Electronic Supplementary Information

for

How does cross-conjugation influence thiol additions to enones? A computational study of thiol trapping by the naturally occurring divinyl ketones zerumbone and α-santonin

Jonathan Y. C. Ting,[a,b] Ras Baizureen Roseli,[a,b] and Elizabeth H. Krenske*[a]

[a] School of Chemistry and Molecular Biosciences, University of Queensland, St Lucia, QLD 4072, Australia. E-mail: e.krenske@uq.edu.au
[b] These authors contributed equally.

Contents

Performance of different QM methods for computing thiol additions

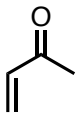
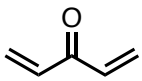
Computations were carried out to compare the performance of several quantum mechanical (QM) methods for modelling the additions of thiols to Michael acceptors. Seven different methods were explored, labelled A–G as listed below. In each method, the solvent (chloroform) was simulated using the CPCM continuum model. The values of ΔG for MeSH addition and $\Delta G^{\ddagger}$ for MeS^- addition to acceptors **8** and **9** were computed with each method. All of the methods except for Method F utilized Truhlar's quasi-harmonic approximation in which low-frequency vibrations (<100 cm^{-1}) were raised to exactly 100 cm^{-1} before evaluation of the vibrational component of the thermal contribution to entropy. Methods A–E all utilized geometries optimized with M06-2X/6-31+G(d), while Methods F and G utilized geometries optimized with B3LYP/6-311G(2d,d,p).

Method A	CBS-QB3//M06-2X/6-31+G(d)
Method B	M06-2X/def2-TZVPP//M06-2X/6-31+G(d)
Method C	M06-2X/6-311+G(d,p)//M06-2X/6-31+G(d)
Method D	ωB97X-D/def2-TZVPP//M06-2X/6-31+G(d)
Method E	ωB97X-D/6-311+G(d,p)//M06-2X/6-31+G(d)
Method F	CBS-QB3 (standard implementation)
Method G	CBS-QB3 (modified to include quasi-harmonic approximation)

Our previous calculations[1] showed that computations with M06-2X/6-311+G(d,p) gave close agreement (within 0.1–0.7 kcal/mol) with the experimental ΔG values for thiol additions to five α-cyanoacrylamides in water. In the present study, no experimental ΔG or $\Delta G^{\ddagger}$ values for **8** or **9** were available, and therefore Method A, comprising CBS-QB3 single-point energy computations on M06-2X optimized geometries, was used as the benchmark against which the other methods were compared. This method was chosen as the benchmark instead of standard CBS-QB3 because previous studies[2] have shown that M06-2X has superior performance compared to B3LYP for computing the geometries of key species in thiol additions (specifically, B3LYP predicts in some cases that the β-thioenolate intermediates are not energy minima, whereas M06-2X correctly identifies these anions as minima). The computed ΔG and $\Delta G^{\ddagger}$ values for thiol addition to **8** and **9** are given in Table S1 overleaf.

1. E. H. Krenske, R. C. Petter and K. N. Houk, *J. Org. Chem.*, 2016, **81**, 11726.
2. J. M. Smith, Y. J. Alahmadi and C. N. Rowley, *J. Chem. Theory Comput.*, 2013, **9**, 4860.

Table S1. Computed ΔG values for MeSH addition and $\Delta G^{\ddagger}$ values for MeS^{-} addition to Michael acceptors **8** and **9**.[a]

Michael Acceptor	 (**8**)		 (**9**)	
	ΔG	$\Delta G^{\ddagger}$	ΔG	$\Delta G^{\ddagger}$
Method A	–8.6	9.1	–9.4	7.4
Method B	–9.2 (–0.6)	6.2 (–2.9)	–9.7 (–0.3)	5.6 (–1.8)
Method C	–10.0 (–1.4)	7.3 (–1.8)	–10.4 (–1.0)	6.4 (–1.0)
Method D	–9.0 (–0.4)	8.1 (–1.0)	–9.3 (+0.1)	6.7 (–0.7)
Method E	–9.4 (–0.8)	9.3 (+0.2)	–9.5 (–0.1)	7.6 (+0.2)
Method F	–9.8 (–1.2)	–	–10.6 (–1.2)	–
Method G	–8.9 (–0.3)	–	–9.9 (–0.5)	–

[a] ΔG and $\Delta G^{\ddagger}$ values in kcal/mol at 1 mol/L and 25 °C. Values in parentheses represent the deviation with respect to Method A.

The following conclusions are drawn from the results in Table S1:

- Comparing the two functionals M06-2X and ωB97X-D (Methods B *vs* D; and C *vs* E): M06-2X predicts ΔG values a few tenths of a kcal/mol more negative, and $\Delta G^{\ddagger}$ values 1–2 kcal/mol smaller, than ωB97X-D.
- Comparing the two basis sets def2-TZVPP and 6-311+G(d,p) with a given functional (Methods B *vs* C; and D *vs* E): the def2-TZVPP basis set predicts ΔG values a few tenths of a kcal/mol less negative, and $\Delta G^{\ddagger}$ values about 1 kcal/mol smaller, than the 6-311+G(d,p) basis set.
- Standard CBS-QB3 (Method F) predicts ΔG values about 1 kcal/mol more negative than Method A. The agreement is improved by applying the quasi-harmonic approximation (Method G). The quasi-harmonic approximation is also a component of Method A. Only ΔG values and not $\Delta G^{\ddagger}$ values were computed with Methods F and G. In these two methods, geometries are optimized with B3LYP, which has known problems in modelling anionic species formed during thiol Michael additions.

The calculations show that Methods B–E are broadly comparable in terms of computing the thermodynamics of MeSH addition to **8** and **9**. The calculated values of ΔG agree to within 0.1–1.8 kcal/mol of the Method A values. For the $\Delta G^{\ddagger}$ of MeS^{-} addition, Methods B–D underestimate the activation barriers by 0.7–2.9 kcal/mol relative to Method A. On the other

hand, Method E overestimates both $\Delta G^{\ddagger}$ values by only 0.2 kcal/mol. Overall, Method E yields the best balance of cost and accuracy for these reactions.

Conformer energies of methyl vinyl ketone 8

The energy difference between the s-*cis* and s-*trans* conformers of methyl vinyl ketone **8** was calculated using five different computational methods (Table S2). Each method predicted that the s-*trans* conformer was more stable than the s-*cis* conformer. The energy differences ranged from 0.2 to 0.7 kcal/mol. These results are in agreement with experimental studies by Durig and Little[3] who showed, based on vibrational spectroscopy, that the s-*trans* conformer was 0.5 kcal/mol more stable than the s-*cis* conformer in the liquid state and 0.8 kcal/mol more stable in the gas phase (ΔH).

Table S2. Relative energies of s-*cis* and s-*trans* conformers of **8**.[a]

Level of Theory	ΔG of s-*cis* conformer relative to s-*trans* conformer
CBS-QB3 in gas phase	0.3
CBS-QB3 in CPCM $CHCl_3$	0.6
CBS-QB3 in CPCM water	0.7
M06-2X/6-31+G(d) in CPCM $CHCl_3$	0.2
M06-2X/6-31+G(d) in CPCM water	0.3

[a] ΔG values in kcal/mol.

Atomic charges in methyl vinyl ketone 8 and divinyl ketone 9

The computed Mulliken atomic charges in **8** and **9** (Fig. S1) are consistent with the resonance schemes shown in Fig. 2 of the paper.

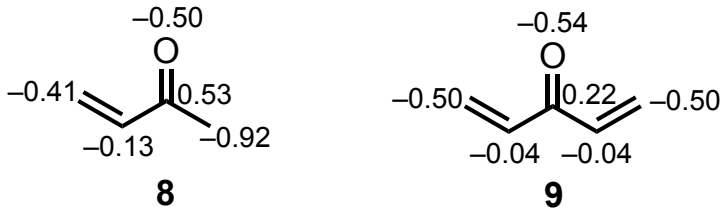
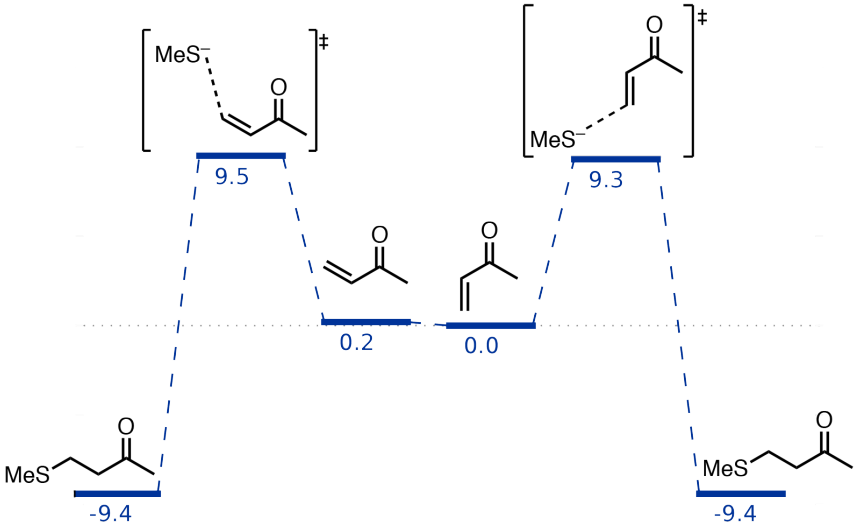


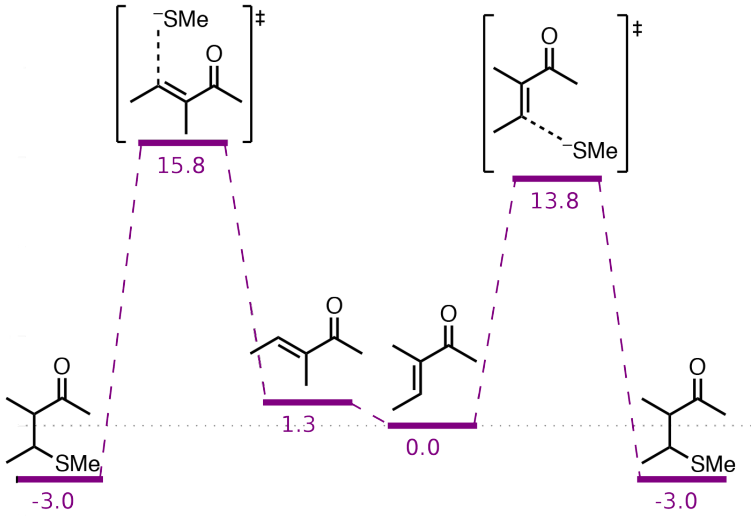
Figure S1. Mulliken charges in **8** and **9**, computed at the M06-2X/6-31+G(d) in CPCM $CHCl_3$.

[3] J. R. Durig and T. S. Little, *J. Chem. Phys.*, 1981, **75**, 3660.

(a) Enone **8**



(b) Enone **11**



(c) Enone **12**

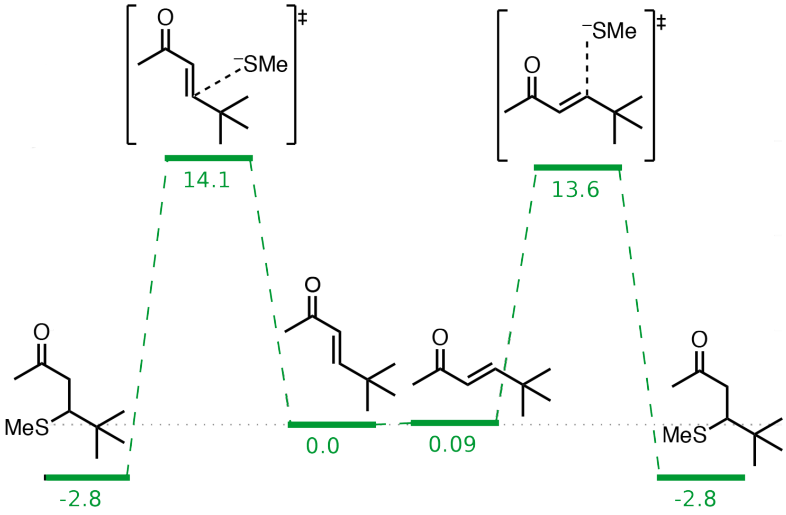


Figure S2. Computed free energy profiles (kcal/mol) for MeSH additions to the s-*cis* and s-*trans* conformers of enones (a) **8**, (b) **11**, and (c) **12**.

