

Supporting Information

for

Why base catalyzed isomerization of *N*-propargyl amides yields mostly allenamides rather than ynamides

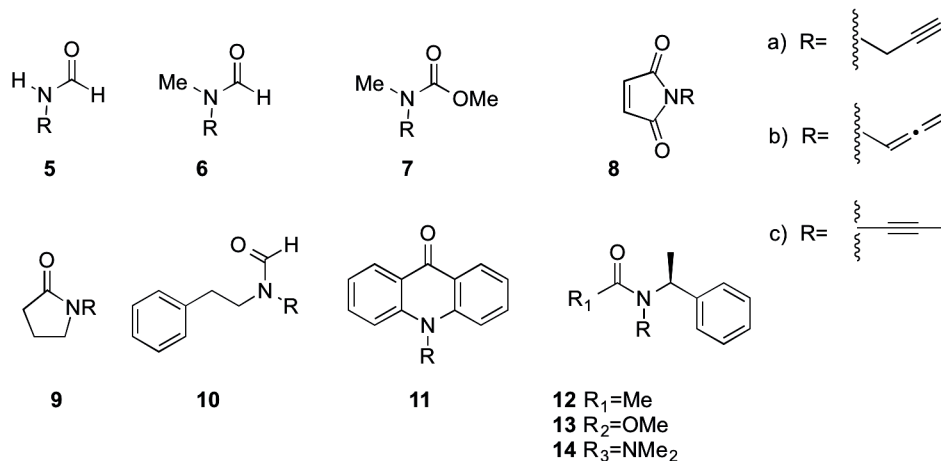
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Computational procedures as well as energies and XYZ coordinates for all computed structures

Computed energies and XYZ coordinates (Å)

**Propadiene****CBS-QB3****E(0 K)= -116.42037 a.u.**

```

7
propadiene CBS-QB3
C      0.000000      0.000000      1.302534
C      0.000000      0.000000      0.000000
C      0.000000      0.000000     -1.302534
H      0.000000      0.927184      1.866962
H      0.000000     -0.927184      1.866962
H     -0.927184      0.000000     -1.866962
H      0.927184      0.000000     -1.866962

```

W1**E(0 K)= -116.62670 a.u.**

```

7
propadiene W1
C      0.000000      0.000000      1.300052
C      0.000000      0.000000      0.000000
C      0.000000      0.000000     -1.300052
H      0.000000      0.925351      1.863005
H      0.000000     -0.925351      1.863005
H     -0.925351      0.000000     -1.863005
H      0.925351      0.000000     -1.863005

```

M05**E(SCF)= -116.56500 a.u.****E(SCF+ZPVE)= -116.50985 a.u.**

```

7
propadiene M05
C      0.000000      0.000000      1.309739
C      0.000000      0.000000      0.000000
C      0.000000      0.000000     -1.309739
H      0.000000      0.930487      1.870783
H      0.000000     -0.930487      1.870783
H     -0.930487      0.000000     -1.870783
H      0.930487      0.000000     -1.870783

```

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M052X

E(SCF)= -116.64304 a.u.

E(SCF+ZPVE)= -116.58684 a.u.

7

propadiene M052X

C	0.000000	0.000000	1.306857
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.306857
H	0.000000	0.930334	1.862332
H	0.000000	-0.930334	1.862332
H	-0.930334	0.000000	-1.862332
H	0.930334	0.000000	-1.862332

M06L

E(SCF)= -116.64464 a.u.

E(SCF+ZPVE)= -116.58967 a.u.

7

propadiene M06L

C	0.000000	0.000000	1.306124
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.306124
H	0.000000	0.927664	1.871905
H	0.000000	-0.927664	1.871905
H	-0.927664	0.000000	-1.871905
H	0.927664	0.000000	-1.871905

M06HF

E(SCF)= -116.62525 a.u.

E(SCF+ZPVE)= -116.56840 a.u.

7

propadiene M06HF

C	0.000000	0.000000	1.308022
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.308022
H	0.000000	0.932071	1.859151
H	0.000000	-0.932071	1.859151
H	-0.932071	0.000000	-1.859151
H	0.932071	0.000000	-1.859151

M06

E(SCF)= -116.56640 a.u.

E(SCF+ZPVE)= -116.51159 a.u.

7

propadiene M06

C	0.000000	0.000000	1.305646
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.305646
H	0.000000	0.929870	1.870846
H	0.000000	-0.929870	1.870846
H	-0.929870	0.000000	-1.870846
H	0.929870	0.000000	-1.870846

M062X

E(SCF)= -116.60306 a.u.

E(SCF+ZPVE)= -116.54733 a.u.

7

propadiene M062X

C	0.000000	0.000000	1.307192
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.307192
H	0.000000	0.931123	1.865448
H	0.000000	-0.931123	1.865448
H	-0.931123	0.000000	-1.865448
H	0.931123	0.000000	-1.865448

WB97

E(SCF)= -116.63180 a.u.

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E(SCF+ZPVE)= -116.57574 a.u.

7

propadiene WB97

C	0.000000	0.000000	1.309396
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.309396
H	0.000000	0.933954	1.867642
H	0.000000	-0.933954	1.867642
H	-0.933954	0.000000	-1.867642
H	0.933954	0.000000	-1.867642

WB97X

E(SCF)= -116.62650 a.u.

E(SCF+ZPVE)= -116.57048 a.u.

7

propadiene WB97X

C	0.000000	0.000000	1.307029
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.307029
H	0.000000	0.931735	1.865715
H	0.000000	-0.931735	1.865715
H	-0.931735	0.000000	-1.865715
H	0.931735	0.000000	-1.865715

WB97XD

E(SCF)= -116.62102 a.u.

E(SCF+ZPVE)= -116.56528 a.u.

7

propadiene WB97XD

C	0.000000	0.000000	1.306714
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.306714
H	0.000000	0.930858	1.866146
H	0.000000	-0.930858	1.866146
H	-0.930858	0.000000	-1.866146
H	0.930858	0.000000	-1.866146

S6

propyne

CBS-QB3

E(0 K)=-116.42168 a.u.

```
7
propyne CBS-QB3
C      0.000000      0.000000      1.420033
C      0.000000      0.000000      0.219037
C      0.000000      0.000000     -1.237554
H      0.000000      0.000000      2.482009
H      0.000000      1.020583     -1.630368
H     -0.883851     -0.510292     -1.630368
H      0.883851     -0.510292     -1.630368
```

W1

E(0 K)= -116.62846 a.u.

```
7
propyne W1
C      0.000000      0.000000      1.417629
C      0.000000      0.000000      0.218596
C      0.000000      0.000000     -1.235649
H      0.000000      0.000000      2.478279
H      0.000000      1.018453     -1.627244
H     -0.882006     -0.509227     -1.627244
H      0.882006     -0.509227     -1.627244
```

M05

E(SCF)= -116.56472 a.u.

E(SCF+ZPVE)= -116.50901 a.u.

```
7
propyne M05
C      0.000000      0.000000      1.427223
C      0.000000      0.000000      0.213880
C      0.000000      0.000000     -1.241230
H      0.000000      0.000000      2.494746
H      0.000000      1.021250     -1.631328
H     -0.884428     -0.510625     -1.631328
H      0.884428     -0.510625     -1.631328
```

M052X

E(SCF)= -116.640922 a.u.

E(SCF+ZPVE)= -116.58422 a.u.

```
7
propyne M052X
C      0.000000      0.000000      1.424721
C      0.000000      0.000000      0.218205
C      0.000000      0.000000     -1.244730
H      0.000000      0.000000      2.490005
H      0.000000      1.021577     -1.626393
H     -0.884711     -0.510788     -1.626393
H      0.884711     -0.510788     -1.626393
```

M06L

E(SCF)= -116.64156 a.u.

E(SCF+ZPVE)= -116.58603 a.u.

```
7
propyne M06L
C      0.000000      0.000000      1.423705
C      0.000000      0.000000      0.212751
C      0.000000      0.000000     -1.235210
H      0.000000      0.000000      2.488605
H      0.000000      1.019432     -1.632028
H     -0.882854     -0.509716     -1.632028
H      0.882854     -0.509716     -1.632028
```

M06HF

E(SCF)= -116.62479 a.u.

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E(SCF+ZPVE)= -116.56747 a.u.

7
propyne M06HF
C 0.000000 0.000000 1.426862
C 0.000000 0.000000 0.223342
C 0.000000 0.000000 -1.254321
H 0.000000 0.000000 2.493165
H 0.000000 1.025125 -1.622821
H -0.887784 -0.512562 -1.622821
H 0.887784 -0.512562 -1.622821

M06

E(SCF)= -116.56600 a.u.

E(SCF+ZPVE)= -116.51058 a.u.

7
propyne M06
C 0.000000 0.000000 1.423712
C 0.000000 0.000000 0.214801
C 0.000000 0.000000 -1.237477
H 0.000000 0.000000 2.490887
H 0.000000 1.021755 -1.632368
H -0.884866 -0.510877 -1.632368
H 0.884866 -0.510877 -1.632368

M062X

E(SCF)= -116.60273 a.u.

E(SCF+ZPVE)= -116.546443 a.u.

7
propyne M062X
C 0.000000 0.000000 1.425096
C 0.000000 0.000000 0.218289
C 0.000000 0.000000 -1.244128
H 0.000000 0.000000 2.491966
H 0.000000 1.022729 -1.629169
H -0.885710 -0.511365 -1.629169
H 0.885710 -0.511365 -1.629169

WB97

E(SCF)= -116.63173 a.u.

E(SCF+ZPVE)= -116.57513 a.u.

7
propyne WB97
C 0.000000 0.000000 1.427337
C 0.000000 0.000000 0.219743
C 0.000000 0.000000 -1.247242
H 0.000000 0.000000 2.497606
H 0.000000 1.025096 -1.632210
H -0.887759 -0.512548 -1.632210
H 0.887759 -0.512548 -1.632210

WB97X

E(SCF)= -116.62531 a.u.

E(SCF+ZPVE)= -116.56881 a.u.

7
WB97X
C 0.000000 0.000000 1.424864
C 0.000000 0.000000 0.218647
C 0.000000 0.000000 -1.243547
H 0.000000 0.000000 2.492506
H 0.000000 1.022560 -1.630764
H -0.885563 -0.511280 -1.630764
H 0.885563 -0.511280 -1.630764

WB97XD

E(SCF)= -116.61839 a.u.

E(SCF+ZPVE)= -116.56224 a.u.

