

Supporting Information

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Antioxidant properties can be tuned in the presence of external electric field: Accurate computation of O-H BDE with range-separated density functionals

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Optimized Structures of Gallic Acid and Caffeic Acid with LC-BLYP/6-311++G(3df,2p)

Gallic Acid (Neutral)

x- 0.010

C -0.9442993342 -1.1425110732 0.0020197783
C -1.6714249843 0.0235205663 0.0001991428
C -1.0335866321 1.2401570759 -0.0041590457
C 0.3402499848 1.2933746176 -0.0067108056
C 1.0538735592 0.1175716864 -0.0048858422
C 0.4199053217 -1.1066690796 -0.0005360855
O -3.0377434478 -0.0063513096 0.0027937994
O -1.774955043 2.3732880527 -0.0058168001
C 2.5410933448 0.0846297597 -0.0074030152
O 3.092602187 1.2867999916 -0.0108334101
O -1.6885387869 -2.2886056774 0.0064807576
O 3.158370364 -0.933888322 -0.0063774063
H 1.0248945092 -2.004409946 0.0007807023
H 0.8471045968 2.2466495479 -0.0100166237
H -1.1106693067 -3.0568416921 0.0083346273
H -3.2991291432 -0.9340271412 0.0064104249
H -2.7046120549 2.1267356648 -0.0028727192
H 4.0584258654 1.1918022781 -0.012113479

x+ 0.10

C -0.9394871461 -1.1749857647 0.0023985575
C -1.6703970723 -0.0011876263 0.0006281601
C -1.0234556773 1.2205078242 -0.0037202539
C 0.347901317 1.264763173 -0.0062928872
C 1.0702392632 0.087993318 -0.0044582733
C 0.4291545701 -1.1390554191 -0.0000917301
O -3.0005633303 0.0189813815 0.0029223391
O -1.7314684186 2.3525646966 -0.0054335896
C 2.5271330905 0.107823203 -0.0071553321
O 3.0617047141 1.3422258937 -0.0118456117
O -1.6905104131 -2.2961194732 0.0066334033
O 3.2589702375 -0.8493894341 -0.0056059683
H 1.0124784696 -2.0491037564 0.0012307941
H 0.8364018567 2.2259679821 -0.0097816953
H -1.166580052 -3.0998415959 0.0073509417
H -3.3847369687 -0.868258537 0.0055377295
H -2.6804739909 2.1629465443 -0.0035792967
H 4.0152505508 1.2053925901 -0.0134432871

x- 0.002

C -0.942994 -1.155173 0.002198
C -1.670193 0.013545 0.000413
C -1.029064 1.23129 -0.003938
C 0.343908 1.280847 -0.00651
C 1.058581 0.104764 -0.004696
C 0.423377 -1.119932 -0.000345
O -3.022444 0.005483 0.002865
O -1.75525 2.364692 -0.005621
C 2.534676 0.093843 -0.007302
O 3.077489 1.309107 -0.011308
O -1.688631 -2.291862 0.006536
O 3.19799 -0.900429 -0.005999
H 1.01862 -2.022999 0.000968
H 0.843598 2.237002 -0.009892
H -1.130319 -3.073309 0.007909
H -3.333149 -0.907439 0.005967
H -2.693024 2.14187 -0.003242
H 4.03839 1.199924 -0.012711

x+ 0.002

C -0.9421149834 -1.1616184288 0.0022907958
C -1.6700527802 0.0085283438 0.0004512641
C -1.0272052488 1.2272909156 -0.0037536595
C 0.3453194413 1.2751043329 -0.0061208183
C 1.0617323131 0.0989365608 -0.0042217648
C 0.4252405124 -1.1262098666 -0.0000287231
O -3.0151316462 0.0106065928 0.0026462515
O -1.7468111462 2.3603118434 -0.0055100804
C 2.5321570274 0.0984950138 -0.0065814694
O 3.0718954963 1.3197525893 -0.0118836895
O -1.6889349602 -2.293252884 0.0064352994
O 3.2182137212 -0.8834906669 -0.006024484
H 1.0160987348 -2.0317980843 0.0013560595
H 0.841149092 2.2329552755 -0.0094221273
H -1.1413677045 -3.0818118732 0.0076044461
H -3.3506294823 -0.8941075488 0.0054481378
H -2.6884664768 2.1489050986 -0.0034951464
H 4.0304690901 1.2026277861 -0.0138962917

x- 0.004

C -0.9433734359 -1.1519912988 0.0021569224
C -1.6703907339 0.0160305501 0.0003654439
C -1.0301203645 1.2334027554 -0.0039871464

C 0.3430617313 1.2838444045 -0.0065556657
C 1.0572092995 0.1078369928 -0.0047406221
C 0.4224742589 -1.1166754239 -0.0003910125
O -3.026170923 0.0026983422 0.0028491618
O -1.7598668101 2.3668296332 -0.0056644408
C 2.536136311 0.0915383332 -0.0073271389
O 3.0808995823 1.3035894731 -0.0111936368
O -1.6885395501 -2.2910722428 0.0065215473
O 3.1880308357 -0.9088343619 -0.0060916785
H 1.0200072693 -2.0184678316 0.0009216964
H 0.8445778921 2.2392356126 -0.0099183115
H -1.1251411234 -3.0691189205 0.0080144879
H -3.3245735957 -0.9140985824 0.0060666107
H -2.6956712616 2.1382315395 -0.0031639108
H 4.0430116181 1.1982460253 -0.0125683063

x+ 0.004

C -0.9415516187 -1.164859682 0.0023049535
C -1.6700270777 0.0061350035 0.0005337479
C -1.0261305084 1.2254390265 -0.0038135228
C 0.3461591147 1.2724037219 -0.0063899451
C 1.0635998247 0.0960397797 -0.004570402
C 0.426202873 -1.1295391667 -0.0002153812
O -3.0114972584 0.0129960796 0.0029021589
O -1.7425415072 2.3584261374 -0.0055109529
C 2.5307088339 0.1007659212 -0.0072273097
O 3.068624802 1.3255800253 -0.0116122663
O -1.6892352595 -2.2941214525 0.0065800608
O 3.228140744 -0.8750701681 -0.0057627288
H 1.0151136915 -2.0362310007 0.0011004886
H 0.8402703172 2.2309996139 -0.0098250149
H -1.147133053 -3.0862333947 0.0076191735
H -3.3590116626 -0.8875799925 0.0057148285
H -2.6860354627 2.1524504242 -0.0034314171
H 4.0259042071 1.203624124 -0.0131024709

x- 0.006

C -0.9437143793 -1.148824781 0.0021139181
C -1.670659935 0.018521748 0.0003140856
C -1.0312227896 1.2355867916 -0.0040403464
C 0.3421705876 1.2869298174 -0.0066043454
C 1.0559726518 0.1109930517 -0.0047873988
C 0.4215943101 -1.1133836272 -0.0004381113
O -3.0299551091 -0.0002064184 0.0028319206
O -1.764684666 2.3689783932 -0.0057118256
C 2.5376859004 0.0892364061 -0.0073527408

O 3.0845482588 1.2980401196 -0.0110754875
O -1.6884965488 -2.2902650265 0.0065077345
O 3.1781121222 -0.9172108104 -0.0061869082
H 1.0215116016 -2.0138651648 0.0008750118
H 0.8454923465 2.2415848446 -0.0099482913
H -1.1201523757 -3.0649809406 0.0081206014
H -3.3160398219 -0.9207546938 0.006174271
H -2.6984826935 2.1345055216 -0.003077506
H 4.04788154 1.1963397689 -0.0124205816

x+ 0.006

C -0.9409452172 -1.1681740514 0.0023369439
C -1.6700885629 0.0036822732 0.0005676153
C -1.0252125652 1.2236772858 -0.0037793396
C 0.3468086804 1.2697619205 -0.0063553486
C 1.0656133237 0.0932801548 -0.0045320153
C 0.4271783518 -1.1327161519 -0.0001742151
O -3.0078689417 0.0151879367 0.0029107242
O -1.7386692455 2.3564125599 -0.0054818022
C 2.5294880085 0.1031029559 -0.0072036854
O 3.066091942 1.3310971905 -0.0116981949
O -1.6895785045 -2.2948234747 0.0065958507
O 3.2383248307 -0.8665426109 -0.0057003378
H 1.0141508808 -2.0405519766 0.0011428951
H 0.8390536915 2.2292088337 -0.0098080461
H -1.1532884708 -3.090688977 0.0075295345
H -3.3676252525 -0.8810447284 0.005647949
H -2.6840192865 2.1559229648 -0.0034838737
H 4.0221473373 1.204432895 -0.013220654

x- 0.008

C -0.9440215227 -1.1456665822 0.0020682887
C -1.671003694 0.0210184111 0.000258734
C -1.032376489 1.237839075 -0.0040976198
C 0.3412337921 1.29010569 -0.0066560391
C 1.054863073 0.1142365604 -0.0048358005
C 0.4207378371 -1.110050135 -0.0004864286
O -3.0338086715 -0.00322474 0.0028134674
O -1.7697113295 2.3711326525 -0.0057626878
C 2.5393347553 0.0869344617 -0.0073781881
O 3.0884454435 1.2924474493 -0.0109548933
O -1.6884977096 -2.2894423735 0.0064942222
O 3.1682272321 -0.9255611299 -0.0062829032
H 1.0231387272 -2.0091821693 0.0008280213

