

# Subtle solvation behaviour of a biofuel additive: The methanol complex with 2,5-dimethylfuran – Supplementary Information –

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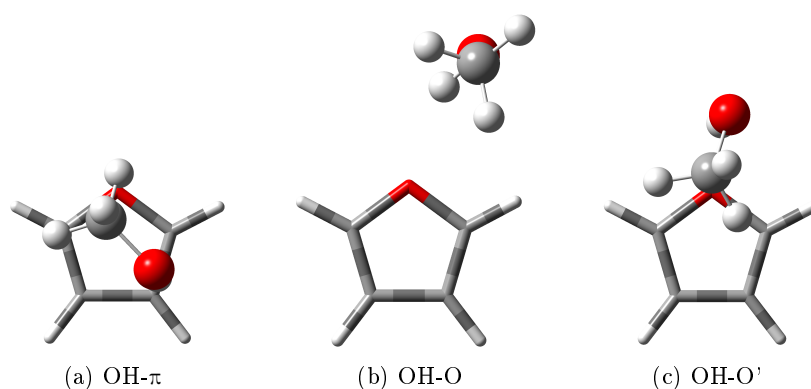


Figure S1: Structures of the most stable methanol/furan dimers at B3LYP-D3/aVTZ level, as well as the OH-O' conformer, which was only located at B2PLYP-D3/aVTZ level.

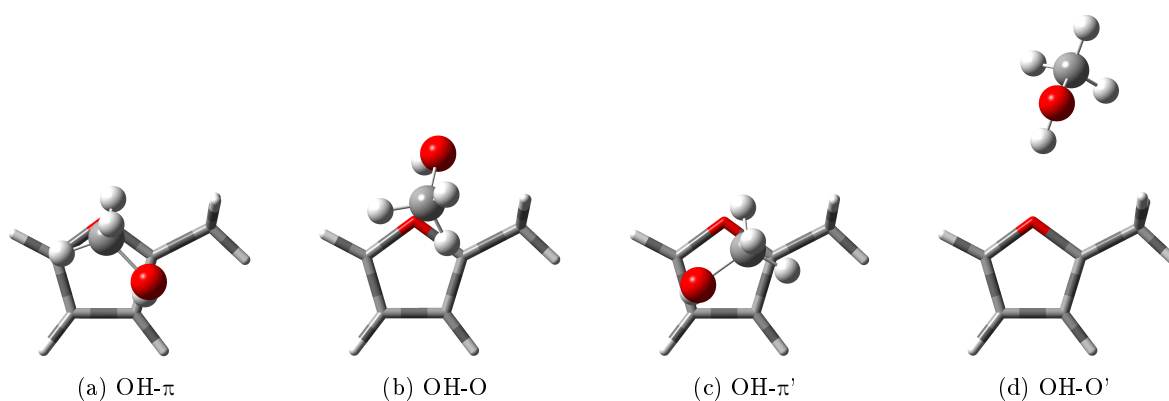


Figure S2: Structures of the most stable methanol/2-methylfuran dimers at B3LYP-D3/aVTZ level.

Table S1: Dissociation energies in  $\text{kJ mol}^{-1}$  without ( $D_e$ ) and with ( $D_0$ ) inclusion of harmonic zero point energy. Dashes mark conformers, which are not stable at the given computational level.

| system            | type                         | B3LYP-D3/aVTZ |       | B2PLYP-D3/aVTZ |       |
|-------------------|------------------------------|---------------|-------|----------------|-------|
|                   |                              | $D_e$         | $D_0$ | $D_e$          | $D_0$ |
| 2,5-dimethylfuran | OH- $\pi$                    | 22.5          | 18.7  | 22.3           |       |
|                   | <b>OH-O</b>                  | 23.3          | 19.0  | 23.1           |       |
|                   | OH-O'                        | 21.6          | 17.5  | 21.2           |       |
| 2-methylfuran     | <b>OH-<math>\pi</math></b>   | 20.0          | 16.5  | 19.9           | 16.6  |
|                   | <b>OH-O</b>                  | 20.9          | 16.5  | 21.0           | 16.7  |
|                   | OH- $\pi'$                   | 19.5          | 16.0  | 19.4           | 16.0  |
|                   | OH-O'                        | 19.5          | 15.4  | 19.3           | 15.2  |
| furan             | <b>OH-<math>\pi</math></b>   | 16.8          | 13.6  | 16.8           | 13.6  |
|                   | OH-O                         | 16.5          | 12.7  | 16.8           | 13.1  |
|                   | OH-O'                        | -             | -     | 16.8           | 13.0  |
| 2,3-benzofuran    | OH-O                         | 20.0          | 15.6  | 20.3           |       |
|                   | <b>OH-<math>\pi_6</math></b> | 21.1          | 17.8  | 21.5           |       |
|                   | OH- $\pi_5$                  | 19.7          | 16.2  | 19.9           |       |
|                   | OH- $\pi_5'$                 | -             | -     | 19.4           |       |

