Assessment of reactivities with explicit and implicit solvent models: QM/MM and gas-phase evaluation of three different Ag-catalyzed furan ring formation routes

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Electronic Supplementary Information

COMPARISON OF THE PRESENT RESULTS WITH EARLIER CALCULATIONS EMPLOYING LARGER BASIS SET.

In an earlier study[1] we have calculated with the Gaussian 09 program[2] the full free energy profiles of several possible routes leading to the formation of polysubstituted furans from terminal alkynes and β-ketoesters. The study concluded that the mechanism can be divided into two parts, a radical and an ionic part where the catalyst Ag salt has different roles. The elementary step scrutinized in the main article is the part of the ionic route. The claculations have been done in the following way: the optimization and vibrational calculations have been carried out with the 6-31+G* basis set for C, O and H, whereas for Ag we have used the LANL2DZbasis set augmented with a set of polarization functions. Then the optimized structures have been recalculated using the larger 6-311++G(3df,3dp) basis set for the C, O H atoms and the LANL2TZ(f) set for the Ag which was further augmented with a set of polarization function in the presence of DMF solvent modeled by the SMD solvent model.[3] For the Ag atom only the valence electrons have been expanded in the basis set, whereas the ionic core has been replaced by the LANL2 effective core potential. Table S1 and Table S2 compare the calculated TS and reaction free energies obtained from two methodologies: the original method from Ref. 1 and the M06/DZVP/i-solv results from the present article. The additional difference between the two methodology that the solven effect has not been taken into account during the optimization in the original calculations, only in the subsequent final calculations with the large basis set.

Table S1. Activation free barriers (kcal/mol) calculated with large basis and with DZVP basis sets and SMD solvent model

reaction	(1)	(2)	(3)
M06/DZVP/SMD	25.0	11.2	19.1
M06/6-311++G(3df,3dp)/SMD//M06/6-31+G*	29.5	15.0	23.9

Table S2. Reaction free energies (kcal/mol) calculated with large basis and with DZVP basis sets and SMD solvent model.

reaction	(1)	(2)	(3)
M06/DZVP/SMD	11.5	-15.2	15.6
M06/6-311++G(3df,3dp)/SMD//M06/6-31+G*	16.5	-11.1	15.1

Comparison of the results shows that the effect of the large basis set is a ca. 4 kcal/mol destabilization for both the TS-s and for the reaction free energies. There is an exception to this trend: reaction 3, where the reaction free energy is shifted only by 0.4 kcal/mol. Hence in the "large-basis"-model the reaction free energies of reactions 1 and 3 are very similar, whereas calculations with DZVP basis set predict reaction 1 more favorable. Apart from this minor discrepancy we can conclude that the trends in the energetics are not affected by the larger basis set.

Initial equilibrium properties of the systems

The QMMM dynamics calculations have been performed on properly equilibrated systems at 353 K. To demonstrate this additional NVE calculations have been performed on the systems and the temperature, the total energy and the root-mean-square displacements (RMSD) of the atoms have been recorded for 50 ps. Figure S1 shows the evolution of the temperature and the total energy in a 3 ps interval for better visibility (note that the results are stable thoroughout the 50 ps); while Figure S2 shoes the evolution of the RMSD for all the three systems. Figure S1 shows the typical fluctiation of an equilibrated system, whereas Figure S2 shows that under NVE conditions the self-diffusivity of the molecules becomes stable within the first 10 ps.

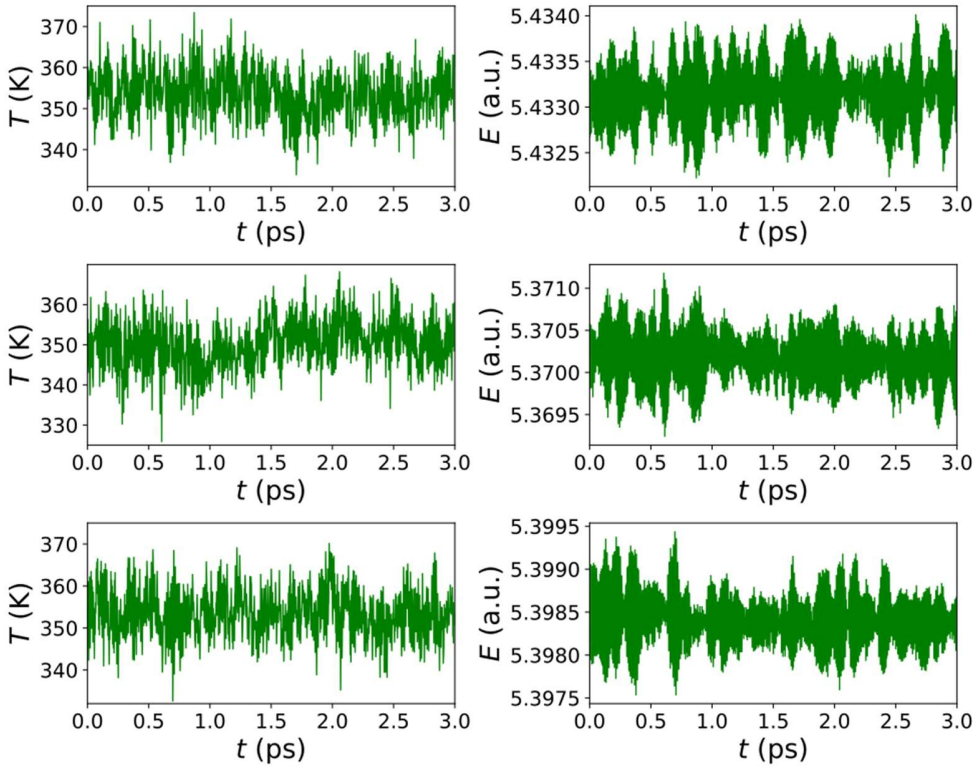

Figure S1. Evolution of the temperature (first column) and the total energy (second column) of the three systems in a 3 ps time-interval under NVE conditions. First row: system **1**; second row: system **2**; bottom row: system **3**.

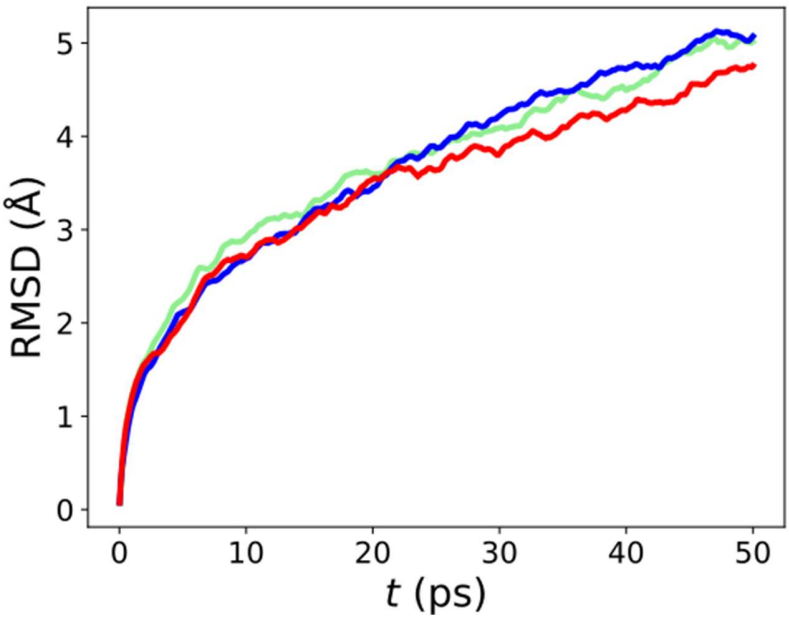

Figure S2. Evolution of the RMSD of the three investigated systems during an NVE simulation of 50 ps. Green: system **1**; blue: system **2**; red: system **3**.

SOLVENT-SOLUTE PAIR-WISE ENERGIES

In Table S3 we present the Kohn-Sham energies of the most favorable DMF-solvent interaction energies for the reactant and product states for all the three reactions. The values show that DMF interact very strongly with the positively charged solute (reaction **3**), and the interaction is the weakest with the negatively charged solute (reaction **1**). The neutral solute (reaction **2**) features intermediate values.