H 0.8463364558 2.2440545057 -0.0099810436
H -1.1153339639 -3.0608900854 0.0082273255
H -3.3075558509 -0.927399503 0.0062892395
H -2.7014616326 2.1306777116 -0.0029810274
H 4.0530145476 1.1941952011 -0.0122686672

x+ 0.008

C -0.9402612899 -1.1715448198 0.002368049
C -1.6702104534 0.0012410259 0.0005988024
C -1.0243204138 1.2220282504 -0.0037483881
C 0.3473936706 1.2672136193 -0.0063227908
C 1.067819431 0.0905970251 -0.0044943858
C 0.4281638575 -1.1358863984 -0.0001329572
O -3.0042287727 0.0171936594 0.0029169007
O -1.734975692 2.3544540375 -0.0054563339
C 2.52829903 0.1054534137 -0.0071793459
O 3.0637763021 1.3366405742 -0.0117750225
O -1.6900005871 -2.2954913824 0.0066135377
O 3.2485921137 -0.8579851635 -0.0056501177
H 1.0132747307 -2.044840608 0.0011863455
H 0.8377683619 2.2275303465 -0.0097931932
H -1.1597550133 -3.0952205465 0.0074413288
H -3.3762032893 -0.8745919966 0.0055888044
H -2.6821608643 2.1594066123 -0.0035330856
H 4.0185898783 1.2050273509 -0.0133341477

Zero Field

C -0.9425689036 -1.1583751222 0.0022362189
C -1.6700658504 0.011065172 0.0004575719
C -1.0280493776 1.22925432 -0.0038924016
C 0.3447081456 1.277936365 -0.0064676475
C 1.0600977975 0.1017716766 -0.0046525344
C 0.4243008292 -1.1231587184 -0.0003002421
O -3.0187617453 0.0081369214 0.0028806848
O -1.7508270708 2.3625705989 -0.0055800614
C 2.5332931073 0.0961522815 -0.0072771279
O 3.0743094117 1.3146066717 -0.0114187473
O -1.6887776535 -2.2926327792 0.0065515926
O 3.2079987558 -0.8919911645 -0.0059090597
H 1.0173434861 -2.0274684264 0.0010141541
H 0.8425550776 2.2348811908 -0.0098678283
H -1.1357067912 -3.0775564628 0.0078040694
H -3.3417566506 -0.9007862264 0.0058742704
H -2.6905368491 2.1454385934 -0.0033111618

H 4.0340052816 1.2013801088 -0.0128477501

y- 0.010

C -0.9480915117 -1.1567939838 0.0019169108
C -1.6803262996 0.0074234381 0.0001609666
C -1.0347662134 1.2278237325 -0.0041583287
C 0.3426785884 1.2681567945 -0.0066679521
C 1.0575016692 0.0941429278 -0.0049104971
C 0.417276531 -1.1291189989 -0.0006237593
O -3.030169041 0.0028505636 0.002641111
O -1.7253846529 2.3649311141 -0.0058649262
C 2.5332820294 0.0881873225 -0.0074277759
O 3.0577318729 1.2984242212 -0.0106901558
O -1.6782742449 -2.3190055427 0.0063632308
O 3.2010881465 -0.9127862567 -0.0066358357
H 1.0089786943 -2.0348788521 0.0007126335
H 0.8356366521 2.2288441634 -0.0098773775
H -1.0754261257 -3.0636718647 0.0088495749
H -3.355417398 -0.9021168301 0.0065925575
H -2.6771965833 2.2098514055 -0.0031082995
H 4.0224388868 1.2389616459 -0.011978077

y+ 0.010

C -0.9387521181 -1.1619640391 0.0023799269
C -1.6615719072 0.0140071433 0.000641806
C -1.0220515437 1.2308800999 -0.0036488198
C 0.3475341557 1.2864202991 -0.0062545768
C 1.0625417995 0.1072156886 -0.0044233549
C 0.4307403319 -1.1202316002 -0.0001111559
O -3.0092855278 0.013275362 0.0029811387
O -1.7734881996 2.362079143 -0.0052810231
C 2.533874874 0.1035799895 -0.0070751731
O 3.089693909 1.3325543391 -0.0121001054
O -1.6983075442 -2.2706507494 0.0065169309
O 3.2166867838 -0.8714789711 -0.0051230317
H 1.0241363127 -2.0247627187 0.0011375028
H 0.850481907 2.2404683669 -0.0097763583
H -1.1937982936 -3.0915045691 0.0072670759
H -3.3300962397 -0.9000495913 0.0053777205
H -2.6996137719 2.0899397977 -0.0034847756
H 4.042836072 1.1714470098 -0.0137297271

y- 0.002

C -0.9435309588 -1.1578677362 0.002183961
C -1.6720156358 0.0104169879 0.0004046481
C -1.0293440921 1.2289624672 -0.0039443781
C 0.3442335484 1.2760986689 -0.0065068473
C 1.0595904048 0.1004252121 -0.0047000591
C 0.4229435026 -1.1241141625 -0.0003555296
O -3.0209031284 0.0070837123 0.0028392304
O -1.7459613249 2.3629209892 -0.0056392546
C 2.5332551179 0.094588685 -0.0073089709
O 3.0711008845 1.3112233427 -0.011269576
O -1.6867537662 -2.2975248411 0.0065236614
O 3.2064322324 -0.8961814879 -0.0060722484
H 1.0158000559 -2.0285715271 0.0009639296
H 0.8410542625 2.2337442282 -0.0098722806
H -1.1237823563 -3.0747453806 0.0079946184
H -3.3442917175 -0.9010272169 0.005996082
H -2.6882163889 2.157532426 -0.0032697723
H 4.0319503599 1.2082606327 -0.012673214

y+ 0.002

C -0.9416730858 -1.1589512917 0.0022817348
C -1.6681941712 0.0116875459 0.0005069472
C -1.0267837909 1.2295466513 -0.0038389702
C 0.3452057594 1.2797582087 -0.0064256771
C 1.060585313 0.1030598296 -0.0046035132
C 0.4256328345 -1.1222976172 -0.0002487477
O -3.0167154666 0.0091796501 0.0029171819
O -1.7555890987 2.3622969449 -0.0055166377
C 2.5333348725 0.0976529129 -0.007237884
O 3.0774868689 1.3180295815 -0.0115765487
O -1.6907249902 -2.2879377162 0.0065699874
O 3.2095935583 -0.887857177 -0.0057324408
H 1.0188263268 -2.0265251592 0.0010601704
H 0.844077684 2.2360337536 -0.0098577257
H -1.1474450587 -3.0803586404 0.0076259013
H -3.3393198321 -0.9005717247 0.0057571395
H -2.692701204 2.1337159365 -0.0033536059
H 4.0359644808 1.1947633114 -0.0130333114

y- 0.004

C -0.9445658328 -1.1574658223 0.0021273732
C -1.6740024272 0.0097278039 0.0003499033
C -1.0306593906 1.2286722297 -0.0039963807