7

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```
propyne WB97XD
C      0.000000    0.000000    1.306714
C      0.000000    0.000000    0.000000
C      0.000000    0.000000   -1.306714
H      0.000000    0.930858    1.866146
H      0.000000   -0.930858    1.866146
H     -0.930858    0.000000   -1.866146
H      0.930858    0.000000   -1.866146
```


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5

5a

CBS-QB3

E(0 K) = -284.88223 a.u.

11

5a CBS-QB3

N	0.560249	0.348651	-0.447269
C	-0.674473	0.924552	0.064535
C	1.604789	-0.045964	0.339729
O	2.587810	-0.628341	-0.055220
H	1.459955	0.250039	1.397958
C	-1.808470	-0.005317	0.061434
C	-2.738185	-0.764425	0.033690
H	0.587922	0.041571	-1.410382
H	-0.935016	1.816578	-0.514849
H	-0.482117	1.266653	1.086117
H	-3.556932	-1.441745	0.017474

M05

E(SCF)= -285.176781 a.u.

E(SCF+ZPVE)= -285.09274 a.u.

11

5a M05

N	0.556058	0.326813	-0.439113
C	-0.668401	0.919479	0.054123
C	1.608971	-0.041528	0.342547
O	2.598917	-0.620364	-0.057140
H	1.474061	0.261786	1.399616
C	-1.809666	0.000999	0.056906
C	-2.757386	-0.754710	0.040690
H	0.589139	0.013902	-1.399425
H	-0.917296	1.805209	-0.540501
H	-0.482664	1.274804	1.072659
H	-3.588089	-1.425916	0.032962

M052X

E(SCF)= -285.31252 a.u.

E(SCF+ZPVE)= -285.22704 a.u.

11

5a M052X

N	0.567260	0.396929	-0.440863
C	-0.666403	0.944457	0.088072
C	1.573042	-0.068555	0.345023
O	2.557493	-0.645636	-0.070106
H	1.418426	0.149043	1.414476
C	-1.788270	-0.007809	0.056191
C	-2.706539	-0.787854	0.013746
H	0.613357	0.144072	-1.416842
H	-0.938422	1.842666	-0.468626
H	-0.481094	1.252251	1.119078
H	-3.514007	-1.482883	-0.019387

M06L

E(SCF)= -285.31587 a.u.

E(SCF+ZPVE)= -285.23237 a.u.

11

5a M06L

N	0.545253	0.260661	-0.459229
C	-0.663865	0.898614	0.023267
C	1.622244	-0.006367	0.330524
O	2.617967	-0.605335	-0.025308
H	1.491807	0.410420	1.353395
C	-1.818765	0.011342	0.063101
C	-2.779049	-0.724965	0.070176
H	0.547517	-0.142561	-1.386184
H	-0.896987	1.779702	-0.588146

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H	-0.446179	1.277780	1.029651
H	-3.620062	-1.379034	0.085942

M06HF**E(SCF)= -285.26142 a.u.****E(SCF+ZPVE)= -285.17515 a.u.**

11

5a M06HF

N	0.582964	0.477310	-0.414953
C	-0.667234	0.975222	0.125584
C	1.536799	-0.116703	0.349270
O	2.519329	-0.664212	-0.097210
H	1.347546	-0.040610	1.427576
C	-1.769376	-0.017830	0.048202
C	-2.657688	-0.825422	-0.023322
H	0.670212	0.346544	-1.415462
H	-0.959953	1.876052	-0.411440
H	-0.506417	1.245205	1.169521
H	-3.441775	-1.546260	-0.086245

M06**E(SCF)= -285.17077 a.u.****E(SCF+ZPVE)= -285.08734 a.u.**

11

5a M06

N	0.547187	0.278742	-0.452064
C	-0.664254	0.907592	0.032663
C	1.616325	-0.018786	0.336220
O	2.607542	-0.608322	-0.036875
H	1.487661	0.356091	1.375008
C	-1.815137	0.008289	0.060009
C	-2.767299	-0.734800	0.061332
H	0.568951	-0.090785	-1.395769
H	-0.900975	1.791628	-0.574819
H	-0.459135	1.281619	1.045082
H	-3.604958	-1.396939	0.068598

M062X**E(SCF)= -285.23009 a.u.****E(SCF+ZPVE)= -285.14536 a.u.**

11

5a M062X

N	-0.082976	-0.864866	0.000000
C	0.000000	0.538843	0.000000
C	1.031599	-1.655009	0.000000
O	2.169336	-1.234813	0.000000
H	0.787179	-2.730601	0.000000
C	-1.044158	1.331606	0.000000
C	-2.077675	2.131994	0.000000
H	-0.994298	-1.300112	0.000000
H	1.017719	0.916580	0.000000
H	-2.521526	2.481047	0.929441
H	-2.521526	2.481047	-0.929441

WB97**E(SCF)= -285.30212 a.u.****E(SCF+ZPVE)= -285.21693 a.u.**

11

5a WB97

N	0.565085	0.378763	-0.441890
C	-0.666157	0.938475	0.080598
C	1.585026	-0.063445	0.345998
O	2.574820	-0.638477	-0.067984
H	1.434218	0.171931	1.419133
C	-1.799512	-0.006423	0.055295
C	-2.725953	-0.778827	0.020307
H	0.610678	0.116928	-1.418818
H	-0.932999	1.840429	-0.483464

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H	-0.481511	1.256645	1.114313
H	-3.544958	-1.468136	-0.007248

WB97(DMSO)**E(SCF)= -285.31564 a.u.****E(SCF+ZPVE)= -285.23033 a.u.**

11

5a WB97 DMSO

N	0.558168	0.325285	-0.435900
C	-0.663009	0.928334	0.072489
C	1.584614	-0.060939	0.347949
O	2.605385	-0.609282	-0.065878
H	1.434942	0.169491	1.418040
C	-1.810586	0.000151	0.052622
C	-2.750993	-0.757640	0.026464
H	0.623668	0.116963	-1.425600
H	-0.903213	1.820087	-0.516652
H	-0.480801	1.262700	1.100244
H	-3.585013	-1.431420	0.005154

WB97X**E(SCF)= -285.27925 a.u.****E(SCF+ZPVE)= -285.19414 a.u.**

11

5a WB97X

N	0.564108	0.372168	-0.440333
C	-0.666155	0.933350	0.079152
C	1.585610	-0.063171	0.345390
O	2.575985	-0.632966	-0.067606
H	1.435061	0.172116	1.416554
C	-1.799061	-0.006088	0.055209
C	-2.727665	-0.773586	0.021060
H	0.611254	0.113627	-1.416893
H	-0.929845	1.833550	-0.486112
H	-0.482037	1.254440	1.110241
H	-3.547449	-1.458211	-0.005481

WB97XD**E(SCF)= -285.25765 a.u.****E(SCF+ZPVE)= -285.17297 a.u.**

11

5a WB97XD

N	0.565981	0.386905	-0.436211
C	-0.669355	0.936834	0.085915
C	1.581092	-0.070961	0.346021
O	2.571573	-0.635652	-0.072627
H	1.424240	0.141926	1.420266
C	-1.795193	-0.007304	0.054898
C	-2.719303	-0.781202	0.014258
H	0.615591	0.148252	-1.417676
H	-0.935536	1.838123	-0.475700
H	-0.489312	1.254973	1.118260
H	-3.532880	-1.470600	-0.017219

B3LYP**E(SCF)= -285.35967 a.u.****E(SCF+ZPVE)= -285.27615 a.u.**

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5a B3LYP

N	0.559239	0.324137	-0.446144
C	-0.672935	0.920125	0.055057
C	1.611435	-0.038447	0.343020
O	2.607538	-0.620307	-0.053356
H	1.479921	0.269525	1.398433
C	-1.817663	-0.000410	0.058124
C	-2.763073	-0.754284	0.042182
H	0.590158	0.005948	-1.407798
H	-0.920129	1.808253	-0.539258

S12

H	-0.479639	1.273497	1.074480
H	-3.591864	-1.425631	0.033703

5b

CBS-QB3

E(0 K)= -284.88908 a.u.

11

5b CBS-QB3

N	0.000000	0.612568	0.000000
C	-0.324081	-0.753113	0.000000
C	-0.922316	1.626758	0.000000
O	-0.645755	2.803295	0.000000
H	-1.960369	1.243585	0.000000
C	0.538216	-1.736953	0.000000
C	1.381604	-2.729696	0.000000
H	0.973311	0.888975	0.000000
H	-1.390941	-0.956878	0.000000
H	1.751747	-3.165999	0.925149
H	1.751747	-3.165999	-0.925149

M05

E(SCF)= -285.18696 a.u.

E(SCF+ZPVE)= -285.10332 a.u.

11

5b M05

N	0.000000	0.606947	0.000000
C	-0.354951	-0.747057	0.000000
C	-0.885954	1.647889	0.000000
O	-0.564961	2.818520	0.000000
H	-1.938452	1.306637	0.000000
C	0.495717	-1.749157	0.000000
C	1.331354	-2.756977	0.000000
H	0.980148	0.854423	0.000000
H	-1.425834	-0.935599	0.000000
H	1.693414	-3.195221	0.928356
H	1.693414	-3.195221	-0.928356

M052X

E(SCF)= -285.32308 a.u.

E(SCF+ZPVE)= -285.23794 a.u.

11

5b M052X

N	0.000000	0.610831	0.000000
C	-0.336669	-0.750741	0.000000
C	-0.920029	1.615032	0.000000
O	-0.637425	2.795476	0.000000
H	-1.957985	1.247661	0.000000
C	0.531588	-1.732336	0.000000
C	1.387741	-2.719583	0.000000
H	0.971930	0.883705	0.000000
H	-1.401558	-0.956139	0.000000
H	1.755614	-3.144545	0.928334
H	1.755614	-3.144545	-0.928334

M06L

E(SCF)= -285.33027 a.u.

E(SCF+ZPVE)= -285.24712 a.u.

11

5b M06L

N	0.000000	0.614816	0.000000
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S13

C	-0.315679	-0.748039	0.000000
C	-0.934482	1.612690	0.000000
O	-0.674930	2.799802	0.000000
H	-1.967903	1.207165	0.000000
C	0.553173	-1.731181	0.000000
C	1.402191	-2.722814	0.000000
H	0.971481	0.896435	0.000000
H	-1.385304	-0.950578	0.000000
H	1.774972	-3.159544	0.925583
H	1.774972	-3.159544	-0.925583

M06HF**E(SCF)= -285.26900 a.u.****E(SCF+ZPVE)= -285.18310 a.u.**

11
5b M06HF

N	0.000000	0.607065	0.000000
C	-0.354682	-0.752326	0.000000
C	-0.904519	1.624929	0.000000
O	-0.598031	2.794948	0.000000
H	-1.947898	1.288072	0.000000
C	0.509804	-1.736276	0.000000
C	1.367422	-2.723604	0.000000
H	0.979533	0.865907	0.000000
H	-1.419886	-0.951429	0.000000
H	1.732177	-3.143963	0.930340
H	1.732177	-3.143963	-0.930340

M06**E(SCF)= -285.18069 a.u.****E(SCF+ZPVE)= -285.09766 a.u.**

11
5b M06

N	0.000000	0.610640	0.000000
C	-0.332679	-0.750358	0.000000
C	-0.918637	1.621081	0.000000
O	-0.638482	2.799891	0.000000
H	-1.961393	1.239400	0.000000
C	0.531436	-1.735482	0.000000
C	1.383536	-2.723993	0.000000
H	0.976801	0.884337	0.000000
H	-1.404618	-0.949897	0.000000
H	1.757560	-3.157466	0.927861
H	1.757560	-3.157466	-0.927861