DFT computed geometries and energies

Cartesian coordinates of structures optimized with M06-2X/6-31+G(d) are listed below, together with the following energies. All calculations were performed in CPCM implicit chloroform.

E: M06-2X/6-31+G(d) electronic potential energy

H: M06-2X/6-31+G(d) enthalpy at 298.15 K

G: M06-2X/6-31+G(d) Gibbs free energy at 298.15 K and 1 mol/L after quasi-harmonic entropy correction

$E_{\omega B97X-D}$: ωB97X-D/6-311+G(d,p)//M06-2X/6-31+G(d) single-point electronic potential energy

H_{tot}: Total ωB97X-D/6-311+G(d,p)//M06-2X/6-31+G(d) enthalpy at 298.15 K

G_{tot}: Total ωB97X-D/6-311+G(d,p)//M06-2X/6-31+G(d) Gibbs free energy at 298.15 K and 1 mol/L

All energies are reported in Hartree.

MeSH

```
S     0.048263   -0.666669    0.000000
H    -1.283176   -0.833102    0.000000
C     0.048263    1.156057    0.000000
H    -0.436485    1.548926    0.894205
H     1.094353    1.465618    0.000000
H    -0.436485    1.548926   -0.894205
0 imaginary frequencies
E = -438.632495
H = -438.581300
G = -438.607591
E_ωB97X-D = -438.709264
H_tot = -438.658069
G_tot = -438.684360
```

MeS$^-$

```
S     0.000000    0.000000    0.710874
C     0.000000    0.000000   -1.130081
H     0.000000    1.019664   -1.531163
H     0.883055   -0.509832   -1.531163
H    -0.883055   -0.509832   -1.531163
0 imaginary frequencies
E = -438.144805
H = -438.103746
G = -438.127280
E_ωB97X-D = -438.212754
H_tot = -438.171695
G_tot = -438.195229
```

8 (s-*trans*)

```
C    -0.542954   -0.184956    0.000021
C     0.870397   -0.650185   -0.000068
H     0.991275   -1.731065   -0.000245
```

O	-1.444567	-1.008203	0.000057
C	1.926384	0.166901	0.000056
H	1.821412	1.248552	0.000229
H	2.938880	-0.224996	-0.000035
C	-0.834485	1.297459	-0.000038
H	-0.398200	1.774391	0.883381
H	-0.398683	1.774142	-0.883841
H	-1.914204	1.449287	0.000231

0 imaginary frequencies
E = -231.137135
H = -231.039756
G = -231.072106
$E_{\omega B97X-D}$ = -231.227537
H_{tot} = -231.130158
G_{tot} = -231.162507

TS8 (s-*trans*)

C	1.721404	-0.007104	0.092236
C	0.790037	0.905822	0.697271
H	0.879795	1.040424	1.773302
O	2.667973	-0.521155	0.716454
C	-0.232293	1.519790	0.000331
H	-0.202056	1.571295	-1.081483
H	-0.800114	2.309667	0.478766
C	1.528353	-0.357253	-1.376626
H	0.490091	-0.648547	-1.575541
H	1.752955	0.507229	-2.012346
H	2.201675	-1.174312	-1.642801
S	-2.244744	0.105609	-0.176878
C	-1.460713	-1.395110	0.471320
H	-0.447670	-1.142197	0.827827
H	-2.016989	-1.808822	1.317625
H	-1.366292	-2.172123	-0.294123

1 imaginary frequency
E = -669.285663
H = -669.146674
G = -669.187193
$E_{\omega B97X-D}$ = -669.441373
H_{tot} = -669.302384
G_{tot} = -669.342903

P8

C	1.958393	-0.074893	0.041968
O	2.237465	-1.151109	0.535580
C	3.008475	0.976670	-0.224094
H	4.006376	0.551029	-0.110063
H	2.889392	1.399778	-1.226142
H	2.881456	1.796505	0.492244
C	0.531775	0.284980	-0.330528
H	0.496078	0.426364	-1.419189
H	0.307569	1.266821	0.106042
C	-0.477739	-0.766748	0.104398
H	-0.230273	-1.732974	-0.343095
H	-0.457304	-0.898786	1.190835
S	-2.182102	-0.403923	-0.416316
C	-2.525340	1.051452	0.612631
H	-1.942055	1.919229	0.297738
H	-3.585890	1.283773	0.497282
H	-2.324814	0.831140	1.664505

0 imaginary frequencies
E = -669.811473
H = -669.657221

G = -669.699095
$E_{\omega B97X-D}$ = -669.974214
H_{tot} = -669.819962
G_{tot} = -669.861836

s-*cis* conformer of 8

C	0.444211	0.161937	0.000020
C	-0.800998	-0.665955	0.000044
H	-0.680389	-1.746869	0.000129
O	0.403139	1.380523	0.000023
C	-2.009628	-0.101056	-0.000038
H	-2.110077	0.981360	-0.000129
H	-2.917304	-0.696066	-0.000012
C	1.748579	-0.593969	-0.000037
H	1.799743	-1.243603	0.880974
H	1.799579	-1.243847	-0.880887
H	2.590352	0.099095	-0.000197

0 imaginary frequencies
E = -231.136313
H = -231.039077
G = -231.071729
$E_{\omega B97X-D}$ = -231.226827
H_{tot} = -231.129591
G_{tot} = -231.162245

s-*cis* conformer of TS8

C	-1.670103	-0.108624	0.161309
C	-0.770217	-0.808870	-0.739016
H	-0.896064	-0.645404	-1.806722
O	-1.595311	-0.178074	1.393728
C	0.254769	-1.575101	-0.266261
H	0.304661	-1.811010	0.790126
H	0.860177	-2.175374	-0.933721
C	-2.736111	0.773069	-0.468361
H	-2.325646	1.780889	-0.605803
H	-3.048864	0.403183	-1.448711
H	-3.599370	0.845123	0.197186
S	2.400596	-0.060198	0.117744
C	1.470127	1.481186	-0.130437
H	0.464839	1.245327	-0.518027
H	1.342982	2.036532	0.804799
H	1.959453	2.138526	-0.856264

1 imaginary frequency
E = -669.283236
H = -669.144344
G = -669.1857073
$E_{\omega B97X-D}$ = -669.440135
H_{tot} = -669.301241
G_{tot} = -669.342605

9 (W-shaped)

C	-0.000001	0.119233	0.000038
C	1.267676	-0.667006	0.000026
H	1.186343	-1.751120	0.000065
C	-1.267675	-0.667000	0.000028
H	-1.186342	-1.751113	0.000083
O	0.000003	1.341692	0.000050
C	2.457164	-0.061403	-0.000057
H	2.521675	1.023639	-0.000107
H	3.383617	-0.626541	-0.000093
C	-2.457166	-0.061404	-0.000059

```
H   -2.521682    1.023638   -0.000122
H   -3.383615   -0.626549   -0.000080
0 imaginary frequencies
E = -269.201695
H = -269.098241
G = -269.133237
E_ωB97X-D = -269.298613
H_tot = -269.195159
G_tot = -269.229641
```

TS9 (W-shaped)

```
C   -1.309536   -0.457296    0.112779
C   -0.311799   -1.122032   -0.722798
H   -0.426501   -1.047287   -1.801481
C   -2.405355    0.260317   -0.615797
H   -2.385312    0.227346   -1.703369
O   -1.278503   -0.464900    1.345898
C    0.765705   -1.733657   -0.179790
H    0.855234   -1.831689    0.895769
H    1.493224   -2.253634   -0.790495
C   -3.366486    0.921481    0.032418
H   -3.373072    0.950298    1.119099
H   -4.156970    1.445093   -0.496373
S    2.789833    0.254562    0.142693
C    1.574379    1.567521   -0.199637
H    1.947089    2.280074   -0.942999
H    0.643590    1.132110   -0.598977
H    1.311969    2.125893    0.705509
1 imaginary frequency
E = -707.351037
H = -707.205918
G = -707.248981
E_ωB97X-D = -707.514839
H_tot = -707.369721
G_tot = -707.412784
```

U-shaped conformer of 9

```
C    0.000060    0.730697    0.000007
C    1.273698    0.000606   -0.247186
H    2.015179    0.569733   -0.803376
C   -1.273660    0.000752    0.247258
H   -2.015000    0.569885    0.803628
O    0.000136    1.954805   -0.000033
C    1.568543   -1.197870    0.263173
H    0.860054   -1.758245    0.866103
H    2.548349   -1.640812    0.112282
C   -1.568747   -1.197610   -0.263218
H   -0.860444   -1.758021   -0.866331
H   -2.548596   -1.640427   -0.112241
0 imaginary frequencies
E = -269.200022
H = -269.096526
G = -269.130538
E_ωB97X-D = -269.297169
H_tot = -269.193673
G_tot = -269.227685
```

U-shaped conformer of TS9

```
C    1.488908    0.606397    0.210545
C    0.518014    0.340491    1.246956
H    0.408038    1.143548    1.973571
```

C	1.778509	-0.407834	-0.858023
H	1.830487	0.003756	-1.865221
O	2.125770	1.672194	0.155361
C	-0.317556	-0.743552	1.302568
H	-0.185810	-1.595953	0.651065
H	-0.931600	-0.905940	2.179995
C	2.087841	-1.686547	-0.636244
H	2.087464	-2.109161	0.365281
H	2.373564	-2.346123	-1.450929
S	-2.536476	-0.324765	-0.007963
C	-1.763547	0.907062	-1.098750
H	-1.544357	0.498139	-2.090774
H	-2.399493	1.788759	-1.225199
H	-0.813857	1.245558	-0.655580

1 imaginary frequency
E = -707.346864
H = -707.201770
G = -707.244470
$E_{\omega B97X-D}$ = -707.510568
H_{tot} = -707.365474
G_{tot} = -707.408174

S-shaped conformer of 9

C	-0.018583	0.469741	0.020102
C	-0.868662	-0.756698	0.055607
H	-0.389164	-1.724473	0.156583
C	1.462765	0.343737	0.020655
H	1.981875	1.298839	0.056066
O	-0.519137	1.586051	-0.010279
C	-2.196961	-0.663897	-0.033213
H	-2.677416	0.305583	-0.134388
H	-2.829263	-1.545505	-0.007531
C	2.148155	-0.801546	-0.038822
H	1.672901	-1.776191	-0.085992
H	3.233871	-0.794684	-0.048481

0 imaginary frequencies
E = -269.201285
H = -269.097632
G = -269.132133
$E_{\omega B97X-D}$ = -269.298260
H_{tot} = -269.194608
G_{tot} = -269.229109

P9

C	-1.639966	-0.544471	0.115506
C	-2.882551	0.271848	0.057649
H	-3.790766	-0.276711	0.296860
O	-1.710492	-1.727432	0.406484
C	-2.918329	1.568394	-0.258933
H	-2.022236	2.132904	-0.502397
H	-3.857943	2.111595	-0.286002
C	-0.306900	0.114358	-0.192242
H	-0.178752	0.960889	0.493645
H	-0.348684	0.539481	-1.202880
C	0.856551	-0.860875	-0.078149
H	0.921931	-1.271829	0.933782
H	0.712493	-1.702682	-0.760578
S	2.460622	-0.131493	-0.528139
C	2.669933	1.045839	0.837687
H	3.683118	1.445998	0.764287
H	2.560107	0.538165	1.799664
H	1.962282	1.874985	0.772845

0 imaginary frequencies
E = -707.877240
H = -707.716754
G = -707.760076
$E_{\omega B97X-D}$ = -708.046366
H_{tot} = -707.885880
G_{tot} = -707.929203

10 (U-shaped conformer)

C	1.214640	-1.214902	-0.246416
C	-0.238156	-0.974076	-0.454797
H	-0.721302	-1.714715	-1.088384
C	2.162168	-0.104688	0.081179
O	1.639308	-2.363346	-0.335102
C	-0.948660	-0.038398	0.187594
H	-0.426750	0.645849	0.859688
C	1.928976	1.132761	-0.391196
H	1.014572	1.293927	-0.959363
C	3.399420	-0.542210	0.819709
H	4.018315	-1.179991	0.180233
H	4.001787	0.303911	1.151547
H	3.129518	-1.140369	1.695797
C	2.809944	2.337327	-0.266006
H	3.124313	2.674919	-1.260487
H	2.250323	3.165804	0.183151
H	3.704277	2.160308	0.332583
C	-2.438379	0.183486	0.104332
C	-3.023804	0.031415	1.518772
H	-4.098248	0.246953	1.505336
H	-2.881371	-0.988031	1.893036
H	-2.546518	0.724718	2.220504
C	-3.129770	-0.793455	-0.847267
H	-4.203616	-0.580230	-0.879629
H	-2.737323	-0.704156	-1.866401
H	-3.002236	-1.830553	-0.517845
C	-2.663857	1.626414	-0.382165
H	-3.736019	1.852466	-0.403539
H	-2.177221	2.348018	0.283992
H	-2.262093	1.765895	-1.391835