Table S3. Gas-phase interaction energies (in kcal/mol) of DMF and solute molecules in the reactant and product stages of the three reactions.

	reactant state	product state
reaction **1**	-16.4	-21.9
reaction **2**	-28.6	-26.1
reaction **3**	-34.6	-36.9

STATISTICAL ERROR CALCULATIONS

The free energy calculations from MD simulations suffer from two main types of error: error in the calculation model and insufficient sampling. In the following the uncertainties from the sampling is addressed whereas the problems of the computational model are discussed in the article. Determining the statistical uncertainties can be done in different ways, from which the method based on block averages has been used here.[4] The following protocol has been followed: The TI (thermodynamic integration) trajectories have been divided into M segments (blocks) of length n. For all segments of a given trajectory the average of the Lagrange multiplier λ (actually the force on the reaction coordinate)

and its standard deviation (σ_n) among the block averages is calculated. Then a running estimate of the overall standard error (*se*) of σ_n for the full trajectory is calculated by $se = {\sigma_n}/{\sqrt{M}}$. For small *M*-s the calculated *se* underestimates the statistical error because of the strongly correlated data in the subsequent blocks. However, when the size of *M* (ie. length *n*) reaches a critical value, the blocks become independent and *se* gives a reliable estimation of the true standard error.[5] In this work for all the constrained values of the blue-moon samplings the *se* values have been plotted against *n* and the converged value has been determined. A typical plot has been given in Figure S3. The converged value from the *se* vs. blocksize (*n*) plot was used to caluclate the error of the computed free energy barriers and reaction free energies. This has been done by using the standard procedure of propagation of the errors associated with the values of the integrand.

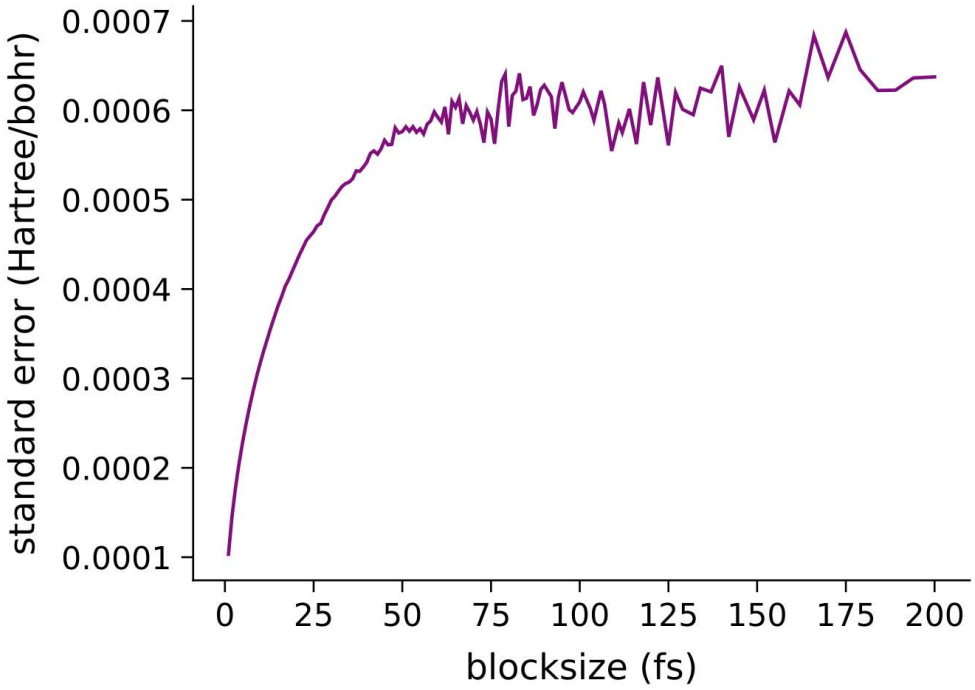

Figure S3. A typical *se* vs blocksize function. This plot belongs to the TI of reaction **3**, where the Ag-O distance was 2.063 Å. It is seen that as the blocksize is increasing the curve becomes noisier because the number of blocks (*M*) are smaller resulting in larger fluctuations. The converged value of the standard error is 0.0006 Ha/bohr in this case.

MINIMAL AG-SOLVENT DISTANCES AT DIFFERENT STAGES OF REACTION 3.

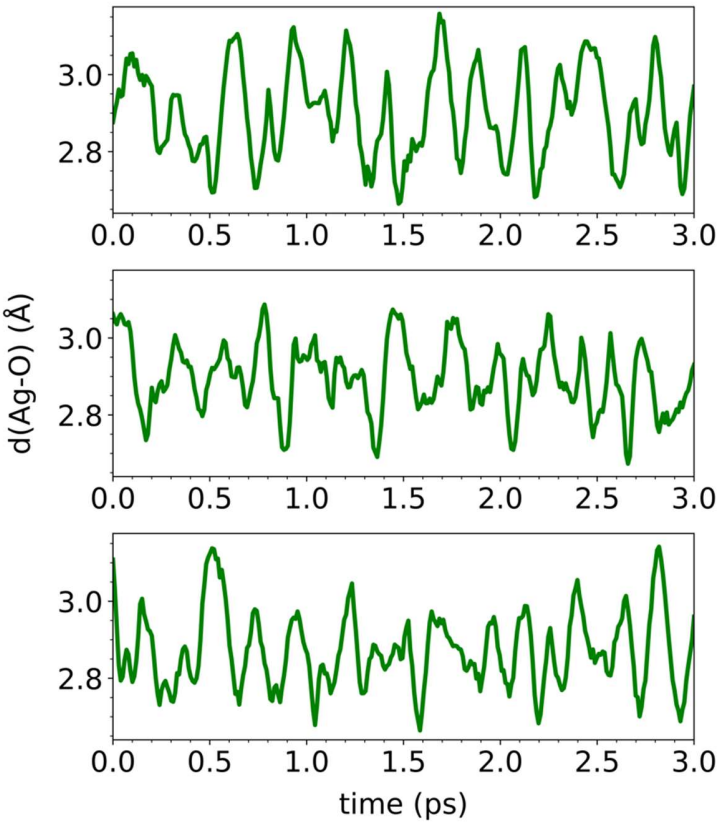

Figure S4. Minimal Ag-solvent distances represented by the instantaneous d(Ag-O) values as a function of time during a 3-ps intervall at different stages of TI simulation of reaction **2**. Top panel: initial stage; middle panel: TS; bottom panel: product stage.

CARTESIAN COORDINATES AND ENERGIES OF THE STRUCTURES DISCUSSED IN THE ARTICLE.

Reactants:

M06/DZVP method

1

30
E = -766.468154908 Ha
C -2.720665 -0.221431 0.059792
C -3.790980 0.696728 0.117683
C -5.104699 0.258758 0.195098
C -5.403641 -1.103489 0.217780
C -4.356776 -2.023431 0.161063

C -3.039691 -1.596110 0.083499
H -3.557203 1.760395 0.100006
H -5.910921 0.992647 0.238606
H -6.437461 -1.443123 0.278766
H -4.571835 -3.093008 0.177713
H -2.222045 -2.314430 0.039109
C -1.383419 0.215487 -0.018471
O 0.406154 3.258155 -0.122816
C 1.338765 2.450801 -0.179992
C 1.117116 1.017045 -0.162232
C -0.221442 0.590584 -0.085801
C 2.746858 3.022275 -0.273758
H 3.270814 2.676017 -1.172763
H 2.651718 4.114016 -0.292368
H 3.367667 2.716545 0.577003
C 2.085866 -0.045055 -0.214104
O 1.851426 -1.246991 -0.218641
O 3.403599 0.389349 -0.261765
C 4.374402 -0.635731 -0.307060
H 5.265100 -0.175747 -0.758767
C 4.686320 -1.172155 1.074497
H 4.027057 -1.448885 -0.958070
H 5.496629 -1.913901 1.036707
H 4.992145 -0.357860 1.744354
H 3.792605 -1.650145 1.490302

2

31
E = -912.197746561 Ha
C -2.854960 0.110326 -0.007697
C -3.614984 1.286797 0.114200
C -4.996657 1.211535 0.203725
C -5.642423 -0.023464 0.174165
C -4.894148 -1.190999 0.053737
C -3.510314 -1.126653 -0.036853
H -3.088826 2.240616 0.135222
H -5.576904 2.127985 0.297925
H -6.727338 -0.075483 0.244907
H -5.391272 -2.159417 0.030015
H -2.923096 -2.043065 -0.131230
C -1.437728 0.254012 -0.095436
O -0.312625 3.372938 0.023036
C 0.804817 2.872895 -0.079580
C 0.943277 1.415412 -0.171858
C -0.305316 0.765557 -0.133147
C 2.018815 3.769295 -0.110267
H 2.597925 3.631550 -1.030883