Table S2: Cartesian coordinates (in  $a_0$ ) of the calculated structures of the methanol/2,5-dimethylfuran dimers at B3LYP-D3/aVTZ level.

| type      | x                 | y                 | z                 |   |
|-----------|-------------------|-------------------|-------------------|---|
| OH- $\pi$ | -2.68812057126807 | -0.30707288272480 | 0.01975574377819  | C |
|           | -2.11783787634909 | 0.33896306912945  | 2.43221426601156  | C |
|           | -0.13834320660907 | 2.19228845962586  | 2.29912037879184  | C |
|           | 0.36970608476702  | 2.55703995875560  | -0.19072829054906 | C |
|           | -1.17865431524359 | 1.03671881335199  | -1.60496810048455 | O |
|           | -2.98941971623967 | -0.41237109108580 | 4.10932113892322  | H |
|           | 0.77215222153549  | 3.13850114372426  | 3.85321955812153  | H |
|           | 2.18762591765144  | 4.16287231527837  | -1.58797005434994 | C |
|           | 3.49928963516906  | 3.01329883491543  | -2.69018337459608 | H |
|           | 1.21555310041490  | 5.43722350908612  | -2.88740764954634 | H |
|           | 3.27900504322790  | 5.29254247922328  | -0.26057924338934 | H |
|           | -4.49529541736808 | -2.10420994056381 | -1.13643956809155 | C |
|           | -5.58845145482256 | -3.03505490732889 | 0.33611015698989  | H |
|           | -5.80300104375046 | -1.14100683681766 | -2.40927777670652 | H |
|           | -3.51180639411972 | -3.55239387213257 | -2.23017151965636 | H |
|           | 2.78424939443717  | -4.13345039313647 | -0.45472256087157 | C |
|           | 2.05249515632656  | -3.34278112102875 | -2.22051759107513 | H |
|           | 4.12292298313675  | -5.62847720442937 | -0.91036083068694 | H |
|           | 1.20942648204826  | -4.95956061897596 | 0.60203838050338  | H |
|           | 4.10728700797154  | -2.30050750604474 | 0.99096341397082  | O |
|           | 2.94239745029396  | -0.97460987226383 | 1.44860167011103  | H |
| OH-O      | 1.61605265886781  | 0.73693629929679  | 2.10500989063254  | C |
|           | 1.63838209292379  | 3.18379513677178  | 1.35686675284520  | C |
|           | 1.63838209292379  | 3.18379513677178  | -1.35686675284520 | C |
|           | 1.61605265886781  | 0.73693629929679  | -2.10500989063254 | C |
|           | 1.60895458896334  | -0.79271833811586 | 0.00000000000000  | O |
|           | 1.65041642688443  | 4.80421850131136  | 2.58650827683682  | H |
|           | 1.65041642688443  | 4.80421850131136  | -2.58650827683682 | H |
|           | 1.57603034483631  | -0.55121021024838 | -4.58993920337172 | C |
|           | 3.23319287704590  | -1.75571649411951 | -4.84055317046204 | H |
|           | -0.09733555800038 | -1.74347977192561 | -4.79053865845833 | H |
|           | 1.55932627766241  | 0.84947793670706  | -6.09565852408381 | H |
|           | 1.57603034483631  | -0.55121021024838 | 4.58993920337172  | C |
|           | 1.55932627766241  | 0.84947793670706  | 6.09565852408381  | H |
|           | -0.09733555800038 | -1.74347977192561 | 4.79053865845833  | H |
|           | 3.23319287704590  | -1.75571649411951 | 4.84055317046204  | H |
|           | -4.54985504795523 | -1.31299097111847 | 0.00000000000000  | C |
|           | -6.54742848892811 | -1.80549661060686 | 0.00000000000000  | H |
|           | -4.15406830905010 | -0.16745833931459 | 1.67664479447650  | H |
|           | -4.15406830905010 | -0.16745833931459 | -1.67664479447650 | H |
|           | -3.16408388603025 | -3.61209284174308 | 0.00000000000000  | O |
|           | -1.39158078839018 | -3.18982735537352 | 0.00000000000000  | H |
| OH-O'     | -1.21882886726137 | 2.35178209273964  | 0.05704798197352  | C |
|           | -3.77249152568336 | 2.41475758493215  | -0.08221628185815 | C |
|           | -4.63096987513123 | -0.16014266779013 | -0.10531183030825 | C |
|           | -2.55119566047724 | -1.64469966182866 | 0.02060015634378  | C |
|           | -0.43926818797549 | -0.12965256146610 | 0.12624405373119  | O |