0 imaginary frequencies
E = -504.981782
H = -504.699172
G = -504.751924
$E_{\omega B97X-D}$ = -505.192087
H_{tot} = -504.909477
G_{tot} = -504.962229

TS10-a

C	0.669165	1.781706	-0.181862
C	-0.765569	1.435220	0.094887
H	-1.385714	2.312740	0.277670
C	1.761208	0.939371	0.220822
O	0.845341	2.878367	-0.768302
C	-1.319282	0.222539	-0.010077
H	-0.680426	-0.634873	-0.232078
C	1.602895	-0.184505	1.034280
H	0.622499	-0.338978	1.474411
C	3.140242	1.298526	-0.276474
H	3.801542	1.663026	0.522145
H	3.628856	0.418458	-0.719768
H	3.076531	2.079252	-1.037676
C	2.741767	-0.677930	1.894267

H	2.909045	0.034523	2.715438
H	2.511826	-1.653739	2.330902
H	3.672243	-0.767941	1.329119
C	-2.779319	-0.131338	0.152727
C	-3.246911	-0.823291	-1.138585
H	-4.286908	-1.157482	-1.039889
H	-3.183131	-0.139017	-1.992098
H	-2.625569	-1.699979	-1.357100
C	-3.663218	1.084110	0.433256
H	-4.707088	0.768999	0.545484
H	-3.362184	1.591278	1.357006
H	-3.614512	1.809824	-0.386523
C	-2.888403	-1.128898	1.319436
H	-3.922909	-1.476061	1.431625
H	-2.249969	-2.003155	1.145673
H	-2.576605	-0.661432	2.260341
S	1.483133	-2.165707	-0.340558
C	1.172276	-1.333727	-1.921797
H	0.194207	-1.593304	-2.341184
H	1.192567	-0.243589	-1.754191
H	1.943746	-1.574860	-2.659246

1 imaginary frequency

E = -943.127318

H = -942.803423

G = -942.862091

$E_{\omega B97X-D}$ = -943.400721

H_{tot} = -943.076826

G_{tot} = -943.135494

P10-a

C	0.017512	1.341256	-0.062490
C	1.069195	0.330837	-0.360641
H	0.799150	-0.488618	-1.022978
O	0.249789	2.353577	0.578084
C	2.295148	0.431545	0.168159
H	2.486710	1.281881	0.827422
C	-1.934780	-0.175830	0.214240
H	-1.197813	-0.987024	0.161994
C	3.459713	-0.499984	-0.039904
C	4.616112	0.320338	-0.639219
H	4.879073	1.163786	0.008698
H	5.503269	-0.313061	-0.751722
H	4.346788	0.714819	-1.624790
C	3.121428	-1.668075	-0.967146
H	2.307447	-2.278419	-0.560008
H	2.825235	-1.315974	-1.961586
H	3.998758	-2.312855	-1.085740
C	3.885775	-1.037560	1.337882
H	3.084427	-1.630515	1.791710
H	4.769869	-1.676350	1.232020
H	4.136631	-0.218469	2.020959
C	-1.382972	1.031664	-0.584901
H	-1.260387	0.696485	-1.624832
C	-2.210159	0.152742	1.679104
H	-2.475609	-0.749168	2.237328
H	-1.318862	0.583483	2.150972
H	-3.032124	0.867895	1.775503
C	-2.280190	2.264308	-0.546331
H	-1.865150	3.052019	-1.181236
H	-3.284937	2.025568	-0.906673
H	-2.357561	2.664985	0.467349
S	-3.424290	-0.798985	-0.658335

C	-3.698863	-2.344924	0.251221
H	-4.460326	-2.904769	-0.295582
H	-4.060198	-2.159493	1.264457
H	-2.781587	-2.938956	0.285595

0 imaginary frequencies
E = -943.651021
H = -943.311494
G = -943.370783
$E_{\omega B97X-D}$ = -943.932766
H_{tot} = -943.593239
G_{tot} = -943.652529

TS10-b

C	1.361866	0.075601	1.320824
C	-0.060774	-0.037669	1.217983
H	-0.601320	0.211401	2.130342
C	2.240876	-0.233427	0.128396
O	1.939931	0.439337	2.368428
C	-0.759729	-0.317328	0.051146
H	-0.180882	-0.683159	-0.791527
C	2.258025	-1.471503	-0.383149
H	1.576342	-2.201561	0.057041
C	3.093262	0.924982	-0.317988
H	3.612567	1.355052	0.544593
H	3.834197	0.643730	-1.068828
H	2.458591	1.713201	-0.742437
C	3.110397	-1.992379	-1.505451
H	3.707982	-2.849119	-1.172181
H	2.480711	-2.347700	-2.330313
H	3.792285	-1.239433	-1.905920
C	-2.186411	-0.857548	0.082239
C	-2.787120	-0.924147	-1.326822
H	-3.730539	-1.483397	-1.306912
H	-2.986794	0.076417	-1.719156
H	-2.104857	-1.435823	-2.017388
C	-3.109695	-0.047733	0.996149
H	-4.124223	-0.464008	0.965314
H	-2.772806	-0.073008	2.038031
H	-3.145641	0.994848	0.664288
C	-2.082918	-2.301209	0.620758
H	-3.071967	-2.776303	0.617040
H	-1.412373	-2.905290	-0.003081
H	-1.693529	-2.309215	1.643692
S	-1.045544	1.794606	-1.238966
C	-0.163519	2.885857	-0.089437
H	-0.833030	3.627839	0.357358
H	0.259789	2.279408	0.726837
H	0.659211	3.416747	-0.578656

1 imaginary frequency
E = -943.122987
H = -942.799358
G = -942.859001
$E_{\omega B97X-D}$ = -943.398222
H_{tot} = -943.074593
G_{tot} = -943.134236

P10-b

C	1.352586	0.402226	0.500184
C	2.789795	0.131440	0.186939
O	1.057869	1.398050	1.143800
C	3.145104	-1.017226	-0.415219
H	2.361320	-1.724100	-0.680440

C	3.736652	1.212527	0.633761
H	3.694971	1.331719	1.721287
H	4.767301	1.002125	0.348110
H	3.445916	2.174849	0.201017
C	4.524436	-1.476116	-0.773058
H	4.588234	-1.660438	-1.851667
H	5.304007	-0.765211	-0.498148
H	4.738853	-2.431100	-0.279631
C	-2.270796	-1.045955	0.217731
C	-2.086231	-1.954693	1.445271
H	-1.985602	-1.363390	2.363545
H	-2.961618	-2.604004	1.558441
H	-1.210876	-2.605655	1.358274
C	-2.274036	-1.903534	-1.052212
H	-3.101443	-2.621519	-1.019023
H	-2.400631	-1.283320	-1.946717
H	-1.343924	-2.474053	-1.155888
C	-3.625503	-0.340104	0.361105
H	-4.428653	-1.081567	0.437151
H	-3.650669	0.277334	1.267928
H	-3.836106	0.300991	-0.500664
C	0.269548	-0.576464	0.054907
H	0.454138	-0.886683	-0.978875
H	0.378927	-1.477460	0.672338
C	-1.135403	0.011565	0.190240
H	-1.178933	0.579396	1.126686
S	-1.327683	1.270408	-1.146095
C	-1.898086	2.694332	-0.177131
H	-2.878929	2.505644	0.265663
H	-1.169805	2.925297	0.603918
H	-1.974893	3.542227	-0.861284

0 imaginary frequencies
E = -943.651716
H = -943.312422
G = -943.372275
$E_{\omega B97X-D}$ = -943.932857
H_{tot} = -943.593563
G_{tot} = -943.653417

11

C	1.218490	-0.041304	-0.000022
C	-0.238440	0.293509	0.000077
O	2.043964	0.860974	-0.000209
C	-1.148581	-0.696362	0.000058
H	-0.787159	-1.723172	0.000107
C	1.678949	-1.485030	0.000091
H	1.311370	-2.014577	0.884241
H	1.311283	-2.014743	-0.883927
H	2.769349	-1.499063	0.000028
C	-2.640254	-0.571843	-0.000127
H	-2.989152	0.461161	-0.000889
H	-3.056979	-1.078048	-0.878497
H	-3.057181	-1.076893	0.878833
C	-0.543279	1.766896	0.000130
H	-1.614842	1.967288	0.000567
H	-0.099534	2.247514	0.877852
H	-0.100176	2.247548	-0.877888

0 imaginary frequencies
E = -309.733868
H = -309.576666
G = -309.616253
$E_{\omega B97X-D}$ = -309.861635

H_{tot} = -309.704434
G_{tot} = -309.744021

TS11

C	1.737208	-0.212562	-0.196678
C	0.688178	0.719274	0.082349
O	2.794284	-0.292467	0.473270
C	-0.446014	0.788879	-0.737276
H	-0.377000	0.310115	-1.708863
C	1.576124	-1.172063	-1.375021
H	0.606131	-1.682698	-1.350929
H	1.645570	-0.641627	-2.331798
H	2.377391	-1.912617	-1.330733
C	-1.312685	2.025976	-0.739097
H	-1.591598	2.324034	0.274842
H	-0.761227	2.858714	-1.198781
H	-2.230511	1.865792	-1.311970
C	0.754781	1.535962	1.347817
H	-0.109963	1.327401	1.997133
H	1.663398	1.291189	1.903312
H	0.755339	2.618409	1.159777
S	-2.099394	-0.723094	-0.008319
C	-1.049133	-1.770988	1.031534
H	-1.450031	-1.854895	2.045957
H	-0.929215	-2.777172	0.617781
H	-0.053009	-1.304268	1.099441

1 imaginary frequency
E = -747.877855
H = -747.679325
G = -747.725741
$E_{\omega B97X-D}$ = -748.069370
H_{tot} = -747.870840
G_{tot} = -747.917256

P11

C	-1.575725	-0.618649	0.232886
O	-1.524508	-0.873224	1.421552
C	-2.355154	-1.464636	-0.738593
H	-3.044285	-0.836736	-1.314567
H	-1.656106	-1.913554	-1.454268
H	-2.905308	-2.247809	-0.215483
C	1.276154	1.988227	-0.175053
H	0.846426	2.816457	0.397746
H	2.340955	1.936236	0.069724
H	1.182744	2.215132	-1.242954
C	-1.693106	1.847152	0.120717
H	-2.750301	1.724934	-0.137261
H	-1.618735	1.976078	1.205629
H	-1.333221	2.755083	-0.369124
S	1.441747	-0.760270	-0.595150
C	2.825096	-0.943089	0.563980
H	3.422603	-1.790689	0.222598
H	3.456462	-0.051806	0.574457
H	2.455985	-1.149807	1.571285
C	-0.879474	0.622148	-0.325182
H	-0.891337	0.572906	-1.422960
C	0.576673	0.674703	0.158361
H	0.575460	0.508564	1.242474

0 imaginary frequencies
E = -748.400879
H = -748.186904
G = -748.235196

$E_{\omega B97X-D}$ = -748.600522
H_{tot} = -748.386547
G_{tot} = -748.433229

12

C	-2.293850	0.173393	0.000009
C	-0.862249	0.556312	-0.000041
H	-0.685988	1.629527	-0.000126
O	-3.151361	1.045414	0.000031
C	0.147196	-0.324182	0.000029
H	-0.083962	-1.391884	0.000118
C	-2.679340	-1.289374	-0.000013
H	-2.277244	-1.794735	-0.883810
H	-2.276883	-1.794922	0.883512
H	-3.766849	-1.369774	0.000199
C	1.622754	-0.012943	0.000002
C	2.239497	-0.657846	1.253791
H	2.050464	-1.737017	1.277139
H	3.324254	-0.502457	1.258634
H	1.823858	-0.216018	2.165723
C	2.239492	-0.657951	-1.253738
H	1.823826	-0.216225	-2.165707
H	3.324243	-0.502532	-1.258617
H	2.050489	-1.737130	-1.276979
C	1.908527	1.489233	-0.000059
H	1.490984	1.975643	-0.888562
H	1.490976	1.975708	0.888405
H	2.990551	1.658654	-0.000060