H 1.667856 4.803364 -0.041155
H 2.699690 3.550871 0.720776
C 2.120884 0.625675 -0.292709
O 2.160010 -0.629132 -0.382548
O 3.276570 1.309060 -0.314503
C 4.490279 0.557761 -0.417980
H 5.214807 1.272387 -0.824389
C 4.930170 0.033940 0.928544
H 4.354741 -0.255862 -1.139452
H 5.904043 -0.464112 0.844208
H 5.025610 0.853875 1.650481
H 4.205000 -0.690920 1.314613
Ag 0.095909 -1.550596 -0.336040

3
32
E = -912.603549378 Ha
C -2.854346 0.476256 -0.067809
C -3.727741 1.350566 0.598227
C -5.058543 0.998081 0.767435
C -5.524687 -0.218819 0.273766
C -4.661628 -1.087055 -0.390811
C -3.327329 -0.747375 -0.563028
H -3.356906 2.309380 0.961421
H -5.737257 1.675914 1.280196
H -6.569706 -0.491020 0.405860
H -5.031288 -2.034096 -0.777312
H -2.644680 -1.417736 -1.081673
C -1.482620 0.835611 -0.240079
O 0.899281 3.114417 1.172242
C 1.361835 2.892433 0.069252
C 1.074587 1.528780 -0.620568
C -0.309472 1.131318 -0.404604
C 2.259096 3.826697 -0.658737
H 1.763535 4.170828 -1.577639
H 2.513987 4.686289 -0.034212
H 3.168654 3.297523 -0.977343
C 2.041332 0.558216 0.075048
O 1.809575 0.080056 1.172385
O 3.135881 0.393192 -0.621759
C 4.204242 -0.412588 -0.030654
H 4.754183 -0.783036 -0.899285
C 5.053237 0.441011 0.873406
H 3.741887 -1.254402 0.494549
H 5.894716 -0.149348 1.253048
H 5.464076 1.300969 0.331597
H 4.480535 0.799684 1.736755
H 1.328942 1.584589 -1.687396

Ag -0.234736 1.109914 2.109522

PBE/DZVP method

1

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E = -766.069000733 Ha
C -2.736068 -0.238918 0.057536
C -3.807541 0.703143 0.117992
C -5.136708 0.280801 0.193614
C -5.460794 -1.088388 0.212617
C -4.418313 -2.031408 0.153938
C -3.084479 -1.623425 0.078065
H -3.558918 1.769064 0.103329
H -5.936004 1.031357 0.238615
H -6.505448 -1.414060 0.272026
H -4.651113 -3.103750 0.167628
H -2.276792 -2.360968 0.032458
C -1.394924 0.181878 -0.019112
O 0.382283 3.252910 -0.121435
C 1.334207 2.444575 -0.176230
C 1.116815 0.995146 -0.164497
C -0.218955 0.561347 -0.087309
C 2.753558 3.028848 -0.255281
H 3.279371 2.706924 -1.170450
H 2.652645 4.126138 -0.243974
H 3.382057 2.697367 0.588862
C 2.102576 -0.069718 -0.220089
O 1.877209 -1.288315 -0.204691
O 3.433082 0.393193 -0.300428
C 4.419634 -0.642316 -0.324800
H 5.304531 -0.184517 -0.803811
C 4.752050 -1.137939 1.082488
H 4.060442 -1.483057 -0.944683
H 5.570559 -1.881405 1.056988
H 5.061002 -0.297163 1.727743
H 3.857501 -1.610033 1.518260

2

31
E = -911.754757316 Ha
C -2.855656 0.049627 -0.007912
C -3.560930 1.278159 0.103300
C -4.955110 1.272912 0.187037
C -5.671204 0.063663 0.162495
C -4.977948 -1.151862 0.053188

C -3.581981 -1.163063 -0.031070
H -2.983437 2.207923 0.121149
H -5.489201 2.225045 0.272534
H -6.763744 0.068972 0.228696
H -5.527731 -2.098617 0.033876
H -3.038364 -2.112004 -0.115278
C -1.431573 0.121197 -0.089620
O -0.395466 3.272943 0.048757
C 0.753957 2.807620 -0.063653
C 0.940526 1.346854 -0.181655
C -0.286565 0.653377 -0.140808
C 1.949863 3.749064 -0.076168
H 2.521620 3.659768 -1.015199
H 1.566564 4.774241 0.035006
H 2.653969 3.517424 0.740565
C 2.152703 0.589222 -0.317514
O 2.239810 -0.682980 -0.398829
O 3.294668 1.324587 -0.363273
C 4.544872 0.593403 -0.441629
H 5.252690 1.333840 -0.847431
C 4.985034 0.092480 0.928226
H 4.436644 -0.237373 -1.157497
H 5.979380 -0.381292 0.855537
H 5.049591 0.926772 1.646418
H 4.270469 -0.653587 1.310215
Ag 0.160363 -1.592163 -0.289636

3

32
E = -912.153835788 Ha
C -2.910203 0.488633 0.063592
C -3.903544 1.493833 0.194701
C -5.253739 1.139378 0.160767
C -5.626307 -0.205873 -0.002414
C -4.647073 -1.205278 -0.133940
C -3.292348 -0.868323 -0.101354
H -3.601615 2.538063 0.317731
H -6.020351 1.913179 0.260380
H -6.686114 -0.476857 -0.027940
H -4.943054 -2.250306 -0.263187
H -2.521081 -1.636995 -0.205626
C -1.535594 0.841922 0.073834
O 1.108646 3.114326 1.529302
C 1.426207 2.907000 0.359185
C 1.018424 1.552154 -0.326196
C -0.328258 1.139871 0.096709

C 2.247051 3.854092 -0.461029
H 1.632459 4.245237 -1.293558
H 2.608838 4.688755 0.155075
H 3.093032 3.314332 -0.924057
C 2.084047 0.547100 0.182309
O 2.009921 -0.001023 1.285810
O 3.082339 0.431370 -0.682868
C 4.232931 -0.408290 -0.272615
H 4.668168 -0.716129 -1.233736
C 5.200122 0.396894 0.576304
H 3.837268 -1.287486 0.258503
H 6.082197 -0.224581 0.804555
H 5.547629 1.295584 0.041023
H 4.739663 0.694914 1.532106
H 1.096390 1.641445 -1.423250
Ag -0.017409 1.009308 2.401687

M06/DZVP/i-solv method

1

30
E = -766.553278891 Ha
C -2.748642 -0.087263 0.001822
C -3.677912 0.961417 0.148562
C -5.041669 0.701313 0.183860
C -5.517519 -0.604776 0.074424
C -4.608687 -1.652152 -0.071589
C -3.243288 -1.401895 -0.107971
H -3.310083 1.983617 0.234469
H -5.741757 1.528452 0.298223
H -6.587544 -0.804622 0.102554
H -4.967921 -2.677220 -0.158278
H -2.536176 -2.223211 -0.222151
C -1.353812 0.170499 -0.034698
O 0.817773 2.932714 0.130583
C 1.648944 2.021026 0.010087
C 1.240180 0.635758 -0.102730
C -0.149142 0.387021 -0.066320
C 3.113845 2.409413 -0.016034
H 3.602335 2.105197 -0.949686
H 3.171466 3.499221 0.086641
H 3.679012 1.935790 0.795511
C 2.064786 -0.542814 -0.252014
O 1.643172 -1.690278 -0.356658
O 3.407307 -0.290784 -0.277471
C 4.261212 -1.427557 -0.394657

H 5.193627 -1.038522 -0.822208
C 4.510796 -2.077254 0.945083
H 3.826311 -2.142666 -1.103430
H 5.224604 -2.905076 0.841960
H 4.927838 -1.353820 1.657832
H 3.577707 -2.476766 1.359985