|                   |                   |                   |   |
|-------------------|-------------------|-------------------|---|
| -4.91844907054935 | 4.09344970885203  | -0.16200776871925 | H |
| -6.55456022044332 | -0.81375785343011 | -0.20642252571586 | H |
| -2.11409434026928 | -4.40932702515389 | 0.06002897472532  | C |
| -0.93068107198939 | -5.00643269821459 | -1.52179023812591 | H |
| -1.17146436445707 | -4.99856216249079 | 1.79942395128401  | H |
| -3.91383907930541 | -5.39646360061043 | -0.06618272099590 | H |
| 0.79077125909178  | 4.29896744503637  | 0.14532709172936  | C |
| -0.05066257457689 | 6.16952749178378  | -0.00329693423784 | H |
| 1.85213333588544  | 4.20618035349669  | 1.91389900141758  | H |
| 2.13556757657418  | 4.05957330430892  | -1.40131933218578 | H |
| 6.18024166318664  | -0.98281393887357 | 0.89286719397345  | C |
| 5.63310053631574  | -2.32268394885755 | 2.37278815457662  | H |
| 8.15067428091886  | -1.32371446868899 | 0.40633768148285  | H |
| 6.02233369427118  | 0.93693930437553  | 1.65310846143622  | H |
| 4.73676552744298  | -1.30323947520706 | -1.34166018295976 | O |
| 2.98060416412643  | -1.02631323743359 | -0.93240324486616 | H |

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Table S3: Cartesian coordinates (in  $a_0$ ) of the calculated structures of the methanol/2-methylfuran dimers at B3LYP-D3/aVTZ level.