0 imaginary frequencies
E = -388.322441
H = -388.105776
G = -388.150046
$E_{\omega B97X-D}$ = -388.488110
H_{tot} = -388.271445
G_{tot} = -388.315715

TS12

C	2.022016	-0.976175	-0.239634
C	0.708411	-0.875444	0.349471
H	0.604842	-1.144064	1.397771
O	2.281963	-0.674757	-1.415400
C	-0.354618	-0.377447	-0.363516
H	-0.188625	-0.230400	-1.428723
C	3.157574	-1.480214	0.639683
H	3.906968	-0.687409	0.740539
H	2.822927	-1.779468	1.636093
H	3.644261	-2.330319	0.150656
C	-1.806367	-0.576992	0.038820
C	-2.146620	-2.043730	-0.307331
H	-3.201224	-2.247020	-0.083116
H	-1.979690	-2.245686	-1.372200
H	-1.526027	-2.735051	0.271953
C	-2.038148	-0.348603	1.534599
H	-3.100300	-0.484047	1.773101
H	-1.468311	-1.056992	2.145905
H	-1.741418	0.669246	1.807069
C	-2.742689	0.327822	-0.770591
H	-2.533281	0.244797	-1.844139
H	-3.785934	0.032470	-0.603648
H	-2.626661	1.374698	-0.478628
S	-0.151070	2.246665	-0.217320
C	1.497011	2.247502	0.543076

H	1.732699	1.231049	0.899777
H	2.279429	2.539423	-0.165453
H	1.542348	2.919872	1.405893

1 imaginary frequency
E = -826.464568
H = -826.206803
G = -826.258915
$E_{\omega B97X-D}$ = -826.694842
H_{tot} = -826.437077
G_{tot} = -826.489189

P12

C	-2.192969	0.435214	-0.129292
O	-2.219482	0.515502	-1.342646
C	-3.451233	0.267483	0.686133
H	-3.459034	-0.735282	1.129675
H	-3.468637	0.984627	1.513375
H	-4.333437	0.393336	0.057204
C	0.711086	-1.346776	-0.071216
C	1.779948	-1.670573	-1.124232
H	1.994823	-2.745138	-1.121824
H	1.432188	-1.397478	-2.127665
H	2.713633	-1.135713	-0.928419
C	1.225522	-1.763990	1.313395
H	1.402178	-2.845279	1.330484
H	2.172175	-1.269641	1.558226
H	0.506215	-1.533662	2.107087
C	-0.545130	-2.165783	-0.405312
H	-0.960593	-1.879272	-1.377332
H	-0.288923	-3.230355	-0.443271
H	-1.327780	-2.049135	0.353857
C	-0.895164	0.550569	0.656124
H	-0.852534	1.606578	0.959255
H	-0.975777	-0.012906	1.592799
S	1.798663	1.181452	0.425900
C	1.382837	2.730664	-0.420234
H	0.411961	3.116412	-0.097089
H	2.151401	3.460507	-0.157993
H	1.377865	2.589936	-1.503740
C	0.365372	0.167550	-0.128232
H	0.199915	0.429074	-1.180671

0 imaginary frequencies
E = -826.988560
H = -826.715447
G = -826.767164
$E_{\omega B97X-D}$ = -827.225933
H_{tot} = -826.952820
G_{tot} = -827.004537

5

C	-2.325042	1.583146	-0.678210
C	-1.162404	2.599068	-0.849260
C	-1.758730	0.194537	-0.742560
H	-3.057772	1.749675	-1.478190
H	-2.845212	1.752486	0.270280
C	-2.046459	-0.882943	0.007330
C	1.149298	1.766591	-0.485800
C	0.008007	2.239640	0.041810
H	-1.535475	3.605568	-0.621930
H	-0.841444	2.593919	-1.897330
C	-0.292463	2.313729	1.517690
H	-0.792384	3.259919	1.756100

H	0.596697	2.233281	2.145380
H	-0.982602	1.508788	1.809940
C	2.294109	1.124023	0.254130
H	1.222748	1.744561	-1.575080
C	2.334301	-0.429317	0.072840
H	2.223548	1.336313	1.326200
H	3.256698	1.526814	-0.087510
C	2.896741	-0.798386	-1.302080
H	3.912091	-0.401455	-1.410190
H	2.279171	-0.392837	-2.110900
H	2.949513	-1.885096	-1.428950
C	3.228482	-1.025306	1.172010
H	2.813331	-0.831756	2.167240
H	4.229051	-0.579244	1.126780
H	3.326233	-2.108656	1.045180
C	0.916321	-0.917059	0.245190
C	0.263093	-1.870210	-0.432430
H	0.351151	-0.371950	1.002840
C	-1.190067	-2.103532	-0.178770
H	0.747434	-2.515209	-1.162990
O	-1.660375	-3.232213	-0.111210
H	-0.940630	0.093118	-1.453530
C	-3.181858	-1.008835	0.984360
H	-3.851577	-1.817476	0.673410
H	-2.813208	-1.266254	1.983900
H	-3.764330	-0.087696	1.051500

0 imaginary frequencies
E = -659.735929
H = -659.379434
G = -659.436416
$E_{\omega B97X-D}$ = -659.997841
H_{tot} = -659.641345
G_{tot} = -659.698328

TS5-disub top face

C	2.670248	-1.111194	-1.363949
C	1.708796	-2.329762	-1.262059
C	1.920701	0.195878	-1.275119
H	3.198408	-1.190375	-2.323819
H	3.432738	-1.184775	-0.582669
C	2.029792	1.149527	-0.336839
C	-0.459573	-1.996298	-0.124229
C	0.844506	-2.296101	-0.017129
H	2.315545	-3.245823	-1.289379
H	1.063826	-2.338921	-2.149269
C	1.576346	-2.498562	1.283251
H	2.170684	-3.420423	1.243781
H	0.899146	-2.558631	2.139081
H	2.279217	-1.674863	1.469411
C	-1.451572	-1.587787	0.941541
H	-0.826653	-1.862518	-1.143859
C	-1.384170	-0.055347	1.301271
H	-1.309053	-2.158767	1.867981
H	-2.460303	-1.824865	0.585681
C	-2.733909	0.438136	1.816511
H	-3.035980	-0.128414	2.706811
H	-3.514199	0.336017	1.057421
H	-2.671427	1.497646	2.092711
C	-0.342069	0.121481	2.423341
H	0.660000	-0.146630	2.074241
H	-0.596991	-0.516428	3.279471
H	-0.307708	1.163871	2.753401

C	-0.831108	0.730652	0.104691
C	-0.277696	2.059741	0.164081
H	-0.124059	0.090011	-0.387429
C	1.061524	2.324039	-0.177729
H	-0.868195	2.903682	0.522041
O	1.587676	3.479318	-0.179459
H	1.121711	0.303499	-2.014709
C	3.096992	1.181186	0.731021
H	3.646224	2.125685	0.660761
H	2.639182	1.156876	1.728871
H	3.810231	0.357424	0.656141
H	-2.870572	-1.569404	-1.757919
H	-4.069641	-0.740702	-0.737129
C	-3.425321	-0.638043	-1.614939
S	-2.327388	0.822325	-1.505509
H	-4.066261	-0.490202	-2.490059

1 imaginary frequency

E = -1097.862727

H = -1097.464614

G = -1097.526861

$E_{\omega B97X-D}$ = -1098.190063

H_{tot} = -1097.791950

G_{tot} = -1097.854197

TS5-disub bottom face

C	-2.903690	1.352622	-0.172740
C	-2.072549	2.641122	0.092240
C	-2.049370	0.301322	-0.835640
H	-3.766320	1.626453	-0.795580
H	-3.306670	0.975222	0.773280
C	-1.935151	-0.993518	-0.505190
C	0.388820	2.473191	-0.112060
C	-0.705160	2.305941	0.648360
H	-2.636659	3.287632	0.778130
H	-1.953809	3.186722	-0.851570
C	-0.718420	1.636011	1.998280
H	-1.225080	2.273822	2.734120
H	0.281680	1.397341	2.367960
H	-1.283620	0.694172	1.950100
C	1.765550	1.898860	0.097920
H	0.240781	2.965221	-1.075420
C	1.978370	0.599870	-0.740920
H	1.948430	1.654410	1.150050
H	2.528551	2.628790	-0.207070
C	1.703420	0.897580	-2.226700
H	2.290610	1.768720	-2.546730
H	0.647170	1.101271	-2.419880
H	1.989889	0.040520	-2.844530
C	3.444309	0.166070	-0.632200
H	3.778819	0.118969	0.408930
H	4.086000	0.881769	-1.161100
H	3.590709	-0.822381	-1.082740
C	0.966279	-0.460029	-0.245900
C	0.470089	-1.513019	-1.086840
H	0.150629	0.029901	0.271220
C	-0.887641	-1.868809	-1.182240
H	1.169928	-2.120169	-1.663330
O	-1.328292	-2.870608	-1.827660
H	-1.370010	0.682272	-1.599560
C	-2.834561	-1.693958	0.483810
H	-3.030622	-2.710918	0.129670
H	-2.357351	-1.777378	1.468960

H	-3.792651	-1.183277	0.613550
H	-0.093962	-2.584079	1.260760
H	0.679088	-2.940649	2.822970
C	0.403658	-2.139439	2.132200
S	1.892069	-1.273010	1.576790
H	-0.296011	-1.464239	2.636200

1 imaginary frequency
E = -1097.881811
H = -1097.484026
G = -1097.546812
$E_{\omega B97X-D}$ = -1098.207407
H_{tot} = -1097.809622
G_{tot} = -1097.872408

P5-disub bottom face

C	3.375126	0.001522	0.226942
C	3.043556	-1.515585	0.325085
C	2.371514	0.684101	-0.657051
H	4.385907	0.105019	-0.185501
H	3.389759	0.443770	1.226931
C	1.460254	1.599336	-0.295888
C	0.746463	-2.189287	-0.286550
C	1.587519	-1.755485	0.664216
H	3.704064	-1.962548	1.079114
H	3.275512	-1.987748	-0.636370
C	1.179968	-1.368656	2.062449
H	1.385376	-0.305567	2.249940
H	1.767675	-1.932407	2.797524
H	0.119913	-1.547871	2.263454
C	-0.758469	-2.249600	-0.262915
H	1.192428	-2.436892	-1.251257
C	-1.402410	-1.008637	-0.953405
H	-1.155909	-2.328338	0.755613
H	-1.093269	-3.143584	-0.805388
C	-0.730237	-0.781010	-2.316787
H	-0.778672	-1.710541	-2.896384
H	0.321815	-0.502999	-2.231855
H	-1.242023	-0.002649	-2.891331
C	-2.884035	-1.301856	-1.236894
H	-3.408251	-1.681256	-0.354180
H	-2.961054	-2.063813	-2.020110
H	-3.406087	-0.404489	-1.589959
C	-1.212065	0.222624	-0.003347
C	-1.075372	1.596924	-0.694298
C	0.327240	1.853315	-1.250737
O	0.503686	2.204926	-2.402589
H	2.300829	0.279296	-1.668532
C	1.381930	2.293767	1.040201
H	1.210910	3.367159	0.899907
H	0.557856	1.916283	1.653868
H	2.305971	2.176457	1.609305
H	-1.266847	2.388326	0.042848
H	-1.803479	1.726641	-1.500538
S	-2.562525	0.230459	1.251996
H	-0.290715	0.047366	0.559806
C	-1.821362	1.237877	2.561569
H	-1.623651	2.261846	2.233094
H	-0.902944	0.780887	2.940465
H	-2.551929	1.274809	3.372785

0 imaginary frequencies
E = -1098.404358
H = -1097.990430

G = -1098.052273
$E_{\omega B97X-D}$ = -1098.738480
H_{tot} = -1098.324552
G_{tot} = -1098.386395

