495487 1.228226 1.845098
C -2.822252 -1.517493 -1.122822
H -2.129527 -1.181289 -1.902145
H -2.506165 -2.518567 -0.803817
H -3.81416 -1.614135 -1.57282

4:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.744500	-673.434186	-673.492458	-673.430140

C -0.364589 -1.736082 0.307933
C 0.941931 -0.813159 -0.715487
C 0.953585 0.574187 -0.419884
C -1.215532 0.479801 1.965246
C -2.0392 -0.015998 1.010312
C -1.639652 -1.139366 0.177852
H 0.12504 -1.684003 1.276769
H -0.276272 0.017626 2.243124

H -1.485583 1.374125 2.518631
H -0.267914 -2.719569 -0.148794
H 0.470602 -1.038841 -1.668973
C 2.243852 -1.576252 -0.463132
H 2.036436 -2.636329 -0.276505
H 2.826386 -1.541498 -1.395371
C 2.007111 1.295888 0.378736
H 1.659507 1.480503 1.40542
C 3.08935 -0.979665 0.669325
C 3.330551 0.513491 0.419667
H 4.04121 -1.519849 0.739998
H 2.58033 -1.117189 1.634971
H 3.856336 0.63146 -0.537989
H 3.983504 0.93711 1.191651
N -0.106146 1.323718 -0.933141
O -1.025972 0.676986 -1.524172
O -0.150523 2.560679 -0.77837
H 2.149878 2.288619 -0.059665
C -2.60438 -1.710774 -0.825325
H -3.389335 -2.289029 -0.314846
H -3.098265 -0.933475 -1.41298
H -2.094768 -2.390374 -1.514471
C -3.352834 0.674892 0.720101
H -3.311851 1.145471 -0.268713
H -4.195659 -0.026369 0.726796
H -3.555759 1.452485 1.461201

5:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.825819	-673.511642	-673.565803	-673.526751

C -0.780165 1.840076 -0.051749
C 0.527579 1.063371 0.244384
C 0.498219 -0.372455 -0.354905
C -0.71526 -0.578017 -1.277716
C -2.011168 -0.20217 -0.58055
C -2.033873 0.990057 0.042669
H -0.710834 2.27263 -1.063877
H -0.548686 0.063624 -2.156755
H -0.736171 -1.608973 -1.636344
H -0.839654 2.694506 0.632673
H 0.610738 0.948009 1.328217
C 1.762818 1.847506 -0.231131
H 1.700396 2.007296 -1.31724
H 1.742771 2.847846 0.219158

C 1.823022 -0.75477 -1.055136
H 1.82594 -0.242052 -2.024938
C 3.081975 1.142899 0.125544
C 3.071598 -0.366076 -0.251461
H 3.260858 1.247099 1.202132
H 3.910134 1.658105 -0.375052
H 3.115026 -0.976582 0.656248
H 3.960711 -0.625101 -0.837297
N 0.364543 -1.417805 0.804029
O 0.808135 -1.133668 1.913009
O -0.109957 -2.51378 0.516499
H 1.813123 -1.828791 -1.271864
C -3.191746 1.580013 0.803182
H -2.909952 1.780724 1.846335
H -3.489424 2.546048 0.371335
H -4.073933 0.936074 0.814561
C -3.123918 -1.212887 -0.649252
H -2.798443 -2.16398 -0.208124
H -4.031473 -0.891295 -0.133155
H -3.392828 -1.426263 -1.693545

6:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.750191	-673.438752	-673.494	-673.440494

C 0.453744 1.780939 0.115906
C -0.861776 0.987891 -0.289345
C -0.782577 -0.49203 -0.067586
C 0.902482 -0.403616 1.768508
C 1.951543 -0.05399 0.948322
C 1.718562 0.979839 -0.000092
H 0.334295 2.128691 1.149112
H 0.144582 0.300456 2.084956
H 0.930827 -1.335101 2.328298
H 0.512431 2.675586 -0.511261
H -0.952711 1.155278 -1.37103
C -2.106468 1.543315 0.419106
H -1.978518 1.427435 1.505145
H -2.190828 2.621909 0.237546
C -1.95014 -1.232209 0.517475
H -1.997055 -1.088467 1.606144
C -3.402409 0.832239 -0.025092
C -3.259031 -0.715021 -0.12062
H -3.710917 1.229037 -1.000078
H -4.201941 1.098673 0.676297

H -3.26808 -1.022637 -1.172722
H -4.11579 -1.208965 0.352499
N 0.125134 -1.143938 -0.846502
O 0.977926 -0.353736 -1.437702
O 0.266989 -2.387481 -0.890833
H -1.814977 -2.301044 0.337529
C 2.802385 1.519553 -0.886914
H 3.262649 2.401747 -0.418281
H 3.588258 0.787445 -1.079355
H 2.381734 1.836793 -1.846066
C 3.166898 -0.94956 0.83108
H 4.09568 -0.39644 1.018135
H 3.116461 -1.763036 1.560118
H 3.229363 -1.39416 -0.167669

7:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-673.793074	-673.479692	-673.536681	-673.490112

C -0.316185 -1.422596 0.218849
C 1.036025 -0.889226 -0.295249
C 1.084084 0.592505 -0.03155
C -2.824309 -0.852114 1.733061
C -2.536349 -0.13698 0.640056
C -1.493459 -0.605044 -0.382246
H -0.315885 -1.339966 1.309537
H -2.310794 -1.773587 1.992552
H -3.612021 -0.539775 2.413499
H -0.425545 -2.485203 -0.028314
H 1.093702 -1.069543 -1.380863
C 2.243307 -1.556974 0.381888
H 2.123622 -1.486417 1.47188
H 2.256967 -2.626966 0.142025
C 2.259728 1.22517 0.647687
H 2.210197 1.037586 1.731601
C 3.573522 -0.907432 -0.041164
C 3.573667 0.64764 0.077215
H 3.786451 -1.191035 -1.079366
H 4.383273 -1.335125 0.560919
H 3.739219 1.088283 -0.912343
H 4.406298 0.983581 0.705012
N 0.042587 1.305211 -0.363083
O -0.960177 0.556284 -1.103043
O -0.193968 2.517245 -0.223234
H 2.214666 2.309621 0.517795

C -2.180286 -1.386775 -1.513946
H -2.659843 -2.28149 -1.105733
H -2.942332 -0.775001 -2.004931
H -1.443504 -1.687217 -2.266592
C -3.279876 1.13433 0.306759
H -4.063512 1.326446 1.045748
H -2.596442 1.988829 0.274994
H -3.748686 1.077247 -0.683787

8:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.425691	-634.144866	-634.20025	-634.132289

C -0.463227 -0.795564 -0.683158
C -0.657318 0.527664 -0.22716
C 2.067983 0.234625 1.250159
C 0.982094 0.595814 1.989038
H 0.951863 1.555952 2.495018
C 2.100987 -0.904361 0.395149
C 0.971288 -1.734664 0.314074
H 1.052583 -2.6394 -0.286565
H 0.101861 -0.839043 -1.609734
O 1.247054 1.106867 -1.366581
O -0.030291 2.709615 -0.576302
N 0.228909 1.506847 -0.755396
H 0.383488 -1.875112 1.215721
H 0.164017 -0.080433 2.205458
C -1.909518 1.05499 0.426504
H -1.675358 1.687546 1.288629
H -2.402755 1.725988 -0.292135
C -1.641052 -1.778978 -0.58198
H -1.475555 -2.495409 0.232599
H -1.676711 -2.375707 -1.501102
C -2.991111 -1.085638 -0.339589
H -3.31483 -0.5623 -1.249855
H -3.754376 -1.841945 -0.119903
C -2.872819 -0.077426 0.807857
H -2.518222 -0.594684 1.711614
H -3.851377 0.348645 1.057302
C 3.262303 -1.118063 -0.538064
H 2.911065 -1.198788 -1.573952
H 3.976385 -0.291395 -0.494077
H 3.795944 -2.047883 -0.299728
H 2.897851 0.933781 1.174568

9:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.424713	-634.143831	-634.199301	-634.131564

```
C -0.797992 -1.657516 0.280624
C 0.528547 -0.771296 -0.75707
C 0.713272 0.575326 -0.354124
C -1.241004 0.574411 2.145321
C -2.167801 0.169629 1.247734
C -1.995393 -0.910492 0.313967
H -0.239642 -1.752301 1.209101
H -0.321312 0.030931 2.329571
H -1.399502 1.465727 2.744081
H -0.843985 -2.593711 -0.273609
H -3.080167 0.753499 1.14612
H -0.032525 -0.859819 -1.684682
C 1.753435 -1.685104 -0.673519
H 1.445571 -2.729897 -0.550621
H 2.262825 -1.632093 -1.646805
C 1.903339 1.115473 0.395806
H 1.666318 1.253805 1.460305
C 2.744532 -1.276932 0.423451
C 3.130461 0.197715 0.263238
H 3.632685 -1.918362 0.37183
H 2.299876 -1.440033 1.41672
H 3.588488 0.337302 -0.72581
H 3.885607 0.486236 1.003623
N -0.278547 1.481758 -0.75238
O -1.302207 0.994854 -1.316817
O -0.151735 2.700792 -0.525027
H 2.119044 2.119017 0.016246
C -3.106923 -1.239749 -0.642283
H -3.757014 -0.378896 -0.816701
H -2.707404 -1.566967 -1.608166
H -3.72434 -2.060706 -0.248658
```

10:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.426914	-634.146345	-634.202165	-634.131232

```
C -0.798038 -1.65753 0.280758
C 0.528568 -0.7713 -0.756977
C 0.713283 0.575315 -0.35403
C -1.241322 0.574396 2.145389
```

C -2.167956 0.169663 1.247602
C -1.995442 -0.910522 0.313934
H -0.239715 -1.752203 1.209262
H -0.321774 0.030779 2.329946
H -1.399866 1.465755 2.744074
H -0.843941 -2.593754 -0.27343
H -0.032514 -0.85983 -1.68458
C 1.753445 -1.685132 -0.673438
H 1.445571 -2.729906 -0.550407
H 2.26273 -1.632231 -1.646785
C 1.903309 1.115395 0.396012
H 1.666319 1.253344 1.460571
C 2.744682 -1.276898 0.423389
C 3.130492 0.197775 0.263131
H 3.632859 -1.918283 0.371635
H 2.300179 -1.440019 1.416722
H 3.58827 0.337434 -0.726023
H 3.885782 0.486333 1.003354
N -0.278481 1.481792 -0.752394
O -1.302092 0.994934 -1.316941
O -0.15165 2.700815 -0.525016
H 2.118888 2.119075 0.016753
H -3.080247 0.753611 1.145755
C -3.10683 -1.239809 -0.642473
H -3.724373 -2.060698 -0.248891
H -3.756839 -0.378928 -0.817064
H -2.707164 -1.567131 -1.60826

11:
E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.425928	-634.145558	-634.200718	-634.126585

C -0.283 -1.86478 -0.300464
C 0.986138 -0.595422 -0.947637
C 0.763366 0.669746 -0.350502
C -1.774355 -0.502302 1.892863
C -2.307311 -0.665827 0.661677
C -1.596081 -1.363399 -0.393867
H 0.122997 -2.028677 0.695333
H -0.823812 -0.935221 2.1862
H -2.292446 0.073403 2.653893
H -0.043731 -2.672741 -0.988981
H 0.622348 -0.658783 -1.969764
C 2.35523 -1.231591 -0.717815
H 2.287901 -2.322065 -0.80851

H 3.012974 -0.900128 -1.534652
C 1.614403 1.301351 0.716257
H 1.130082 1.194811 1.698166
C 2.987138 -0.832435 0.6225
C 3.02656 0.694685 0.757548
H 3.997311 -1.253328 0.692845
H 2.410515 -1.263632 1.454183
H 3.625842 1.106518 -0.066258
H 3.525862 0.990192 1.687445
N -0.405202 1.321158 -0.712694
O -1.176949 0.693113 -1.516031
O -0.707925 2.431972 -0.228623
H 1.654234 2.380562 0.534573
H -2.153653 -1.560393 -1.304321
C -3.642414 -0.059007 0.298315
H -3.483686 0.75707 -0.414931
H -4.297119 -0.797961 -0.180508
H -4.158258 0.335479 1.17812

12:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.508855	-634.223485	-634.276981	-634.230197