| type       | x                 | y                 | z                 |   |
|------------|-------------------|-------------------|-------------------|---|
| OH- $\pi$  | 2.14009410254246  | -2.49234195546242 | -1.23401782248343 | C |
|            | 2.35698642228875  | -2.50836258034699 | 1.31346728397670  | C |
|            | 2.02609703951405  | 0.06193430008711  | 2.11458724287769  | C |
|            | 1.62975757399981  | 1.45875019406001  | -0.00743703835366 | C |
|            | 1.69493086657269  | -0.09214977326245 | -2.07424592547259 | O |
|            | 2.70583801638269  | -4.13168274227160 | 2.48711764305879  | H |
|            | 2.09472299261719  | 0.77755407864491  | 4.01779525601533  | H |
|            | 1.13364892608820  | 4.17396055608175  | -0.47436409385932 | C |
|            | -0.72342842346944 | 4.45182401428193  | -1.32870810345610 | H |
|            | 2.54462519157543  | 4.98188993750618  | -1.74372072467581 | H |
|            | 1.18410387639469  | 5.20562681733277  | 1.30351992124005  | H |
|            | -4.74770708130210 | -1.21427927908846 | -0.80285319744167 | C |
|            | -3.81050670713132 | -0.29346198530685 | -2.40006490821587 | H |
|            | -6.78115989235511 | -1.15640147170152 | -1.11177884113339 | H |
|            | -4.14590124112417 | -3.19201320670389 | -0.73824230455513 | H |
|            | -4.26360791626383 | 0.05510937634091  | 1.51384914130159  | O |
|            | -2.46807187914855 | 0.01571587065603  | 1.82242160925835  | H |
|            | 2.23925633339045  | -3.93169963126563 | -2.66242739864312 | H |
| OH-O       | 2.17189611955882  | -2.30553607786503 | -1.27029645632021 | C |
|            | 3.65185042095498  | -1.93525827854799 | 0.77830627802065  | C |
|            | 3.17394049687795  | 0.59799116815841  | 1.61691199982843  | C |
|            | 1.43445406339699  | 1.60268481947908  | 0.02419820996824  | C |
|            | 0.80058148313431  | -0.16666913908338 | -1.76862823828586 | O |
|            | 4.93047813232308  | -3.28625703474994 | 1.60001476044474  | H |
|            | 4.02068747609560  | 1.54612907166953  | 3.20451001256928  | H |
|            | 0.14296087855201  | 4.08108284495414  | -0.14164294299680 | C |
|            | -1.90386950679369 | 3.86126137767455  | -0.00290341979827 | H |
|            | 0.55421878339744  | 5.01936069963130  | -1.93308848831758 | H |
|            | 0.78132942488261  | 5.29712245345199  | 1.38886142172472  | H |
|            | -4.38039141270971 | -1.63949133827515 | 1.51326148857848  | C |
|            | -3.98817907071994 | -3.65785199113182 | 1.28679219496216  | H |
|            | -6.12943731124351 | -1.42988751709513 | 2.57624913235354  | H |
|            | -2.84042003613286 | -0.78828351976365 | 2.60106571153368  | H |
|            | -4.73740042991347 | -0.41455709825130 | -0.85079815227731 | O |
|            | -3.15117790406760 | -0.45485323032077 | -1.74432796767673 | H |
|            | 1.87289647739497  | -3.86775264180089 | -2.53202929615003 | H |
| OH- $\pi'$ | 2.15972201326251  | 0.94616806917604  | 0.24597370963204  | C |
|            | 1.81358332332603  | -0.71649548242640 | 2.16945022191410  | C |
|            | 1.16472993061119  | -3.09624133949346 | 1.04272222511280  | C |
|            | 1.16261902168935  | -2.70971647623392 | -1.48956686447816 | C |
|            | 1.76438714291132  | -0.25644791190205 | -2.01071707790712 | O |
|            | 1.98668049849596  | -0.30330983506009 | 4.15304695691700  | H |
|            | 0.76980744705527  | -4.84896248210314 | 1.99607737173842  | H |
|            | -4.43083531186152 | 1.76795164083706  | -0.23622961138865 | C |
|            | -3.42351730312805 | 2.09684686290582  | -2.01291648829965 | H |
|            | -6.30657600511064 | 2.60106279623470  | -0.38420012647353 | H |
|            | -3.40768567921387 | 2.71681081073705  | 1.29126863697540  | H |

|       |                   |                   |                   |   |
|-------|-------------------|-------------------|-------------------|---|
|       | -4.76460379038586 | -0.84741440094827 | 0.25776777703216  | O |
|       | -3.12271494396793 | -1.62929895994907 | 0.36896030452260  | H |
|       | 0.79995713369106  | -3.90165723709270 | -3.09276118184012 | H |
|       | 2.81072538342896  | 3.66561291510491  | 0.12757346091970  | C |
|       | 4.53981107262560  | 3.97506146928493  | -0.95433208897296 | H |
|       | 1.30525031092129  | 4.75198825732917  | -0.77337150570974 | H |
|       | 3.09164621334669  | 4.39782254235804  | 2.02850703678084  | H |
| OH-O' | 1.67176476337100  | 1.45546692094449  | -0.01505651429814 | C |
|       | 4.22075849898910  | 1.23500498036347  | 0.12797196731137  | C |
|       | 4.79585669836138  | -1.41403159613815 | 0.06958172354122  | C |
|       | 2.55899612693524  | -2.63343344819370 | -0.10422826102516 | C |
|       | 0.62231102061488  | -0.91577959075557 | -0.16188101508148 | O |
|       | 5.54202719640828  | 2.77540668130950  | 0.26094726003177  | H |
|       | 6.63443553447330  | -2.27899478861424 | 0.15012156565484  | H |
|       | -0.10166965009627 | 3.62180059258523  | -0.05138753754065 | C |
|       | 0.94248146518800  | 5.37485923446081  | 0.20254455773819  | H |
|       | -1.11761733899959 | 3.72853342357590  | -1.84544258906981 | H |
|       | -1.50628841062848 | 3.46273270797882  | 1.45042087558570  | H |
|       | -6.11964378726776 | -0.65979081994089 | -0.87638248087121 | C |
|       | -5.98736244959763 | -2.27846381085216 | -2.15896671375245 | H |
|       | -8.09135811234642 | -0.41661179767343 | -0.33975093295861 | H |
|       | -5.50875415752395 | 1.03759090308968  | -1.89297731729818 | H |
|       | -4.72099930497088 | -1.04181943092213 | 1.37829551290337  | O |
|       | -2.96433619961960 | -1.25132086714963 | 0.93771341525121  | H |
|       | 2.01816969215031  | -4.58796180841940 | -0.19665930534225 | H |