TS5-trisub-1 bottom face

C	-1.668830	1.722950	-0.991050
C	-0.373500	2.187350	-1.716450
C	-1.409511	0.423180	-0.238200
H	-2.474020	1.605730	-1.724320
H	-1.980170	2.516280	-0.300250
C	-1.697221	-0.867130	-0.796290
C	1.804149	1.334569	-0.881990
C	0.793960	2.206339	-0.751630
H	-0.556300	3.184930	-2.139750
H	-0.154650	1.505830	-2.546930
C	0.610760	3.099479	0.452400
H	0.146900	4.047739	0.155320
H	1.554180	3.328289	0.952970
H	-0.062560	2.632640	1.186270
C	2.794759	0.934509	0.180900
H	1.811529	0.717489	-1.782320
C	2.785959	-0.615911	0.425080
H	2.550739	1.432839	1.126050
H	3.824969	1.222298	-0.077010
C	3.586409	-1.306271	-0.683790
H	4.638539	-1.006002	-0.618740
H	3.227129	-1.043341	-1.684060
H	3.534848	-2.396271	-0.583260
C	3.462869	-0.897241	1.772580
H	2.885319	-0.465741	2.598310
H	4.470139	-0.463392	1.799000
H	3.549589	-1.976181	1.945110
C	1.335269	-1.062461	0.468810
C	0.689609	-1.685211	-0.522430
H	0.779299	-0.705681	1.340960
C	-0.780921	-1.942360	-0.747240
H	1.273389	-2.056261	-1.367400
O	-1.076882	-3.125930	-1.100760
H	-0.428521	0.462630	0.212180
C	-3.080831	-1.167500	-1.310910
H	-3.051961	-1.840320	-2.174890
H	-3.696991	-1.663459	-0.542850
H	-3.609821	-0.251499	-1.595150
H	-3.375321	-1.319240	2.636210
C	-2.407991	-0.944000	2.291640
H	-1.697061	-0.975110	3.121740
H	-2.044301	-1.604020	1.490190
S	-2.573091	0.724720	1.604380

1 imaginary frequency
E = -1097.874368
H = -1097.476683
G = -1097.540343
$E_{\omega B97X-D}$ = -1098.200202
H_{tot} = -1097.802518
G_{tot} = -1097.866178

TS5-trisub-1 top face

C	1.500912	1.978318	-0.435510
C	0.387492	2.776849	0.282170
C	1.401000	0.494268	-0.084950
H	2.476762	2.404407	-0.174710

H	1.393722	2.096428	-1.521830
C	1.624739	-0.536052	-1.057390
C	-1.731829	1.556291	0.732320
C	-0.984768	2.279430	-0.117740
H	0.494313	3.842059	0.036290
H	0.525332	2.669269	1.365240
C	-1.347728	2.532340	-1.561320
H	-1.042037	3.542570	-1.858430
H	-2.416998	2.430831	-1.758250
H	-0.819209	1.832690	-2.222660
C	-2.973290	0.771222	0.401770
H	-1.345599	1.424610	1.745510
C	-2.719751	-0.770498	0.343440
H	-3.372419	1.081782	-0.570240
H	-3.763149	0.954233	1.143960
C	-2.561552	-1.333958	1.757800
H	-3.461821	-1.128388	2.348800
H	-1.701221	-0.892419	2.273320
H	-2.417483	-2.419959	1.734760
C	-3.933152	-1.427757	-0.331510
H	-4.037421	-1.086117	-1.367810
H	-4.857221	-1.177106	0.204880
H	-3.824583	-2.517927	-0.342100
C	-1.476731	-0.984380	-0.493700
C	-0.408042	-1.735461	-0.216140
H	-1.435451	-0.368190	-1.396660
C	0.840678	-1.710012	-1.068150
H	-0.389353	-2.385741	0.660350
O	1.090667	-2.737532	-1.769410
H	0.520840	0.302979	0.518340
C	2.834189	-0.472394	-1.951440
H	3.698039	-0.997504	-1.512550
H	2.638529	-0.938663	-2.922960
H	3.147730	0.565226	-2.120590
S	2.840170	0.364336	1.573960
H	3.476518	-1.819514	2.392700
C	2.583568	-1.395793	1.925750
H	2.403008	-1.918833	0.977520
H	1.726688	-1.560323	2.586570

1 imaginary frequency
E = -1097.881189
H = -1097.483708
G = -1097.548312
$E_{\omega B97X-D}$ = -1098.207497
H_{tot} = -1097.810016
G_{tot} = -1097.874620

P5-trisub-1 top face

C	-1.605761	1.565118	-0.316031
C	-0.648511	1.969939	-1.458061
C	-1.740360	0.036468	-0.193311
H	-1.235081	1.979339	0.629549
H	-2.591911	2.019488	-0.471861
C	-1.778210	-0.474532	1.273139
C	1.546560	0.786810	-1.563061
C	0.795439	1.774759	-1.050411
H	-0.884231	1.379789	-2.352541
H	-0.820601	3.024799	-1.706371
C	1.266279	2.712250	0.037799
H	0.925779	2.378250	1.027069
H	2.353749	2.801210	0.081199
H	0.851418	3.714330	-0.119451

C	2.917720	0.380401	-1.087841
H	1.100300	0.163210	-2.339931
C	2.906800	-0.829359	-0.087621
H	3.548340	0.086411	-1.937141
H	3.420459	1.219611	-0.595411
C	4.304610	-0.961269	0.531749
H	4.565380	-0.068459	1.110949
H	5.056871	-1.089218	-0.254901
H	4.354681	-1.829029	1.198299
C	2.547991	-2.116750	-0.832601
H	2.476271	-2.964420	-0.141821
H	1.595701	-2.030010	-1.366991
H	3.325291	-2.345059	-1.569681
C	1.903370	-0.471450	0.975029
C	0.690680	-1.015031	1.126219
H	2.141110	0.416090	1.566529
C	-0.378010	-0.292061	1.861339
H	0.380341	-1.866541	0.524569
O	-0.155720	0.470509	2.788089
C	-2.856600	0.178708	2.125659
H	-3.840260	0.020387	1.674879
H	-2.860790	-0.249352	3.131869
H	-2.686481	1.254448	2.225849
H	-1.946029	-1.561012	1.236379
S	-3.194670	-0.491722	-1.172071
H	-0.876960	-0.418241	-0.692801
C	-2.823339	-2.256712	-1.365921
H	-2.892879	-2.793022	-0.416671
H	-3.564669	-2.669813	-2.053051
H	-1.827279	-2.393432	-1.796581

0 imaginary frequencies
E = -1098.409278
H = -1097.995432
G = -1098.058712
$E_{\omega B97X-D}$ = -1098.744116
H_{tot} = -1098.330270
G_{tot} = -1098.393550

TS5-trisub-2 bottom face

C	2.534704	0.978784	-0.969800
C	2.031111	2.372186	-0.536500
C	2.305300	-0.081415	0.125000
H	2.010303	0.676386	-1.884500
H	3.598205	1.030679	-1.235200
C	1.671994	-1.396312	-0.391000
C	-0.268789	2.490497	0.433500
C	0.526411	2.460393	-0.646400
H	2.361512	2.574385	0.490700
H	2.489414	3.131984	-1.183400
C	-0.007289	2.376895	-2.059800
H	-0.263894	1.340197	-2.315900
H	-0.903786	2.985699	-2.204500
H	0.746812	2.715992	-2.778900
C	-1.771489	2.440303	0.411400
H	0.205411	2.509694	1.417100
C	-2.449895	1.067107	0.774400
H	-2.172185	3.172505	1.126900
H	-2.141887	2.734505	-0.577300
C	-3.950394	1.262413	0.526100
H	-4.160694	1.346314	-0.546800
H	-4.295890	2.181215	1.016200
H	-4.525798	0.421116	0.920300

C	-2.221197	0.755005	2.255400
H	-2.625801	-0.234093	2.496900
H	-1.160096	0.771701	2.524900
H	-2.733593	1.500808	2.875300
C	-1.848700	0.018104	-0.146500
C	-0.649903	-0.594402	0.131800
C	0.250795	-1.058606	-0.885600
O	-0.012105	-1.121305	-2.098000
C	2.506290	-2.103716	-1.449600
H	3.489289	-2.369521	-1.048600
H	2.004286	-3.016914	-1.782200
H	2.648893	-1.470117	-2.330300
H	1.547291	-2.061512	0.475200
S	3.896299	-0.322223	1.009100
H	1.622702	0.341888	0.870100
C	3.336494	-1.304720	2.427600
H	3.092489	-2.329319	2.138300
H	4.153094	-1.329224	3.152300
H	2.463996	-0.837216	2.893600
H	-2.085699	0.158505	-1.200700
H	-0.298903	-0.652903	1.159400
S	-3.631808	-1.846688	-0.094400
C	-2.442715	-3.207593	-0.249000
H	-2.643718	-4.000893	0.478000
H	-1.428413	-2.820498	-0.052600
H	-2.444717	-3.647893	-1.251500

1 imaginary frequency
E = -1536.554399
H = -1536.099419
G = -1536.169989
$E_{\omega B97X-D}$ = -1536.953321
H_{tot} = -1536.498340
G_{tot} = -1536.568910

TS5-trisub-2 top face

C	-2.579174	1.162603	0.221357
C	-2.067542	2.421921	-0.519604
C	-1.872205	-0.103346	-0.299879
H	-2.398914	1.268625	1.297816
H	-3.666729	1.082566	0.099661
C	-1.313365	-1.058564	0.787082
C	0.382362	2.372479	-0.955901
C	-0.631293	2.704838	-0.140079
H	-2.156940	2.254795	-1.600959
H	-2.708681	3.274377	-0.261493
C	-0.444689	3.221688	1.267994
H	-1.260070	3.906680	1.528693
H	-0.461554	2.400230	1.996011
H	0.497148	3.759851	1.396083
C	1.836940	2.304995	-0.575392
H	0.129579	2.011122	-1.956135
C	2.443427	0.854399	-0.597685
H	2.450968	2.919293	-1.250370
H	1.971552	2.701511	0.435397
C	3.756639	0.889245	0.187621
H	3.586632	1.139174	1.240732
H	4.425653	1.650062	-0.233940
H	4.249622	-0.085839	0.140456
C	2.728006	0.450939	-2.048665
H	3.189490	-0.540189	-2.092462
H	1.805895	0.420193	-2.642569
H	3.409797	1.170607	-2.517247

C	1.406337	-0.078710	0.017604
C	0.941045	0.080834	1.306543
C	-0.375395	-0.289887	1.742852
O	-0.806811	0.025773	2.868424
C	-2.407206	-1.773709	1.573932
H	-2.987747	-2.427692	0.917255
H	-1.967468	-2.378056	2.372968
H	-3.089313	-1.054420	2.038856
H	-0.695142	-1.809042	0.273976
S	-2.995183	-0.931985	-1.493091
H	-1.029795	0.229378	-0.907709
C	-1.859124	-2.169618	-2.179973
H	-1.649080	-2.965064	-1.460378
H	-2.338199	-2.605458	-3.059273
H	-0.919131	-1.698760	-2.484728
H	1.539162	0.613738	2.045451
S	2.453564	-2.368055	-0.271454
C	1.700926	-3.078888	1.219468
H	0.902846	-3.789656	0.979140
H	1.263321	-2.266360	1.823260
H	2.442834	-3.590705	1.839946
H	0.710526	-0.463807	-0.716751

1 imaginary frequency

E = -1536.554872

H = -1536.099658

G = -1536.169950

$E_{\omega B97X-D}$ = -1536.953517

H_{tot} = -1536.498303

G_{tot} = -1536.568595

P5-trisub-2 bottom face

C	2.607865	-0.486352	1.053179
C	2.029499	-1.914702	1.031311
C	2.362237	0.272594	-0.269108
H	2.161062	0.067861	1.886967
H	3.681757	-0.531869	1.263515
C	1.551683	1.585418	-0.113895
C	-0.255272	-2.180348	0.076184
C	0.519822	-1.943696	1.146385
H	2.348847	-2.421232	0.112016
H	2.457808	-2.475810	1.872619
C	0.003982	-1.709604	2.545045
H	0.174867	-2.602517	3.160597
H	0.543477	-0.883245	3.019753
H	-1.058863	-1.465223	2.581373
C	-1.756820	-2.286719	0.055452
H	0.248462	-2.361870	-0.876809
C	-2.571880	-1.175816	-0.668478
H	-2.023172	-3.234379	-0.434808
H	-2.136312	-2.358955	1.080456
C	-2.382747	-1.264740	-2.189536
H	-1.330518	-1.278412	-2.490219
H	-2.839466	-2.188009	-2.563283
H	-2.867853	-0.420659	-2.693598
C	-4.046751	-1.474300	-0.352802
H	-4.272569	-1.289731	0.703476
H	-4.261601	-2.526540	-0.570814
H	-4.725796	-0.864794	-0.957499
C	-2.158237	0.214697	-0.103229
C	-0.823358	0.742869	-0.647925
C	0.159634	1.225952	0.401510
O	-0.123535	1.321606	1.579839