2

31
E = -912.235917243 Ha
C -2.716492 0.377121 0.064672
C -3.386674 1.613977 0.104066
C -4.771451 1.660198 0.182993
C -5.515914 0.482088 0.223485
C -4.860720 -0.746847 0.185007
C -3.474763 -0.803839 0.106216
H -2.799708 2.531105 0.072607
H -5.274405 2.625727 0.213079
H -6.602090 0.521937 0.285269
H -5.433800 -1.672375 0.216372
H -2.965557 -1.769152 0.077210
C -1.291857 0.386360 -0.012669
O 0.401857 3.265741 -0.043468
C 1.398581 2.538159 -0.095291
C 1.257042 1.086552 -0.109034
C -0.084206 0.646483 -0.059990
C 2.760487 3.190012 -0.144893
H 3.309699 2.916389 -1.053724
H 2.612140 4.275237 -0.122036
H 3.388117 2.889317 0.702298
C 2.287568 0.091046 -0.162536
O 2.097978 -1.141661 -0.180131
O 3.543593 0.566275 -0.203277
C 4.615743 -0.388054 -0.223644
H 5.456914 0.159065 -0.663734
C 4.947863 -0.873982 1.164596
H 4.353744 -1.217166 -0.890248
H 5.816540 -1.543752 1.129499
H 5.193027 -0.031837 1.824228
H 4.106389 -1.426117 1.599819
Ag -0.138291 -1.815678 -0.155606

3

32
E = -912.698348774 Ha

C -2.768526 0.735713 0.172343
C -3.433984 -0.499469 0.192839
C -4.803295 -0.552884 -0.029317
C -5.518525 0.618658 -0.270293
C -4.862483 1.847516 -0.288991
C -3.492611 1.912276 -0.069257
H -2.865385 -1.410263 0.388145
H -5.315584 -1.513025 -0.013585
H -6.592049 0.573227 -0.445043
H -5.421021 2.762438 -0.477850
H -2.972019 2.868248 -0.083533
C -1.359548 0.800887 0.401158
O 1.297661 -1.280833 1.626741
C 1.720391 -0.154543 1.811690
C 1.259774 1.004022 0.885994
C -0.161970 0.895746 0.598544
C 2.708095 0.204882 2.857583
H 2.238456 0.902516 3.565656
H 3.063991 -0.683886 3.385358
H 3.551818 0.745335 2.405162
C 2.095566 0.835713 -0.385359
O 1.818821 0.030487 -1.255519
O 3.153622 1.614655 -0.368874
C 4.127469 1.444628 -1.439416
H 4.638405 2.410045 -1.485178
C 5.067288 0.317474 -1.108119
H 3.586989 1.281296 -2.377409
H 5.830913 0.237425 -1.891189
H 5.575008 0.498982 -0.152815
H 4.538613 -0.642062 -1.050559
H 1.501584 1.965892 1.355596
Ag -0.106093 -1.476050 -0.491871

PBE/DZVP/i-solv method

1

30
E = -766.151946666 Ha
C -2.761783 -0.099274 0.001804
C -3.694413 0.968578 0.151278
C -5.070231 0.719252 0.188413
C -5.565892 -0.592525 0.078947
C -4.659189 -1.657513 -0.069092
C -3.280845 -1.422415 -0.107797
H -3.316179 1.992791 0.237128
H -5.764850 1.559063 0.304116
H -6.643882 -0.782211 0.108497

H -5.030838 -2.684901 -0.155677
H -2.581494 -2.257297 -0.223306
C -1.367545 0.147308 -0.036754
O 0.799282 2.943098 0.116853
C 1.646862 2.024976 0.004333
C 1.238182 0.624283 -0.109407
C -0.148799 0.368838 -0.070834
C 3.125486 2.418068 -0.004981
H 3.621136 2.131014 -0.948279
H 3.181142 3.511531 0.121576
H 3.690830 1.921695 0.802049
C 2.076447 -0.562037 -0.255969
O 1.658625 -1.728887 -0.329677
O 3.433759 -0.283330 -0.321129
C 4.303521 -1.433694 -0.404987
H 5.224126 -1.051088 -0.877257
C 4.595492 -2.018388 0.970855
H 3.848545 -2.190958 -1.065620
H 5.321269 -2.847083 0.886565
H 5.022172 -1.251867 1.641102
H 3.670933 -2.410473 1.425859

2

31
E = -911.791731499 Ha
C -2.736351 0.306914 0.045869
C -3.362448 1.582752 0.101260
C -4.755011 1.678642 0.180936
C -5.552019 0.520283 0.206370
C -4.940158 -0.743781 0.152175
C -3.547726 -0.855554 0.072802
H -2.732494 2.477828 0.081811
H -5.222900 2.668135 0.223926
H -6.641876 0.602637 0.268869
H -5.552688 -1.651526 0.171992
H -3.065906 -1.839975 0.032271
C -1.314131 0.254581 -0.031101
O 0.245476 3.191610 -0.033925
C 1.293716 2.511844 -0.086755
C 1.227675 1.041923 -0.123076
C -0.088433 0.532265 -0.079261
C 2.635849 3.232309 -0.106183
H 3.201861 3.011854 -1.027313
H 2.438107 4.314099 -0.045216
H 3.277604 2.923722 0.736404
C 2.312416 0.086981 -0.187534

O 2.180985 -1.171987 -0.191259
O 3.554939 0.633340 -0.258727
C 4.682005 -0.286768 -0.263504
H 5.496127 0.300090 -0.717940
C 5.042120 -0.734910 1.144326
H 4.449757 -1.144100 -0.915461
H 5.947108 -1.366862 1.112213
H 5.250346 0.134102 1.791818
H 4.223594 -1.323522 1.590164
Ag -0.091593 -1.810533 -0.118940

3

32
E = -912.248952275 Ha
C -2.814152 0.689384 -0.018267
C -3.506746 -0.546334 -0.047444
C -4.893779 -0.565916 -0.224381
C -5.605246 0.636648 -0.370893
C -4.924163 1.864668 -0.341019
C -3.536469 1.899820 -0.166844
H -2.944015 -1.480170 0.071286
H -5.422131 -1.524204 -0.247813
H -6.690870 0.616294 -0.509897
H -5.476341 2.802824 -0.455602
H -3.000942 2.853430 -0.143956
C -1.398647 0.737044 0.166555
O 1.350071 -0.909542 1.917698
C 1.724172 0.257493 1.815198
C 1.228047 1.131872 0.603996
C -0.179609 0.872276 0.320696
C 2.673650 0.922336 2.757419
H 2.145397 1.748196 3.270108
H 3.063639 0.206267 3.494691
H 3.501912 1.386267 2.191266
C 2.129403 0.701610 -0.576045
O 1.918725 -0.310027 -1.248271
O 3.167085 1.524372 -0.706509
C 4.199378 1.145231 -1.692436
H 4.683994 2.102786 -1.931931
C 5.168505 0.148067 -1.086766
H 3.695257 0.753155 -2.589093
H 5.969698 -0.059688 -1.816796
H 5.631592 0.553345 -0.171436
H 4.667485 -0.804160 -0.845811
H 1.396611 2.198504 0.826865
Ag -0.091370 -1.556521 -0.163486

Transition states:

M06/DZVP method

1

30
E = -766.426575760 Ha
C 0.426334 -0.151499 -0.078202
C 0.108070 0.113463 1.268060
C 1.101633 0.426355 2.185815
C 2.441576 0.488353 1.807155
C 2.769537 0.227288 0.475491
C 1.787856 -0.086084 -0.450168
H -0.935646 0.066861 1.569030
H 0.821439 0.626568 3.221820
H 3.215693 0.735022 2.533965
H 3.811579 0.269433 0.153223
H 2.037497 -0.290266 -1.490691
C -0.531161 -0.477076 -1.079031
O -2.201798 -0.486064 -0.311147
C -2.887723 -0.783638 -1.348062
C -2.163294 -0.968716 -2.552072
C -0.757670 -0.773519 -2.325375
C -4.370469 -0.898423 -1.140257
H -4.741503 -1.884451 -1.444910
H -4.601639 -0.730344 -0.082430
H -4.915774 -0.169516 -1.752498
C -2.707285 -1.301847 -3.846000
O -2.096582 -1.492548 -4.883164
O -4.096367 -1.400120 -3.841185
C -4.682786 -1.714774 -5.087442
H -5.658396 -2.162701 -4.849897
C -4.849834 -0.482713 -5.952284
H -4.068374 -2.461088 -5.608665
H -5.373335 -0.724290 -6.888035
H -5.425734 0.286210 -5.420837
H -3.863964 -0.072939 -6.198178