C -0.501588 2.067139 0.57934
C 0.615262 0.988271 0.484044
C 0.177279 -0.263531 -0.328834
C -1.071176 0.005993 -1.187889
C -2.20572 0.534139 -0.331861
C -1.900466 1.506927 0.535484
H -0.374239 2.772147 -0.259423
H -0.777001 0.753194 -1.940694
H -1.355149 -0.899527 -1.727934
H -0.343746 2.658735 1.487872
H -2.6578 1.925885 1.195401
H 0.830845 0.636824 1.496275
C 1.910719 1.588273 -0.090227
H 1.726391 1.915991 -1.123614
H 2.159802 2.498233 0.469611
C 1.334029 -0.86123 -1.167581
H 1.404017 -0.269378 -2.089188
C 3.096477 0.605678 -0.050972
C 2.674897 -0.83955 -0.424778
H 3.539749 0.606515 0.951866
H 3.877599 0.964533 -0.732007
H 2.584851 -1.449021 0.480938

H 3.442131 -1.318789 -1.043181
N -0.209274 -1.414623 0.663413
O 0.315687 -1.44712 1.77236
O -0.970735 -2.281011 0.240779
H 1.061153 -1.877466 -1.472633
C -3.56947 -0.075784 -0.488531
H -3.536701 -1.153792 -0.284198
H -4.296271 0.384255 0.188802
H -3.941787 0.04112 -1.51606

13:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.430074	-634.148097	-634.200667	-634.139339

C -0.383708 -1.947449 -0.411221
C 0.826346 -0.914961 -0.51336
C 0.500204 0.460199 -0.015896
C -1.240351 -0.215503 1.623513
C -2.178818 -0.533284 0.664958
C -1.723802 -1.290318 -0.434821
H -0.266411 -2.510214 0.523278
H -0.411391 -0.870086 1.860099
H -1.433321 0.571599 2.34831
H -0.289856 -2.665094 -1.230453
H 1.016911 -0.837608 -1.591754
C 2.088513 -1.427864 0.194604
H 1.868604 -1.555114 1.264472
H 2.349625 -2.424753 -0.181088
C 1.504817 1.228891 0.793362
H 1.511644 0.885144 1.837123
C 3.288476 -0.470358 0.026217
C 2.909947 1.031015 0.182366
H 3.738073 -0.629506 -0.961486
H 4.057555 -0.747273 0.756939
H 2.924396 1.52032 -0.798552
H 3.653309 1.551311 0.797492
N -0.452407 1.119452 -0.736425
O -1.126965 0.351516 -1.54728
O -0.794228 2.309245 -0.54725
H 1.217626 2.282766 0.801479
H -2.42714 -1.568182 -1.213413
C -3.500241 0.198872 0.569999
H -4.302137 -0.479622 0.255675
H -3.785582 0.633361 1.532556
H -3.433806 1.005252 -0.167778

14:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.476368	-634.192043	-634.246373	-634.191019

C -0.373315 -1.556856 -0.263078
C 0.962637 -0.840336 -0.551695
C 0.88325 0.554077 0.015456
C -2.975577 -1.408296 1.21793
C -2.708703 -0.504888 0.268697
C -1.560604 -0.675524 -0.718895
H -0.430074 -1.738298 0.814612
H -2.368663 -2.29329 1.383091
H -3.842307 -1.298105 1.864335
H -0.401833 -2.532453 -0.76161
H 1.09669 -0.782038 -1.643604
C 2.174874 -1.559987 0.059992
H 1.985324 -1.727972 1.129269
H 2.28313 -2.552734 -0.393256
C 1.967549 1.099275 0.893802
H 1.869864 0.684006 1.908934
C 3.475972 -0.756525 -0.119258
C 3.351319 0.736848 0.311442
H 3.775767 -0.805064 -1.17345
H 4.275591 -1.249826 0.444995
H 3.536684 1.382593 -0.554235
H 4.120062 0.987597 1.050659
N -0.182207 1.262053 -0.245095
O -1.082539 0.617296 -1.190992
O -0.516655 2.401717 0.116647
H 1.849258 2.181854 0.988232
H -1.977841 -1.07456 -1.652613
C -3.580772 0.706435 0.046695
H -4.438274 0.69908 0.725976
H -3.00855 1.627643 0.197551
H -3.955596 0.739757 -0.984991

15:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.508362	-634.223007	-634.276951	-634.228954

C -1.270378 -1.558722 -0.104078
C 0.15029 -0.967019 -0.326542
C 0.375266 0.380744 0.414619

C -0.69318 0.63642 1.494702
C -2.075272 0.511567 0.904531
C -2.356898 -0.524404 0.104914
H -1.241424 -2.214314 0.781731
H -0.530694 -0.118423 2.280088
H -0.531176 1.613684 1.952296
H -1.512302 -2.214443 -0.9489
H -2.810646 1.284488 1.114663
H 0.257865 -0.751663 -1.392472
C 1.233565 -1.991612 0.055512
H 1.167755 -2.199442 1.133311
H 1.016137 -2.943335 -0.445005
C 1.810291 0.516119 0.976434
H 1.844532 -0.045936 1.918311
C 2.654843 -1.521401 -0.305831
C 2.872987 -0.017008 0.007815
H 2.839936 -1.701528 -1.371419
H 3.381568 -2.134953 0.240092
H 2.832867 0.567852 -0.918005
H 3.869566 0.149372 0.431764
N 0.248434 1.565867 -0.608606
O 0.405118 1.347524 -1.806426
O 0.061246 2.682294 -0.134538
H 1.991549 1.565115 1.233121
C -3.689435 -0.738617 -0.556983
H -3.587162 -0.765836 -1.650657
H -4.130762 -1.700474 -0.260328
H -4.400045 0.053822 -0.301189

16:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.433338	-634.151575	-634.203249	-634.142903

C -0.894455 -1.623611 -0.00127
C 0.481263 -0.936649 -0.383848
C 0.591039 0.505085 0.023212
C -0.930212 0.381779 1.97622
C -2.059442 0.220603 1.212333
C -2.045087 -0.662761 0.10789
H -0.767257 -2.137584 0.959814
H -0.230181 -0.425441 2.152066
H -0.826766 1.238465 2.636804
H -1.108527 -2.395498 -0.746651
H -2.847682 0.968329 1.251095
H 0.499433 -0.9667 -1.482