C 0.343796653 1.2741924529 -0.0065467162
C 1.0590798626 0.0989804006 -0.0047499522
C 0.4215637664 -1.1251898383 -0.0004145283
O -3.0231024847 0.0060441386 0.0027963331
O -1.7409900101 2.3633266376 -0.0056971068
C 2.5332359755 0.0930251971 -0.0073412013
O 3.0678334981 1.3079270397 -0.0111250753
O -1.6846991039 -2.3026013607 0.0064930472
O 3.204977833 -0.9003289956 -0.0062219914
H 1.0141941445 -2.0298652652 0.0009104738
H 0.8396272842 2.2325586615 -0.009876832
H -1.1118251739 -3.071967311 0.0081879368
H -3.3469333709 -0.901258976 0.0061267775
H -2.685736231 2.1699943778 -0.0032284553
H 4.0297660078 1.2154536297 -0.0124996054

y+ 0.004

C -0.9408435413 -1.1595576076 0.0022964888
C -1.6665898855 0.0123487948 0.000521351
C -1.0255137859 1.2298967198 -0.0037804878
C 0.345859611 1.2813094827 -0.00632979
C 1.0612146184 0.1039880758 -0.0044944149
C 0.4269290277 -1.1219435827 -0.0001866565
O -3.014756219 0.0101213388 0.0028764428
O -1.7598681127 2.362318151 -0.0054537006
C 2.5334222099 0.0991945159 -0.0070828186
O 3.0801033653 1.322033069 -0.0117480365
O -1.6929303562 -2.2833668588 0.0065082577
O 3.2113660268 -0.8837098094 -0.0056444535
H 1.0202236961 -2.026140927 0.0011083932
H 0.845831441 2.2369558241 -0.0097541863
H -1.1593517331 -3.0830320839 0.0075948565
H -3.3365734399 -0.9005975148 0.0056088179
H -2.6942504116 2.1225126581 -0.0033976062
H 4.0372884889 1.1888947543 -0.013348457

y- 0.006

C -0.9456708114 -1.1571525915 0.002064783
C -1.6760490252 0.0090009884 0.0002918374
C -1.0320012605 1.2283851324 -0.0040488268
C 0.3433912334 1.2722364838 -0.0065866779
C 1.0585607789 0.0974534533 -0.0048014364
C 0.4201595371 -1.1263793559 -0.0004782539
O -3.0253794404 0.0049967681 0.0027499207

O -1.7359070017 2.3637972519 -0.0057535328
C 2.5332333274 0.0914351263 -0.0073717302
O 3.0645182106 1.3046943872 -0.0109820512
O -1.6825978127 -2.3078720029 0.0064567719
O 3.2036002535 -0.9044807178 -0.0063639906
H 1.0125233139 -2.0313434938 0.0008517089
H 0.8382479587 2.2313499617 -0.0098797187
H -1.0997736966 -3.0691976716 0.0083921741
H -3.3496718199 -0.9015114455 0.006267771
H -2.6830815761 2.1828543544 -0.0031878984
H 4.027458831 1.2229583717 -0.0123268503

y+ 0.006

C -0.9400688011 -1.1602557774 0.0023260302
C -1.6648656066 0.0129175784 0.0005623816
C -1.0243425085 1.2302138824 -0.0037378227
C 0.3463856798 1.283021745 -0.0063072007
C 1.0616739706 0.1051241441 -0.0044731295
C 0.4282230911 -1.1212931651 -0.0001615899
O -3.0128690755 0.0111496573 0.0029139327
O -1.7644677103 2.3621706297 -0.0053966777
C 2.5335569443 0.1006980877 -0.0070853416
O 3.0833237669 1.3254790978 -0.0118640813
O -1.6947978391 -2.278961954 0.0065139148
O 3.2130785278 -0.8796199903 -0.0054713316
H 1.0215767507 -2.0255422439 0.0011176281
H 0.8473130783 2.2381179839 -0.0097644179
H -1.1709129042 -3.0858062118 0.0074818279
H -3.3343046534 -0.9004364135 0.0055314715
H -2.6961516383 2.1114064426 -0.0034242619
H 4.0392099277 1.1828415072 -0.013467332

y- 0.008

C -0.9468460249 -1.1569285654 0.001995133
C -1.678156587 0.0082337767 0.000229308
C -1.0333700818 1.2281020316 -0.0041024764
C 0.3430182653 1.2702261549 -0.0066268856
C 1.0580344098 0.0958418037 -0.0048547094
C 0.4187305695 -1.127687498 -0.0005475259
O -3.0277347809 0.0039347394 0.0026986238
O -1.730706982 2.3643323397 -0.0058092487
C 2.5332484448 0.0898215071 -0.0074004982
O 3.0611520234 1.3015264317 -0.0108382637
O -1.6804545981 -2.3133392954 0.006413912

O 3.202302766 -0.908634052 -0.0065007837
H 1.0107855286 -2.0330125624 0.0007864383
H 0.8369173413 2.2301134352 -0.0098799324
H -1.0876375789 -3.0664336684 0.0086109478
H -3.3525018356 -0.9017940085 0.0064218219
H -2.6802396209 2.1961328607 -0.0031479788
H 4.0250197416 1.2307895694 -0.012153882

y+ 0.008

C -0.9393717053 -1.1610594893 0.0023538493
C -1.6631937032 0.0134693601 0.0006024994
C -1.0231891592 1.2305432099 -0.0036937518
C 0.3469444775 1.2847231718 -0.0062817507
C 1.0621177322 0.1061986884 -0.0044489734
C 0.4294939532 -1.1207247362 -0.0001361165
O -3.0110445009 0.0121986511 0.0029485196
O -1.7690065038 2.362089712 -0.005338862
C 2.5337125049 0.1021611296 -0.0070821917
O 3.0865189263 1.3289845798 -0.0119825948
O -1.6965905698 -2.2747229266 0.0065165399
O 3.2148522704 -0.8755450984 -0.0052964537
H 1.0228814765 -2.02508516 0.0011276431
H 0.84886393 2.2392868838 -0.0097712467
H -1.182401152 -3.0886308274 0.0073721102
H -3.3321461261 -0.9002549612 0.0054539685
H -2.6979382649 2.1005565473 -0.0034533062
H 4.0410574141 1.1770362655 -0.0135958823

z- 0.010

C -0.930908127 -1.1675574132 -0.0831303471
C -1.6657370725 -0.0030506931 -0.0930591191
C -1.0294380152 1.2203377146 -0.102039088
C 0.3419399082 1.2754088489 -0.0911848528
C 1.0653943822 0.1029750387 -0.1082602657
C 0.4368866107 -1.1243991985 -0.1144277316
O -3.0136471474 -0.0147611944 -0.0691063727
O -1.7586738099 2.3507535842 -0.1032646835
C 2.5397297155 0.1118582573 -0.0974487734
O 3.058121846 1.2784741477 0.273907753
O -1.6629927649 -2.3169680169 -0.055058351
O 3.2242661835 -0.8256502774 -0.3933388045
H 1.0295736547 -2.0283850885 -0.113044588
H 0.8338092341 2.2343295583 -0.0357265536
H -1.2209174644 -2.9986059225 0.459602004

H -3.319539375 -0.8974288393 0.1762128997
H -2.6703855815 2.1465188526 0.1386750796
H 4.014078823 1.1673756416 0.3659857946

z+ 0.010

C -0.9306028172 -1.1670676409 0.0878671242
C -1.6654351497 -0.0025659418 0.0942186996
C -1.0291356637 1.2208573502 0.0943792941
C 0.3422157322 1.27584346 0.0783029344
C 1.0657407668 0.1035328772 0.099026756
C 0.4372765669 -1.1237787895 0.1140152452
O -3.0134877157 -0.0145157043 0.0751321681
O -1.7582917011 2.351280081 0.0922101217
C 2.5400910448 0.1122647414 0.0827769267
O 3.057043505 1.2767977468 -0.296635418
O -1.662674293 -2.3168040779 0.0684141086
O 3.2254881208 -0.8238413458 0.3811381208
H 1.0299996815 -2.0277415113 0.1153212007
H 0.8338743146 2.234457197 0.0159581019
H -1.2224387491 -3.0006300419 -0.4449003665
H -3.3200007726 -0.8984434785 -0.1647325718
H -2.6708259736 2.1459967128 -0.1456586972
H 4.0127241031 1.1655833655 -0.3915397486

z- 0.002

C -0.9420441638 -1.1588823774 -0.0207153872
C -1.6698780743 0.010299877 -0.0232755423
C -1.0281146354 1.2287677216 -0.0257280833
C 0.3445546775 1.2777688555 -0.0240608451
C 1.0603353527 0.1017269017 -0.0262518903
C 0.4248903995 -1.1233242989 -0.0269426218
O -3.0185421972 0.0068228725 -0.0169834359
O -1.7512702494 2.3618986506 -0.0247678382
C 2.5335781521 0.0967433161 -0.0238252793
O 3.0736720693 1.3135917642 0.0446704229
O -1.6875615346 -2.2940099181 -0.0147054177
O 3.2087488971 -0.8896567482 -0.0777663414
H 1.0179219457 -2.0276018152 -0.0268132843
H 0.8421504042 2.2347998631 -0.0130323254
H -1.1403304395 -3.0731522381 0.1100766518
H -3.3401744789 -0.9000964851 0.0516061468
H -2.6895583917 2.1450952328 0.028879316
H 4.0331832666 1.2004338258 0.0649297548
z+ 0.002