2

31
E = -912.186666386 Ha
C 0.210550 -0.395261 -0.567200
C -0.080955 0.148917 0.694857

C 0.852725 0.951821 1.332570
C 2.088639 1.213884 0.746090
C 2.383168 0.674062 -0.503093
C 1.452732 -0.113621 -1.164452
H -1.051025 -0.061183 1.137212
H 0.612253 1.374904 2.306671
H 2.818055 1.838504 1.258480
H 3.343952 0.876758 -0.974000
H 1.674738 -0.523506 -2.149715
C -0.721951 -1.224921 -1.235613
O -2.803540 -0.920313 -0.233333
C -3.423313 -1.702089 -0.975078
C -2.711311 -2.394863 -2.024717
C -1.333456 -2.029945 -1.998856
C -4.899852 -1.891189 -0.742985
H -5.136076 -2.942032 -0.539892
H -5.201431 -1.271227 0.106012
H -5.477184 -1.610350 -1.631285
C -3.183952 -3.334191 -2.989515
O -2.477190 -3.901978 -3.850498
O -4.501518 -3.604731 -2.929562
C -5.026090 -4.526223 -3.889974
H -5.940028 -4.913007 -3.424844
C -5.323256 -3.840769 -5.202617
H -4.319348 -5.353239 -4.022893
H -5.801115 -4.540358 -5.899699
H -5.999812 -2.990956 -5.051371
H -4.397962 -3.475354 -5.661617
Ag -0.264546 -3.139661 -3.532094

3

32
E = -912.574373138 Ha
C 0.469823 -0.329103 -0.210191
C 0.196895 0.856523 0.487365
C 1.140884 1.370668 1.361949
C 2.360527 0.718575 1.537127
C 2.636875 -0.458901 0.846157
C 1.691680 -0.993241 -0.016952
H -0.757422 1.358846 0.343804
H 0.929169 2.286687 1.908651
H 3.099040 1.128931 2.222720
H 3.585772 -0.969750 0.993286
H 1.883104 -1.925096 -0.547450
C -0.456808 -0.873801 -1.152773
O -2.141845 -0.769806 -0.395857

C -2.879136 -1.315679 -1.221030
C -2.148011 -1.891935 -2.428097
C -0.727485 -1.479250 -2.263185
C -4.332832 -1.442515 -0.972144
H -4.708924 -2.417776 -1.299282
H -4.550835 -1.270959 0.085090
H -4.863095 -0.692475 -1.574261
C -2.712263 -1.607667 -3.824568
O -2.004932 -1.442648 -4.794960
O -4.029135 -1.633733 -3.835601
C -4.692669 -1.439899 -5.122495
H -5.658698 -1.934273 -4.989445
C -4.833691 0.027003 -5.431149
H -4.114607 -1.973161 -5.884058
H -5.397157 0.153037 -6.362614
H -5.379234 0.548309 -4.635906
H -3.854858 0.501259 -5.564465
H -2.246187 -2.990937 -2.313518
Ag 0.521573 -1.515199 -4.011065

PBE/DZVP method

1

30
E = -766.035305710 Ha
C 0.436243 -0.147255 -0.064099
C 0.122353 0.122353 1.297365
C 1.125961 0.427986 2.221657
C 2.477562 0.479294 1.837720
C 2.804000 0.214926 0.493997
C 1.811863 -0.091569 -0.439095
H -0.926445 0.084171 1.602252
H 0.847487 0.630531 3.264138
H 3.259237 0.719591 2.567635
H 3.852048 0.248774 0.169165
H 2.059561 -0.297984 -1.485062
C -0.542518 -0.465061 -1.055343
O -2.211452 -0.464846 -0.303298
C -2.899669 -0.768768 -1.362969
C -2.149956 -0.960964 -2.565228
C -0.740152 -0.765321 -2.322887
C -4.393578 -0.870058 -1.161259
H -4.762180 -1.879611 -1.413104
H -4.641019 -0.639504 -0.112563
H -4.934121 -0.178933 -1.830529
C -2.690239 -1.301029 -3.870250
O -2.071476 -1.462535 -4.925116

O -4.100250 -1.450093 -3.850607
C -4.683067 -1.752005 -5.121241
H -5.641590 -2.252067 -4.890196
C -4.908865 -0.488253 -5.951190
H -4.028516 -2.451207 -5.672007
H -5.426967 -0.724177 -6.899450
H -5.518085 0.241634 -5.390051
H -3.934291 -0.031083 -6.184350

2

31
E = -911.749370760 Ha
C 0.268455 -0.368126 -0.601220
C -0.106439 0.401459 0.533513
C 0.842874 1.193710 1.182807
C 2.171463 1.245872 0.730314
C 2.548049 0.488411 -0.390270
C 1.615024 -0.312342 -1.053072
H -1.143281 0.348858 0.872806
H 0.538353 1.779970 2.056212
H 2.907362 1.870788 1.245796
H 3.580819 0.519767 -0.753319
H 1.908363 -0.904552 -1.926859
C -0.695423 -1.168416 -1.253531
O -2.934378 -1.010271 -0.073413
C -3.510411 -1.793210 -0.867335
C -2.767273 -2.385568 -1.975948
C -1.413547 -1.938269 -1.970100
C -4.983735 -2.098013 -0.641495
H -5.143579 -3.177127 -0.481381
H -5.323604 -1.533242 0.238483
H -5.584926 -1.821677 -1.523346
C -3.206451 -3.294073 -2.997086
O -2.482148 -3.755684 -3.935362
O -4.512794 -3.672877 -2.917828
C -5.000620 -4.551778 -3.962634
H -5.886116 -5.028058 -3.511678
C -5.364612 -3.773059 -5.220669
H -4.240394 -5.321097 -4.174354
H -5.812776 -4.450037 -5.968634
H -6.093656 -2.978215 -4.990638
H -4.463796 -3.315807 -5.659492
Ag -0.348903 -2.819451 -3.623273

3

32

E = -912.137544359 Ha
C 0.517963 -0.316732 -0.214458
C 0.298200 0.940134 0.401637
C 1.235945 1.441044 1.306332
C 2.397658 0.705041 1.598377
C 2.620046 -0.543339 0.993694
C 1.681133 -1.065406 0.100632
H -0.609474 1.503643 0.168336
H 1.065755 2.409679 1.785020
H 3.130722 1.104735 2.305662
H 3.521514 -1.116068 1.230157
H 1.831908 -2.043639 -0.365537
C -0.410379 -0.845381 -1.162940
O -2.146906 -0.766471 -0.389602
C -2.870735 -1.324186 -1.240328
C -2.121376 -1.875604 -2.462367
C -0.700354 -1.438500 -2.288800
C -4.336328 -1.468325 -1.004555
H -4.687524 -2.468982 -1.303477
H -4.576846 -1.261739 0.047609
H -4.873064 -0.751852 -1.652581
C -2.705238 -1.565139 -3.867398
O -2.005112 -1.293787 -4.836487
O -4.032553 -1.699709 -3.880396
C -4.712964 -1.470514 -5.174139
H -5.641273 -2.050923 -5.072220
C -4.972975 0.009515 -5.390101
H -4.086099 -1.905205 -5.967713
H -5.545895 0.143239 -6.323017
H -5.565719 0.435998 -4.564177
H -4.028842 0.568722 -5.487926
H -2.205288 -2.983258 -2.372055
Ag 0.559618 -1.424954 -3.982098

M06/DZVP/i-solv method

1

30
E = -766.515201929 Ha
C -2.588897 -0.222227 -0.000004
C -3.324330 0.972852 0.101061
C -4.711210 0.947340 0.185044
C -5.409142 -0.258875 0.170590
C -4.691425 -1.450799 0.069362
C -3.306668 -1.437957 -0.015017
H -2.787161 1.918007 0.114081
H -5.255138 1.888768 0.263472