C	2.227488	2.624059	0.778325
H	2.404987	2.232521	1.783261
H	3.186046	2.933347	0.352560
H	1.593415	3.510483	0.874142
H	1.423326	1.999095	-1.123150
S	3.914324	0.677175	-1.162830
H	1.805483	-0.381845	-0.952083
C	4.482857	-1.009203	-1.508860
H	5.404965	-0.927726	-2.087802
H	4.696067	-1.553152	-0.584813
H	3.740196	-1.555972	-2.096454
H	-2.071921	0.115941	0.986172
H	-0.980279	1.574225	-1.350259
S	-3.491301	1.461761	-0.377981
C	-2.763181	2.876722	0.492067
H	-2.539148	2.617175	1.528954
H	-3.508612	3.674494	0.470645
H	-1.854435	3.236453	0.001722
H	-0.301234	-0.016463	-1.236122

0 imaginary frequencies
E = -1537.075428
H = -1536.604634
G = -1536.674927
$E_{\omega B97X-D}$ = -1537.481035
H_{tot} = -1537.010240
G_{tot} = -1537.080533

P5-trisub-2 top face

C	-2.709187	0.922937	0.074508
C	-2.175369	2.049928	-0.837392
C	-1.923108	-0.394376	-0.107092
H	-2.646882	1.250436	1.118508
H	-3.771690	0.758054	-0.133692
C	-1.189516	-0.914587	1.153108
C	0.294828	1.912790	-0.933392
C	-0.796063	2.467507	-0.384392
H	-2.151675	1.695128	-1.875392
H	-2.866656	2.900639	-0.795692
C	-0.778447	3.454606	0.750508
H	-1.485652	3.162418	1.534308
H	0.205054	3.567291	1.209908
H	-1.093732	4.437111	0.375808
C	1.713630	2.025367	-0.447492
H	0.140618	1.279392	-1.808692
C	2.544210	0.728754	-0.630492
H	2.249743	2.819959	-0.986992
H	1.725935	2.315767	0.609408
C	3.913513	0.959933	0.024908
H	4.593900	0.120322	-0.151792
H	3.832916	1.110334	1.106808
H	4.376627	1.856825	-0.401492
C	2.760106	0.476051	-2.131892
H	1.828701	0.205565	-2.641192
H	3.156220	1.380345	-2.607492
H	3.473493	-0.335060	-2.299792
C	1.800991	-0.485234	0.007908
C	1.329194	-0.244727	1.460108
C	-0.142901	0.077996	1.679808
O	-0.470786	1.004002	2.396808
C	-2.143722	-1.273472	2.298208
H	-1.581427	-1.630181	3.166908
H	-2.725008	-0.401763	2.610008

H	-2.834634	-2.064061	1.993108
H	-0.652330	-1.820396	0.847308
S	-2.967730	-1.769559	-0.740192
H	-1.167806	-0.245887	-0.885692
C	-3.350619	-1.084353	-2.374592
H	-3.951630	-1.825244	-2.905492
H	-3.928204	-0.159944	-2.289992
H	-2.434016	-0.896367	-2.940492
H	0.933487	-0.710821	-0.625892
S	2.870167	-1.982551	-0.102292
C	1.615047	-3.264631	0.148308
H	2.114732	-4.228039	0.026608
H	0.819348	-3.182019	-0.597892
H	1.186848	-3.223724	1.154008
H	1.917307	0.537864	1.946708
H	1.488180	-1.159129	2.049808

0 imaginary frequencies
E = -1537.071699
H = -1536.600995
G = -1536.670938
$E_{\omega B97X-D}$ = -1537.478029
H_{tot} = -1537.007325
G_{tot} = -1537.077268

13

C	1.132431	0.021693	0.018909
C	0.378217	1.291397	-0.055640
C	-0.961352	1.318770	0.027349
H	0.967003	2.199813	-0.151190
H	-1.472810	2.279884	0.021174
O	2.350612	-0.000214	-0.081550
C	-1.810537	0.083557	0.133925
H	-2.112459	-0.041978	1.184884
H	-2.737292	0.228442	-0.431373
C	-1.063574	-1.158149	-0.353539
H	-0.962294	-1.109352	-1.444941
H	-1.633693	-2.062704	-0.121897
C	0.327068	-1.235008	0.279063
H	0.232311	-1.330635	1.371180
H	0.900811	-2.095324	-0.075833

0 imaginary frequencies
E = -308.539606
H = -308.403786
G = -308.437680
$E_{\omega B97X-D}$ = -308.655644
H_{tot} = -308.519824
G_{tot} = -308.553719

TS13

C	-1.660253	-0.638674	-0.193196
C	-0.593499	-0.528834	-1.130882
C	0.283050	0.556263	-1.161057
H	-0.463466	-1.354675	-1.827966
H	0.849725	0.718939	-2.072871
O	-2.466780	-1.597495	-0.172930
C	-0.062879	1.794898	-0.367032
H	-0.799644	2.374438	-0.946644
H	0.819695	2.426771	-0.240631
C	-0.664488	1.410231	0.981175
H	-0.943531	2.303763	1.550595
H	0.101971	0.879444	1.560035
C	-1.883988	0.508707	0.786939

H	-2.224280	0.079627	1.735909
H	-2.725389	1.097536	0.391476
H	1.669106	-1.082375	2.014998
S	2.364609	-0.068714	-0.097915
C	1.695162	-1.380253	0.962144
H	2.274676	-2.303813	0.876548
H	0.663012	-1.594295	0.640094

1 imaginary frequency
E = -746.702575
H = -746.525290
G = -746.566960
$E_{\omega B97X-D}$ = -746.865671
H_{tot} = -746.688386
G_{tot} = -746.730057

P13

C	1.992986	-0.636107	0.044197
O	2.800618	-1.379472	0.568140
C	-0.160714	1.309277	-0.296388
H	-0.204198	1.321552	-1.394264
H	-0.918713	2.010494	0.067640
C	1.224596	1.754380	0.179706
H	1.240705	1.792719	1.276441
H	1.438530	2.766540	-0.177071
C	2.319681	0.796525	-0.314432
H	2.376262	0.853709	-1.411043
H	3.303003	1.047977	0.090571
C	0.589495	-1.101587	-0.299668
H	0.432598	-2.099212	0.118303
H	0.525415	-1.172201	-1.396086
C	-0.470005	-0.104739	0.195330
H	-0.478119	-0.113497	1.293839
S	-2.098208	-0.725260	-0.354765
C	-3.200094	0.388247	0.561889
H	-3.161984	1.407717	0.173732
H	-4.214646	0.003859	0.439710
H	-2.948141	0.384302	1.625536

0 imaginary frequencies
E = -747.207733
H = -747.015107
G = -747.057595
$E_{\omega B97X-D}$ = -747.395894
H_{tot} = -747.203268
G_{tot} = -747.245756

14

C	0.332449	-1.258107	-0.000048
C	-1.008120	-1.255050	-0.000015
C	-1.008056	1.255109	-0.000045
C	0.332501	1.258116	-0.000056
C	1.105065	-0.000021	-0.000000
H	0.907267	-2.179830	-0.000213
H	-1.555239	-2.195182	-0.000043
H	-1.555169	2.195246	-0.000098
H	0.907364	2.179811	-0.000008
O	2.333174	-0.000036	0.000069
C	-1.817691	-0.000015	0.000074
H	-2.493122	0.000003	0.868585
H	-2.493381	0.000044	-0.868233

0 imaginary frequencies
E = -307.322673
H = -307.211299

G = -307.244350
$E_{\omega B97X-D}$ = -307.426447
H_{tot} = -307.315073
G_{tot} = -307.348124

TS14

C	-1.649847	0.357564	0.954650
C	-0.962153	1.507017	0.921145
C	0.265773	0.683026	-1.095741
C	-0.629190	-0.386040	-1.179901
C	-1.606802	-0.620820	-0.167579
H	-2.294474	0.099079	1.792177
H	-1.042776	2.222632	1.737557
H	0.853894	0.915660	-1.977857
H	-0.521195	-1.139433	-1.956537
O	-2.416253	-1.579272	-0.166529
C	-0.117492	1.878924	-0.260410
H	0.763152	2.445167	0.051613
H	-0.710771	2.557119	-0.900231
H	0.680855	-1.793499	0.225536
S	2.248884	0.015829	0.063237
C	1.658456	-1.580314	0.686099
H	1.524414	-1.568271	1.772079
H	2.342317	-2.393697	0.426517

1 imaginary frequency
E = -745.465383
H = -745.312397
G = -745.353515
$E_{\omega B97X-D}$ = -745.633639
H_{tot} = -745.480653
G_{tot} = -745.521771

P14

C	2.424322	0.450012	0.204129
C	1.722979	1.593150	0.178829
C	1.779641	-0.851592	-0.064785
H	3.493253	0.434543	0.397032
H	2.238068	2.538841	0.335513
O	2.403532	-1.899641	-0.010121
C	0.240105	1.657950	-0.058236
H	0.062294	1.948273	-1.105478
H	-0.199196	2.447916	0.559677
C	0.315062	-0.816697	-0.465851
H	-0.118963	-1.798091	-0.257481
H	0.275638	-0.656428	-1.553407
S	-2.184485	0.431945	-0.266375
C	-2.827469	-1.107075	0.449247
H	-3.913518	-1.077605	0.342426
H	-2.448066	-1.986719	-0.073984
H	-2.579018	-1.168300	1.511743
C	-0.433201	0.316875	0.234628
H	-0.415619	0.147838	1.319165

0 imaginary frequencies
E = -745.988099
H = -745.819695
G = -745.861505
$E_{\omega B97X-D}$ = -746.163503
H_{tot} = -745.995099
G_{tot} = -746.036909

15

C	-1.057936	0.593429	0.002922
C	0.277006	0.807841	-0.002316
C	0.664159	-1.683178	0.015004
C	-0.653525	-1.905206	0.013377
C	-1.605465	-0.782840	0.000624
H	1.360937	-2.521571	0.023622
H	-1.077227	-2.905537	0.020350
O	-2.818826	-0.985060	-0.010457
C	1.290944	-0.320978	0.000110
C	-2.094541	1.683924	0.005300
H	-2.688095	1.649272	-0.915087
H	-2.795635	1.536376	0.832891
H	-1.654011	2.677030	0.095448
C	0.830508	2.215967	-0.005521
H	0.446076	2.786087	-0.857404
H	0.537529	2.751007	0.904688
H	1.919385	2.235249	-0.060312
C	2.171916	-0.240311	-1.269229
H	2.731376	0.698451	-1.306578
H	2.895655	-1.062044	-1.270713
H	1.557551	-0.317505	-2.171554
C	2.188656	-0.213347	1.255118
H	2.917694	-1.030361	1.261321
H	2.741724	0.730008	1.267449
H	1.587307	-0.277796	2.167205

0 imaginary frequencies
E = -464.508261
H = -464.277610
G = -464.323481
$E_{\omega B97X-D}$ = -464.686247
H_{tot} = -464.455596
G_{tot} = -464.501467

TS15-a

C	1.346273	0.792455	-0.346365
C	1.169912	-0.542363	-0.446354
C	-0.843154	-0.360634	1.028653
C	-0.472717	0.948539	1.354908
C	0.609355	1.587915	0.694897
H	-1.536296	-0.861103	1.702819
H	-1.067775	1.544872	2.041922
O	0.973800	2.768321	0.932970
C	0.237464	-1.287597	0.497698
C	2.302647	1.565287	-1.225611
H	2.144521	2.635350	-1.082187
H	3.350234	1.350970	-0.978510
H	2.159679	1.327843	-2.284640
C	1.954352	-1.385476	-1.417266
H	1.299977	-1.792205	-2.199226
H	2.754542	-0.823547	-1.901446
H	2.407581	-2.246386	-0.909637
C	-0.351347	-2.563985	-0.121560
H	0.418912	-3.331632	-0.252193
H	-1.116967	-2.970932	0.549727
H	-0.817431	-2.370983	-1.090233
C	1.079716	-1.732770	1.725480
H	0.450326	-2.281937	2.436367
H	1.889402	-2.399887	1.407079
H	1.511806	-0.868123	2.235727
H	-2.812758	1.848731	-1.701514
S	-2.414161	-0.332031	-0.715909

C	-2.780766	1.442837	-0.686574
H	-3.732299	1.662354	-0.192556
H	-1.977693	1.957296	-0.138138

1 imaginary frequency
E = -902.647271
H = -902.375586
G = -902.428285
$E_{\omega B97X-D}$ = -902.888685
H_{tot} = -902.617000
G_{tot} = -902.669699