C -0.9419672785 -1.1587484294 0.0252620956
C -1.6698019551 0.0104293921 0.0242456037
C -1.0280452199 1.2288869707 0.017964336
C 0.3446136014 1.2778593366 0.0111294236
C 1.0604054503 0.1018412859 0.0169685044
C 0.424976548 -1.1231801156 0.0264069571
O -3.0184937135 0.006911822 0.0228028669
O -1.7511893925 2.3620080345 0.0136043622
C 2.5336430339 0.0968153713 0.0092746315
O 3.0734603622 1.3132643294 -0.0675493078
O -1.687475156 -2.2939212034 0.027929592
O 3.2089678353 -0.8893270502 0.0659648852
H 1.0180184726 -2.0274479167 0.0289400817
H 0.8421620166 2.2348134387 -0.006731705
H -1.1406302361 -3.0736592453 -0.0947905719
H -3.3403202928 -0.9003604278 -0.0398938267
H -2.6896677685 2.1449762081 -0.0355668902
H 4.0329046925 1.2000631992 -0.0906670383

z- 0.004

C -0.9403778105 -1.1602352031 -0.0412640407
C -1.6691288391 0.0082377464 -0.0450214767
C -1.028161241 1.2274353816 -0.046401006
C 0.3442535959 1.2773137995 -0.0409016807
C 1.0610944647 0.101713413 -0.0472329824
C 0.4266951581 -1.1236457628 -0.0519393708
O -3.0177986929 0.003377846 -0.0350017119
O -1.7523483262 2.3601485324 -0.0437445269
C 2.5343571342 0.0986470146 -0.0410979369
O 3.0714005692 1.3099852562 0.10175703
O -1.6839822724 -2.297788764 -0.0323309244
O 3.2110867604 -0.8819991331 -0.1530247241
H 1.0196650953 -2.0278654881 -0.0528449476
H 0.8410710964 2.2345559621 -0.016348403
H -1.1533633247 -3.0614198113 0.2082667071
H -3.3363237682 -0.8985630351 0.092334811
H -2.6869575559 2.1443779771 0.0586102235
H 4.0303789565 1.1969492684 0.1414789605

z+ 0.004

C -0.9402319005 -1.1599794744 0.045822203
C -1.6689842839 0.0084864236 0.0460167287
C -1.0280286767 1.2276684322 0.038668889

C 0.3443668365 1.2774935616 0.0279912173
C 1.0612313022 0.1019424338 0.0379584716
C 0.4268619929 -1.1233635191 0.0514101121
O -3.017709472 0.003538812 0.0408469494
O -1.7521922429 2.3603665068 0.0326355696
C 2.5344876254 0.0987969805 0.0265423578
O 3.0709746741 1.3093126826 -0.1247003974
O -1.6838224973 -2.2976290025 0.0455451976
O 3.2115345501 -0.8813106342 0.1412727574
H 1.0198525708 -2.0275641831 0.0549767497
H 0.8410914449 2.2345874987 -0.003392201
H -1.1539524954 -3.0624062669 -0.1930370573
H -3.3365830051 -0.89907067 -0.0806874171
H -2.6871641319 2.1441550086 -0.0653362199
H 4.0298287088 1.1962004098 -0.1672399107

z- 0.006

C -0.9378623008 -1.1622307712 -0.0579876892
C -1.6681073767 0.0051985138 -0.0634256925
C -1.0283443632 1.2255366928 -0.0657297046
C 0.3437532862 1.2767062349 -0.0575480923
C 1.0622835881 0.1018582526 -0.0678135452
C 0.429443709 -1.1239835114 -0.0746284675
O -3.0166192956 -0.0015978048 -0.0491032145
O -1.753952663 2.3575500822 -0.062853167
C 2.5358051663 0.1018884014 -0.0596532324
O 3.0679746665 1.3029607998 0.1601167936
O -1.6784933485 -2.3031699574 -0.0441764885
O 3.2146697829 -0.8685941759 -0.2331100924
H 1.0222871442 -2.0281472765 -0.0757772689
H 0.8393369378 2.234311372 -0.0212121678
H -1.1725431764 -3.0441646432 0.2994623385
H -3.3312442386 -0.8973049256 0.1254266262
H -2.6830128554 2.1438887355 0.0854917044
H 4.0261863374 1.1905189809 0.2178153599

z+ 0.006

C -0.9376546852 -1.1618787678 0.0626102869
C -1.6679021216 0.0055413805 0.0644773165
C -1.0281522074 1.2258723797 0.0580191524
C 0.3439203358 1.2769731727 0.0446438175
C 1.06248991 0.1022000772 0.0585583305
C 0.4296903034 -1.1235755916 0.07415028
O -3.0164981934 -0.0013921637 0.0550123874

O -1.7537241909 2.357869319 0.0517501272
C 2.5360102485 0.1021248994 0.0450813645
O 3.0673294362 1.3019340881 -0.183067211
O -1.6782640849 -2.3029863908 0.057451977
O 3.2153707384 -0.867515816 0.2213230374
H 1.0225622155 -2.0277143154 0.0779824601
H 0.8393685166 2.2343686585 0.0014534852
H -1.1734551349 -3.0455383964 -0.2844826473
H -3.3315856557 -0.8980109823 -0.1138455457
H -2.683309164 2.1435586607 -0.0922552566
H 4.0253647337 1.1893947882 -0.243569362

z- 0.008

C -0.9347170873 -1.164685443 -0.0716597137
C -1.6670037526 0.0014143896 -0.0790993324
C -1.0288076944 1.2231934503 -0.0842506778
C 0.3429464219 1.2760961283 -0.0744777582
C 1.0637250148 0.1023074408 -0.0882288682
C 0.4328545094 -1.12422016 -0.0954530836
O -3.0152124107 -0.0076728754 -0.0599009716
O -1.7560977636 2.3543606378 -0.0827676183
C 2.5376854607 0.1063406569 -0.0786193391
O 3.0636526052 1.2923520149 0.2178480713
O -1.6715424749 -2.3095563718 -0.0511346729
O 3.2191248396 -0.8497001624 -0.3139494624
H 1.0255974522 -2.0283039712 -0.0957717208
H 0.8368714067 2.2342612002 -0.0279878587
H -1.1953609881 -3.0229439894 0.3827704829
H -3.3254792442 -0.8969493313 0.1527176915
H -2.6775160761 2.1443087775 0.1120641134
H 4.0208407814 1.1806226084 0.2931947186

z+ 0.008

C -0.9344593409 -1.1642554756 0.0763334227
C -1.6667480306 0.0018366353 0.0801951946
C -1.0285589623 1.2236263568 0.0765608901
C 0.3431687107 1.2764502601 0.0615877036
C 1.0640004254 0.1027598205 0.0789889743
C 0.4331736148 -1.123699076 0.0950086812
O -3.0150710723 -0.0074360274 0.0658572898
O -1.7557930483 2.3547842938 0.0716789982
C 2.5379674661 0.106661962 0.0640027874
O 3.0627885457 1.2909906215 -0.2406984049
O -1.6712672973 -2.3093692261 0.0644380551

O 3.2200840444 -0.8482523689 0.3019673664
H 1.0259508591 -2.0277563545 0.0980118331
H 0.8369203279 2.234353354 0.008230349
H -1.1965560561 -3.0246805716 -0.3678898379
H -3.3258919364 -0.8978101062 -0.1412122191
H -2.6778944893 2.143874292 -0.1188958466
H 4.0197472394 1.1791466104 -0.3188712369

Gallic Acid (Radical)

x- 0.010

C -0.9375246767 -1.1953215858 0.0031379567
C -1.7291355106 0.0065417479 0.0013884811
C -1.0077569867 1.2625598589 -0.0034246076
C 0.351826471 1.3219908564 -0.0063917847
C 1.0510429742 0.1274058153 -0.0046833925
C 0.4129691803 -1.1146252412 0.0000471043
O -2.9647093355 0.0383147809 0.0038073082
O -1.7894212152 2.3334596098 -0.0047138875
C 2.5413275205 0.0865030526 -0.0078693846
O 3.0939318085 1.2852467698 -0.0117440755
O -1.6213135738 -2.3459029911 0.007832762
O 3.1443221263 -0.9395921557 -0.0071079889
H 1.0404594363 -1.9972895421 0.0011533034
H 0.8730992761 2.2670285689 -0.009953619
H -1.007713898 -3.0882401068 0.009123968
H -2.6973105667 1.9780911583 -0.0017689072
H 4.0609989701 1.1969524039 -0.0135382363

x+ 0.010

C -0.9313042359 -1.2225942532 0.0032506285
C -1.7287188595 -0.005680612 0.0017427196
C -1.0046971955 1.2578340038 -0.0033646504
C 0.3587790794 1.2992993515 -0.0063530692
C 1.0614230281 0.1025582618 -0.0044846183
C 0.4243557129 -1.1462055773 0.0002418842
O -2.9416760509 0.0140494038 0.0043525821
O -1.7459098951 2.336027335 -0.0047692244
C 2.5220730591 0.1090654191 -0.0074794187
O 3.0669327835 1.3362622397 -0.0125364288
O -1.6408510575 -2.3358333155 0.007672809
O 3.2351665716 -0.8605878117 -0.0058928891
H 1.0325390323 -2.0399096794 0.001363048
H 0.8676427842 2.2494907964 -0.0101226199
H -1.0957995234 -3.1280303489 0.0081403904
H -2.6850687472 2.0616276326 -0.0021301477