M062X**E(SCF)= -285.23927 a.u.****E(SCF+ZPVE)= -285.15491 a.u.**

11
5b M062X

N	0.000000	0.610773	0.000000
C	-0.335849	-0.751205	0.000000
C	-0.919809	1.619842	0.000000
O	-0.636893	2.797906	0.000000
H	-1.960885	1.249186	0.000000
C	0.531249	-1.734599	0.000000
C	1.386403	-2.722950	0.000000
H	0.975858	0.882259	0.000000
H	-1.403664	-0.955532	0.000000
H	1.755936	-3.150549	0.929197
H	1.755936	-3.150549	-0.929197

WB97**E(SCF)= -285.31011 a.u.****E(SCF+ZPVE)= -285.22538 a.u.**

11
5b Wb97

N	0.000000	0.611761	0.000000
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S14

C	-0.338648	-0.754498	0.000000
C	-0.920253	1.620650	0.000000
O	-0.635371	2.803414	0.000000
H	-1.965288	1.252847	0.000000
C	0.530338	-1.737485	0.000000
C	1.389145	-2.725492	0.000000
H	0.975601	0.883365	0.000000
H	-1.408572	-0.960598	0.000000
H	1.758868	-3.152151	0.932113
H	1.758868	-3.152151	-0.932113

WB97(DMSO)

E(SCF)= -285.32083 a.u.

E(SCF+ZPVE)= -285.23603 a.u.

11

5b WB97 DMSO

N	0.000000	0.612858	0.000000
C	-0.348922	-0.755495	0.000000
C	-0.912303	1.613185	0.000000
O	-0.621459	2.806493	0.000000
H	-1.957867	1.258430	0.000000
C	0.523537	-1.735696	0.000000
C	1.381855	-2.724525	0.000000
H	0.980193	0.872884	0.000000
H	-1.419359	-0.956693	0.000000
H	1.751855	-3.150692	0.932291
H	1.751855	-3.150692	-0.932291

WB97X

E(SCF)= -285.28873 a.u.

E(SCF+ZPVE)= -285.20400 a.u.

11

5b WB97X

N	0.000000	0.610546	0.000000
C	-0.339439	-0.752799	0.000000
C	-0.915476	1.620960	0.000000
O	-0.627615	2.800670	0.000000
H	-1.959862	1.257601	0.000000
C	0.526178	-1.736025	0.000000
C	1.381039	-2.724551	0.000000
H	0.975215	0.879474	0.000000
H	-1.407786	-0.956799	0.000000
H	1.749772	-3.152487	0.929952
H	1.749772	-3.152487	-0.929952

WB97XD

E(SCF)= -285.26879 a.u.

E(SCF+ZPVE)= -285.18441 a.u.

11

5b WB97XD

N	-0.080925	-0.859448	0.000000
C	0.000000	0.544545	0.000000
C	1.026775	-1.657927	0.000000
O	2.171703	-1.251595	0.000000
H	0.770654	-2.731204	0.000000
C	-1.043589	1.336057	0.000000
C	-2.076365	2.136540	0.000000
H	-0.992242	-1.292858	0.000000
H	1.015943	0.926074	0.000000
H	-2.521216	2.485800	0.929169
H	-2.521216	2.485800	-0.929169

B3LYP

E(SCF)= -285.37407 a.u.

E(SCF+ZPVE)= -285.29077 a.u.

11

5b b3lyp

N	0.000000	0.610826	0.000000
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S15

C	-0.343535	-0.753415	0.000000
C	-0.906141	1.636589	0.000000
O	-0.603727	2.818040	0.000000
H	-1.953922	1.283232	0.000000
C	0.516012	-1.746730	0.000000
C	1.360343	-2.746719	0.000000
H	0.979405	0.872687	0.000000
H	-1.414027	-0.946262	0.000000
H	1.729143	-3.184059	0.927120
H	1.729143	-3.184059	-0.927120

5c**CBS-QB3****E(0 K)= -284.88748 a.u.**

11

5c CBS-QB3

N	-0.805135	0.553084	0.000047
C	0.521727	0.298223	0.000260
C	-1.793526	-0.418193	0.000106
O	-2.971699	-0.165744	-0.000227
H	-1.367704	-1.435844	0.000504
C	1.700283	0.056495	0.000535
C	3.130265	-0.226278	0.000115
H	-1.131179	1.512621	-0.000305
H	3.414516	-0.851711	-0.851217
H	3.441071	-0.736880	0.916338
H	3.700334	0.704698	-0.069930

M05**E(SCF)= -285.18651 a.u.****E(SCF+ZPVE)= -285.10276 a.u.**

11

5c M05

N	-0.808737	0.547745	0.000135
C	0.518367	0.293589	0.000532
C	-1.795952	-0.418317	0.000603
O	-2.978344	-0.160146	-0.000641
H	-1.378055	-1.439661	0.000542
C	1.709187	0.054984	0.000822
C	3.139216	-0.222610	0.000354
H	-1.131610	1.507379	-0.000475
H	3.408760	-0.906111	-0.809553
H	3.463230	-0.664677	0.946640
H	3.700685	0.704153	-0.146840

M052X**E(SCF)= -285.31857 a.u.****E(SCF+ZPVE)= -285.23348 a.u.**

11

5c M052X

N	0.815068	-0.562228	0.000006
C	-0.515404	-0.300016	-0.000038
C	1.780734	0.417746	-0.000007
O	2.966034	0.175715	0.000014
H	1.355683	1.430532	-0.000027
C	-1.699029	-0.062854	0.000037
C	-3.134003	0.226466	0.000048
H	1.141183	-1.518688	0.000013
H	-3.616803	-0.194255	-0.882671
H	-3.293086	1.305613	-0.007713
H	-3.614515	-0.181382	0.890005

M06L**E(SCF)= -285.32663 a.u.****E(SCF+ZPVE)= -285.24342 a.u.**

11

5c M06L

S16

N	-0.806870	0.554528	0.000134
C	0.517906	0.299928	0.000625
C	-1.788184	-0.417721	0.000569
O	-2.974470	-0.168357	-0.000677
H	-1.355920	-1.436113	0.000806
C	1.705841	0.057327	0.000902
C	3.126367	-0.226626	0.000274
H	-1.130036	1.514803	-0.000557
H	3.400710	-0.910943	-0.808820
H	3.456282	-0.673165	0.943830
H	3.701223	0.693135	-0.144999

M06HF**E(SCF)= -285.26524 a.u.****E(SCF+ZPVE)= -285.17926 a.u.**

11

5c M06HF

N	0.820327	-0.564447	-0.000007
C	-0.514148	-0.299879	-0.000003
C	1.781248	0.419512	-0.000005
O	2.961657	0.177042	0.000001
H	1.364124	1.431276	0.000017
C	-1.694531	-0.063219	0.000067
C	-3.144149	0.227896	0.000034
H	1.145131	-1.524509	-0.000002
H	-3.613206	-0.200925	-0.884450
H	-3.291828	1.307511	-0.009894
H	-3.610291	-0.184423	0.893808

M06**E(SCF)= -285.17993 a.u.****E(SCF+ZPVE)= -285.09680 a.u.**

11

5c M06

N	-0.810241	0.559539	-0.000036
C	0.516700	0.300091	0.000600
C	-1.785377	-0.416755	0.000164
O	-2.968759	-0.173417	-0.000374
H	-1.350356	-1.435060	0.000878
C	1.701807	0.056979	0.001112
C	3.127041	-0.227592	0.000331
H	-1.141057	1.519716	-0.000491
H	3.398690	-0.912624	-0.810563
H	3.454667	-0.673354	0.946215
H	3.698790	0.695541	-0.146033

M062X**E(SCF)= -285.23721 a.u.****E(SCF+ZPVE)= -285.15276 a.u.**

11

5c M062X

N	0.814538	-0.562351	0.000010
C	-0.516606	-0.301523	-0.000052
C	1.784296	0.418088	-0.000009
O	2.967519	0.175844	0.000022
H	1.356424	1.433963	-0.000053
C	-1.700407	-0.063252	0.000012
C	-3.134458	0.227173	0.000064
H	1.140092	-1.522409	0.000028
H	-3.621096	-0.192883	-0.883751
H	-3.295508	1.308292	-0.007606
H	-3.618782	-0.180167	0.891044

WB97**E(SCF)= -285.30844 a.u.****E(SCF+ZPVE)= -285.22364 a.u.**

11

5c WB97

S17

N	0.818457	-0.565619	-0.000003
C	-0.518640	-0.302517	-0.000030
C	1.784446	0.417679	-0.000010
O	2.973588	0.178794	0.000019
H	1.355617	1.436351	-0.000040
C	-1.702246	-0.063540	0.000040
C	-3.140741	0.228233	0.000051
H	1.143614	-1.525113	0.000013
H	-3.627711	-0.193430	-0.885508
H	-3.301114	1.311536	-0.008357
H	-3.625223	-0.179493	0.893457

WB97(DMSO)

E(SCF)= -285.31781 a.u.

E(SCF+ZPVE)= -285.23313 a.u.

11
5c WB97 DMSO

N	0.822349	-0.565674	-0.000009
C	-0.516791	-0.300007	0.000135
C	1.775967	0.415096	0.000028
O	2.975164	0.180866	-0.000092
H	1.353523	1.433847	0.000219
C	-1.701362	-0.063441	0.000326
C	-3.140880	0.227609	-0.000015
H	1.138725	-1.529769	-0.000192
H	-3.629223	-0.213639	-0.874787
H	-3.301723	1.310124	-0.030238
H	-3.620660	-0.163314	0.902957

WB97X

E(SCF)= -285.28581 a.u.

E(SCF+ZPVE)= -285.20112 a.u.

11
5c WB97X

N	-0.815253	0.560982	-0.000011
C	0.517847	0.297448	0.000617
C	-1.784266	-0.416846	0.000211
O	-2.970073	-0.173529	-0.000443
H	-1.360559	-1.435364	0.000970
C	1.699639	0.056907	0.001182
C	3.135735	-0.227275	0.000196
H	-1.138196	1.520231	-0.000609
H	3.398833	-0.912977	-0.810185
H	3.454570	-0.670549	0.947793
H	3.698977	0.698609	-0.147578

WB97XD

E(SCF)= -285.264109 a.u.

E(SCF+ZPVE)= -285.17985 a.u.

11
5c WB97XD

N	-0.812863	0.558851	0.000001
C	0.517617	0.297162	0.000617
C	-1.785433	-0.417124	0.000219
O	-2.970432	-0.171415	-0.000449
H	-1.362950	-1.435304	0.000972
C	1.700490	0.056748	0.001151
C	3.134101	-0.226836	0.000210
H	-1.134241	1.518968	-0.000592
H	3.398182	-0.912101	-0.810306
H	3.453795	-0.670658	0.947341
H	3.698056	0.698766	-0.147006

S18

6

6a

CBS-QB3

E(0 K)=-324.10551 a.u.

14

6a CBS-QB3

C	0.601571	1.543039	0.019159
N	0.470162	0.122039	0.306461
C	1.458541	-0.751564	-0.054374
O	2.506568	-0.450814	-0.583137
H	1.198820	-1.795649	0.205250
C	-0.771300	-0.357447	0.896719
C	-1.931093	-0.253005	0.003314
C	-2.881647	-0.158993	-0.724144
H	1.588372	1.702595	-0.410600
H	0.503043	2.129751	0.938257
H	-0.163608	1.868397	-0.691611
H	-0.976484	0.200125	1.819067
H	-0.629474	-1.402830	1.187200
H	-3.720771	-0.082327	-1.371739

WB97

E(SCF)= -324.60816 a.u.

E(SCF+ZPVE)= -324.49447 a.u.

14

6a WB97

C	0.562566	1.531497	0.054800
N	0.473231	0.107504	0.324908
C	1.464903	-0.740509	-0.068653
O	2.505778	-0.403160	-0.607957
H	1.236806	-1.799190	0.165554
C	-0.757144	-0.399406	0.900508
C	-1.917702	-0.260486	-0.002337
C	-2.865404	-0.137622	-0.739296
H	1.553004	1.736575	-0.357611