P15-a

C	1.924066	0.505444	-0.112080
C	1.425391	-0.753320	-0.087836
C	1.052272	1.667240	0.177706
O	1.476875	2.814658	0.167412
C	-0.056431	-1.100780	0.085487
C	-0.382829	1.380852	0.553905
H	-0.974556	2.275259	0.341112
H	-0.420865	1.219422	1.639395
S	-2.684909	-0.126149	0.242904
C	-3.436960	1.137044	-0.821189
H	-3.203253	0.946008	-1.871278
H	-4.517443	1.069692	-0.679841
H	-3.111143	2.142292	-0.545047
C	-0.918136	0.156666	-0.177010
H	-0.892072	0.350222	-1.258370
C	2.363596	-1.923385	-0.256692
H	2.444457	-2.200337	-1.316096
H	3.366597	-1.688222	0.103618
H	2.010264	-2.807618	0.279068
C	3.379654	0.808705	-0.369873
H	3.994082	0.608375	0.516497
H	3.775756	0.207824	-1.192843
H	3.497779	1.864076	-0.620600
C	-0.277619	-1.648903	1.509479
H	-0.092333	-0.887156	2.272907
H	-1.304429	-2.012780	1.623728
H	0.391678	-2.491196	1.707704
C	-0.438628	-2.184425	-0.940326
H	-1.513050	-2.379626	-0.889678
H	-0.195807	-1.859952	-1.958758
H	0.081619	-3.126002	-0.746697

0 imaginary frequencies
E = -903.172165
H = -902.884826
G = -902.938097
$E_{\omega B97X-D}$ = -903.422065
H_{tot} = -903.134726
G_{tot} = -903.187997

TS15-b

C	-0.899507	-0.435182	0.737721
C	0.364019	0.219345	0.642710
C	0.874433	-1.190701	-1.362587
C	-0.397542	-1.601153	-1.388594
C	-1.326495	-1.354801	-0.254585
H	1.552305	-1.414887	-2.187554
H	-0.805942	-2.154113	-2.232295
O	-2.436064	-1.964079	-0.257255
C	1.465928	-0.508280	-0.156243
C	-1.895177	0.005262	1.777824

H	-2.088533	1.088285	1.705484
H	-2.841015	-0.520355	1.624008
H	-1.562416	-0.188059	2.807024
C	0.862893	0.871383	1.923403
H	0.099010	1.521786	2.350313
H	1.103066	0.099036	2.667200
H	1.757198	1.477171	1.754970
C	2.651221	0.366260	-0.591055
H	3.123585	0.860832	0.263711
H	3.410866	-0.270641	-1.060587
H	2.343193	1.128982	-1.307664
C	2.050010	-1.635775	0.741347
H	2.744839	-2.248893	0.156569
H	2.606573	-1.212476	1.584876
H	1.253873	-2.278765	1.127778
H	-2.353165	2.643483	-0.845160
S	0.012437	2.170669	-0.533187
C	-1.649825	1.878843	-1.188480
H	-1.652880	1.857211	-2.282239
H	-2.000787	0.902138	-0.826162

1 imaginary frequency
E = -902.644293
H = -902.372965
G = -902.424479
$E_{\omega B97X-D}$ = -902.884775
H_{tot} = -902.613447
G_{tot} = -902.664962

P15-b

C	2.220027	1.110405	-0.365127
C	1.137495	1.892832	-0.291166
C	2.107550	-0.355125	-0.275851
H	3.220997	1.515629	-0.484508
H	1.256360	2.973731	-0.377296
O	3.103694	-1.060946	-0.244327
C	-0.285651	1.410031	-0.130790
C	0.703519	-0.961926	-0.272667
C	-0.302201	-0.041345	0.470434
C	0.774296	-2.406140	0.231679
H	-0.221815	-2.815140	0.413954
H	1.284561	-3.032375	-0.503554
H	1.345706	-2.469703	1.161468
C	-1.022992	2.412107	0.775314
H	-2.038499	2.062638	0.986929
H	-0.501749	2.573589	1.722854
H	-1.096203	3.378874	0.266107
C	-0.928224	1.497334	-1.530697
H	-2.009097	1.339267	-1.461512
H	-0.761712	2.496594	-1.946734
H	-0.500485	0.774587	-2.231830
S	-2.015649	-0.760416	0.432225
C	-2.193124	-1.544869	-1.195786
H	-3.183635	-2.006298	-1.183607
H	-2.153333	-0.829198	-2.017305
H	-1.450555	-2.331247	-1.350903
C	0.033024	-0.010875	1.971754
H	0.132697	-1.026045	2.361426
H	0.971660	0.525816	2.149870
H	-0.753351	0.486132	2.546551
H	0.416981	-0.977192	-1.335484

0 imaginary frequencies
E = -903.162965

H = -902.875583
G = -902.925958
$E_{\omega B97X-D}$ = -903.411794
H_{tot} = -903.124412
G_{tot} = -903.174788

4

C	3.452801	-0.258407	-0.538831
C	2.875140	1.090632	-0.428441
C	2.746802	-1.343818	-0.213581
C	1.454820	1.221411	0.015119
C	0.754841	0.105550	0.311119
C	1.337262	-1.308469	0.288449
O	3.551389	2.075413	-0.709571
C	0.497563	-2.242460	-0.637851
C	-1.011897	-2.213171	-0.362471
C	-1.466708	-0.766292	-0.396471
H	-1.248976	-2.660691	0.611519
H	-1.530766	-2.805182	-1.123801
C	-0.706989	0.048099	0.656869
C	0.927139	2.636090	0.073279
H	0.217609	2.830460	-0.736741
H	1.761588	3.330201	-0.032261
H	0.412269	2.835120	1.013449
C	1.375993	-1.891869	1.725589
C	-2.905358	-0.381333	-0.068631
H	-1.216378	-0.337501	-1.380541
O	-1.424960	1.290178	0.713509
H	-0.830348	-0.428211	1.639679
C	-2.716020	1.071647	0.355059
O	-3.534641	1.953566	0.382879
C	-3.933398	-0.543404	-1.177921
H	-3.229828	-0.927193	0.831549
H	-4.906819	-0.160875	-0.860521
H	-4.045197	-1.599254	-1.440041
H	-3.624159	0.005156	-2.073271
H	1.900244	-2.852869	1.714819
H	0.376483	-2.067600	2.130399
H	1.909192	-1.213539	2.398339
H	0.668613	-1.934040	-1.677151
H	0.887094	-3.262010	-0.536541
H	4.478861	-0.315676	-0.890351
H	3.194253	-2.334798	-0.290831

0 imaginary frequencies
E = -807.801286
H = -807.477243
G = -807.532463
$E_{\omega B97X-D}$ = -808.087219
H_{tot} = -807.763177
G_{tot} = -807.818397

TS4-disub bottom face

C	-2.486049	0.227378	1.446370
C	-1.756280	1.403479	1.220950
C	-2.274599	-0.933272	0.650140
C	-0.608510	1.339079	0.236310
C	-0.165199	0.146490	-0.208990
C	-0.847998	-1.176171	0.152630
O	-1.948601	2.500728	1.820790
C	-0.028908	-1.800170	1.332180
C	1.471482	-1.971249	1.016420
C	2.031531	-0.662939	0.480450

H	1.637663	-2.773739	0.286800
H	2.002002	-2.263659	1.930070
C	1.217181	-0.149939	-0.717830
C	0.056629	2.663660	-0.049130
H	0.822059	2.894490	0.703630
H	-0.692772	3.455689	0.014590
H	0.532299	2.682700	-1.028280
C	-0.846058	-2.195371	-1.006240
C	3.447571	-0.576238	-0.077910
H	1.932821	0.106021	1.264010
O	2.030230	0.927921	-1.229660
H	1.191791	-0.906599	-1.510700
C	3.326220	0.681572	-0.935500
O	4.212450	1.404603	-1.320580
C	4.585451	-0.494947	0.928260
H	3.616442	-1.413358	-0.774120
H	5.541201	-0.335216	0.421820
H	4.649102	-1.422577	1.504440
H	4.423501	0.333803	1.625200
H	-1.591767	-2.970921	-0.797020
H	0.117863	-2.695550	-1.125810
H	-1.118028	-1.726151	-1.953330
H	-0.139128	-1.146160	2.205180
H	-0.466867	-2.772431	1.593440
H	-3.344619	0.281277	2.112030
H	-2.706048	-1.855152	1.043890
H	-4.953370	1.066766	-1.541420
H	-3.243200	1.358868	-1.948160
C	-3.920880	0.888697	-1.229590
H	-3.767670	1.353817	-0.247750
S	-3.625339	-0.891143	-1.085880

1 imaginary frequency
E = -1245.938801
H = -1245.573875
G = -1245.635931
$E_{\omega B97X-D}$ = -1246.288490
H_{tot} = -1245.923564
G_{tot} = -1245.985620

TS4-disub top face

C	-3.125501	-0.026032	-0.379659
C	-2.624202	1.283878	-0.391049
C	-2.248711	-1.146342	-0.309889
C	-1.115692	1.449249	-0.353879
C	-0.307501	0.391419	-0.573599
C	-0.892941	-0.966041	-0.994169
O	-3.341532	2.326428	-0.424389
C	0.008460	-2.208231	-0.765019
C	1.507829	-1.984460	-0.996949
C	1.898009	-0.781170	-0.163069
H	1.742909	-1.799870	-2.054819
H	2.064920	-2.877980	-0.692849
C	1.190198	0.459029	-0.696669
C	-0.629582	2.860309	-0.122439
H	-0.309073	3.008249	0.915131
H	-1.455343	3.544718	-0.322929
H	0.218307	3.114389	-0.762029
C	-1.147571	-0.888881	-2.526209
C	3.338689	-0.286610	-0.103409
H	1.548089	-0.940900	0.870321
O	1.849448	1.541680	0.005261
H	1.452808	0.578890	-1.763089

C	3.110688	1.163990	0.306921
O	3.889138	1.917030	0.840231
C	4.287579	-1.023109	0.829101
H	3.754189	-0.260490	-1.123909
H	5.262919	-0.530019	0.859171
H	4.430109	-2.053159	0.489571
H	3.883949	-1.048080	1.846471
H	-1.695891	-1.776772	-2.862769
H	-0.195361	-0.856971	-3.069839
H	-1.729461	-0.001402	-2.783239
H	-0.108780	-2.547341	0.266631
H	-0.362470	-3.012421	-1.413029
H	-4.199401	-0.162053	-0.276429
H	-2.696511	-2.109622	-0.561989
H	-1.365132	0.533478	2.736281
H	-2.723481	-0.275632	3.562421
C	-2.255311	-0.085712	2.593111
H	-2.964352	0.463888	1.961381
S	-1.856001	-1.658732	1.793251

1 imaginary frequency
E = -1245.941907
H = -1245.577022
G = -1245.63927
$E_{\omega B97X-D}$ = -1246.293015
H_{tot} = -1245.928130
G_{tot} = -1245.990378

P4-disub top face

C	2.319739	0.982501	-0.968741
C	1.451099	2.146081	-0.556611
C	2.339829	-0.060609	0.138839
C	0.155409	1.817801	0.104629
C	-0.101381	0.532611	0.434059
C	0.928789	-0.617889	0.449489
O	1.765239	3.295271	-0.822121
C	0.510799	-1.717449	-0.567231
C	-0.945011	-2.187919	-0.416971
C	-1.855001	-0.974829	-0.398921
H	-1.078461	-2.769299	0.504159
H	-1.199211	-2.850639	-1.250891
C	-1.465351	-0.020749	0.740379
C	-0.791001	2.985341	0.256179
H	-1.467271	3.066481	-0.602031
H	-0.203291	3.904261	0.300369
H	-1.399211	2.903631	1.154779
C	0.987409	-1.219499	1.873539
C	-3.352741	-1.117399	-0.149851
H	-1.720991	-0.416389	-1.339981
O	-2.564211	0.902191	0.796279
H	-1.460671	-0.560899	1.694679
C	-3.686731	0.285531	0.345579
O	-4.755551	0.838811	0.356409
C	-4.211271	-1.545279	-1.330451
H	-3.515331	-1.795699	0.702939
H	-5.271101	-1.521049	-1.064161
H	-3.954701	-2.562939	-1.637721
H	-4.055941	-0.876279	-2.182841
H	0.124889	-1.844399	2.112789
H	1.879059	-1.848009	1.956399
H	1.053489	-0.424969	2.624799
H	0.651809	-1.335769	-1.586991
H	1.181799	-2.575719	-0.449631