C 1.687592 -1.714868 0.163404
H 1.636806 -1.718756 1.261837
H 1.626324 -2.765643 -0.145407
C 1.888941 1.034815 0.562977
H 2.013282 0.76399 1.620918
C 3.036138 -1.110807 -0.286832
C 3.057769 0.444123 -0.255234
H 3.263661 -1.455652 -1.302882
H 3.827821 -1.515647 0.354747
H 2.987236 0.835899 -1.276758
H 4.010693 0.805049 0.149088
N -0.282105 1.343988 -0.600065
O -1.275406 0.730966 -1.188601
O -0.269558 2.591123 -0.507228
H 1.873019 2.125536 0.506846
C -3.283778 -0.925363 -0.696215
H -3.770303 -1.845414 -0.343206
H -3.999687 -0.103348 -0.612996
H -3.03204 -1.066288 -1.752052

17:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-634.474010	-634.190333	-634.245054	-634.189267

C -0.688829 -1.354277 0.136074
C 0.702008 -0.883227 -0.340311
C 0.858465 0.583724 -0.035453
C -2.875594 -0.259421 1.974965
C -2.633425 0.241769 0.764203
C -1.795202 -0.37326 -0.340617
H -0.672865 -1.406811 1.228805
H -2.447676 -1.194897 2.326539
H -3.532947 0.255454 2.669938
H -0.887134 -2.366826 -0.234164
H -3.09979 1.179558 0.465619
H 0.758032 -1.032704 -1.430651
C 1.852294 -1.655911 0.324758
H 1.73202 -1.595281 1.415361
H 1.782551 -2.719571 0.066561
C 2.090762 1.110129 0.635117
H 2.049184 0.905285 1.716177
C 3.234526 -1.107741 -0.077024
C 3.342162 0.444154 0.023184
H 3.452723 -1.41937 -1.105961
H 3.996499 -1.583865 0.550736

H 3.494991 0.864842 -0.977219
H 4.220239 0.729581 0.613075
N -0.117903 1.38694 -0.360426
O -1.185917 0.722632 -1.097403
O -0.261597 2.607811 -0.204746
H 2.127346 2.197143 0.524972
C -2.712624 -1.017784 -1.389659
H -3.251748 -1.858549 -0.942185
H -3.442407 -0.292859 -1.76257
H -2.12084 -1.382193 -2.236274

18:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.512375	-1126.134693	-1126.213798	-1126.041988

C 1.485691 -0.212803 -1.756537
C 0.656606 0.772303 -0.366307
C 0.681134 0.086458 0.882515
C 2.360638 -2.090464 0.184972
H 2.66032 -2.693491 1.03795
H 1.247679 0.4049 -2.621328
H -0.311729 0.683849 -0.854393
C 1.206806 2.201548 -0.388324
H 1.593892 2.447028 -1.383391
H 0.350262 2.87145 -0.223661
C 1.435198 0.557729 2.104917
H 2.391378 0.026826 2.192266
C 2.255446 2.483964 0.692633
C 1.716375 2.068926 2.06453
H 2.515678 3.549257 0.67991
H 3.181321 1.930152 0.479067
H 0.791873 2.625005 2.271764
H 2.426587 2.326525 2.858909
N -0.272538 -0.937699 1.059962
O -0.857346 -1.388715 0.0257
O -0.510436 -1.392248 2.189002
H 0.854432 0.288837 2.990686
C 3.27861 -1.316247 -0.470342
C 2.859262 -0.409507 -1.502357
H 1.352477 -2.250313 -0.171353
H 0.814802 -1.062365 -1.652963
C 4.731953 -1.338898 -0.041413
H 5.386838 -1.638071 -0.869238
H 5.078397 -0.354098 0.296782
H 4.887228 -2.048549 0.775564

C 3.882225 0.443742 -2.206908
H 4.478064 1.047397 -1.509955
H 4.597869 -0.184695 -2.755076
H 3.412865 1.11822 -2.927304
H -2.618847 -1.823885 0.469267
O -3.595704 -1.844004 0.384673
C -3.929435 -1.114628 -0.759112
H -4.937506 -1.404417 -1.075219
H -3.244893 -1.2869 -1.602032
C -3.964149 0.389248 -0.515055
F -4.853983 0.736468 0.430739
F -2.757542 0.875199 -0.125046
F -4.303087 1.03975 -1.656832

19:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.522139	-1126.144722	-1126.221368	-1126.053039

C -2.060385 1.917277 -0.541557
C -2.443434 0.067526 -1.132319
C -2.064938 -0.868165 -0.144322
C -1.289816 1.295224 2.180017
C -0.370998 1.753636 1.298032
C -0.736334 2.046229 -0.086624
H -2.868058 1.993 0.179648
H -2.342467 1.189875 1.947541
H -0.997235 1.017828 3.188221
H -2.286553 2.401316 -1.488941
H -1.741238 0.146393 -1.95686
C -3.915493 0.108519 -1.526459
H -4.185533 1.102721 -1.899666
H -4.039764 -0.576273 -2.378816
C -3.006568 -1.644854 0.739315
H -3.037826 -1.206531 1.746715
C -4.856631 -0.328424 -0.396801
C -4.427243 -1.694413 0.151769
H -5.885913 -0.368382 -0.772331
H -4.848612 0.417275 0.412014
H -4.460838 -2.429234 -0.664391
H -5.127652 -2.043777 0.918761
N -0.701641 -1.066131 0.012149
O 0.081227 -0.343143 -0.668487
O -0.266855 -1.919458 0.835052
H -2.603857 -2.653596 0.875155
H 1.538007 -1.547394 1.041879

O 2.503054 -1.378295 1.114346
C 3.054725 -1.547118 -0.164001
H 2.295727 -1.529425 -0.9538
H 3.624219 -2.485886 -0.246252
C 4.030846 -0.424236 -0.462591
F 3.428911 0.79188 -0.495526
F 5.021597 -0.348715 0.445115
F 4.601499 -0.615955 -1.676892
C 1.072915 1.895294 1.723932
H 1.163885 1.791861 2.808556
H 1.697564 1.124256 1.261402
H 1.484658 2.871527 1.443468
C 0.31124 2.557771 -1.037845
H 0.524886 3.615875 -0.82408
H 1.251964 2.010064 -0.95562
H -0.038661 2.498121 -2.072483

20:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.517088	-1126.139786	-1126.219538	-1126.044559