H	0.425372	2.100500	0.983273
H	-0.205824	1.834805	-0.667914
H	-0.968644	0.131233	1.839745
H	-0.617973	-1.458051	1.152127
H	-3.704896	-0.033960	-1.396004

WB97(DMSO)

E(SCF)= -324.61998 a.u.

E(SCF+ZPVE)= -324.50632 a.u.

14

6a WB97-DMSO

C	0.557589	1.534056	0.068198
N	0.470763	0.100517	0.298715
C	1.463193	-0.737432	-0.070267
O	2.521005	-0.394639	-0.600899
H	1.244746	-1.795445	0.158009
C	-0.754353	-0.413389	0.891668
C	-1.919834	-0.262717	-0.002772
C	-2.874808	-0.130965	-0.730736
H	1.548829	1.763458	-0.326908
H	0.404161	2.072013	1.011059
H	-0.205118	1.851155	-0.653382
H	-0.950150	0.114509	1.834070
H	-0.614519	-1.472565	1.135064
H	-3.722054	-0.016953	-1.378266

6b

CBS-QB3

E(0 K)= -324.11330 a.u.

14

6b CBS-QB3

S19

C	-1.448497	0.351211	0.000000
N	0.000000	0.510557	0.000000
C	0.554072	1.769490	0.000000
O	-0.069247	2.807172	0.000000
H	1.658510	1.732328	0.000000
C	0.829345	-0.622831	0.000000
C	0.425235	-1.868763	0.000000
C	0.072378	-3.123015	0.000000
H	-1.889433	1.345212	0.000000
H	-1.768036	-0.199927	0.888130
H	-1.768036	-0.199927	-0.888130
H	1.892154	-0.398235	0.000000
H	-0.083191	-3.673639	-0.925002
H	-0.083191	-3.673639	0.925002

WB97

E(SCF)= -324.61703 a.u.**E(SCF+ZPVE)= -324.50361 a.u.**

14

6b WB97

C	-1.437385	0.306207	0.000000
N	0.000000	0.513940	0.000000
C	0.523088	1.779347	0.000000
O	-0.132190	2.806034	0.000000
H	1.630146	1.780788	0.000000
C	0.856924	-0.602262	0.000000
C	0.457086	-1.854310	0.000000
C	0.100610	-3.114235	0.000000
H	-1.919491	1.285869	0.000000
H	-1.734474	-0.258596	0.891837
H	-1.734474	-0.258596	-0.891837
H	1.921223	-0.368091	0.000000
H	-0.053675	-3.657853	-0.931790
H	-0.053675	-3.657853	0.931790

WB97(DMSO)

E(SCF)= -324.62607 a.u.**E(SCF+ZPVE)= 324.51282 a.u.**

14

6b WB97-DMSO

C	-1.437545	0.295181	0.000000
N	0.000000	0.517542	0.000000
C	0.521906	1.771567	0.000000
O	-0.137501	2.808361	0.000000
H	1.625434	1.779834	0.000000
C	0.865627	-0.598782	0.000000
C	0.460145	-1.848872	0.000000
C	0.098724	-3.107632	0.000000
H	-1.936112	1.265508	0.000000
H	-1.726652	-0.271654	0.892231
H	-1.726652	-0.271654	-0.892231
H	1.928523	-0.360907	0.000000
H	-0.058836	-3.649788	-0.932084
H	-0.058836	-3.649788	0.932084

6c

CBS-QB3

E(0 K)= -324.10954 a.u.

14

6c CBS-QB3

C	1.201652	1.559504	-0.000064
N	0.637568	0.203176	0.000123
C	1.480515	-0.899776	0.000068
O	2.686318	-0.837240	-0.000194
H	0.908774	-1.842239	0.000272
C	-0.705163	0.041207	0.000284
C	-1.902384	-0.083505	0.000437
C	-3.351979	-0.238282	0.000027

S20

H	0.876613	2.100330	-0.890959
H	0.876475	2.100592	0.890619
H	2.285018	1.459771	0.000014
H	-3.838808	0.739812	-0.054705
H	-3.692360	-0.824408	-0.858778
H	-3.705074	-0.733057	0.909718

WB97

E(SCF)= -324.61324 a.u.**E(SCF+ZPVE)= -324.49991 a.u.**

14

6c WB97

C	1.200454	1.559335	-0.000074
N	0.649735	0.205392	0.000154
C	1.478813	-0.897828	0.000057
O	2.692480	-0.838446	-0.000194
H	0.911240	-1.845635	0.000251
C	-0.703663	0.038505	0.000282
C	-1.905588	-0.084748	0.000406
C	-3.365547	-0.238263	0.000003
H	0.869066	2.097029	-0.894621
H	0.869068	2.097298	0.894311
H	2.289349	1.472375	-0.000073
H	-3.843802	0.745757	-0.049171
H	-3.699244	-0.820543	-0.865403
H	-3.710479	-0.738455	0.911134

WB97(DMSO)

E(SCF)= -324.62116 a.u.**E(SCF+ZPVE)= -324.50800 a.u.**

14

6c WB97-DMSO

C	1.192422	1.565169	-0.000084
N	0.654790	0.202735	0.000171
C	1.474694	-0.894470	0.000056
O	2.697111	-0.839166	-0.000202
H	0.913940	-1.843864	0.000233
C	-0.701162	0.032197	0.000309
C	-1.903820	-0.087752	0.000399
C	-3.364875	-0.238323	-0.000033
H	0.853718	2.096229	-0.894849
H	0.853951	2.096455	0.894635
H	2.281696	1.496754	-0.000214
H	-3.840562	0.746623	-0.048334
H	-3.697963	-0.819895	-0.865619
H	-3.708742	-0.739043	0.910693

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7a

CBS-QB3

E(0 K)=-438.48928 a.u.

18

7a CBS-QB3

C	-0.854145	2.015356	-0.057051
N	-0.301276	0.732933	0.357952
C	0.959534	0.394063	-0.059771
O	1.716013	1.129368	-0.656901
O	1.280186	-0.876667	0.300777
C	2.600441	-1.295701	-0.075802
C	-1.222883	-0.233163	0.951505
C	-2.159012	-0.825217	-0.012998
C	-2.926939	-1.301518	-0.804135
H	-0.043944	2.634733	-0.432308
H	-1.325249	2.510078	0.797648
H	-1.603220	1.886816	-0.845972
H	2.681871	-2.327482	0.260369
H	3.355834	-0.674887	0.408496
H	2.729779	-1.234332	-1.157119
H	-0.643004	-1.020175	1.430441
H	-1.792322	0.278083	1.736059
H	-3.602383	-1.727900	-1.504790

WB97

E(SCF)= -439.14555 a.u.

E(SCF+ZPVE)= -438.99792 a.u.

18

7a WB97

C	-0.893352	1.996199	-0.097713
N	-0.307061	0.764604	0.406774
C	0.933063	0.402458	-0.047982
O	1.670321	1.118487	-0.705153
O	1.270425	-0.848415	0.345069
C	2.575249	-1.270935	-0.071095
C	-1.223206	-0.202660	0.990643
C	-2.091130	-0.853804	-0.013239
C	-2.800905	-1.373424	-0.840010
H	-0.091846	2.654150	-0.437258
H	-1.453051	2.486416	0.707681
H	-1.575324	1.795221	-0.936283
H	2.683242	-2.289207	0.307655
H	3.341879	-0.615659	0.353687
H	2.650469	-1.253148	-1.162454
H	-0.651777	-0.961866	1.529818
H	-1.852149	0.323987	1.720155
H	-3.426304	-1.839696	-1.573376

WB97(DMSO)

E(SCF)= -439.15508 a.u.

E(SCF+ZPVE)= -439.007881a .u.

18

7a WB97(DMSO)

C	-0.881742	2.041836	-0.139454
N	-0.316010	0.807039	0.386928
C	0.913100	0.410234	-0.049126
O	1.676404	1.106937	-0.711898
O	1.217356	-0.840645	0.351686
C	2.522240	-1.309698	-0.026771
C	-1.248228	-0.134080	0.994241
C	-2.039175	-0.880166	-0.007965
C	-2.681796	-1.482099	-0.835756
H	-0.071964	2.718682	-0.415105
H	-1.496786	2.510951	0.635236
H	-1.505534	1.847751	-1.023266
H	2.589659	-2.323473	0.370594
H	3.296645	-0.673953	0.411981

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H	2.621386	-1.317298	-1.115896
H	-0.700195	-0.835616	1.627511
H	-1.926163	0.435241	1.640543
H	-3.251454	-2.018050	-1.569416

7b

CBS-QB3

E(0 K)=-438.49664 a.u.

18

7b CBS-QB3

C	0.861287	1.768868	-0.000146
N	0.247018	0.446106	-0.000405
C	-1.128825	0.359184	0.000003
O	-1.878546	1.310780	0.000408
O	-1.550425	-0.928679	-0.000247
C	-2.977188	-1.097302	0.000116
C	1.081164	-0.688097	-0.000105
C	2.391861	-0.654718	-0.000399
C	3.694722	-0.685403	0.000439
H	0.069848	2.512314	-0.000156
H	1.488093	1.891998	-0.887567
H	1.487951	1.891762	0.887380
H	-3.138901	-2.173207	-0.005888
H	-3.418808	-0.638158	-0.885283
H	-3.417025	-0.648680	0.891859
H	0.557337	-1.633896	0.000045
H	4.267353	-0.698294	0.925371
H	4.268677	-0.698579	-0.923658

WB97

E(SCF)=-439.15402 a.u.

E(SCF+ZPVE)= -439.00672 a.u.

18

7b WB97

C	0.097037	1.949855	0.000000
N	0.000000	0.499344	0.000000
C	1.153055	-0.247062	0.000000
O	2.278803	0.220759	0.000000
O	0.900218	-1.574642	0.000000
C	2.070916	-2.403160	0.000000
C	-1.282661	-0.085758	0.000000
C	-2.402629	0.604005	0.000000
C	-3.545252	1.244325	0.000000
H	1.152050	2.226220	0.000000
H	-0.396338	2.356662	0.891273
H	-0.396338	2.356662	-0.891273
H	1.697286	-3.428922	0.000000
H	2.673766	-2.209615	0.892285
H	2.673766	-2.209615	-0.892285
H	-1.301598	-1.170990	0.000000
H	-4.038779	1.521011	-0.931472
H	-4.038779	1.521011	0.931472

WB97(DMSO)

E(SCF)= -439.16096 a.u.

E(SCF+ZPVE)= -439.01416 a.u.

18

7b WB97-DMSO

C	-0.886929	1.743620	-0.000003
N	-0.244278	0.437442	-0.000030
C	1.122351	0.355191	0.000000
O	1.872426	1.324956	0.000018
O	1.559979	-0.916872	0.000006
C	2.989250	-1.077957	0.000006
C	-1.068988	-0.709687	-0.000027
C	-2.383795	-0.662664	-0.000009
C	-3.693923	-0.670527	0.000027

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H	-0.116722	2.514688	-0.000027
H	-1.515857	1.848870	0.891851
H	-1.515920	1.848870	-0.891813
H	3.155648	-2.156007	-0.000160
H	3.421556	-0.622673	0.895403
H	3.421590	-0.622384	-0.895226
H	-0.548466	-1.662207	-0.000049
H	-4.259488	-0.671876	-0.931668
H	-4.259435	-0.671902	0.931754

CBS-QB3**E(0 K)=-438.49164 a.u.**

18

7c CBS-QB3

C	0.025697	2.344351	0.000002
N	0.017145	0.875457	-0.000015
C	-1.204405	0.214213	-0.000006
O	-2.277533	0.773046	0.000003
O	-1.032234	-1.119155	-0.000013
C	-2.246495	-1.887125	0.000007
C	1.203380	0.225813	0.000028
C	2.295353	-0.279143	0.000008
C	3.600068	-0.929398	0.000013
H	-1.006973	2.683359	0.000183
H	0.538566	2.713911	-0.890485
H	0.538879	2.713872	0.890322
H	-1.926843	-2.926806	-0.000059