H 4.020205514 1.1957501544 -0.0143359955

x- 0.002

C -0.9359505577 -1.2053004404 0.0031713275
C -1.7280854976 0.0021305776 0.0015232805
C -1.006170687 1.2596225748 -0.0033947997
C 0.3553222822 1.3114470414 -0.0063940788
C 1.0533207794 0.1162457591 -0.0046289482
C 0.4173239359 -1.127013187 0.0000955225
O -2.9545519294 0.0300192994 0.0040037061
O -1.77008206 2.3346291565 -0.0047108419
C 2.5329011093 0.0950140743 -0.0077226747
O 3.080283256 1.3053734219 -0.0120988293
O -1.6286275244 -2.3419954662 0.0077583093
O 3.1803655676 -0.9083514315 -0.0064998359
H 1.0357067264 -2.0147404033 0.0012173023
H 0.871741234 2.258250018 -0.0100364524
H -1.0393191291 -3.1028084496 0.00873184
H -2.6910100309 2.0117201999 -0.0018729034
H 4.0419245255 1.1988802551 -0.013846924

x+ 0.002

C -0.9348108878 -1.2106379909 0.0031927976
C -1.7279917933 -0.0003130091 0.0015889409
C -1.0056421297 1.2585928263 -0.003380614
C 0.3566739528 1.3068823322 -0.0063798694
C 1.0553150509 0.111284706 -0.0045833957
C 0.4195932903 -1.1332450642 0.0001369622
O -2.950053967 0.025213048 0.0041067543
O -1.7614432243 2.3351206667 -0.0047210078
C 2.5292007066 0.0994781294 -0.0076365777
O 3.0749813013 1.3153901927 -0.0122626561
O -1.6325135106 -2.3400080875 0.007724082
O 3.198472987 -0.8925997392 -0.0062608593
H 1.0341185368 -2.0231819007 0.0012630011
H 0.870565849 2.2547428253 -0.0100599477
H -1.0566816276 -3.1106831704 0.0085367915
H -2.6886250335 2.028436186 -0.0019500832
H 4.0339324988 1.1986510494 -0.0140193188

x- 0.004

C -0.9364160832 -1.2027421487 0.0031619226
C -1.7282477685 0.0032930995 0.0014900863

C -1.0064909204 1.2602667513 -0.0034020674
C 0.3545542257 1.3139077375 -0.0063965952
C 1.0525489855 0.1188783786 -0.0046457894
C 0.4162139693 -1.1239200248 0.0000800227
O -2.9569283501 0.0322460035 0.0039522205
O -1.7746516679 2.3343634042 -0.0047090373
C 2.5348655529 0.0928415715 -0.0077598411
O 3.0833051814 1.3003743417 -0.0120142077
O -1.6267476822 -2.3429743284 0.0077755752
O 3.1713469813 -0.9161879805 -0.0066361915
H 1.03669856 -2.0104625527 0.0011989718
H 0.8722205511 2.2602210488 -0.0100191835
H -1.0310824871 -3.0990398376 0.0088286339
H -2.6923865525 2.0033405342 -0.0018410676
H 4.0462895048 1.1987170017 -0.0137684525

x+ 0.004

C -0.9341059016 -1.2134499986 0.0032051761
C -1.7280649568 -0.0015955336 0.0016232351
C -1.0054126339 1.2582275296 -0.0033742251
C 0.3572661527 1.3047833342 -0.0063700735
C 1.056560469 0.108953628 -0.0045562476
C 0.4207570342 -1.1364066689 0.0001623291
O -2.9479034527 0.0226075822 0.0041600234
O -1.757351117 2.3353558809 -0.0047295023
C 2.5274168565 0.1017897585 -0.007589785
O 3.0726791983 1.3204671438 -0.012341848
O -1.6345250317 -2.3389917138 0.0077076093
O 3.2075819842 -0.8846546669 -0.0061551701
H 1.033521589 -2.0273702443 0.0012896064
H 0.8698853746 2.2532066616 -0.0100694653
H -1.0658840135 -3.1148182095 0.0084368829
H -2.6875935205 2.0367814905 -0.0019936365
H 4.0302639692 1.1982370263 -0.0141099089

x- 0.006

C -0.9368288814 -1.2002337446 0.0031532904
C -1.7284781947 0.0044163842 0.0014562688
C -1.0068579701 1.260978633 -0.0034095358
C 0.3537187647 1.3164864643 -0.0063965948
C 1.0519148888 0.1216151658 -0.0046598839
C 0.4151174826 -1.1208284715 0.0000671764
O -2.95940598 0.0343696143 0.0039017642
O -1.7793969894 2.3340806014 -0.0047093436

C 2.5369211651 0.0906995521 -0.0077956286
O 3.0865828076 1.2953575605 -0.0119256561
O -1.6249044437 -2.3439502236 0.007793795
O 3.1623369732 -0.924008478 -0.0067857816
H 1.0378210795 -2.0061318453 0.0011827452
H 0.8726149806 2.2623395763 -0.0099989438
H -1.0230858999 -3.095361258 0.0089267979
H -2.6938942337 1.9949396362 -0.001813822
H 4.0509164508 1.1983538329 -0.0136916478

x+ 0.006

C -0.9332938976 -1.2163709167 0.0032190675
C -1.7282115463 -0.0029180901 0.0016600906
C -1.0051876926 1.2579713237 -0.0033692628
C 0.3578095814 1.3028154028 -0.006361601
C 1.0579850721 0.1067226335 -0.0045299695
C 0.4219393337 -1.1396120954 0.0001887558
O -2.9457988806 0.019868866 0.004217472
O -1.753398607 2.3355879027 -0.0047405418
C 2.5256432692 0.1041592446 -0.0075473445
O 3.0705833288 1.3256243737 -0.0124143355
O -1.6365835935 -2.337959053 0.0076937476
O 3.2167300145 -0.8766618364 -0.0060596433
H 1.0330566186 -2.0315482477 0.0013159007
H 0.8691590121 2.2518185704 -0.0100820194
H -1.0754566884 -3.1190876099 0.0083373822
H -2.6866558682 2.0451044352 -0.0020387533
H 4.0267725438 1.1976080967 -0.0141939454

x- 0.008

C -0.9371963908 -1.1977630179 0.0031453442
C -1.7287738445 0.0054996766 0.00142236
C -1.0072777069 1.2617458824 -0.0034170741
C 0.3528113499 1.3191812979 -0.0063948676
C 1.0514136629 0.124457232 -0.004672248
C 0.4140351147 -1.117731976 0.0000563049
O -2.961995724 0.0363929202 0.0038533706
O -1.7843194428 2.3337795099 -0.0047111004
C 2.5390727697 0.0885867345 -0.0078317496
O 3.0901219092 1.2903168392 -0.011835379
O -1.6230940475 -2.3449259487 0.0078128303
O 3.1533296779 -0.9318106621 -0.0069437253
H 1.0390741126 -2.0017423718 0.0011676063
H 0.8729124675 2.2646076595 -0.0099768842

H -1.0153022558 -3.0917631064 0.0090253563
H -2.6955347382 1.9865210404 -0.0017900037
H 4.0558150862 1.1977712904 -0.0136151405

x+ 0.008

C -0.9323643057 -1.2194124812 0.0032342572
C -1.7284283558 -0.0042795806 0.001700186
C -1.0049529435 1.2578348048 -0.0033660936
C 0.3583113776 1.3009854918 -0.0063564996
C 1.0596007534 0.1045909672 -0.0045067382
C 0.4231388127 -1.14287345 0.0002149835
O -2.9437271567 0.0170119334 0.0042819126
O -1.7495837634 2.335814247 -0.004753575
C 2.5238652544 0.1065840531 -0.007511813
O 3.0686715914 1.3308816037 -0.0124798234
O -1.6386913603 -2.3369081592 0.0076824156
O 3.2259205781 -0.8686355154 -0.005970347
H 1.0327269939 -2.0357245609 0.0013400996
H 0.8684052418 2.2505798149 -0.0101005916
H -1.0854162077 -3.1234895866 0.008238193
H -2.6858112828 2.0533889089 -0.0020835779
H 4.0234267724 1.1967745089 -0.0142679882