Table S4: Cartesian coordinates (in  $a_0$ ) of the calculated structures of the methanol/furan dimers at B3LYP-D3/aVTZ level.

| type                 | x                 | y                 | z                 |   |
|----------------------|-------------------|-------------------|-------------------|---|
| OH- $\pi$            | -2.21962084453628 | 2.04555122905537  | 0.87112123299057  | C |
|                      | -2.33415573447433 | -0.12478968649616 | 2.22423547200234  | C |
|                      | -2.20431011364885 | -2.14629056489136 | 0.42299785279504  | C |
|                      | -2.01906533806706 | -1.03948849807435 | -1.88334837660616 | C |
|                      | -2.02491254363411 | 1.52299649465129  | -1.64407024059466 | O |
|                      | -2.24176803064077 | 4.01303927377802  | 1.37180537645758  | H |
|                      | -2.48499981275526 | -0.28377769008423 | 4.24532612490203  | H |
|                      | -2.25863162945472 | -4.14361903083868 | 0.80259412133421  | H |
|                      | -1.87602585575188 | -1.75999999470018 | -3.77636704335547 | H |
|                      | 4.57353171583944  | 1.09978973266212  | -0.03017069903609 | C |
|                      | 6.61158710134132  | 1.37688886540769  | -0.08481944858150 | H |
|                      | 3.81419518926942  | 2.10865543521018  | 1.60832344703573  | H |
|                      | 3.75245581816192  | 1.91193831191916  | -1.74579557276322 | H |
|                      | 4.14025461114998  | -1.54501931923086 | 0.13594042373147  | O |
|                      | 2.34200016477424  | -1.83136312060663 | 0.13408001341977  | H |
| OH-O                 | -1.20350554429714 | 1.76192562032972  | 0.71908580435517  | C |
|                      | -3.59697695056892 | 2.12876143252383  | -0.10387396022947 | C |
|                      | -4.62399839249740 | -0.33034339031120 | -0.59667925801811 | C |
|                      | -2.77746932492338 | -2.00919175846785 | -0.03660965407092 | C |
|                      | -0.66548922608796 | -0.76511833097856 | 0.77457539015276  | O |
|                      | 0.29883430782896  | 2.99304114440187  | 1.31169410369434  | H |
|                      | -4.52885419246305 | 3.92102375060673  | -0.33439859478513 | H |
|                      | -6.48883072646227 | -0.77353356951989 | -1.27499130481148 | H |
|                      | -2.65007053997398 | -4.03451898798150 | -0.09679824449532 | H |
|                      | 5.51069886138296  | -0.11887873924503 | -1.44157599565470 | C |
|                      | 7.36153039134451  | 0.77618984884444  | -1.52395060393763 | H |
|                      | 4.16049206424771  | 1.07146368646876  | -2.46301099643193 | H |
|                      | 5.62836294776266  | -1.95175016632033 | -2.39484969282893 | H |
|                      | 4.86671175597589  | -0.37273917019096 | 1.15166540900937  | O |
|                      | 3.18400297169713  | -1.06063945118886 | 1.25507813503950  | H |
| OH-O'<br>(B2PLYP-D3) | 1.904330          | -1.760773         | -1.315495         | C |
|                      | 3.483198          | -1.549398         | 0.691037          | C |
|                      | 3.344320          | 1.029596          | 1.500690          | C |
|                      | 1.691889          | 2.192591          | -0.074431         | C |
|                      | 0.789089          | 0.514075          | -1.818595         | O |
|                      | 1.381906          | -3.291364         | -2.540102         | H |
|                      | 4.607695          | -3.036971         | 1.496242          | H |
|                      | 4.341336          | 1.893583          | 3.045133          | H |
|                      | 0.973343          | 4.084384          | -0.215835         | H |
|                      | -4.330995         | -0.818917         | 1.517949          | C |
|                      | -6.031271         | -0.676938         | 2.661088          | H |
|                      | -2.744670         | -0.054721         | 2.595775          | H |
|                      | -3.967312         | -2.813795         | 1.127930          | H |
|                      | -4.776430         | 0.575949          | -0.733709         | O |
|                      | -3.218759         | 0.617043          | -1.670319         | H |