S	3.540729	-1.399829	-0.234651
C	5.067869	-0.545229	0.244189
H	5.890379	-1.239789	0.062659
H	5.230489	0.352941	-0.355651
H	5.048459	-0.285519	1.305249
H	3.319969	1.360291	-1.194391
H	1.909309	0.551411	-1.891471
H	2.706339	0.417331	1.058119

0 imaginary frequencies
E = -1246.462635
H = -1246.081882
G = -1246.144846
$E_{\omega B97X-D}$ = -1246.820581
H_{tot} = -1246.439829
G_{tot} = -1246.502793

P4-disub bottom face

C	2.690360	1.216928	0.260380
C	1.657571	2.237319	-0.151500
C	2.261040	-0.178732	-0.163400
C	0.218900	1.841969	-0.066480
C	-0.097820	0.575829	0.287930
C	0.911210	-0.583091	0.474970
O	1.994511	3.360688	-0.489680
C	0.414829	-1.867621	-0.254380
C	-1.044021	-2.265630	-0.004060
C	-1.914591	-1.064680	-0.316530
H	-1.201851	-2.580600	1.036190
H	-1.300311	-3.119080	-0.640690
C	-1.492720	0.093830	0.585720
C	-0.763829	2.961149	-0.331670
H	-1.277009	3.269000	0.583450
H	-1.527929	2.665420	-1.051410
H	-0.219839	3.819939	-0.726080
C	1.080869	-0.874411	1.982410
C	-3.417811	-1.095190	-0.060560
H	-1.748040	-0.756260	-1.361320
O	-2.562390	1.044550	0.469560
H	-1.506150	-0.254290	1.629240
C	-3.703640	0.389171	0.138870
O	-4.753090	0.968941	0.029920
C	-4.288721	-1.727109	-1.135570
H	-3.607421	-1.577430	0.911840
H	-4.114511	-1.247799	-2.104160
H	-5.347551	-1.621309	-0.885900
H	-4.060081	-2.792329	-1.230620
H	1.394190	0.016899	2.534180
H	1.830629	-1.657731	2.134140
H	0.152309	-1.232891	2.432940
H	0.540639	-1.712511	-1.334810
H	1.081299	-2.689611	0.022560
S	3.585139	-1.406902	0.174990
C	4.642859	-1.078303	-1.262510
H	5.499269	-1.751043	-1.186370
H	5.007110	-0.048643	-1.265600
H	4.107619	-1.286832	-2.191800
H	2.808790	1.266048	1.350660
H	3.646990	1.503888	-0.183730
H	2.120450	-0.184402	-1.252690

0 imaginary frequencies
E = -1246.463684
H = -1246.083038

G = −1246.146138
$E_{\omega B97X-D}$ = −1246.821823
H_{tot} = −1246.441177
G_{tot} = −1246.504277

TS4-tetrasub top face

C	3.264941	0.743503	0.082039
C	2.934201	−0.540368	−0.605281
C	2.350330	1.695762	0.296509
C	1.568402	−0.867449	−0.736921
C	0.580831	0.019721	−0.173461
C	0.951640	1.531051	−0.243221
O	3.906762	−1.262107	−0.991141
C	−0.053881	2.450880	0.483459
C	−1.505271	2.258109	0.011179
C	−1.848770	0.784609	0.141359
H	−1.634701	2.589379	−1.027611
H	−2.180441	2.864879	0.625419
C	−0.866289	−0.094950	−0.629491
C	1.193663	−2.247369	−1.208451
H	0.707853	−2.834549	−0.414001
H	2.100113	−2.772778	−1.520851
H	0.492223	−2.238249	−2.053201
C	1.031530	2.003741	−1.725931
C	−3.175759	0.229338	−0.367491
H	−1.775729	0.506839	1.202539
O	−1.482158	−1.403391	−0.569801
H	−0.884359	0.187350	−1.693851
C	−2.817598	−1.250622	−0.478411
O	−3.570367	−2.196052	−0.478031
C	−4.405379	0.477277	0.491969
H	−3.353119	0.587448	−1.394611
H	−5.275299	−0.046643	0.086569
H	−4.632490	1.546787	0.531189
H	−4.237289	0.122627	1.514189
H	1.386679	3.040451	−1.745461
H	0.064200	1.980160	−2.235881
H	1.732660	1.382751	−2.287291
H	−0.001741	2.258220	1.560419
H	0.258169	3.491250	0.325379
H	4.302570	0.866133	0.387269
H	2.610109	2.646822	0.762929
H	1.740752	−2.051239	3.100749
H	2.772512	−0.791808	2.369139
C	1.892782	−1.423588	2.218199
H	2.074302	−2.066438	1.352509
S	0.395431	−0.437179	1.970619

1 imaginary frequency
E = −1245.942152
H = −1245.577722
G = −1245.639215
$E_{\omega B97X-D}$ = −1246.290053
H_{tot} = −1245.925623
G_{tot} = −1245.987116

TS4-tetrasub bottom face

C	2.982690	0.902430	0.979701
C	2.166550	−0.140600	1.658511
C	2.507780	1.627190	−0.036589
C	0.975670	−0.551700	1.020601
C	0.601230	0.004920	−0.257749

C	1.097690	1.458720	-0.539869
O	2.605260	-0.596060	2.758941
C	0.214600	2.459320	0.283801
C	-1.293750	2.339870	0.017261
C	-1.695740	0.896590	0.266091
H	-1.539180	2.626650	-1.014539
H	-1.840300	3.021040	0.679811
C	-0.872570	-0.024030	-0.633399
C	0.241570	-1.733790	1.603391
H	-0.766760	-1.491840	1.970871
H	0.817500	-2.121120	2.448241
H	0.114550	-2.537300	0.866111
C	1.062700	1.893700	-2.017069
C	-3.109290	0.407020	-0.030679
H	-1.456460	0.639840	1.309471
O	-1.555300	-1.294930	-0.543819
H	-0.983910	0.291250	-1.677489
C	-2.847470	-1.083130	-0.235019
O	-3.639280	-1.991750	-0.139529
C	-4.171150	0.681620	1.022961
H	-3.434440	0.800280	-1.007469
H	-5.121110	0.214460	0.749381
H	-4.332060	1.758580	1.129091
H	-3.859660	0.282110	1.993871
H	1.359760	2.947470	-2.077629
H	0.072990	1.811690	-2.473899
H	1.762430	1.306410	-2.614389
H	0.396910	2.274740	1.348831
H	0.560770	3.476680	0.064351
H	3.981350	1.064640	1.380531
H	3.105350	2.417020	-0.493179
H	1.819430	-3.426490	-0.902459
H	2.464590	-2.102640	0.099381
C	2.346360	-2.468770	-0.929059
H	3.340100	-2.614410	-1.359929
S	1.438220	-1.224580	-1.878809

1 imaginary frequency

E = -1245.945576

H = -1245.580963

G = -1245.642208

$E_{\omega B97X-D}$ = -1246.294498

H_{tot} = -1245.929885

G_{tot} = -1245.991130

P4-tetrasub bottom face

C	-3.237281	0.548050	-0.926690
C	-2.499391	-0.632490	-1.420050
C	-2.644040	1.463730	-0.152460
C	-0.983041	-0.602510	-1.225170
C	-0.656521	-0.073810	0.202790
C	-1.221800	1.397480	0.352560
O	-3.064931	-1.536950	-2.009700
C	-0.393480	2.416470	-0.497900
C	1.122280	2.375780	-0.247100
C	1.596360	0.946610	-0.453750
H	1.363710	2.705160	0.772190
H	1.624220	3.063470	-0.935660
C	0.838089	0.027720	0.495790
C	-0.330221	-1.916050	-1.645830
H	-0.781301	-2.252960	-2.581850
H	-0.477581	-2.693280	-0.892030
H	0.742609	-1.790910	-1.803530

C	-1.251390	1.886400	1.814350
C	3.035499	0.541480	-0.138670
H	1.387500	0.642010	-1.490860
O	1.566749	-1.213060	0.459860
H	0.958589	0.418910	1.514280
C	2.857049	-0.950130	0.132380
O	3.683929	-1.823090	0.073170
C	4.083290	0.828190	-1.203000
H	3.335920	0.994550	0.819560
H	4.186330	1.906570	-1.353160
H	3.799999	0.370940	-2.156510
H	5.055049	0.425920	-0.905610
H	-1.640170	2.909580	1.840400
H	-0.261570	1.905750	2.277830
H	-1.909710	1.260800	2.423030
H	-0.574950	2.236630	-1.564080
H	-0.784980	3.418520	-0.288840
H	-4.277360	0.635100	-1.228230
H	-3.210360	2.340690	0.162250
S	-1.482781	-1.264670	1.367980
C	-0.453721	-1.257090	2.863990
H	-0.935421	-1.968910	3.538410
H	-0.432381	-0.279840	3.349920
H	0.558979	-1.603720	2.652150
H	-0.658711	0.175630	-1.931480

0 imaginary frequencies
E = -1246.458035
H = -1246.077494
G = -1246.138335
$E_{\omega B97X-D}$ = -1246.815746
H_{tot} = -1246.435205
G_{tot} = -1246.496046

Cysteamine

H	1.580152	-0.086656	1.302361
S	1.457737	-0.320275	-0.015328
C	0.111952	0.880672	-0.316941
C	-1.211012	0.500001	0.353647
H	0.438774	1.873665	0.003779
H	-0.007811	0.903252	-1.404933
H	-1.934564	1.298460	0.152071
N	-1.801180	-0.764625	-0.068400
H	-1.069784	0.466853	1.440177
H	-1.133085	-1.519955	0.078601
H	-1.994852	-0.742884	-1.068242

0 imaginary frequencies
E = -533.256909
H = -533.156091
G = -533.188116
$E_{\omega B97X-D}$ = -533.375820
H_{tot} = -533.271983
G_{tot} = -533.307027

Cysteamine analogue of P4-disub bottom face

C	1.947290	2.050731	0.333310
C	0.782299	2.727451	-0.347300
C	1.849470	0.540011	0.193140
C	-0.548210	2.048200	-0.294950
C	-0.647660	0.831330	0.287230
C	0.541241	-0.015270	0.802280
O	0.923629	3.818351	-0.876310
C	0.406981	-1.498600	0.344990

C	-0.962808	-2.151400	0.559540
C	-2.007989	-1.261501	-0.083020
H	-1.184778	-2.276730	1.627770
H	-0.961378	-3.150880	0.111970
C	-1.944369	0.119329	0.567850
C	-1.695611	2.855699	-0.860910
H	-2.279070	2.278249	-1.579120
H	-1.292741	3.737050	-1.360650
H	-2.379051	3.186659	-0.074490
C	0.581291	0.052001	2.344730
C	-3.494678	-1.573781	0.053010
H	-1.775879	-1.141401	-1.153590
O	-3.158550	0.764389	0.154150
H	-2.021169	-0.006531	1.658250
C	-4.094919	-0.181782	-0.109690
O	-5.216989	0.115248	-0.428890
C	-4.079298	-2.588462	-0.917600
H	-3.704388	-1.878552	1.090940
H	-3.883138	-2.289782	-1.952220
H	-5.160868	-2.671472	-0.783670
H	-3.633088	-3.572942	-0.751180
H	0.625970	1.084551	2.703750
H	1.456491	-0.486949	2.722340
H	-0.298269	-0.415900	2.793570
H	0.636351	-1.545009	-0.729040
H	1.182322	-2.076989	0.856590
H	1.944070	2.339921	1.392480
H	2.871850	2.437152	-0.104440
H	5.011142	-3.019847	-0.793660
S	3.351881	-0.269348	0.879910
H	4.341060	0.641822	-1.127310
N	4.052152	-2.810298	-1.066800
H	3.491842	-2.877098	-0.217600
C	4.371691	-0.335388	-0.632180
C	3.968971	-1.454638	-1.597910
H	5.396641	-0.493827	-0.280720
H	2.943811	-1.290778	-1.950220
H	4.614701	-1.391108	-2.481230
H	1.835531	0.294561	-0.876220

0 imaginary frequencies
E = -1341.088317
H = -1340.658215
G = -1340.725565
$E_{\omega B97X-D}$ = -1341.489571
H_{tot} = -1341.056450
G_{tot} = -1341.126819