C -2.825583 1.044565 0.643526
C -2.779646 -0.423584 -0.6449
C -1.660038 -1.249525 -0.390206
C -1.612536 1.766118 0.725556
H -3.081908 0.456881 1.523056
H -3.677509 1.557273 0.205992
H -2.651075 0.249985 -1.486665
C -4.153626 -1.075686 -0.545749
H -4.91987 -0.321269 -0.33421
H -4.392418 -1.478122 -1.541501
C -1.702326 -2.579641 0.307661
H -1.418775 -2.453305 1.365797
C -4.207709 -2.215654 0.480219
C -3.09084 -3.231216 0.210799
H -5.189913 -2.700913 0.437657
H -4.102924 -1.811093 1.497462
H -3.22694 -3.651492 -0.79512
H -3.152019 -4.070128 0.913214
N -0.427466 -0.673533 -0.599564
O -0.395748 0.529005 -1.005632
O 0.63385 -1.294867 -0.301739
H -0.930756 -3.228956 -0.118137
C -1.416077 3.01637 -0.01336
C -0.414558 3.85935 0.309995

H -0.284897 4.798978 -0.218861
H 0.304365 3.64554 1.092149
C -0.615582 1.340576 1.771641
H 0.420721 1.469409 1.451678
H -0.774303 1.918823 2.693533
H -0.763317 0.286875 2.029556
C -2.366877 3.361299 -1.13836
H -2.369184 2.575407 -1.902058
H -3.399184 3.489497 -0.788855
H -2.064701 4.29377 -1.622383
H 1.843168 0.162014 -0.155293
O 2.479187 0.743567 0.316491
C 3.437875 -0.089772 0.90907
H 3.004451 -1.006731 1.33155
H 3.933686 0.462844 1.714057
C 4.516716 -0.513669 -0.077977
F 3.998943 -1.193302 -1.121874
F 5.195198 0.539237 -0.574502
F 5.416091 -1.324756 0.534583

21:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.595088	-1126.213021	-1126.29023	-1126.141535

C 3.611884 0.593899 -0.199999
C 2.195634 1.177892 -0.418526
C 1.135403 0.463294 0.476937
C 1.781556 -0.58039 1.406137
C 2.720583 -1.508906 0.656283
C 3.62752 -0.922325 -0.146078
H 4.027205 1.002643 0.736089
H 2.337027 -0.007246 2.163834
H 1.005441 -1.133866 1.937862
H 4.263648 0.961275 -1.001288
H 1.918247 0.979429 -1.457354
C 2.170239 2.704969 -0.229922
H 2.528 2.962799 0.777562
H 2.885327 3.156311 -0.928924
C 0.253801 1.457036 1.272408
H 0.893455 1.838297 2.07747
C 0.769342 3.286283 -0.465007
C -0.302513 2.629579 0.448232
H 0.499549 3.12629 -1.515135
H 0.790778 4.371201 -0.311831
H -1.149359 2.282703 -0.150032

H -0.710963 3.363697 1.152431
N 0.126674 -0.291131 -0.43978
O -0.161649 0.191249 -1.526137
O -0.409168 -1.309676 0.0117
H -0.561343 0.907521 1.755069
H -1.998703 -1.625037 -1.12409
O -2.918426 -1.831534 -1.379073
C -3.718471 -1.687415 -0.240366
H -3.30353 -2.179087 0.651845
H -4.694993 -2.133838 -0.452236
C -3.96196 -0.229441 0.126403
F -4.755506 -0.143684 1.219741
F -4.548457 0.462069 -0.863711
F -2.797922 0.408969 0.42698
C 4.666157 -1.618501 -0.984513
H 4.639305 -2.706461 -0.890878
H 4.538533 -1.370394 -2.047497
H 5.676146 -1.284626 -0.707868
C 2.539238 -2.983354 0.89688
H 3.2393 -3.600946 0.329695
H 2.670964 -3.224135 1.961369
H 1.519703 -3.290823 0.63013

22:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.529413	-1126.150991	-1126.224902	-1126.064095

C -1.904966 1.89059 -0.727242
C -2.567043 0.448584 -0.85043
C -2.123245 -0.535427 0.189118
C -1.49398 1.173773 1.92551
C -0.384393 1.641726 1.255345
C -0.529157 1.911292 -0.131456
H -2.573542 2.508862 -0.116382
H -2.506904 1.417169 1.634016
H -1.390736 0.732437 2.913497
H -1.89125 2.334221 -1.726737
H -2.216652 0.075388 -1.821976
C -4.101169 0.529721 -0.854447
H -4.436929 0.96747 0.096618
H -4.435832 1.218128 -1.639848
C -3.126829 -1.419876 0.869942
H -3.685245 -0.85629 1.630039
C -4.760275 -0.8519 -1.048408
C -4.114492 -1.973176 -0.182418

H -4.699267 -1.129903 -2.107548
H -5.828589 -0.761391 -0.820326
H -3.567607 -2.670661 -0.827161
H -4.888271 -2.562212 0.322919
N -0.821896 -0.905398 0.100709
O -0.090292 -0.162518 -0.661682
O -0.297752 -1.819241 0.810766
H -2.602356 -2.226981 1.385265
H 1.47348 -1.584196 0.924503
O 2.44771 -1.44121 0.976091
C 2.945436 -1.458143 -0.333904
H 3.37907 -2.433934 -0.605525
H 2.181229 -1.200513 -1.076504
C 4.061883 -0.440447 -0.466894
F 3.635459 0.828724 -0.239895
F 4.569708 -0.468714 -1.723094
F 5.075374 -0.672787 0.38686
C 0.591392 2.464205 -0.95942
H 0.581789 3.563461 -0.90614
H 1.569157 2.114858 -0.625642
H 0.462388 2.186441 -2.009681
C 0.978826 1.617848 1.912157
H 1.46909 2.595603 1.832701
H 0.885281 1.384336 2.976532
H 1.640839 0.871616 1.461451

23:
E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-1126.565415	-1126.185033	-1126.261462	-1126.109336

C 1.990909 1.553121 0.701591
C 2.569463 0.132047 0.849017
C 2.155059 -0.681117 -0.348994
C 0.607342 3.589137 -0.976441
C 0.035138 2.397044 -0.772351
C 0.466263 1.515545 0.406097
H 2.517216 2.048648 -0.119149
H 1.425662 3.966503 -0.36899
H 0.255665 4.249705 -1.764146
H 2.184813 2.132446 1.611445
H 2.141868 -0.328214 1.754578
C 4.102585 0.118855 0.957218
H 4.517896 0.675546 0.106016
H 4.413136 0.659922 1.858703
C 3.144754 -1.510708 -1.106322