Table S5: Cartesian coordinates (in  $a_0$ ) of the calculated structures of the methanol/2,3-benzofuran dimers at B3LYP-D3/aVTZ level.

| type        | x                 | y                 | z                 |   |
|-------------|-------------------|-------------------|-------------------|---|
| OH- $\pi$ 6 | 1.19812401981534  | -1.06199526558450 | 1.28848228473357  | C |
|             | 1.11245448020534  | -1.20285412536927 | -1.35822874516689 | C |
|             | -1.10023584412526 | -2.06244351917840 | -2.51797789850951 | C |
|             | -3.12450521283447 | -2.73841565601617 | -0.99401342019160 | C |
|             | -2.97728239385037 | -2.57078977738965 | 1.64846703965460  | C |
|             | -0.79782946532329 | -1.72442788535194 | 2.84090288422745  | C |
|             | 4.85800232046118  | 0.28215935108518  | -0.11055514262771 | C |
|             | 3.53840392582907  | -0.30926662751218 | -2.21293693715897 | C |
|             | -1.23873139519247 | -2.18487815817577 | -4.55260980740047 | H |
|             | -4.85542917665431 | -3.40112430627624 | -1.85336984003054 | H |
|             | -4.59526974930089 | -3.10105524765161 | 2.77649537711344  | H |
|             | -0.66278518703092 | -1.57506115820194 | 4.87219866078939  | H |
|             | 6.73186447055492  | 1.01239088496672  | 0.17871092367671  | H |
|             | 4.19183486405743  | -0.13176288647944 | -4.13047294966291 | H |
|             | 3.49208302637449  | -0.15146088935445 | 2.05348863424483  | O |
|             | -3.42866907295747 | 3.85489329211053  | -1.09823009098180 | O |
|             | -3.23250591574711 | 2.04628014580223  | -1.14565918786238 | H |
|             | -1.43441327556420 | 4.89727126290402  | 0.36521856475997  | C |
|             | 0.42199680026867  | 4.45716727326560  | -0.43220861425905 | H |
|             | -1.68482314223746 | 6.93970759137415  | 0.35581400928205  | H |
|             | -1.48563182848657 | 4.23516224448054  | 2.32365203609334  | H |
| OH-O        | 0.53166323424722  | 0.17094500607204  | -0.60978364734409 | C |
|             | 2.83647725695668  | 1.14437816678113  | 0.25678560577841  | C |
|             | 4.82311575933557  | -0.52910897757694 | 0.73173587460839  | C |
|             | 4.41917619556828  | -3.08517856384075 | 0.32373322490794  | C |
|             | 2.08518222969240  | -3.99289855975343 | -0.54207798035974 | C |
|             | 0.08107191204383  | -2.36830746569360 | -1.02976479564973 | C |
|             | 0.07983904713398  | 4.29664092538752  | -0.30471017674028 | C |
|             | 2.47593318902039  | 3.84051117850608  | 0.43335246319345  | C |
|             | 6.63000058221439  | 0.15099079973670  | 1.40110925669583  | H |
|             | 5.93138317022372  | -4.41268345203178 | 0.67915281122934  | H |
|             | 1.83758212178052  | -5.99915699785952 | -0.83753941865764 | H |
|             | -1.73339159225493 | -3.03138656483028 | -1.69029778970061 | H |
|             | -1.01271897526551 | 6.00036308814936  | -0.48034803261729 | H |
|             | 3.82898333090392  | 5.23712525280336  | 1.02947354038047  | H |
|             | -1.16559640712252 | 2.10622333121042  | -0.95705122325198 | O |
|             | -6.12583173983057 | -0.46198087757667 | -0.81629955192999 | O |
|             | -4.79000434073581 | 0.74045590856046  | -1.11169552295721 | H |
|             | -6.23558031017972 | -0.95564875803868 | 1.82038469790531  | C |
|             | -6.73773208496666 | 0.73334971173953  | 2.90474423813415  | H |
|             | -7.69716198906751 | -2.37389753343332 | 2.11316797042938  | H |
|             | -4.44504343948783 | -1.69921313160141 | 2.54351255326157  | H |
| OH- $\pi$ 5 | -0.70786351356304 | -1.58082478898168 | 1.05955748265411  | C |
|             | -0.34598710718111 | -1.13154696174089 | -1.52736774135386 | C |
|             | -2.15065497977528 | 0.27587584299123  | -2.84453466554277 | C |
|             | -4.23202016410615 | 1.16729553143245  | -1.52878941041375 | C |
|             | -4.53921963466622 | 0.68343867888976  | 1.05897393621670  | C |