H -6.495937 -0.271114 0.237292
H -5.217200 -2.405464 0.056095
H -2.752150 -2.373099 -0.093046
C -1.164443 -0.274001 -0.084858
O -0.486179 1.520485 -0.029865
C 0.755562 1.250367 -0.101664
C 1.114806 -0.125049 -0.184218
C -0.063546 -0.945988 -0.169669
C 1.693926 2.420852 -0.090928
H 2.323612 2.437250 -0.988399
H 1.118170 3.351138 -0.038003
H 2.379693 2.374430 0.763634
C 2.448469 -0.684095 -0.265140
O 2.723401 -1.873886 -0.337051
O 3.433344 0.264062 -0.260070
C 4.776568 -0.215351 -0.309906
H 5.359029 0.613465 -0.730781
C 5.283360 -0.591605 1.061411
H 4.836296 -1.066678 -0.998925
H 6.338115 -0.891962 1.010237
H 5.203355 0.256966 1.753321
H 4.706600 -1.429782 1.470535

2

31
E = -912.219389797 Ha
C -2.754633 0.430217 0.061806
C -3.501241 1.599701 -0.161611
C -4.886485 1.570951 -0.072101
C -5.557725 0.386657 0.224855
C -4.823828 -0.778000 0.442822
C -3.437869 -0.762902 0.371993
H -2.974101 2.521129 -0.394721
H -5.448901 2.488032 -0.242933
H -6.644409 0.371038 0.287636
H -5.335069 -1.710385 0.678902
H -2.866122 -1.673139 0.553596
C -1.336910 0.410338 -0.027857
O -0.617433 2.492703 -0.042146
C 0.607086 2.227562 -0.096192
C 1.014742 0.852128 -0.118945
C -0.130252 0.001245 -0.079230
C 1.576526 3.376136 -0.131881
H 2.200948 3.340143 -1.032390
H 1.018512 4.317717 -0.113605
H 2.261153 3.342977 0.723894
C 2.332560 0.280089 -0.175868

O 2.571147 -0.934480 -0.201883
O 3.334231 1.180977 -0.207070
C 4.674961 0.670555 -0.229857
H 5.268653 1.477556 -0.673814
C 5.159442 0.335770 1.158446
H 4.720570 -0.200789 -0.893003
H 6.208027 0.013751 1.123546
H 5.093047 1.211418 1.816694
H 4.565962 -0.476075 1.595761
Ag 0.340637 -2.139142 -0.145086

3

32
E = -912.667905270 Ha
C -2.429391 0.803659 0.004134
C -2.879743 1.883473 0.775360
C -4.240830 2.068913 0.975202
C -5.159851 1.178260 0.423536
C -4.716614 0.101658 -0.341391
C -3.358510 -0.082344 -0.563750
H -2.160540 2.573903 1.210849
H -4.586934 2.911591 1.570770
H -6.225774 1.326450 0.587620
H -5.432855 -0.591279 -0.779004
H -3.002473 -0.910106 -1.176310
C -1.030896 0.551383 -0.202762
O -0.197654 2.209281 -0.411015
C 0.974323 1.902092 -0.649642
C 1.243365 0.407565 -0.754328
C -0.036964 -0.249532 -0.388690
C 2.025292 2.919531 -0.839374
H 2.653974 2.670712 -1.701911
H 1.588845 3.915488 -0.950193
H 2.681525 2.913890 0.044445
C 2.454870 -0.035976 0.059459
O 2.386548 -0.611350 1.118554
O 3.575278 0.306405 -0.567963
C 4.820055 0.065792 0.134334
H 5.565344 -0.026826 -0.661199
C 5.126327 1.209377 1.064317
H 4.744267 -0.890429 0.663011
H 6.089076 1.034750 1.560076
H 5.193473 2.155765 0.513016
H 4.357494 1.306402 1.841483
H 1.490606 0.233468 -1.817497
Ag -0.336553 -2.344714 -0.004259

PBE/DZVP/i-solv method

1

30
E = -766.122358291 Ha
C -2.608658 -0.226914 0.001438
C -3.354407 0.981212 0.087393
C -4.751250 0.959602 0.167100
C -5.457698 -0.256129 0.163175
C -4.734863 -1.460103 0.077624
C -3.339019 -1.452874 -0.002319
H -2.812350 1.930116 0.091678
H -5.296671 1.908286 0.233041
H -6.550829 -0.266202 0.225963
H -5.265400 -2.419376 0.073113
H -2.784346 -2.394927 -0.067828
C -1.181268 -0.258203 -0.078596
O -0.471337 1.568359 -0.020398
C 0.779656 1.266317 -0.094923
C 1.119677 -0.128729 -0.182107
C -0.071432 -0.938394 -0.164539
C 1.746354 2.428673 -0.076587
H 2.344312 2.464418 -1.003271
H 1.189587 3.372660 0.031700
H 2.470157 2.333406 0.750209
C 2.455824 -0.706457 -0.267586
O 2.722081 -1.915080 -0.312908
O 3.459753 0.253809 -0.304728
C 4.812194 -0.253843 -0.328652
H 5.404063 0.550778 -0.796746
C 5.319454 -0.563261 1.073859
H 4.855385 -1.150976 -0.969235
H 6.377046 -0.880312 1.035277
H 5.248876 0.327190 1.722655
H 4.728816 -1.377154 1.526034

2

31
E = -911.783782858 Ha
C -2.764557 0.411749 0.051910
C -3.492864 1.632797 0.053178
C -4.888620 1.621143 0.135419

C -5.596028 0.409554 0.215765
C -4.884709 -0.802906 0.214184
C -3.489306 -0.812618 0.134482
H -2.937252 2.571470 -0.008829
H -5.430505 2.573188 0.135897
H -6.688829 0.409169 0.279289
H -5.422012 -1.755511 0.276702
H -2.936044 -1.758284 0.134557
C -1.350544 0.405031 -0.027458
O -0.480557 2.632656 -0.078096
C 0.730581 2.274040 -0.134179
C 1.063832 0.860742 -0.144592
C -0.117109 0.060407 -0.085861
C 1.792542 3.358364 -0.186300
H 2.391214 3.282327 -1.109649
H 1.301172 4.342327 -0.147170
H 2.500063 3.263698 0.654279
C 2.354640 0.211498 -0.193987
O 2.530626 -1.035634 -0.178180
O 3.417085 1.062765 -0.269891
C 4.740731 0.462045 -0.244734
H 5.384217 1.217594 -0.723416
C 5.191126 0.172982 1.179011
H 4.737851 -0.451279 -0.861349
H 6.226777 -0.210187 1.171754
H 5.166128 1.089959 1.792590
H 4.543627 -0.586324 1.647873
Ag 0.248682 -2.060754 -0.102856

3

32
E = -912.232304519 Ha
C -2.506787 0.716402 0.012018
C -2.972632 1.754835 0.854021
C -4.345664 1.923336 1.057524
C -5.265048 1.058600 0.439949
C -4.808658 0.025425 -0.395846
C -3.439488 -0.142111 -0.624776
H -2.253440 2.423916 1.334159
H -4.700790 2.730842 1.705426
H -6.338607 1.192224 0.607506
H -5.523542 -0.646188 -0.881658
H -3.074061 -0.936273 -1.283213
C -1.106023 0.503218 -0.201900
O -0.262246 2.259538 -0.394607

C 0.917468 1.951090 -0.654471
C 1.205822 0.446971 -0.788328
C -0.064423 -0.241647 -0.417130
C 1.965351 2.989779 -0.844027
H 2.604957 2.744296 -1.706827
H 1.512886 3.984965 -0.958193
H 2.621947 2.992052 0.047284
C 2.443277 -0.023676 0.005419
O 2.390082 -0.724357 1.005724
O 3.563336 0.436401 -0.578851
C 4.826659 0.159390 0.119238
H 5.579774 0.197977 -0.681847
C 5.086084 1.198514 1.194900
H 4.781105 -0.861359 0.530190
H 6.064854 0.997155 1.663896
H 5.111987 2.214779 0.766886
H 4.314340 1.158867 1.981609
H 1.448675 0.293092 -1.861750
Ag -0.197768 -2.301697 -0.001301

Products:

M06/DZVP method

1

30
E = -766.438700814 Ha
C -2.520693 -0.104096 0.019167
C -3.350707 1.029625 0.093016
C -4.733888 0.902773 0.156563
C -5.338231 -0.351631 0.149020
C -4.523565 -1.485634 0.076114
C -3.145782 -1.367544 0.012578
H -2.891183 2.016949 0.099676
H -5.350369 1.802413 0.213092
H -6.423355 -0.447406 0.198912
H -4.976705 -2.478969 0.068790
H -2.488681 -2.235511 -0.045105
C -1.080742 -0.040051 -0.049584
O -0.566863 1.300836 -0.037585
C 0.755590 1.159456 -0.107305
C 1.076265 -0.190782 -0.160777
C -0.121785 -1.012756 -0.124289
C 1.527524 2.432234 -0.110116
H 2.150868 2.526945 -1.009377