H 3.740442 -0.862849 -1.767209
C 4.679362 -1.309805 0.977116
C 4.071076 -2.243807 -0.111964
H 4.50586 -1.750103 1.966509
H 5.767135 -1.247989 0.8606
H 3.48966 -3.0384 0.36935
H 4.865574 -2.744865 -0.675125
N 0.905613 -0.628491 -0.708457
O 0.055047 0.115426 0.16582
O 0.313323 -1.2073 -1.6586
H 2.614658 -2.215413 -1.751842
H -1.543302 -1.216864 -1.488171
O -2.513886 -1.300459 -1.383464
C -2.778999 -1.665221 -0.057434
H -3.15945 -2.695734 0.015185
H -1.902138 -1.578089 0.594647
C -3.855572 -0.769779 0.531872
F -4.132865 -1.156362 1.801346
F -5.001679 -0.816116 -0.168746
F -3.475575 0.532964 0.589713
C -0.358541 1.854841 1.656568
H -0.202441 2.904149 1.92244
H -1.423192 1.690468 1.473315
H -0.050429 1.223502 2.497393
C -1.103963 1.905525 -1.631031
H -1.44101 2.699231 -2.30415
H -0.795496 1.04604 -2.236098
H -1.955483 1.562 -1.036619

24:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-468.671390	-468.375468	-468.426827	-468.439619

C -0.325934 1.377929 -0.021072
C 0.670197 0.552845 0.834249
C 0.60104 -0.877601 0.377975
C -1.901483 -0.57087 0.104621
C -1.695771 0.733962 -0.159038
H 0.095432 1.557295 -1.023298
H -0.442822 2.377071 0.427347
H 0.28609 0.602664 1.86621
C 2.098077 1.137938 0.826085
H 2.049693 2.231957 0.910243
H 2.627629 0.780523 1.720204
C 2.912192 0.726996 -0.409556

H 3.925402 1.14336 -0.341598
C -0.755835 -1.497295 0.517436
H -0.819427 -2.42362 -0.073704
H -0.937976 -1.813457 1.562471
C 2.968385 -0.801347 -0.534121
H 3.576766 -1.098102 -1.397672
H 3.459493 -1.215597 0.357904
H 2.463247 1.150866 -1.319814
C 1.555234 -1.393515 -0.660595
H 1.594688 -2.492085 -0.623439
H 1.169819 -1.156034 -1.673548
C -3.233602 -1.277471 0.034869
H -4.079187 -0.610531 -0.145093
H -3.232991 -2.039631 -0.757722
H -3.429405 -1.812399 0.974988
C -2.761684 1.701923 -0.617002
H -3.72397 1.23202 -0.829831
H -2.929273 2.486301 0.135047
H -2.438098 2.218432 -1.531799

25:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-468.667279	-468.372727	-468.424189	-468.4339259

C -0.609132 -1.426668 0.292198
C 0.611267 -0.746428 -0.358995
C 0.648013 0.704294 0.014488
C -1.905022 0.676198 -0.104787
C -1.904114 -0.652415 0.11493
H -0.415221 -1.576649 1.367129
H -0.729954 -2.436462 -0.128663
H 0.453353 -0.822769 -1.45341
C 1.941458 -1.447479 -0.044331
H 2.043267 -1.588882 1.042324
H 1.951151 -2.449218 -0.492586
C 3.107087 -0.602679 -0.570271
H 2.940438 -0.415633 -1.640633
C -0.617565 1.487414 -0.14073
H -0.676796 2.267815 0.6383
H -0.602906 2.065607 -1.08864
C 3.224957 0.739591 0.18289
H 3.865638 0.603794 1.062907
H 3.740961 1.465226 -0.456845
H 4.054263 -1.151236 -0.497442
C 1.857154 1.325753 0.647902

H 1.84185 2.412147 0.482
H 1.788051 1.218036 1.74788
C -3.137513 1.524569 -0.309232
H -3.224435 2.285286 0.480141
H -3.071323 2.074384 -1.25881
H -4.068494 0.954963 -0.323996
C -3.137875 -1.515955 0.229781
H -4.075474 -0.956848 0.21379
H -3.173743 -2.255641 -0.582888
H -3.112916 -2.091086 1.16639

26:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-468.674942	-468.379343	-468.4313	-468.441878

C 0.618765 -1.443728 -0.203179
C -0.625356 -0.724262 0.344851
C -0.6454 0.715638 -0.079557
C 1.922652 0.674352 0.005596
C 1.916175 -0.669086 -0.066693
H 0.456147 -1.681016 -1.267607
H 0.720758 -2.416579 0.299373
H -0.548774 -0.749802 1.453115
C -1.920268 -1.471445 -0.035459
H -1.914902 -1.65793 -1.119583
H -1.930822 -2.455403 0.451762
C -3.18284 -0.676992 0.320462
C -3.171197 0.690426 -0.375006
H -3.23728 -0.53467 1.410423
H -4.078115 -1.243828 0.034283
C 0.640608 1.484181 -0.048203
H 0.686957 2.167211 -0.916836
H 0.634579 2.1786 0.818554
H -4.077098 1.258973 -0.12971
H -3.177566 0.538257 -1.46353
C -1.923127 1.498379 0.019705
H -2.054172 1.849134 1.064401
H -1.853806 2.415701 -0.583014
C 3.156695 1.536321 0.126902
H 3.226454 2.236178 -0.718297
H 3.108157 2.155219 1.034265
H 4.088939 0.969896 0.164716
C 3.143042 -1.549221 -0.064782
H 4.085494 -0.99838 -0.077793
H 3.149907 -2.204693 0.817882

H 3.136654 -2.214241 -0.94021

27:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-592.361708	-591.94094	-592.018387	-592.037165