H	-2.839897	-1.668121	-0.888887
H	-2.839808	-1.668212	0.888984
H	4.183916	-0.664153	0.886780
H	4.186660	-0.658326	-0.883172
H	3.482027	-2.017124	-0.003795

WB97**E(SCF)= -439.14847 a.u.****E(SCF+ZPVE)= -439.00134 a.u.**

18

7c WB97

C	-0.003948	2.342390	0.000000
N	0.000000	0.879995	0.000000
C	1.204170	0.201313	0.000000
O	2.292564	0.747098	0.000000
O	1.020375	-1.127970	0.000000
C	2.231077	-1.895289	0.000000
C	-1.201284	0.235536	0.000000
C	-2.300814	-0.263357	0.000000
C	-3.621774	-0.903575	0.000000
H	1.033277	2.682502	0.000000
H	-0.517739	2.712014	0.894081
H	-0.517739	2.712014	-0.894081
H	1.909684	-2.938448	0.000000
H	2.823454	-1.671668	0.892707
H	2.823454	-1.671668	-0.892707
H	-4.197516	-0.623408	-0.888819
H	-4.197516	-0.623408	0.888819
H	-3.507431	-1.993024	0.000000

WB97(DMSO)**E(SCF)= -439.15682 a.u.****E(SCF+ZPVE)= -439.01007 a.u.**

18

7c WB97-DMSO

C	0.027928	2.347958	0.000004
N	0.001874	0.882957	-0.000012
C	-1.200843	0.210933	-0.000003
O	-2.290405	0.765955	0.000007
O	-1.029412	-1.116708	-0.000007
C	-2.242087	-1.892839	0.000004
C	1.197914	0.225758	-0.000003

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C	2.293810	-0.283950	0.000005
C	3.615086	-0.926666	0.000006
H	-1.001599	2.708068	-0.000111
H	0.545787	2.708224	-0.894496
H	0.545589	2.708219	0.894621
H	-1.915662	-2.933457	0.000003
H	-2.829877	-1.673760	-0.895737
H	-2.829864	-1.673757	0.895752
H	4.189046	-0.645318	0.888912
H	4.189528	-0.644270	-0.888257
H	3.501631	-2.015784	-0.000675

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8

8a

CBS-QB3

E(OK)=-474.15830 a.u.

15

8a CBS-QB3

C	0.471680	-2.105251	0.666243
C	0.471680	-2.105251	-0.666243
C	0.403633	-0.684744	-1.152926
N	0.358780	0.107277	0.000000
C	0.403633	-0.684744	1.152926
O	0.403633	-0.279799	2.288141
O	0.403633	-0.279799	-2.288141
C	0.252014	1.561445	0.000000
C	-1.130033	2.045108	0.000000
C	-2.255747	2.460593	0.000000
H	0.518189	-2.937709	1.352961
H	0.518189	-2.937709	-1.352961
H	0.773797	1.927742	-0.887326
H	0.773797	1.927742	0.887326
H	-3.254711	2.822848	0.000000

WB97

E(SCF)=-474.82325 a.u.

E(SCF+ZPVE)= -474.71558 a.u.

15

8a WB97

C	-0.389558	2.110025	0.666351
C	-0.389558	2.110025	-0.666351
C	-0.389650	0.682287	-1.148575
N	-0.405548	-0.108814	0.000000
C	-0.389650	0.682287	1.148575
O	-0.389650	0.271555	2.287300
O	-0.389650	0.271555	-2.287300
C	-0.322455	-1.556965	0.000000
C	1.067307	-2.046501	0.000000
C	2.203021	-2.452092	0.000000
H	-0.392224	2.946075	1.357589
H	-0.392224	2.946075	-1.357589
H	-0.845479	-1.919580	-0.891747
H	-0.845479	-1.919580	0.891747
H	3.211894	-2.810568	0.000000

WB97(DMSO)

E(SCF)= -474.83574 a.u.

E(SCF+ZPVE)= -474.72826 a.u.

15

8a WB97 DMSO

C	-0.314228	2.132243	0.666329
C	-0.314228	2.132243	-0.666329
C	-0.353937	0.706150	-1.143613
N	-0.394831	-0.086506	0.000000
C	-0.353937	0.706150	1.143613
O	-0.353937	0.288081	2.284273
O	-0.353937	0.288081	-2.284273
C	-0.398240	-1.537361	0.000000
C	0.963084	-2.104576	0.000000
C	2.076908	-2.570846	0.000000
H	-0.290800	2.970484	1.354038
H	-0.290800	2.970484	-1.354038
H	-0.945374	-1.872422	-0.887233
H	-0.945374	-1.872422	0.887233

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H	3.066613	-2.983895	0.000000
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8b

CBS-QB3

E(0 K)= -474.16033 a.u.

15

8b CBS-QB3

C	-2.262306	-0.278537	0.000000
C	-2.199886	1.069392	0.000000
C	-0.754318	1.486658	0.000000
N	0.000000	0.286011	0.000000
C	-0.861504	-0.838541	0.000000
O	-0.516260	-2.004701	0.000000
O	-0.286035	2.611381	0.000000
C	1.411593	0.290446	0.000000
C	2.211708	-0.765043	0.000000
C	3.091865	-1.743807	0.000000
H	-3.142626	-0.936824	0.000000
H	-3.014011	1.807988	0.000000
H	1.812411	1.321762	0.000000
H	3.469837	-2.185930	0.943320
H	3.469837	-2.185930	-0.943320

WB97

E(SCF)= -474.826367721 a.u.

E(SCF+ZPVE)= -474.71933 a.u.

15

8b WB97 vacuo

C	-2.241840	-0.309088	0.000000
C	-2.206435	1.022199	0.000000
C	-0.768521	1.463482	0.000000
N	0.000000	0.291960	0.000000
C	-0.829249	-0.836063	0.000000
O	-0.465857	-1.988470	0.000000
O	-0.329243	2.591041	0.000000
C	1.414324	0.319799	0.000000
C	2.203244	-0.728583	0.000000
C	3.064676	-1.710845	0.000000
H	-3.095809	-0.978100	0.000000
H	-3.021873	1.737448	0.000000
H	1.811321	1.333198	0.000000
H	3.424982	-2.141123	0.932919
H	3.424982	-2.141123	-0.932919

WB97(DMSO)

E(SCF)= -474.83702 a.u.

E(SCF+ZPVE)= -474.73022 a.u.

15

8b WB97 DMSO

C	-2.252678	-0.276696	0.000000
C	-2.195873	1.053839	0.000000
C	-0.753147	1.468068	0.000000
N	0.000000	0.286947	0.000000
C	-0.850454	-0.821599	0.000000
O	-0.498743	-1.982345	0.000000
O	-0.288307	2.588890	0.000000
C	1.414018	0.294302	0.000000
C	2.196090	-0.759974	0.000000
C	3.063852	-1.738522	0.000000
H	-3.119491	-0.928415	0.000000
H	-3.002370	1.778710	0.000000
H	1.826958	1.301226	0.000000
H	3.430227	-2.164511	0.933054
H	3.430227	-2.164511	-0.933054

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8c

CBS-QB3

E(0 K)= -474.15518 a.u.

CBSQB3

15

8c CBS-QB3

C	-0.693087	2.378508	0.000000
C	0.638943	2.394695	0.000000
C	1.157011	0.989684	0.000000
N	0.000000	0.162472	0.000000
C	-1.176740	0.961321	0.000000
O	-2.304714	0.553140	0.000000
O	2.294618	0.609286	0.000000
C	0.015728	-1.187598	0.000000
C	0.028589	-2.388187	0.000000
C	0.038093	-3.844268	0.000000
H	-1.386765	3.206458	0.000000
H	1.312266	3.239278	0.000000
H	-0.985153	-4.230272	0.000000
H	0.544597	-4.238550	0.885563
H	0.544597	-4.238550	-0.885563

WB97

E(SCF)= -474.82067 a.u.

E(SCF+ZPVE)= -474.71351 a.u.

15

8c WB97

C	2.396797	-0.665641	-0.001157
C	2.396381	0.666661	-0.001029
C	0.976670	1.160958	0.000222
N	0.172951	-0.000156	0.001619
C	0.977390	-1.160817	0.000469
O	0.577243	-2.297506	-0.000181
O	0.575814	2.297414	-0.000125
C	-1.189091	-0.000454	0.002522
C	-2.393899	-0.000850	0.003324
C	-3.859988	-0.000367	-0.001237
H	3.235184	-1.354074	-0.002221
H	3.234329	1.355632	-0.002000
H	-4.237952	-0.846769	-0.583722
H	-4.234709	0.922678	-0.455870
H	-4.257525	-0.072564	1.016243

WB97

E(SCF)= -474.83323 a.u.

E(SCF+ZPVE)= -474.72628 a.u.

15

8c WB97(DMSO)

C	-0.679853	2.395087	0.000000
C	0.652821	2.403181	0.000000
C	1.151739	0.988884	0.000000
N	0.000000	0.175724	0.000000
C	-1.161502	0.974838	0.000000
O	-2.295061	0.553524	0.000000
O	2.290377	0.581545	0.000000
C	0.007941	-1.186168	0.000000
C	0.014661	-2.392775	0.000000
C	0.019393	-3.860032	0.000000
H	-1.369487	3.231943	0.000000
H	1.332259	3.248324	0.000000
H	-1.008958	-4.235057	0.000000
H	0.526231	-4.246959	0.889468
H	0.526231	-4.246959	-0.889468

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9

9a

WB97

E(SCF)= -402.04006 a.u.

E(SCF+ZPVE)= -401.88909 a.u.

18

9a WB97

C	2.092581	0.041731	-0.606964
C	1.874899	-1.344315	0.012670
C	0.361926	-1.390985	0.287570
N	0.026357	0.012473	0.478988
C	0.932756	0.875442	-0.081462
O	0.803698	2.088743	-0.150144
C	-1.295647	0.450128	0.869906
C	-2.343990	-0.018943	-0.058028
C	-3.196807	-0.420218	-0.812353
H	2.009457	0.025294	-1.701681
H	3.046722	0.511516	-0.352944
H	2.200645	-2.165130	-0.633478
H	2.421941	-1.421223	0.959796
H	0.109244	-1.972738	1.183278
H	-0.202510	-1.808892	-0.561130
H	-1.524110	0.093475	1.883441
H	-1.273148	1.546258	0.887266
H	-3.956631	-0.762862	-1.484349

WB97 (DMSO)

E(SCF)= -402.05194 a.u.

E(SCF+ZPVE)= -401.90106 a.u.

18

9a WB97 DMSO

C	2.071719	0.176595	-0.623204
C	1.972644	-1.244085	-0.053286
C	0.474889	-1.416677	0.246439
N	0.033306	-0.044363	0.481656
C	0.860038	0.891961	-0.052750
O	0.637073	2.105348	-0.078430
C	-1.302354	0.268344	0.943169
C	-2.336974	-0.079267	-0.053190
C	-3.178288	-0.374306	-0.868855
H	1.972539	0.191641	-1.716670
H	2.991822	0.706982	-0.362380
H	2.343629	-2.010006	-0.739707
H	2.543906	-1.314097	0.879281
H	0.282564	-2.034104	1.131387
H	-0.071960	-1.848797	-0.605234
H	-1.500105	-0.269149	1.878640
H	-1.336368	1.342649	1.153617
H	-3.925788	-0.632745	-1.593025

9b

WB97

E(SCF)=-402.048360 a.u.

E(SCF+ZPVE)=-401.897791 a.u.

18

9b WB97

C	-2.319087	-0.266258	0.168330
C	-1.621784	-1.584565	-0.190238
C	-0.133480	-1.313757	0.093248
N	-0.028016	0.129663	-0.057671