H 0.836512 3.282979 -0.066745
H 2.216300 2.492290 0.743544
C 2.432127 -0.712856 -0.241638
O 2.786139 -1.871903 -0.301584
O 3.378698 0.303589 -0.247997
C 4.726142 -0.120159 -0.319755
H 5.279307 0.726899 -0.749329
C 5.267418 -0.483769 1.046737
H 4.807478 -0.977762 -1.000867
H 6.334510 -0.740661 0.992977
H 5.146905 0.354960 1.744606
H 4.720052 -1.346704 1.441703

2

31
E = -912.238571227 Ha
C -2.697941 0.606907 -0.009830
C -3.523219 1.729297 0.140460
C -4.903844 1.589703 0.204330
C -5.491237 0.331493 0.119980
C -4.679129 -0.790654 -0.029606
C -3.300320 -0.655633 -0.093827
H -3.071806 2.716698 0.206991
H -5.526697 2.475623 0.321388
H -6.573540 0.224356 0.170194
H -5.125739 -1.781977 -0.097057
H -2.666316 -1.534789 -0.211266
C -1.251304 0.741682 -0.078120
O -0.774773 2.045153 0.013282
C 0.564076 2.005009 -0.065707
C 0.963249 0.696228 -0.206374
C -0.212865 -0.128580 -0.214375
C 1.268360 3.306374 0.010557
H 1.836044 3.507520 -0.906737
H 0.541757 4.111704 0.160022
H 1.991175 3.320583 0.835360
C 2.320289 0.181253 -0.329631
O 2.611607 -0.999974 -0.451020
O 3.248763 1.155352 -0.301980
C 4.617638 0.741585 -0.405953
H 5.141811 1.622129 -0.793438
C 5.160625 0.316166 0.937257
H 4.690841 -0.068213 -1.141143
H 6.228361 0.077496 0.858662
H 5.041473 1.118195 1.675648
H 4.635408 -0.574948 1.298664

Ag 0.152461 -2.186389 -0.422099

3

32
E = -912.581221789 Ha
C -2.492792 0.740978 -0.012080
C -3.092121 1.816316 0.654055
C -4.433081 1.752863 1.009264
C -5.186598 0.623313 0.705951
C -4.597340 -0.446680 0.036060
C -3.260561 -0.387728 -0.327369
H -2.509613 2.701540 0.900511
H -4.891605 2.591818 1.528132
H -6.237168 0.578651 0.984847
H -5.187892 -1.324561 -0.217161
H -2.804738 -1.207663 -0.882395
C -1.087443 0.755737 -0.373285
O -0.521495 2.130397 -0.426570
C 0.706586 2.075819 -0.741725
C 1.097577 0.663818 -1.001676
C -0.132118 -0.125136 -0.677690
C 1.478292 3.316892 -0.856694
H 2.193535 3.259175 -1.684184
H 0.817548 4.181797 -0.963469
H 2.081690 3.438079 0.055226
C 2.399040 0.131037 -0.385529
O 2.563386 -1.042691 -0.162841
O 3.280824 1.095436 -0.202855
C 4.588955 0.704114 0.322149
H 5.252043 1.502080 -0.022744
C 4.548553 0.594950 1.822989
H 4.875282 -0.237427 -0.157561
H 5.552815 0.370910 2.200264
H 4.220098 1.535284 2.280441
H 3.881783 -0.212644 2.145089
H 1.287265 0.631221 -2.096984
Ag 0.024133 -2.232442 -0.491161

PBE/DZVP method

1

30
E = -766.041442853 Ha
C -2.540763 -0.106686 0.014857
C -3.379779 1.036977 0.096320

C -4.772978 0.907885 0.160513
C -5.381982 -0.357666 0.146183
C -4.560704 -1.500463 0.065574
C -3.172130 -1.381286 0.001223
H -2.917613 2.029055 0.108258
H -5.393501 1.811743 0.222802
H -6.473053 -0.454084 0.196659
H -5.016530 -2.499214 0.053051
H -2.510302 -2.252213 -0.061919
C -1.095157 -0.044602 -0.054171
O -0.572301 1.323339 -0.030372
C 0.764975 1.169118 -0.102207
C 1.080944 -0.199740 -0.167360
C -0.125817 -1.022097 -0.135743
C 1.553546 2.442820 -0.093516
H 2.121935 2.575505 -1.032699
H 0.877849 3.304852 0.037679
H 2.305182 2.444730 0.715820
C 2.441494 -0.729626 -0.248722
O 2.799673 -1.904654 -0.280737
O 3.402954 0.308322 -0.293714
C 4.762605 -0.137838 -0.338285
H 5.326196 0.692581 -0.801218
C 5.295225 -0.453233 1.059093
H 4.835948 -1.033374 -0.981080
H 6.366243 -0.726078 1.021886
H 5.177654 0.418779 1.725651
H 4.729473 -1.299098 1.480617

2

31
E = -911.801789050 Ha
C -2.716291 0.596237 -0.015192
C -3.544111 1.731802 0.150620
C -4.935409 1.597562 0.217935
C -5.535238 0.333207 0.122095
C -4.722815 -0.800512 -0.043020
C -3.332944 -0.672580 -0.111211
H -3.085085 2.721116 0.226362
H -5.555909 2.490931 0.346713
H -6.623955 0.230968 0.175112
H -5.176934 -1.794390 -0.119986
H -2.703402 -1.559351 -0.241261
C -1.264910 0.729320 -0.085988
O -0.780669 2.044386 0.009868
C 0.575616 2.001237 -0.070114
C 0.979525 0.678893 -0.216882

C -0.207288 -0.141849 -0.225343
C 1.283417 3.310368 0.006164
H 1.752867 3.569760 -0.959671
H 0.571422 4.105640 0.276781
H 2.094392 3.275840 0.751764
C 2.346809 0.163476 -0.338637
O 2.651107 -1.029916 -0.445833
O 3.278081 1.164887 -0.326926
C 4.664313 0.740676 -0.408321
H 5.190134 1.619797 -0.813824
C 5.200643 0.344921 0.961545
H 4.740648 -0.094994 -1.123172
H 6.275335 0.103130 0.891718
H 5.076185 1.168919 1.683861
H 4.668531 -0.543045 1.337943
Ag 0.051147 -2.187085 -0.418470

3

32
E = -912.144318970 Ha
C -2.506340 0.728689 -0.019949
C -3.092336 1.797471 0.695440
C -4.440658 1.737966 1.063510
C -5.218508 0.620725 0.724719
C -4.644815 -0.439900 0.004622
C -3.300621 -0.386546 -0.372790
H -2.491332 2.668847 0.969738
H -4.884887 2.568442 1.619973
H -6.272816 0.579037 1.013871
H -5.252508 -1.304825 -0.277467
H -2.861550 -1.195721 -0.965681
C -1.098592 0.746362 -0.388811
O -0.519218 2.117722 -0.418981
C 0.724225 2.060322 -0.764382
C 1.107537 0.641321 -1.032598
C -0.136043 -0.144227 -0.717069
C 1.494375 3.314442 -0.867069
H 2.149423 3.298045 -1.753673
H 0.828064 4.189003 -0.886951
H 2.172336 3.388450 0.004839
C 2.419535 0.103261 -0.374549
O 2.566610 -1.073886 -0.099553
O 3.317359 1.081215 -0.235739
C 4.629527 0.692755 0.335314
H 5.304826 1.471800 -0.046960
C 4.569177 0.664986 1.851439
H 4.906259 -0.283385 -0.091656

H 5.575569 0.448650 2.247605
H 4.246449 1.637813 2.257017
H 3.887290 -0.123285 2.208090
H 1.334408 0.591779 -2.124626
Ag -0.097902 -2.222077 -0.596668