C 3.135437 0.743424 -0.862459
C 1.589704 0.843839 -0.821712
C 1.093027 0.255308 0.478899
C 2.957333 -1.47313 0.293475
C 3.697531 -0.59023 -0.403307
H 3.581723 1.545039 -0.252715
H 3.476438 0.942503 -1.890411
H 1.216591 0.212049 -1.643513
C 1.093181 2.28559 -1.056275
H 1.620156 2.722506 -1.915358
H 0.029279 2.250718 -1.32847
C 1.24984 3.183612 0.181115
H 0.834954 4.177943 -0.028354
C 1.506809 -1.181257 0.673058
H 1.34457 -1.485466 1.718194
H 0.861027 -1.850905 0.075796
C 0.554733 2.56368 1.40096
H 0.682522 3.20338 2.28336
H -0.525586 2.507209 1.206533
H 2.314899 3.336409 0.406856
C 1.091022 1.152558 1.694347
H 0.509141 0.683346 2.500594
H 2.121645 1.239364 2.088864
C 3.425998 -2.829455 0.763105
H 4.421697 -3.100597 0.406491
H 3.436592 -2.88108 1.861383
H 2.729861 -3.610511 0.425462
C 5.141701 -0.791047 -0.799715
H 5.59471 -1.691028 -0.379163
H 5.243563 -0.843328 -1.893283
H 5.748927 0.066169 -0.475649
Sn -2.376247 -0.362668 -0.117645
C -2.571783 -1.910597 -1.615337
H -2.07729 -2.833074 -1.29417
H -3.628521 -2.136413 -1.79682
H -2.123949 -1.596996 -2.563893
C -3.317442 -1.045518 1.705434
H -4.377549 -1.26215 1.532985
H -2.839631 -1.958575 2.075267

H -3.249569 -0.284685 2.48985
C -3.426429 1.394694 -0.814332
H -4.480486 1.164013 -1.00432
H -3.383599 2.198263 -0.071724
H -2.988281 1.769109 -1.745408
H -0.605476 0.041353 0.190339

28:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-592.364984	-591.944607	-592.022379	-592.041961

C 2.136917 -0.242807 1.369377
C 2.153625 1.040891 0.524671
C 1.382184 0.855376 -0.759989
C 2.155086 -1.589243 -0.742727
C 2.325335 -1.532299 0.591837
H 1.185983 -0.300548 1.923198
H 2.915938 -0.173954 2.143574
H 3.210038 1.227193 0.237907
C 1.683937 2.265993 1.331847
H 0.700227 2.04752 1.772599
H 2.370618 2.435688 2.171932
C 1.572227 3.525648 0.462756
C 0.62168 3.287463 -0.718939
H 2.567934 3.800696 0.082982
H 1.224285 4.372764 1.067808
C 1.755516 -0.369067 -1.552446
H 0.924791 -0.641583 -2.224912
H 2.58816 -0.119866 -2.241935
H 0.551343 4.186216 -1.344614
H -0.388581 3.092683 -0.332841
C 1.081175 2.093562 -1.570282
H 1.994652 2.386285 -2.12415
H 0.332881 1.86343 -2.342999
C 2.34173 -2.823553 -1.593781
H 1.395922 -3.115399 -2.072695
H 3.048906 -2.620994 -2.410825
H 2.716631 -3.688151 -1.042844
C 2.693107 -2.704623 1.471339
H 2.708735 -3.663262 0.949198
H 3.681944 -2.554603 1.92823
H 1.981219 -2.794035 2.304246
H -0.219609 0.389625 -0.251138
Sn -1.910283 -0.273249 0.066964
C -1.981942 -1.253062 1.992816

H -1.755256 -0.550071 2.801128
H -2.979146 -1.668787 2.175099
H -1.257818 -2.072777 2.040274
C -3.378417 1.314991 0.058591
H -4.382806 0.909784 0.2248
H -3.172214 2.044184 0.849015
H -3.379991 1.843922 -0.900035
C -2.445631 -1.712181 -1.45595
H -2.465574 -1.246657 -2.446782
H -1.726105 -2.537065 -1.481137
H -3.438129 -2.132283 -1.257994

29:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-469.332131	-469.022119	-469.071739	-469.102613

C -0.212697 1.360858 0.142732
C 0.727227 0.468225 0.972486
C 0.617611 -1.00852 0.539493
C -1.880192 -0.507521 0.10638
C -1.593603 0.788579 -0.11674
H 0.244667 1.608538 -0.82778
H -0.319635 2.330194 0.653559
H 0.391149 0.528713 2.018273
C 2.192585 0.948311 0.914852
H 2.248904 2.016185 1.167249
H 2.763853 0.416575 1.689744
C 2.855907 0.69189 -0.449443
H 3.917609 0.966545 -0.401252
C -0.841371 -1.479421 0.639778
H -0.952813 -2.442483 0.118304
H -1.08216 -1.698347 1.693314
C 2.707092 -0.773959 -0.885621
H 3.128861 -0.916637 -1.888964
H 3.293833 -1.412207 -0.207758
H 2.408369 1.342847 -1.213034
C 1.239638 -1.231768 -0.852443
H 1.172922 -2.296173 -1.115412
H 0.661847 -0.690026 -1.613938
C -3.234001 -1.145073 -0.099418
H -4.020797 -0.437975 -0.369328
H -3.18957 -1.91386 -0.884093
H -3.555061 -1.660821 0.816941
C -2.562817 1.813387 -0.657922
H -3.526854 1.39769 -0.957057

H -2.753143 2.602165 0.084132
H -2.134353 2.316619 -1.536475
H 1.21009 -1.60747 1.248772

30:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-469.336341	-469.026684	-469.076801	-469.105419

C -0.633693 1.469393 -0.093474
C 0.624505 0.698004 0.324562
C 0.624441 -0.697977 -0.324422
C -1.924562 -0.671496 0.046068
C -1.924532 0.671452 -0.046106
H -0.497086 1.861945 -1.115865
H -0.741723 2.363141 0.540111
H 0.587469 0.550798 1.41707
C 1.908433 1.47788 -0.006413
H 1.914574 1.709651 -1.082802
H 1.903137 2.44388 0.516949
C 3.177551 0.68755 0.342224
C 3.177547 -0.687573 -0.342353
H 3.233789 0.549098 1.432237
H 4.069917 1.258408 0.054662
C -0.633677 -1.469347 0.093887
H -0.741562 -2.363408 -0.539275
H -0.497066 -1.861381 1.116477
H 4.069882 -1.258463 -0.054765
H 3.233816 -0.549097 -1.432357
C 1.908412 -1.477908 0.006257
H 1.91468 -1.709912 1.082591
H 1.903039 -2.443795 -0.517316
C -3.159189 -1.537783 0.128481
H -3.241713 -2.186806 -0.755303
H -3.096017 -2.209364 0.996568
H -4.090618 -0.975269 0.217277
C -3.159142 1.537783 -0.128723
H -4.090406 0.975333 -0.21967
H -3.242915 2.18533 0.756032
H -3.094878 2.21079 -0.995611
H 0.58712 -0.550741 -1.416935

31:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-429.355778	-429.090792	-429.140728	-429.1410989