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C	-1.234983	0.788727	0.008374
O	-1.375921	2.000014	-0.031405
C	1.192310	0.819128	-0.070288
C	2.369668	0.237336	-0.010850
C	3.557792	-0.311418	0.046251
H	-2.649537	-0.240620	1.215142
H	-3.181255	-0.021557	-0.458074
H	-1.997091	-2.441210	0.377648
H	-1.757650	-1.801389	-1.256237
H	0.536950	-1.818209	-0.612980
H	0.162654	-1.609225	1.111667
H	1.083248	1.900827	-0.132873
H	4.090892	-0.601439	-0.858963
H	4.052649	-0.490075	1.000643

WB97 (DMSO)

E(SCF)= -402.05815 a.u.

E(SCF+ZPVE)=-401.90781 a.u.

18

9b WB97 DMSO

C	-2.316579	-0.269143	0.166139
C	-1.618066	-1.587399	-0.189705
C	-0.131454	-1.314078	0.091986
N	-0.030500	0.135992	-0.052650
C	-1.233008	0.780725	0.009455
O	-1.380144	2.002443	-0.030645
C	1.192677	0.825302	-0.072471
C	2.368273	0.239064	-0.011719
C	3.554373	-0.313768	0.046814
H	-2.647664	-0.244415	1.212772
H	-3.177530	-0.028761	-0.463836
H	-1.990699	-2.439024	0.385656
H	-1.755686	-1.808090	-1.254060
H	0.538034	-1.809739	-0.619976
H	0.166507	-1.606691	1.109091
H	1.093541	1.906942	-0.143402
H	4.082255	-0.615806	-0.857493
H	4.048601	-0.490125	1.001963

9c

WB97

E(SCF)= -402.040714899 a.u.

E(SCF+ZPVE)= -401.890063 a.u

18

9c WB97

C	-2.390507	0.454095	0.140805
C	-2.347179	-1.036366	-0.213985
C	-0.912430	-1.460684	0.138974
N	-0.156616	-0.217202	-0.029125
C	-0.949694	0.923392	0.002329
O	-0.541016	2.064990	-0.049814
C	1.201893	-0.181146	-0.017078
C	2.409257	-0.167101	-0.009515
C	3.875882	-0.120314	-0.002776
H	-2.690311	0.622655	1.183764
H	-3.044968	1.055821	-0.495442
H	-3.092982	-1.631842	0.321269
H	-2.514598	-1.169946	-1.289297
H	-0.515231	-2.234492	-0.526417
H	-0.826955	-1.814634	1.176759
H	4.292387	-0.607311	-0.891059
H	4.282281	-0.613167	0.886958
H	4.211482	0.922156	0.003325

WB97 (DMSO)

E(SCF)= -402.05333 a.u.

E(SCF+ZPVE)=-401.90286 a.u

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18

9c WB97 DMSO

C	-2.389851	0.457495	0.133063
C	-2.349718	-1.035068	-0.215323
C	-0.918149	-1.464156	0.139789
N	-0.159679	-0.213172	-0.020270
C	-0.950408	0.914726	0.004121
O	-0.530154	2.064401	-0.047541
C	1.199751	-0.171231	-0.012725
C	2.408690	-0.155879	-0.010067
C	3.877408	-0.131089	-0.007417
H	-2.694595	0.630056	1.173828
H	-3.039286	1.056060	-0.511338
H	-3.094857	-1.621966	0.328070
H	-2.519665	-1.173355	-1.288932
H	-0.517752	-2.230620	-0.530403
H	-0.831584	-1.815424	1.176420
H	4.280629	-0.560528	-0.930266
H	4.274788	-0.696514	0.841721
H	4.234970	0.900495	0.074478

10

10a

WB97

E(SCF)= -594.942254 a.u.**E(SCF+ZPVE)**= -594.71663 a.u.

27

10a WB97 vacuo

C	-2.945769	1.135751	0.459515
C	-3.302820	0.637392	-0.794959
C	-2.647003	-0.484409	-1.302537
C	-1.634441	-1.098317	-0.562863
C	-1.260950	-0.601594	0.690639
C	-1.933308	0.519019	1.194032
C	-0.101957	-1.210839	1.445530
C	1.200939	-0.422560	1.238453
N	1.559856	-0.287128	-0.170198
C	1.264124	0.953419	-0.869213
C	2.056388	2.093480	-0.368232
C	2.695168	3.028236	0.049879
C	2.136564	-1.336594	-0.811136
O	2.372396	-2.417950	-0.291286
H	2.378284	-1.122619	-1.870934
H	-3.458723	2.005826	0.867089
H	-4.093432	1.117109	-1.369793
H	-2.925576	-0.885409	-2.276222
H	-1.123606	-1.976043	-0.961255
H	-1.657763	0.914078	2.173360
H	-0.317968	-1.236613	2.522178
H	0.065275	-2.244135	1.118261
H	2.023920	-0.935052	1.749797
H	1.115925	0.589613	1.654409
H	1.472839	0.806740	-1.936090
H	0.193587	1.186501	-0.780348
H	3.267468	3.855590	0.416577

WB97 (DMSO)

E(SCF)= -594.95575 a.u.**E(SCF+ZPVE)**= -594.73015 a.u.

27

10a WB97 dms0

C	3.418852	-0.383035	0.220955
C	3.298512	0.978829	0.508635
C	2.130824	1.656743	0.155822
C	1.088866	0.976565	-0.479555
C	1.198419	-0.388240	-0.771887
C	2.375787	-1.058567	-0.413700
C	0.053093	-1.146634	-1.406065
C	-0.848482	-1.815602	-0.355627
N	-1.583261	-0.866179	0.476661
C	-2.818504	-0.276374	-0.023427
C	-2.623655	0.981675	-0.773340
C	-2.487001	2.012406	-1.388985
C	-1.093932	-0.448353	1.665198
O	-1.619538	0.411638	2.374621
H	-0.166015	-0.967819	1.962154
H	4.328425	-0.919357	0.488236
H	4.112066	1.508101	1.002527
H	2.028753	2.718898	0.374738
H	0.176534	1.509373	-0.750931
H	2.477217	-2.121557	-0.638204
H	-0.550267	-0.476695	-2.032122
H	0.444302	-1.937737	-2.058680
H	-0.241785	-2.445672	0.306769
H	-1.579475	-2.469551	-0.845860
H	-3.314361	-1.011076	-0.667419
H	-3.473700	-0.079884	0.831954
H	-2.359237	2.926653	-1.934893

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10b

WB97

E(SCF)= -594.95038 a.u.

E(SCF+ZPVE)= -594.72512 a.u.

27

10b WB97 vacuo

C	-2.417233	0.489611	1.465823
C	-3.555303	0.310042	0.679208
C	-3.487469	-0.492915	-0.459820
C	-2.285659	-1.109226	-0.809349
C	-1.137631	-0.936233	-0.027866
C	-1.218475	-0.130894	1.114169
C	0.179681	-1.547736	-0.445223
C	1.002800	-0.593403	-1.327111
N	1.377301	0.638257	-0.648146
C	2.417085	0.633275	0.304354
C	3.150108	-0.414365	0.608681
C	3.895346	-1.437677	0.945420
C	0.661418	1.796547	-0.828245
O	0.879221	2.844837	-0.246492
H	-0.145534	1.682718	-1.575812
H	-2.460397	1.117413	2.354393
H	-4.491781	0.793239	0.953075
H	-4.372714	-0.641916	-1.076583
H	-2.239173	-1.738878	-1.699533
H	-0.330049	0.014916	1.730650
H	0.770992	-1.821985	0.437612
H	0.006345	-2.469504	-1.016354
H	0.423399	-0.319178	-2.217855
H	1.921813	-1.088864	-1.666535
H	2.577462	1.599032	0.779823
H	3.611910	-2.098290	1.764965
H	4.824842	-1.657355	0.420867

WB97 (DMSO)

E(SCF)= -594.96159 a.u.

E(SCF+ZPVE)= -594.73656 a.u.

27

10b WB97 DMSO

C	-2.410108	0.287794	1.559452
C	-3.528072	0.249309	0.724207
C	-3.441255	-0.386066	-0.516618
C	-2.241989	-0.976805	-0.918003
C	-1.114008	-0.944488	-0.088328
C	-1.212763	-0.305388	1.153689
C	0.200248	-1.530729	-0.551064
C	1.021948	-0.523668	-1.371417
N	1.359484	0.682424	-0.620202
C	2.375516	0.642200	0.362440
C	3.124178	-0.408099	0.614897
C	3.877791	-1.439468	0.903034
C	0.637394	1.825294	-0.775571
O	0.815473	2.862048	-0.139551
H	-0.141272	1.738406	-1.552488
H	-2.469410	0.779671	2.529430
H	-4.463354	0.709532	1.039332
H	-4.310098	-0.424024	-1.172373
H	-2.180500	-1.473003	-1.887738
H	-0.341330	-0.273554	1.809835
H	0.789921	-1.867274	0.310903
H	0.024013	-2.408162	-1.186098
H	0.458703	-0.214751	-2.259640
H	1.956055	-0.984429	-1.714920
H	2.501599	1.574558	0.907917
H	3.577815	-2.161293	1.662686
H	4.824417	-1.608355	0.390666

10c

WB97

E(SCF)= -594.94601 a.u.

E(SCF+ZPVE)= -594.72102 a.u.

S33

27

10c wb97

C	-3.458776	-0.144455	0.039392
C	-3.196628	-1.205128	-0.828547
C	-1.931086	-1.790913	-0.838815
C	-0.934018	-1.318081	0.015433
C	-1.187096	-0.255947	0.890197
C	-2.459644	0.325014	0.890596
C	-0.090408	0.287030	1.778649
C	0.673157	1.446071	1.125758
N	1.303300	1.046899	-0.136362
C	2.287015	0.103821	-0.120831
C	3.157015	-0.734710	-0.085147
C	4.225726	-1.740931	-0.046841
C	0.837979	1.530873	-1.346055
O	-0.045075	2.356626	-1.455077
H	1.372624	1.087101	-2.205104
H	-4.443884	0.319585	0.052429
H	-3.975973	-1.572857	-1.494202
H	-1.718311	-2.619334	-1.513255
H	0.056165	-1.777208	0.004470
H	-2.669644	1.157014	1.564388
H	-0.512415	0.654305	2.723540
H	0.618720	-0.512675	2.032238
H	1.454499	1.818744	1.800092
H	-0.003539	2.269700	0.875931
H	4.388389	-2.074160	0.983680
H	5.168327	-1.329723	-0.423378
H	3.963131	-2.617653	-0.648402

10c

WB97 (DMSO)

E(SCF)= -594.95709 a.u.

E(SCF+ZPVE)= -594.73215 a.u.

27

10c WB97 DMSO

C	-3.488965	-0.138972	0.096440
C	-3.239044	-1.166946	-0.815695
C	-1.968595	-1.742221	-0.875198
C	-0.954755	-1.289915	-0.027765
C	-1.193826	-0.258493	0.888644
C	-2.472530	0.310075	0.940744
C	-0.080019	0.264499	1.767755
C	0.682178	1.426101	1.118838
N	1.308097	1.031131	-0.150654
C	2.322718	0.115729	-0.126903
C	3.215130	-0.698204	-0.077684
C	4.302922	-1.683523	-0.020827
C	0.831549	1.476257	-1.357782
O	-0.093704	2.266186	-1.483788
H	1.381753	1.050952	-2.213804
H	-4.478690	0.312409	0.152420
H	-4.031736	-1.519682	-1.473830
H	-1.765671	-2.546585	-1.581092
H	0.036168	-1.745044	-0.075567
H	-2.673671	1.112866	1.651628
H	-0.484334	0.626467	2.721359
H	0.627266	-0.542399	2.001657
H	1.470356	1.788789	1.788512
H	0.008063	2.255614	0.886097
H	4.502092	-1.957786	1.020241
H	5.224515	-1.275827	-0.448347
H	4.036257	-2.593497	-0.567807