|                             |                   |                   |                   |   |
|-----------------------------|-------------------|-------------------|-------------------|---|
|                             | -2.76953417499012 | -0.70780820329671 | 2.40744465509191  | C |
|                             | 2.89023878647589  | -3.35965161962806 | 0.02502614024846  | C |
|                             | 2.02868617887010  | -2.32115491976265 | -2.14529617149266 | C |
|                             | -1.92287192663442 | 0.67078057495870  | -4.83603938658904 | H |
|                             | -5.64971785960757 | 2.26402935027111  | -2.50951888848947 | H |
|                             | -6.18481564419911 | 1.41273395383860  | 2.02518080904784  | H |
|                             | -2.97717372012442 | -1.08525413643012 | 4.40269245795829  | H |
|                             | 4.56477243948268  | -4.42034329361576 | 0.47180718575911  | H |
|                             | 2.94745262846622  | -2.39693421488326 | -3.95854644569648 | H |
|                             | 1.27512898199188  | -2.94737236741037 | 2.00889744829886  | O |
|                             | 4.27690351982905  | 3.37214274614190  | -0.30092951075304 | O |
|                             | 3.86154105214740  | 1.65461436887624  | -0.73613681912980 | H |
|                             | 2.34043387158801  | 4.34002129034831  | 1.29347428767047  | C |
|                             | 2.23731201341948  | 3.31800000073198  | 3.08835270372399  | H |
|                             | 2.81326248476345  | 6.30369318292593  | 1.68531402475922  | H |
|                             | 0.48554762758622  | 4.27099923442677  | 0.38630562103102  | H |
| OH- $\pi 5'$<br>(B2PLYP-D3) | -0.340226         | 1.703564          | -1.088495         | C |
|                             | -0.134575         | 1.201123          | 1.506573          | C |
|                             | -2.182348         | 0.094842          | 2.760393          | C |
|                             | -4.334650         | -0.459377         | 1.372924          | C |
|                             | -4.478160         | 0.065522          | -1.223785         | C |
|                             | -2.470322         | 1.164049          | -2.509813         | C |
|                             | 3.442263          | 2.916781          | 0.061199          | C |
|                             | 2.369607          | 2.014764          | 2.204071          | C |
|                             | -2.088743         | -0.323115         | 4.757004          | H |
|                             | -5.937954         | -1.316274         | 2.301943          | H |
|                             | -6.184996         | -0.395985         | -2.244033         | H |
|                             | -2.551803         | 1.572934          | -4.506460         | H |
|                             | 5.270114          | 3.709931          | -0.329470         | H |
|                             | 3.239852          | 1.948406          | 4.039804          | H |
|                             | 1.847631          | 2.760610          | -1.971419         | O |
|                             | 3.617935          | -3.834889         | -0.240761         | O |
|                             | 3.360702          | -2.187664         | 0.484747          | H |
|                             | 1.229724          | -5.052935         | -0.443332         | C |
|                             | -0.100532         | -3.958687         | -1.578167         | H |
|                             | 1.560324          | -6.857708         | -1.366400         | H |
|                             | 0.386776          | -5.402651         | 1.407751          | H |