Zero Field

C -0.935420728 -1.2079259816 0.0031815602
C -1.7279982316 0.0009288345 0.0015559347
C -1.0058907439 1.2590604727 -0.0033875545
C 0.35602737 1.3091050018 -0.0063882655
C 1.0542388876 0.1137152289 -0.0046080576
C 0.4184493634 -1.1301175347 0.0001144897
O -2.9522651021 0.0276801007 0.0040550371
O -1.7656828123 2.3348801648 -0.0047147385
C 2.5310193695 0.0972226265 -0.0076817137
O 3.0775112761 1.3103694229 -0.0121815562
O -1.6305481775 -2.3410085303 0.007741139
O 3.1894031945 -0.9004940515 -0.0063750481
H 1.0348466846 -2.0189756722 0.001238617
H 0.8711870871 2.2564243794 -0.0100496579
H -1.0478367048 -3.1066833091 0.0086349554
H -2.6897596155 2.020082578 -0.0019094648
H 4.0378108826 1.1988592691 -0.0139306763

y- 0.010

C -0.9376047882 -1.2063536515 0.003086067
C -1.741501189 -0.0058528947 0.0013496159
C -1.0189631217 1.2529117274 -0.0033782533
C 0.3580719881 1.3015860927 -0.006364463
C 1.0525250735 0.120036718 -0.004721963
C 0.4056882546 -1.1299060982 0.0000261835
O -2.965854309 -0.0022890486 0.0037333805
O -1.7416937063 2.3376702877 -0.0047622677
C 2.5304942627 0.092665716 -0.0079095738
O 3.0731507992 1.2920411035 -0.0116812173
O -1.620212971 -2.3684081911 0.0078395345
O 3.1731287392 -0.9237769818 -0.0072502851
H 1.0243859447 -2.017823086 0.0011874806
H 0.862805628 2.2561750841 -0.0098681412
H -0.9915280212 -3.0933614178 0.0094617681
H -2.6854079391 2.0964076069 -0.0019829874
H 4.0376073555 1.2214000334 -0.0134698784

y+ 0.010

C -0.9367769233 -1.2100095258 0.0031149555
C -1.7193334762 0.0067510187 0.0015278281
C -0.995223427 1.264294012 -0.0033484377
C 0.3532354108 1.3134934912 -0.0063307457
C 1.0573561055 0.1035126471 -0.0045011805
C 0.4319996207 -1.1304306048 0.0001105807
O -2.9439187832 0.0567495244 0.0044279556
O -1.7860938124 2.335242549 -0.0045439869
C 2.532440481 0.0995511984 -0.0073730938
O 3.0805496216 1.3296018022 -0.0128460495
O -1.6375210225 -2.3190636588 0.0075195972
O 3.209721251 -0.8776833477 -0.0052128202
H 1.0437246031 -2.0231957545 0.0012677228
H 0.8783200649 2.2548144914 -0.0100757542
H -1.0985496863 -3.1212561387 0.0080704683
H -2.690909263 1.9581490175 -0.0018947897
H 4.0360712354 1.1826022784 -0.0146172501

y- 0.002

C -0.9356172312 -1.2075752008 0.0031730117
C -1.7303080176 -0.0003127495 0.0015224013
C -1.0082583357 1.257934939 -0.003388978
C 0.3565447051 1.3078651532 -0.0063863062
C 1.0538028103 0.1153092513 -0.004629867

C 0.4158237636 -1.1300413091 0.0001029947
O -2.9545424829 0.0219103166 0.0040034591
O -1.7612337553 2.335146082 -0.0047342445
C 2.5308635617 0.0965026775 -0.0077303308
O 3.0767417475 1.306672262 -0.0120652106
O -1.6287635395 -2.3460356726 0.0077722176
O 3.1858483034 -0.9050726361 -0.0065810309
H 1.0328126665 -2.018518489 0.0012320179
H 0.8697700776 2.2564768474 -0.0100186088
H -1.0370785994 -3.1039801876 0.008779113
H -2.68924686 2.0339608368 -0.0019327531
H 4.037933186 1.2028808787 -0.0138228854

y+ 0.002

C -0.9353441555 -1.208342613 0.0031871372
C -1.7259242411 0.0021336926 0.0015855657
C -1.0036339644 1.2601952589 -0.0033847165
C 0.3554917203 1.3102216068 -0.0063838757
C 1.0547367814 0.1119955617 -0.0045788596
C 0.42110466 -1.1301991447 0.0001285801
O -2.9502020224 0.0333910536 0.0040946436
O -1.7699998119 2.3347287082 -0.0046946168
C 2.531271785 0.0978603295 -0.007619688
O 3.0782641659 1.3140674059 -0.012300857
O -1.6322171882 -2.3361756382 0.0077042915
O 3.1931090977 -0.8959749248 -0.0061729817
H 1.036863252 -2.0195291024 0.0012498004
H 0.8725563778 2.2563138959 -0.0100711793
H -1.0585022259 -3.1094906906 0.0084985296
H -2.6901422431 2.0067429113 -0.0018875656
H 4.0376600125 1.1951846893 -0.0140592082

y- 0.004

C -0.9359314521 -1.2072519974 0.0031592998
C -1.73284043 -0.001611002 0.0014836261
C -1.0107656576 1.2567537468 -0.0033882498
C 0.3570311262 1.3064807323 -0.0063791454
C 1.0534235759 0.1167767765 -0.0046472713
C 0.4132131989 -1.1299783274 0.0000912735
O -2.9570564537 0.0160439156 0.0039418784
O -1.7566041714 2.3355394738 -0.0047502617
C 2.5307634777 0.0957060154 -0.0077691822
O 3.0759597212 1.3029745632 -0.0119562504
O -1.6268521362 -2.3512992647 0.0077959217

O 3.1824320268 -0.9096984368 -0.0067799643
H 1.0307471411 -2.0181587189 0.001226971
H 0.8682178692 2.2564841885 -0.0099791722
H -1.0260939562 -3.1013262535 0.0089340346
H -2.6885712294 2.0485143228 -0.0019555521
H 4.0380193498 1.2071732658 -0.0137329555

y+ 0.004

C -0.9354261734 -1.2088167783 0.0031897576
C -1.7240506018 0.0033305742 0.0016128356
C -1.0014354133 1.2613705432 -0.0033795247
C 0.3549298312 1.3112486061 -0.006372454
C 1.0552872652 0.1101098195 -0.0045406993
C 0.4238120069 -1.130264838 0.0001464978
O -2.9483283777 0.0390910332 0.0041197589
O -1.7742289446 2.3347050802 -0.004672079
C 2.531589235 0.0983935234 -0.0075410472
O 3.0789638116 1.3178177851 -0.012434569
O -1.6337589866 -2.3315044007 0.0076591199
O 3.1970052615 -0.8914707259 -0.0059602867
H 1.0388298845 -2.020195432 0.0012677108
H 0.873975797 2.2561165478 -0.0100828079
H -1.0691026226 -3.1124043632 0.0083618849
H -2.6904121948 1.9937795688 -0.0018633152
H 4.037442222 1.1918164566 -0.0142157825

y- 0.006

C -0.9363700633 -1.2069364599 0.0031397631
C -1.735561371 -0.0029658896 0.0014409299
C -1.0133964985 1.2555081304 -0.0033857266
C 0.3574603575 1.3049626647 -0.006371363
C 1.0530898307 0.118074621 -0.0046662116
C 0.4106392477 -1.1299305973 0.0000756656
O -2.9597927049 0.0100697929 0.0038745641
O -1.7517963177 2.3360813696 -0.0047602147
C 2.5306757981 0.0948110229 -0.0078078528
O 3.0751225793 1.2992979397 -0.0118582315
O -1.6247956048 -2.3567934804 0.0078132044
O 3.179168154 -0.9143564636 -0.0069571202
H 1.0286456329 -2.017914228 0.0012192456
H 0.8665278461 2.2564398685 -0.0099381311
H -1.0148279545 -3.098677457 0.0090990873
H -2.6877150929 2.0637662332 -0.0019723433
H 4.0380181614 1.2116859329 -0.0136502652