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11a

WB97

E(SCF)=-746.14764 a.u.

E(SCF+ZPVE)= -745.91894 a.u.

29

11a WB97

C	1.128781	0.173631	3.668339
C	-0.262548	0.003403	3.632059
C	-0.935210	-0.176160	2.433289
C	-0.221063	-0.198851	1.215894
C	1.172647	0.000702	1.249017
C	1.829981	0.178640	2.475935
N	-0.873376	-0.413840	0.000000
C	-0.221063	-0.198851	-1.215894
C	1.172647	0.000702	-1.249017
C	1.963372	0.042737	0.000000
C	-0.935210	-0.176160	-2.433289
C	-0.262548	0.003403	-3.632059
C	1.128781	0.173631	-3.668339
C	1.829981	0.178640	-2.475935
O	3.187626	0.139452	0.000000
C	-2.248391	-0.891772	0.000000
C	-3.256573	0.185324	0.000000
C	-4.081128	1.066305	0.000000
H	1.642807	0.313322	4.616805
H	-0.836457	0.024987	4.557589
H	-2.018973	-0.257192	2.445587
H	2.908947	0.321376	2.443022
H	-2.018973	-0.257192	-2.445587
H	-0.836457	0.024987	-4.557589
H	1.642807	0.313322	-4.616805
H	2.908947	0.321376	-2.443022
H	-2.393988	-1.534797	0.874230
H	-2.393988	-1.534797	-0.874230
H	-4.806771	1.853930	0.000000

WB97 (DMSO)

E(SCF)= -746.16052 a.u.

E(SCF+ZPVE)= -745.93196 a.u.

29

11a WB97 DMSO

C	1.125159	0.166062	3.668644
C	-0.265728	-0.031316	3.632052
C	-0.935173	-0.217566	2.434719
C	-0.223599	-0.219428	1.212392
C	1.168471	0.004263	1.245330
C	1.823512	0.187943	2.477301
N	-0.875081	-0.433481	0.000000
C	-0.223599	-0.219428	-1.212392
C	1.168471	0.004263	-1.245330
C	1.951535	0.062882	0.000000
C	-0.935173	-0.217566	-2.434719
C	-0.265728	-0.031316	-3.632052
C	1.125159	0.166062	-3.668644
C	1.823512	0.187943	-2.477301
O	3.182672	0.183976	0.000000
C	-2.265694	-0.880709	0.000000
C	-3.233554	0.232546	0.000000
C	-4.023767	1.145911	0.000000
H	1.636603	0.311060	4.617519
H	-0.838681	-0.028354	4.557940
H	-2.014920	-0.332500	2.454044
H	2.899359	0.351345	2.454247

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H	-2.014920	-0.332500	-2.454044
H	-0.838681	-0.028354	-4.557940
H	1.636603	0.311060	-4.617519
H	2.899359	0.351345	-2.454247
H	-2.429879	-1.521247	0.870891
H	-2.429879	-1.521247	-0.870891
H	-4.723592	1.958681	0.000000

11b

WB97

E(SCF)= -746.15154 a.u.

E(SCF+ZPVE)= -745.92416 a.u.

29

11b WB97

C	3.792659	-0.832152	0.026824
C	3.636187	0.536723	-0.240699
C	2.379413	1.107821	-0.352675
C	1.223381	0.311541	-0.204384
C	1.377135	-1.061484	0.064257
C	2.662930	-1.614589	0.178630
N	-0.048979	0.876542	-0.317511
C	-1.204567	0.095422	-0.218776
C	-1.111285	-1.281793	0.058497
C	0.200880	-1.940307	0.231241
C	-2.484024	0.664280	-0.398478
C	-3.617465	-0.124397	-0.294977
C	-3.527978	-1.495527	-0.008381
C	-2.277389	-2.058091	0.163870
O	0.306513	-3.137477	0.486660
C	-0.154437	2.262792	-0.668134
C	-0.402346	3.187019	0.228740
C	-0.672619	4.110137	1.112578
H	4.786062	-1.266685	0.114782
H	4.514374	1.169989	-0.360326
H	2.285710	2.172618	-0.546655
H	2.725141	-2.680859	0.390068
H	-2.582347	1.722888	-0.619460
H	-4.593528	0.336944	-0.440123
H	-4.427316	-2.102126	0.072832
H	-2.147299	-3.116700	0.382656
H	-0.015237	2.521427	-1.719785
H	-1.702523	4.378480	1.340701
H	0.124866	4.623674	1.645797

WB97 (DMSO)

E(SCF)= -746.16338 a.u.

E(SCF+ZPVE)= -745.93627 a.u.

29

11b WB97-DMSO

C	3.728081	-1.025372	0.019021
C	3.639040	0.349737	-0.266308
C	2.414031	0.981115	-0.381273
C	1.217014	0.246001	-0.217030
C	1.300974	-1.132582	0.064385
C	2.563026	-1.747680	0.181354
N	-0.020730	0.873537	-0.329469
C	-1.208829	0.154439	-0.223298
C	-1.188182	-1.226389	0.060410
C	0.085030	-1.943275	0.235912
C	-2.458385	0.793464	-0.398663
C	-3.631530	0.069873	-0.287927
C	-3.616215	-1.306984	0.002429
C	-2.399825	-1.936722	0.172252
O	0.130306	-3.151705	0.501629
C	-0.066352	2.269300	-0.677564
C	-0.170276	3.199466	0.240928
C	-0.283896	4.135560	1.144813
H	4.699162	-1.507119	0.109160

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H	4.547407	0.935513	-0.398740
H	2.372557	2.045080	-0.595183
H	2.583553	-2.813203	0.402688
H	-2.498607	1.855698	-0.620026
H	-4.581452	0.583281	-0.428945
H	-4.547639	-1.862066	0.089013
H	-2.339161	-3.000376	0.394991
H	-0.009707	2.515169	-1.738629
H	-1.264405	4.481263	1.467294
H	0.598727	4.585959	1.594982

11c

WB97 (DMSO)

E(SCF)= -746.15557 a.u.
E(SCF+ZPVE)= -745.92777 a.u.

29

11c WB97			
C	3.674906	-1.260800	0.000000
C	3.643402	0.142008	0.000000
C	2.441894	0.831829	0.000000
C	1.227948	0.121550	0.000000
C	1.249770	-1.282333	0.000000
C	2.480519	-1.958124	0.000000
N	0.000000	0.811446	0.000000
C	-1.229672	0.124433	0.000000
C	-1.254557	-1.279407	0.000000
C	-0.003309	-2.070185	0.000000
C	-2.442006	0.837404	0.000000
C	-3.645005	0.150200	0.000000
C	-3.679635	-1.252553	0.000000
C	-2.486815	-1.952498	0.000000
O	-0.004711	-3.297094	0.000000
C	0.002149	2.175950	0.000000
C	0.004749	3.383396	0.000000
C	0.012857	4.851491	0.000000
H	4.625549	-1.789729	0.000000
H	4.575110	0.705938	0.000000
H	2.428890	1.918383	0.000000
H	2.448758	-3.046329	0.000000
H	-2.426601	1.923913	0.000000
H	-4.575439	0.716231	0.000000
H	-4.631448	-1.779379	0.000000
H	-2.457472	-3.040767	0.000000
H	-0.488504	5.247047	0.889598
H	-0.488504	5.247047	-0.889598
H	1.044170	5.220104	0.000000

WB97 (DMSO)

E(SCF)= -746.16548 a.u.
E(SCF+ZPVE)= -745.93804 a.u.

29

11c WB97 DMSO			
C	3.648747	-1.332184	-0.000092
C	3.642700	0.073209	0.000010
C	2.454374	0.783844	0.000066
C	1.225864	0.095551	0.000020
C	1.220500	-1.310148	-0.000080
C	2.442833	-2.007243	-0.000135
N	0.015235	0.808130	0.000078
C	-1.224615	0.147593	0.000030
C	-1.278567	-1.257127	-0.000071
C	-0.045631	-2.066999	-0.000126
C	-2.422887	0.887155	0.000086
C	-3.640185	0.227327	0.000040
C	-3.705603	-1.176573	-0.000061
C	-2.529314	-1.901958	-0.000114
O	-0.071769	-3.301422	-0.000235

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C	0.045417	2.175171	0.000195
C	0.075511	3.382477	0.000276
C	0.118475	4.850021	0.000151
H	4.589713	-1.877784	-0.000135
H	4.584185	0.619965	0.000046
H	2.463778	1.870471	0.000144
H	2.402784	-3.094777	-0.000212
H	-2.385935	1.973198	0.000164
H	-4.557666	0.813465	0.000083
H	-4.668832	-1.681826	-0.000095
H	-2.535545	-2.990226	-0.000191
H	-0.374512	5.254983	0.889557
H	-0.374872	5.254877	-0.889107
H	1.158710	5.191412	-0.000091

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12

12a

WB97 (PCM=DMSO)

E(SCF)=-634.27096 a.u.

E(SCF+ZPVE)= -634.01789 a.u.

30

12a WB97 DMSO

N	-1.059575	-0.280985	0.069280
C	-1.224478	0.596666	-1.085930
C	-2.314810	1.582514	-0.934629
C	-0.036478	0.088411	1.061694
C	1.349706	0.036968	0.421462
C	-0.385138	1.411383	1.741925
C	1.750404	-1.150063	-0.210345
C	3.008013	-1.259255	-0.797273
C	3.892772	-0.176044	-0.762896
C	3.505616	1.006756	-0.137778
C	2.240486	1.112459	0.451812
C	-1.866248	-1.361268	0.281858
O	-1.736592	-2.088400	1.275490
C	-2.924247	-1.654264	-0.761128
C	-3.215483	2.380444	-0.825541
H	-1.395933	0.005025	-1.991393
H	-0.276688	1.125159	-1.243008
H	-0.082460	-0.705840	1.813723
H	-0.373030	2.255891	1.041383
H	-1.387764	1.344461	2.177862
H	0.326074	1.625371	2.547382
H	1.062337	-1.996190	-0.240685
H	3.301800	-2.189684	-1.281115
H	4.877067	-0.257848	-1.221407
H	4.186058	1.856505	-0.106158
H	1.959676	2.046416	0.935748
H	-3.541025	-0.774503	-0.974094
H	-2.458049	-1.979283	-1.698773
H	-3.556271	-2.460013	-0.384341
H	-4.012713	3.090381	-0.723392

12b

WB97 (PCM=DMSO)

E(SCF)= -634.27636 a.u.

E(SCF+ZPVE)= -634.02420 a.u.

30

12b WB97 DMSO

N	-1.457049	0.136969	-0.026745
C	-1.291430	1.338560	-0.760495
C	-0.270190	2.161730	-0.685167
C	0.711303	3.028288	-0.653286
C	-0.477289	-0.224402	1.013029
C	0.913056	-0.445557	0.412277
C	-0.533070	0.755920	2.188542
C	1.038851	-1.053128	-0.843414
C	2.294476	-1.319137	-1.387527
C	3.451217	-0.984074	-0.679680
C	3.336181	-0.383299	0.573344
C	2.075964	-0.116843	1.115033
C	-2.584961	-0.608124	-0.295143
O	-3.397436	-0.249412	-1.152631
C	-2.809951	-1.887078	0.483849
H	-2.112691	1.547247	-1.440423
H	0.700796	3.869656	0.039749
H	1.575814	2.924440	-1.308883

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H	-0.793526	-1.196559	1.399761
H	-0.116923	1.735592	1.932059
H	0.022643	0.355788	3.042910
H	-1.575101	0.887450	2.499870
H	0.143219	-1.308812	-1.410039
H	2.369559	-1.787501	-2.367933
H	4.433231	-1.188731	-1.103259
H	4.229856	-0.115298	1.135237