C 0.279989 -1.454009 -0.177794
C -0.927771 -0.716384 0.41658
C -0.928905 0.722994 0.006539
C 1.603282 0.67376 0.014717
C 1.58199 -0.671439 -0.061263
H 0.087822 -1.671741 -1.241212
H 0.401254 -2.43338 0.306851
H -0.847146 -0.795945 1.51969
C -2.327816 -1.207249 -0.015983
C 0.33076 1.511158 -0.024683
H 0.361335 2.159422 -0.920296
H 0.364412 2.234006 0.816978
C -3.222103 0.041496 0.132806
C -2.311298 1.220346 -0.2945
H -2.563993 2.156275 0.228957
H -2.434528 1.444296 -1.370135
C 2.850222 1.519382 0.120605
H 3.777165 0.943487 0.128035
H 2.907952 2.231765 -0.714948
H 2.828879 2.124431 1.038307
C 2.805217 -1.557579 -0.078053
H 3.75101 -1.013418 -0.108984
H 2.823418 -2.210944 0.806018
H 2.779256 -2.225019 -0.951279
H -3.511639 0.164343 1.18439
H -4.145841 -0.021776 -0.452317
H -2.687173 -2.063427 0.565943
H -2.293585 -1.517228 -1.069822

32:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-553.042317	-552.651794	-552.728506	-552.735030

C 3.074451 0.948982 -0.82973
C 1.541423 1.076194 -0.687701
C 1.090763 0.459541 0.617013
C 2.964592 -1.260111 0.352484
C 3.632486 -0.413131 -0.453616
H 3.571314 1.716778 -0.214841
H 3.359001 1.1833 -1.866643
H 1.084934 0.562842 -1.547161
C 1.062474 2.53792 -0.576503
H 1.616599 3.222034 -1.230217
H 0.005147 2.596869 -0.864201

C 1.221497 2.880459 0.922148
C 1.598999 -0.919118 0.942718
H 1.639013 -1.061195 2.033979
H 0.886744 -1.687896 0.590061
C 0.956275 1.546661 1.67095
C 3.449266 -2.627877 0.772292
H 4.386198 -2.928343 0.299736
H 3.594167 -2.673951 1.861339
H 2.696597 -3.391484 0.529718
C 4.996001 -0.677207 -1.049125
H 5.464273 -1.597894 -0.696
H 4.93902 -0.728561 -2.145955
H 5.680125 0.151271 -0.816077
H -0.521536 0.141594 0.260811
H 1.660389 1.397991 2.502502
H -0.047116 1.537426 2.12531
H 2.243562 3.22389 1.122353
H 0.550331 3.685647 1.239469
Sn -2.280988 -0.282631 -0.1155
C -2.398248 -2.101195 -1.280449
H -1.96662 -2.946073 -0.734003
H -3.441975 -2.342665 -1.510752
H -1.857232 -1.995931 -2.226412
C -3.393788 -0.568944 1.716905
H -4.441597 -0.802296 1.497237
H -2.977573 -1.394365 2.303601
H -3.369222 0.333982 2.335674
C -3.21867 1.308903 -1.241142
H -4.259739 1.054931 -1.469831
H -3.214824 2.2459 -0.67464
H -2.69573 1.481286 -2.187525

33:

E(UB3LYP)	H(UB3LYP)	G(UB3LYP)	E(UM06-2X)
-553.043562	-552.65336	-552.728523	-552.738780

C 2.078203 0.07003 1.428202
C 2.091869 1.337237 0.573961
C 1.372964 1.123453 -0.730084
C 2.263366 -1.240622 -0.719563
C 2.364009 -1.193987 0.625337
H 1.100276 -0.034237 1.923961
H 2.81333 0.149768 2.242367
H 3.152468 1.568743 0.343804
C 1.437525 2.615476 1.124755

C 1.22037 3.477692 -0.142031
C 1.833425 -0.037843 -1.552833
H 1.04872 -0.354208 -2.259719
H 2.680808 0.266523 -2.199964
C 0.966462 2.465049 -1.300103
H 1.552374 2.723911 -2.196004
H -0.086345 2.46827 -1.620526
C 2.559331 -2.455291 -1.568963
H 1.654364 -2.797194 -2.091609
H 3.288653 -2.203617 -2.352061
H 2.960146 -3.301902 -1.008721
C 2.751622 -2.362984 1.501859
H 2.837267 -3.31141 0.968287
H 3.710973 -2.172257 2.004159
H 2.009469 -2.50003 2.30111
H -0.145575 0.513712 -0.244775
Sn -1.814122 -0.238957 0.031055
C -1.859621 -1.305749 1.91154
H -1.648519 -0.636421 2.752001
H -2.846971 -1.752157 2.074023
H -1.11703 -2.110227 1.921069
C -3.363687 1.271113 0.076199
H -4.344533 0.809339 0.236175
H -3.189923 1.987308 0.886006
H -3.398958 1.826233 -0.866832
C -2.268581 -1.63965 -1.553346
H -2.308963 -1.135976 -2.524687
H -1.506984 -2.424453 -1.607652
H -3.238533 -2.118438 -1.378154
H 2.042193 3.124218 1.883989
H 0.473303 2.363528 1.586277
H 2.127423 4.058315 -0.350064
H 0.40314 4.196988 -0.024779

34:

E(B3LYP)	H(B3LYP)	G(B3LYP)	E(M06-2X)
-430.009836	-429.730165	-429.778834	-429.798781

C -0.044829 1.352331 -0.175534
C -1.053572 0.443264 -0.899862
C -0.924521 -1.016694 -0.426672
C 1.591899 -0.545709 -0.080667
C 1.342328 0.772038 0.033345
H -0.444475 1.645633 0.809294
H 0.041788 2.298772 -0.729791

H -0.883853 0.518829 -1.981683
C -2.508207 0.7893 -0.523905
C 0.512661 -1.545874 -0.45566
H 0.595726 -2.4237 0.204052
H 0.741035 -1.931675 -1.4626
C -2.772357 0.032567 0.813822
C -1.615814 -0.997512 0.954872
H -1.969708 -1.992036 1.248782
H -0.90184 -0.676732 1.72316
C 2.943569 -1.192858 0.112098
H 3.756578 -0.483412 0.276964
H 2.925607 -1.886221 0.965249
H 3.206825 -1.797111 -0.767821
C 2.36409 1.819657 0.409114
H 3.338517 1.412049 0.684573
H 2.518584 2.527868 -0.41771
H 2.004249 2.41613 1.259692