y+ 0.006

C -0.9356929083 -1.2093115806 0.0031883886
C -1.7223473077 0.0045242451 0.0016381239
C -0.9992846996 1.2625334359 -0.0033714031
C 0.3543601861 1.3121778055 -0.0063550896
C 1.0558896815 0.1080630957 -0.0044955494
C 0.426548892 -1.1303116329 0.0001666567
O -2.9466553178 0.0448157419 0.0041314228
O -1.7783376728 2.3348172342 -0.00464542
C 2.5319197702 0.0988328229 -0.0074475483
O 3.0795929898 1.3216706141 -0.012586869
O -1.6351744635 -2.3270264319 0.0076042342
O 3.2010960316 -0.8869310441 -0.0057284299
H 1.0406911331 -2.0209895256 0.001291094
H 0.8754485997 2.2558251107 -0.0100865417
H -1.0795453741 -3.115399308 0.0082244889
H -2.6905480969 1.9811624183 -0.0018337657
H 4.037130557 1.1886699988 -0.0143987924

y- 0.008

C -0.9369299093 -1.2066330925 0.0031152406
C -1.7384501747 -0.0043778031 0.0013962189
C -1.0161312926 1.2542198919 -0.0033824449
C 0.357812268 1.3033276463 -0.0063667016
C 1.0527925265 0.1191674586 -0.0046915063
C 0.4081267794 -1.1299038932 0.0000536464
O -2.962730062 0.0039695327 0.0038054017
O -1.7468240344 2.336788496 -0.0047642924
C 2.5305853685 0.0937998164 -0.0078552857
O 3.0741917841 1.2956542246 -0.0117656827
O -1.6225838698 -2.3624992153 0.0078278033
O 3.1760665044 -0.9190472394 -0.0071141984
H 1.0265208018 -2.0177997526 0.0012057223
H 0.8647204393 2.256337916 -0.0099014525
H -1.0032967586 -3.0960217058 0.0092757461
H -2.6866656477 2.0797204891 -0.001981444
H 4.0378872772 1.2164202301 -0.0135617708

y+ 0.008

C -0.9361575046 -1.2095500698 0.0031385294
C -1.7206889841 0.0056178573 0.0015377841
C -0.9971847114 1.2633851537 -0.003362086

C 0.353732983 1.31288229 -0.0063488782
C 1.0566006538 0.1057453005 -0.0045256171
C 0.4293329815 -1.1303543262 0.0001156117
O -2.9451424904 0.0508095107 0.0043589523
O -1.7823349736 2.334985237 -0.0045870406
C 2.5320776094 0.0992025114 -0.007444872
O 3.0799766091 1.3255677778 -0.0126883663
O -1.6363049459 -2.3229977822 0.007580819
O 3.2053164782 -0.8823162265 -0.0054863217
H 1.0422018753 -2.022086363 0.0012627907
H 0.8769052889 2.2552815878 -0.0100788985
H -1.088778584 -3.1181745459 0.0081734111
H -2.6909527067 1.9697643986 -0.001900667
H 4.0364924216 1.1853606889 -0.0144501508

z- 0.010

C -0.9296267286 -1.2116542505 -0.0036238443
C -1.7249808588 -0.0050285404 -0.0582916355
C -1.0069849059 1.2552052633 -0.022425327
C 0.3550366029 1.3083215648 -0.012079387
C 1.0560716438 0.115055488 -0.0394495926
C 0.4240336494 -1.1308262979 -0.0273008995
O -2.9468719804 0.0170554906 -0.1386578385
O -1.7669040855 2.331510213 -0.0278651406
C 2.5310544033 0.1101079434 -0.1127583919
O 3.0795509611 1.2780454506 0.1975576259
O -1.6212528994 -2.3471033895 0.0454628754
O 3.1790396896 -0.8412123545 -0.4419937181
H 1.0395628192 -2.0199852248 -0.0182082152
H 0.8678550299 2.2563718282 0.0299501947
H -1.069940678 -3.0822026868 0.3330409588
H -2.690407309 2.0226540136 0.0328655316
H 4.0398566465 1.166808489 0.2190718039

z+ 0.010

C -0.9295975584 -1.2115636182 0.0101197504
C -1.7247773765 -0.0047228081 0.0615203231
C -1.006970825 1.2552760459 0.0156495957
C 0.3550669544 1.3083602663 -0.0007736637
C 1.0561946046 0.1153453347 0.0301634528
C 0.4240633898 -1.1306177301 0.027554972
O -2.9463610695 0.0177143221 0.1469808482
O -1.7667727516 2.3316229652 0.0183867797
C 2.531539733 0.110621511 0.0972474884

O 3.0787035595 1.2767120593 -0.2217072636
O -1.621309242 -2.3474892661 -0.0297997883
O 3.1806014495 -0.8391231624 0.4289339907
H 1.0396120096 -2.0197867069 0.0207326117
H 0.8676595371 2.2561877962 -0.0501623765
H -1.0709707629 -3.0837475182 -0.316223622
H -2.6905605065 2.0226397783 -0.0367602788
H 4.0389708549 1.1656937309 -0.2465678199

z- 0.002

C -0.935108496 -1.2080990305 0.0016948324
C -1.7278675368 0.0006401836 -0.0102442235
C -1.005853174 1.2589217541 -0.0068752288
C 0.3560591935 1.3091309965 -0.0071864838
C 1.05433336 0.1138151978 -0.0113677605
C 0.4186893481 -1.1301484408 -0.0054653201
O -2.9520218075 0.027185862 -0.0240499605
O -1.7657529042 2.334785543 -0.0090298624
C 2.5309078727 0.0977283976 -0.0283621257
O 3.0775719019 1.3093146846 0.0279895824
O -1.6302052945 -2.3412571774 0.0151642772
O 3.1887837538 -0.8984870005 -0.0911390564
H 1.0350987446 -2.0189699743 -0.0030834023
H 0.8711462168 2.2564909159 -0.0015789363
H -1.0486609265 -3.1057527873 0.072085557
H -2.6898667807 2.0202406956 0.0047145319
H 4.0378385288 1.1975831802 0.0320285794

z+ 0.002

C -0.9351009202 -1.2080771871 0.0046862415
C -1.7278270938 0.0007062553 0.0133613683
C -1.0058489364 1.2589352913 0.0001012722
C 0.356066057 1.3091369457 -0.0056217774
C 1.0543593221 0.1138687955 0.0021064955
C 0.4186981827 -1.1301089559 0.0056875572
O -2.9519203478 0.0273362306 0.0322057848
O -1.7657329293 2.3348037735 -0.0003868933
C 2.5310023259 0.0978224062 0.012925705
O 3.077397175 1.3090517388 -0.0523469905
O -1.6302245095 -2.341322485 0.0003778058
O 3.1890869868 -0.8980865207 0.0783874171
H 1.0351131517 -2.0189319211 0.0055757215
H 0.8711084357 2.2564524711 -0.0185679385
H -1.0488414534 -3.106059392 -0.0548998364

H -2.6898972686 2.0202278888 -0.0085031166
H 4.0376538222 1.197367665 -0.0597938164

z- 0.004

C -0.9344375908 -1.2085336379 0.0004646486
C -1.7275159492 -0.0000664222 -0.0220603154
C -1.0059868327 1.2584807273 -0.0105576791
C 0.3559376448 1.309046213 -0.0080927605
C 1.054534943 0.1139666594 -0.0181719648
C 0.419341303 -1.1302323919 -0.0109249684
O -2.9514076767 0.0258938485 -0.0522933403
O -1.7658979231 2.3343952091 -0.0137951013
C 2.5308849638 0.0992324476 -0.0495185481
O 3.0778732729 1.3056119273 0.0701638419
O -1.6291252917 -2.3419253786 0.0230203198
O 3.1874395624 -0.8916514204 -0.1789557031
H 1.0356408411 -2.0190899157 -0.0072675984
H 0.8707722853 2.2564877565 0.0066810074
H -1.0511322707 -3.1028733812 0.136518334
H -2.689952945 2.0205554395 0.0110224207
H 4.0381236636 1.1938253195 0.079062407

z+ 0.004

C -0.9344048127 -1.2085567835 0.0056123722
C -1.7275725266 0.0001375077 0.0249791211
C -1.0060267167 1.258574643 0.0039775933
C 0.3558691171 1.3090832358 -0.0044193523
C 1.0545505029 0.1140964861 0.0088587985
C 0.4193750389 -1.1301769091 0.011006921
O -2.9512841914 0.0264225276 0.0602068267
O -1.7659650643 2.3343542829 0.0042120245
C 2.5311747747 0.099332997 0.0336504343
O 3.0777251262 1.3049936021 -0.0943100163
O -1.6293486096 -2.3418725761 -0.0077872067
O 3.1882032937 -0.8909613424 0.165674218
H 1.0357061104 -2.0190699697 0.0099249515
H 0.8705756459 2.2565086499 -0.026521035
H -1.0516535394 -3.103499827 -0.1184116077
H -2.6898774281 2.0200343545 -0.0147619429
H 4.0380452789 1.1937221211 -0.1065971001