H	2.013096	0.361147	2.090750
H	-3.743078	-2.325242	0.126117
H	-2.895724	-1.695090	1.558840
H	-1.997284	-2.604700	0.325340

12c

WB97 (PCM=DMSO)

E(SCF)= -634.27636 a.u.

E(SCF+ZPVE)= -634.02420 a.u.

30

12c WB97 DMSO			
N	-1.243140	-0.343365	0.186013
C	-1.293388	1.007888	-0.008355
C	-0.132966	-0.879455	1.008927
C	1.199421	-0.534357	0.353433
C	-0.290683	-0.426685	2.456551
C	2.174594	0.240091	0.984594
C	3.383528	0.524203	0.339771
C	3.627437	0.036630	-0.942266
C	2.655908	-0.740328	-1.581848
C	1.454691	-1.021647	-0.936463
C	-2.213435	-1.183650	-0.332321
O	-2.165617	-2.397606	-0.142128
C	-3.310565	-0.527900	-1.133172
C	-1.297262	2.207872	-0.155948
C	-1.323314	3.664196	-0.347335
H	-0.264437	-1.965261	0.960959
H	-0.247555	0.665896	2.543763
H	0.498833	-0.857819	3.081660
H	-1.258250	-0.765620	2.841799
H	2.003400	0.631039	1.986163
H	4.133566	1.130544	0.845605
H	4.568620	0.257808	-1.443307
H	2.837984	-1.128624	-2.582879
H	0.698704	-1.628005	-1.438150
H	-3.860180	0.190114	-0.515097
H	-3.988849	-1.305151	-1.488842
H	-2.892000	0.019401	-1.984513
H	-0.406668	4.011770	-0.834603
H	-1.428157	4.184808	0.610029
H	-2.171896	3.942350	-0.981058

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13

13a

WB97 (PCM=DMSO)

E(SCF)= -709.48889 a.u.

E(SCF+ZPVE)= -709.23056 a.u.

31

13a WB97 DMSO

N	-0.798442	0.026274	0.096380
C	-0.851949	0.864406	-1.096470
C	0.280713	0.252657	1.069784
C	1.632834	-0.036404	0.418505
C	0.157650	1.632537	1.714530
C	1.833776	-1.290954	-0.176540
C	3.049690	-1.613837	-0.772456
C	4.092591	-0.681364	-0.784347
C	3.903891	0.566940	-0.196350
C	2.679960	0.887553	0.402396
C	-1.787417	-0.864512	0.381310
O	-1.826158	-1.581667	1.378377
O	-2.736285	-0.882934	-0.576027
C	-3.806875	-1.819240	-0.366608
C	-1.763686	2.020396	-0.970835
C	-2.509809	2.966757	-0.882540
H	-1.152580	0.260693	-1.958152
H	0.165455	1.222782	-1.293666
H	0.120410	-0.503361	1.845905
H	0.291468	2.442714	0.986747
H	-0.835793	1.737968	2.163683
H	0.907067	1.754255	2.504340
H	1.022085	-2.019855	-0.171665
H	3.187419	-2.593794	-1.227215
H	5.044884	-0.930331	-1.250073
H	4.708475	1.300902	-0.201395
H	2.555191	1.869197	0.856222
H	-4.471423	-1.691751	-1.222360
H	-4.332882	-1.591530	0.564811
H	-3.417274	-2.840712	-0.332797
H	-3.172066	3.806096	-0.800117

13b

WB97 (PCM=DMSO)

E(SCF)= -709.49158 a.u.

E(SCF+ZPVE)=-709.23403 a.u.

31

13b WB97 DMSO

N	-1.297435	0.219708	-0.013196
C	-2.461767	-0.396816	-0.530572
C	-2.835814	-1.636066	-0.302131
C	-3.255872	-2.861388	-0.102199
C	-0.412623	-0.533876	0.898323
C	0.996354	-0.668580	0.326067
C	-0.504915	-0.017404	2.333354
C	1.147968	-1.047658	-1.014678
C	2.414128	-1.226698	-1.567808
C	3.554874	-1.034497	-0.782886
C	3.412803	-0.663917	0.553266
C	2.140457	-0.482721	1.104642
C	-1.078523	1.526908	-0.370668
O	-1.799225	2.169195	-1.127598
O	0.023882	2.028107	0.205107
C	0.336656	3.389888	-0.136622
H	-3.059094	0.253998	-1.164021
H	-2.953702	-3.677010	-0.759097

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H	-3.917502	-3.103814	0.729381
H	-0.836156	-1.545779	0.896415
H	-0.053125	0.973980	2.438274
H	-0.003323	-0.709766	3.018484
H	-1.558851	0.041637	2.626879
H	0.261326	-1.198917	-1.632366
H	2.512004	-1.519133	-2.612395
H	4.545972	-1.173621	-1.211995
H	4.294426	-0.510222	1.174119
H	2.052397	-0.185888	2.148253
H	1.251708	3.619108	0.411195
H	0.500728	3.481680	-1.213951
H	-0.474373	4.054328	0.174604

13c

WB97 (PCM=DMSO)
E(SCF)=-709.49157 a.u.
E(SCF+ZPVE)=-709.23403

31

13c	WB97-DMSO		
N	-0.966618	0.006758	0.525369
C	-1.124448	1.267170	0.024898
C	0.227934	-0.286295	1.359437
C	1.474339	-0.335179	0.486078
C	0.305238	0.686359	2.531534
C	2.219240	0.812167	0.189809
C	3.335440	0.736025	-0.645729
C	3.721682	-0.488896	-1.192597
C	2.986088	-1.639038	-0.900240
C	1.870020	-1.559508	-0.066340
C	-1.791935	-1.030002	0.138348
O	-1.637090	-2.191068	0.489770
O	-2.783048	-0.609134	-0.655880
C	-3.696473	-1.632074	-1.095212
C	-1.208345	2.402454	-0.381002
C	-1.326769	3.776660	-0.887054
H	0.046803	-1.292741	1.746947
H	0.393526	1.726244	2.198042
H	1.177416	0.447001	3.149147
H	-0.595992	0.600012	3.148081
H	1.932369	1.775132	0.610657
H	3.906126	1.636716	-0.867463
H	4.594539	-0.547375	-1.841119
H	3.283030	-2.599636	-1.318706
H	1.294558	-2.457833	0.160414
H	-4.421440	-1.116009	-1.725685
H	-3.161372	-2.394372	-1.668176
H	-4.191923	-2.090119	-0.234674
H	-1.614486	4.469390	-0.089477
H	-0.378481	4.115871	-1.316711
H	-2.089315	3.822976	-1.671557

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14a

WB97 (PCM=DMSO)

E(SCF)= -728.92222 a.u.

E(SCF+ZPVE)= -728.62265 a.u.

35

14a WB97 DMSO

N	0.639916	-0.599686	-0.295170
C	0.550735	0.341617	-1.351471
C	1.033112	1.564546	-1.361060
C	1.565106	2.759188	-1.439040
C	-0.567663	-1.419965	-0.059525
C	-1.805540	-0.544266	0.133600
C	-0.696635	-2.485952	-1.147163
C	-2.932674	-0.635202	-0.686720
C	-4.041705	0.190749	-0.470174
C	-4.034879	1.116900	0.570308
C	-2.910663	1.215170	1.397011
C	-1.808645	0.392084	1.179074
C	1.561399	-0.468243	0.750265
O	1.236359	-0.685185	1.928059
N	2.828273	-0.106576	0.408830
C	3.433835	-0.356310	-0.891981
C	3.755161	0.241571	1.474995
H	-0.003233	-0.010726	-2.221578
H	1.018381	3.643662	-1.113829
H	2.573900	2.905421	-1.827221
H	-0.378623	-1.926407	0.892309
H	-0.856172	-2.056032	-2.143759
H	-1.538449	-3.153433	-0.931077
H	0.219159	-3.085387	-1.176550
H	-2.961653	-1.351965	-1.505914
H	-4.911143	0.105468	-1.120730
H	-4.898029	1.759128	0.739233
H	-2.895962	1.934906	2.214575
H	-0.930026	0.464578	1.821171
H	2.780359	-0.979407	-1.505887
H	4.380063	-0.890145	-0.739750
H	3.639298	0.581047	-1.425140
H	3.210422	0.686330	2.309962
H	4.300256	-0.641414	1.837765
H	4.477592	0.968375	1.087622

14b

WB97 (PCM=DMSO)

E(SCF)= -728.92853 a.u.

E(SCF+ZPVE)= -728.62993 a.u.

35

14b WB97 DMSO

N	-0.868597	-0.430396	-0.028123
C	-0.770975	-0.635631	1.368320
C	0.332865	-0.828297	2.057174
C	1.383928	-1.069296	2.801118
C	0.214874	-0.885057	-0.914739
C	1.485026	-0.066365	-0.680795
C	0.397139	-2.402206	-0.847004
C	2.756516	-0.646125	-0.708769
C	3.901777	0.134490	-0.528267
C	3.791750	1.508568	-0.318641
C	2.525367	2.098959	-0.297932
C	1.386332	1.316905	-0.480959
C	-2.114375	-0.182006	-0.603652
O	-2.395672	-0.603442	-1.733319
N	-3.011638	0.523067	0.156686
C	-4.378687	0.599181	-0.339559
C	-2.623239	1.640240	1.016025
H	-1.725088	-0.659137	1.892202
H	1.755618	-2.084603	2.942873
H	1.930673	-0.261403	3.287437

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H	-0.141862	-0.645635	-1.922398
H	0.811992	-2.725331	0.114799
H	1.064273	-2.746140	-1.644771
H	-0.575881	-2.884172	-0.990386
H	2.868437	-1.718518	-0.857567
H	4.882937	-0.338201	-0.547588
H	4.683856	2.115946	-0.173423
H	2.424782	3.171735	-0.138292
H	0.401682	1.784576	-0.458898
H	-4.487046	1.378809	-1.107528
H	-5.038562	0.836903	0.501493
H	-4.674623	-0.360760	-0.767467
H	-1.537166	1.715258	1.096502
H	-3.001099	2.576753	0.584127
H	-3.045694	1.522612	2.021569

14c

WB97 (PCM=DMSO)
E(SCF)= -728.93041 a.u.
E(SCF+ZPVE)= -728.63186 a.u.

35

WB97 DMSO

N	-0.715917	-0.250159	0.312816
C	-0.601238	1.103620	0.436805
C	-0.459543	2.298730	0.560145
C	-0.305839	3.754516	0.692252
C	0.385177	-1.070098	0.870675
C	1.683216	-0.703934	0.157579
C	0.424877	-0.970216	2.392309
C	1.731619	-0.798079	-1.241065
C	2.896181	-0.490029	-1.939003
C	4.039783	-0.080032	-1.245368
C	4.001997	0.017025	0.143607
C	2.828839	-0.292630	0.841289
C	-1.975410	-0.855168	0.149028
O	-2.213354	-1.951772	0.667528
N	-2.888607	-0.170073	-0.590470
C	-2.543164	0.748764	-1.671857
C	-4.255149	-0.673432	-0.608780
H	0.729885	4.048748	0.492925
H	-0.946189	4.271210	-0.030733
H	-0.574456	4.097529	1.696835
H	0.127559	-2.099510	0.598529
H	0.629464	0.056874	2.719318
H	1.197350	-1.628221	2.805718
H	-0.544164	-1.280091	2.796755
H	0.839961	-1.113097	-1.785002
H	2.914946	-0.570311	-3.024985
H	4.952551	0.161525	-1.787881
H	4.885993	0.336978	0.693469
H	2.820743	-0.207870	1.926552
H	-2.813534	1.782157	-1.423344
H	-3.089866	0.443260	-2.572250
H	-1.474047	0.705306	-1.891083
H	-4.500268	-1.116865	0.358214
H	-4.932134	0.165086	-0.802465
H	-4.393355	-1.431128	-1.392917