M06/DZVP/i-solv method

1

30
E = -766.534827162 Ha
C -2.529020 -0.125676 0.016863
C -3.340249 1.021269 0.083521
C -4.726075 0.917454 0.148893
C -5.347863 -0.328987 0.149959
C -4.555365 -1.476595 0.085352
C -3.173300 -1.377317 0.019955
H -2.872891 2.004626 0.082854
H -5.327440 1.825496 0.198804
H -6.432991 -0.407298 0.200953
H -5.022284 -2.461784 0.086216
H -2.555301 -2.273824 -0.028813
C -1.079598 -0.061918 -0.055453
O -0.570210 1.264622 -0.028329
C 0.757213 1.144112 -0.104155
C 1.088425 -0.200724 -0.177712
C -0.111189 -1.023806 -0.148569
C 1.514411 2.421646 -0.090915
H 2.144026 2.527959 -0.983319
H 0.819125 3.268129 -0.050907
H 2.188514 2.484654 0.773324
C 2.454798 -0.717690 -0.267146
O 2.778299 -1.889289 -0.342354
O 3.381005 0.279214 -0.263981
C 4.753323 -0.120010 -0.319947
H 5.281256 0.741516 -0.745558
C 5.283902 -0.460873 1.050996
H 4.858235 -0.967126 -1.008519
H 6.354615 -0.696460 0.996747
H 5.154485 0.383787 1.739981
H 4.761430 -1.331353 1.465702

2

31

E = -912.266369207 Ha
C -2.557116 0.707890 0.041645
C -3.361508 1.857453 0.077933
C -4.746556 1.755294 0.146037
C -5.363369 0.507603 0.179243
C -4.574339 -0.641581 0.143968
C -3.191289 -0.544203 0.075733
H -2.894656 2.840080 0.052477
H -5.348689 2.662844 0.172817
H -6.448151 0.429661 0.232312
H -5.041706 -1.625455 0.169274
H -2.582225 -1.449313 0.047807
C -1.105460 0.803861 -0.030445
O -0.605987 2.102140 -0.069497
C 0.732699 2.024960 -0.135235
C 1.102744 0.697810 -0.138289
C -0.089245 -0.106955 -0.069748
C 1.459053 3.314225 -0.188183
H 2.028510 3.415443 -1.120973
H 0.748461 4.145392 -0.122727
H 2.179116 3.402290 0.634594
C 2.459479 0.157129 -0.199229
O 2.735917 -1.031212 -0.191445
O 3.390421 1.124313 -0.274860
C 4.765419 0.705786 -0.312525
H 5.290516 1.529231 -0.808412
C 5.300187 0.468927 1.076985
H 4.850667 -0.190568 -0.937412
H 6.367563 0.218803 1.029849
H 5.186929 1.367336 1.696800
H 4.775699 -0.361049 1.565762
Ag 0.037042 -2.216932 -0.049640

3

32
E = -912.677025633 Ha
C -2.416446 0.801392 0.041240
C -3.045873 2.020768 0.322301
C -4.400113 2.055759 0.636156
C -5.145300 0.881575 0.674559
C -4.526048 -0.335174 0.392607
C -3.176075 -0.377127 0.074675
H -2.478145 2.948275 0.300484
H -4.873903 3.011787 0.852802
H -6.205446 0.912583 0.919962
H -5.101420 -1.259307 0.413455

H -2.699228 -1.330116 -0.157904
C -0.997562 0.728621 -0.277045
O -0.391911 2.063723 -0.464503
C 0.847139 1.931807 -0.725614
C 1.188728 0.488047 -0.811739
C -0.075173 -0.222452 -0.442273
C 1.664152 3.121158 -0.948086
H 2.368996 2.955284 -1.769699
H 1.038651 3.998661 -1.135279
H 2.269051 3.301457 -0.046008
C 2.470487 0.007457 -0.130390
O 2.571884 -1.077030 0.388292
O 3.434502 0.906885 -0.246287
C 4.720654 0.582092 0.347323
H 5.433517 1.188037 -0.219151
C 4.728609 0.923864 1.812689
H 4.929721 -0.477173 0.164527
H 5.726958 0.735965 2.226167
H 4.488024 1.982771 1.969116
H 4.008781 0.312375 2.370056
H 1.384549 0.338221 -1.897768
Ag -0.132531 -2.327961 -0.153387

PBE/DZVP/i-solv method

1

30
E = -766.136009418 Ha
C -2.546184 -0.123947 0.019061
C -3.363436 1.036499 0.074400
C -4.759966 0.935807 0.136413
C -5.390674 -0.319559 0.145487
C -4.594583 -1.479494 0.092772
C -3.201240 -1.385031 0.030638
H -2.890292 2.023181 0.066768
H -5.362273 1.851059 0.176706
H -6.482266 -0.394653 0.193464
H -5.067091 -2.468791 0.100379
H -2.581149 -2.287284 -0.009081
C -1.091517 -0.065144 -0.051269
O -0.572249 1.281084 -0.023888
C 0.770441 1.147754 -0.102041
C 1.094846 -0.215717 -0.176887
C -0.114483 -1.037902 -0.144041
C 1.544100 2.426307 -0.087896
H 2.114501 2.564303 -1.023870

H 0.861918 3.283201 0.036676
H 2.285014 2.438898 0.730313
C 2.465391 -0.743925 -0.267936
O 2.789866 -1.932643 -0.310452
O 3.405097 0.271291 -0.310183
C 4.790813 -0.147206 -0.336755
H 5.324061 0.687173 -0.821794
C 5.321206 -0.397971 1.068259
H 4.887028 -1.049407 -0.963933
H 6.397250 -0.644280 1.028846
H 5.194127 0.497258 1.701434
H 4.789179 -1.241325 1.539032

2

31
E = -911.831026275 Ha
C -2.553663 0.717497 0.041463
C -3.347763 1.891393 0.064084
C -4.744295 1.811793 0.136739
C -5.387213 0.564753 0.188115
C -4.610641 -0.606836 0.166501
C -3.215637 -0.533969 0.094126
H -2.862562 2.870720 0.024314
H -5.334162 2.734834 0.152630
H -6.479085 0.505181 0.244802
H -5.096155 -1.588212 0.206528
H -2.619596 -1.454131 0.078544
C -1.096450 0.795095 -0.033735
O -0.575976 2.100396 -0.071963
C 0.778192 2.007324 -0.139234
C 1.139239 0.662027 -0.145009
C -0.070631 -0.128873 -0.075606
C 1.522019 3.296226 -0.191274
H 2.037339 3.422744 -1.160186
H 0.826692 4.139208 -0.051725
H 2.298649 3.337700 0.590618
C 2.500663 0.108734 -0.201224
O 2.779343 -1.093947 -0.164174
O 3.442497 1.090444 -0.309261
C 4.832406 0.656836 -0.313298
H 5.363385 1.461924 -0.845387
C 5.357638 0.484212 1.103337
H 4.916235 -0.276788 -0.892981
H 6.431538 0.229267 1.072539
H 5.239775 1.416061 1.682530
H 4.824008 -0.327692 1.624730

Ag -0.028429 -2.204324 -0.053908

3

32
E = -912.241094741 Ha
C -2.402385 0.839910 0.024549
C -2.981778 2.086738 0.356447
C -4.345109 2.172923 0.666653
C -5.152022 1.025378 0.651561
C -4.584804 -0.215881 0.316566
C -3.226016 -0.310608 0.000520
H -2.366589 2.990232 0.378287
H -4.776353 3.145927 0.923377
H -6.217008 1.096762 0.894861
H -5.206795 -1.116684 0.292649
H -2.793387 -1.278187 -0.276326
C -0.979679 0.718868 -0.282594
O -0.322568 2.036186 -0.482388
C 0.929203 1.853955 -0.752554
C 1.225581 0.391478 -0.799437
C -0.072869 -0.272240 -0.430992
C 1.790782 3.020050 -0.984916
H 2.433938 2.848419 -1.864205
H 1.198584 3.939083 -1.102918
H 2.474149 3.133820 -0.120242
C 2.493873 -0.074363 -0.032122
O 2.507274 -1.029612 0.724889
O 3.538339 0.692947 -0.371225
C 4.814760 0.408571 0.307061
H 5.568974 0.784690 -0.399602
C 4.879671 1.121310 1.644582
H 4.918552 -0.682875 0.408620
H 5.870399 0.945191 2.098235
H 4.745745 2.209265 1.520827
H 4.111676 0.741162 2.338399
H 1.467299 0.183738 -1.870180
Ag -0.245719 -2.321984 -0.134126

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