z- 0.006

C -0.9333132077 -1.2092642392 -0.0005852
C -1.7269201852 -0.0012273327 -0.0338982268
C -1.0062136703 1.2577319744 -0.0144253622
C 0.3557342235 1.3088783593 -0.009152192
C 1.0548866746 0.1142058186 -0.0250138725
C 0.4204496553 -1.130385708 -0.0162459682
O -2.950350185 0.0238150343 -0.0807722889
O -1.7661312335 2.3337303925 -0.0188334037
C 2.5308808998 0.1018147114 -0.0709164155
O 3.0782816014 1.29902985 0.1136206111
O -1.627300844 -2.3430794032 0.0311338061
O 3.1852596462 -0.8796161624 -0.2686672988
H 1.0365464638 -2.0193270986 -0.0111376531
H 0.8701302401 2.2564550626 0.0146771131
H -1.0553063449 -3.0980571264 0.2016030819
H -2.6900815643 2.0210747735 0.0173131088
H 4.0385398301 1.187344094 0.1265951607

z+ 0.006

C -0.9333028005 -1.2092076268 0.0070011221
C -1.7268036566 -0.0010409526 0.037060914
C -1.0062069162 1.2577770941 0.007644514
C 0.3557503465 1.3088990699 -0.003674335
C 1.0549564309 0.114374067 0.0157487713
C 0.4204637529 -1.1302618961 0.0164767149
O -2.9500531071 0.0242123213 0.0889873116
O -1.7660510749 2.3338057409 0.0093879627
C 2.5311721839 0.1021232147 0.0554685303
O 3.0777682118 1.2982288062 -0.13789436
O -1.6273496811 -2.3433042885 -0.015570267
O 3.1862022707 -0.878355588 0.2558074611
H 1.0365754067 -2.0192057487 0.0136244961
H 0.8700157509 2.2563397593 -0.0348453871
H -1.0558765144 -3.0990078703 -0.1845115647
H -2.6901672207 2.0210832462 -0.0211412351
H 4.0379986173 1.1866636513 -0.1542756492

z- 0.008

C -0.9317105714 -1.2102887789 -0.001999454
C -1.726060587 -0.0028646747 -0.0459856418
C -1.006528666 1.2566449528 -0.0183374128
C 0.355442913 1.3086324743 -0.0104128516
C 1.0553855392 0.1145632965 -0.0320607967

C 0.4220055984 -1.1305802319 -0.0217195671
O -2.9488170421 0.0209125138 -0.109548567
O -1.7664541439 2.3327610024 -0.0234413532
C 2.5309035712 0.1054282799 -0.0919330841
O 3.0787996012 1.2898837624 0.1557307733
O -1.6246860295 -2.3447732042 0.0385263842
O 3.1824003685 -0.8628690022 -0.3558916739
H 1.0378396689 -2.0196254913 -0.0148066051
H 0.8691813999 2.2564032333 0.0225305216
H -1.0614439187 -3.0911919041 0.2669724355
H -2.6902302649 2.0217548816 0.0245915371
H 4.0390645632 1.1783318902 0.1730803556

z+ 0.008

C -0.9316936029 -1.2102136203 0.0084506734
C -1.725902789 -0.0026173538 0.0491750819
C -1.0065194731 1.256704192 0.0115580007
C 0.3554644036 1.3086624261 -0.0024218553
C 1.0554797116 0.1147920226 0.0227889323
C 0.4220250547 -1.1304129217 0.02196052
O -2.9484157869 0.0214404066 0.1178092237
O -1.7663485682 2.3328576113 0.0139774914
C 2.531291803 0.1058383472 0.0764501568
O 3.0781198882 1.2888189019 -0.179926416
O -1.6247430662 -2.3450760815 -0.0229182531
O 3.1836565908 -0.8611994315 0.3429034652
H 1.0378773994 -2.0194632079 0.0173088929
H 0.8690255918 2.2562532172 -0.042714625
H -1.0622276616 -3.0924485343 -0.2499803747
H -2.6903478471 2.0217556846 -0.0284585656
H 4.0383503519 1.1774313414 -0.2006673488

Gallic Acid (Anion)

x- 0.010

C -0.9647452657 -1.1384746789 0.0029842583
C -1.7424171039 0.0232216194 0.0013995355
C -1.0105410229 1.2360247706 -0.0033856657
C 0.3489609301 1.3071490233 -0.0063855838
C 1.0764193444 0.1233213666 -0.0047392845
C 0.4050102346 -1.0809655405 -0.0000689657
O -3.025725337 0.1005283491 0.00336863
O -1.8229488289 2.3271362997 -0.0045463591
C 2.5382755926 0.0795011998 -0.0078108215
O 3.1256105767 1.2821730592 -0.0119272242

O -1.6116858422 -2.3564827733 0.007697723
O 3.1924652126 -0.9267922069 -0.0070126719
H 1.0006617659 -1.9874353106 0.0011303538
H 0.8553616779 2.2614267401 -0.0098925684
H -0.9313559794 -3.033568436 0.0090849862
H -2.6997581431 1.8764687075 -0.0011040808
H 4.0815031883 1.129890811 -0.0134992613

x+ 0.010

C -0.9375111015 -1.187063432 0.0033092162
C -1.7320878268 0.009494836 0.0018404122
C -0.9929934461 1.2495671278 -0.0033886301
C 0.3475101504 1.2981123838 -0.0064816411
C 1.1075691193 0.1003929368 -0.0046653433
C 0.4089241675 -1.1277671051 0.0002652783
O -2.9582232875 0.0512948427 0.0044108185
O -1.7805057044 2.3402418751 -0.0047888576
C 2.5031970556 0.1045431908 -0.0075307486
O 3.093228204 1.3529008134 -0.0123010395
O -1.6490545041 -2.3453232938 0.0079520363
O 3.2962486877 -0.8430290223 -0.0062867461
H 0.9880745728 -2.0442347585 0.0015201365
H 0.8408137885 2.2589048934 -0.0103939077
H -1.0560887614 -3.0975876216 0.0076379917
H -2.6906576999 1.9790533957 -0.0018594269
H 4.0266475858 1.1236219378 -0.0139465488

x- 0.002

C -0.95653227 -1.1536388975 0.0030392095
C -1.7375694162 0.0192312336 0.0014410257
C -1.0021396377 1.2390896198 -0.00332693
C 0.3509715599 1.3019335807 -0.0062263373
C 1.0851195009 0.1135554309 -0.0045103142
C 0.4060337801 -1.0967447795 0.0001106496
O -2.9976589108 0.0873086644 0.0037307542
O -1.8042839322 2.3302479163 -0.0046149866
C 2.5241882435 0.0884234813 -0.0073724169
O 3.108438209 1.3073403699 -0.012328003
O -1.6260838897 -2.3522573502 0.0076705231
O 3.2292658497 -0.8941733255 -0.006727208
H 0.9935976902 -2.0079864664 0.0013829078
H 0.8523574361 2.2585353992 -0.0097808181
H -0.9750367192 -3.0561070201 0.0084991773
H -2.6924064186 1.9073203952 -0.0016083189

H 4.056829925 1.1310447479 -0.0140859141

x+ 0.002

C -0.9504950109 -1.1636482578 0.0030879294
C -1.734989376 0.0163382784 0.0014869268
C -0.9984600906 1.242106243 -0.0033083859
C 0.3506995564 1.3001480666 -0.0061675871
C 1.0916879149 0.1089429358 -0.0044022197
C 0.4071055501 -1.1060299942 0.0002161342
O -2.9830639262 0.077422596 0.0038680289
O -1.7963322537 2.3325603672 -0.0046574305
C 2.5165740031 0.0935391416 -0.0071717409
O 3.1021144946 1.3214819066 -0.0125057727
O -1.6334311675 -2.3499497283 0.0076694595
O 3.2497683651 -0.8771715371 -0.0066273105
H 0.9912999396 -2.0193330343 0.0015109459
H 0.8491485421 2.2581822737 -0.0097674921
H -1.0002877655 -3.0693751511 0.0082135825
H -2.692143488 1.9290959358 -0.0018111697
H 4.0458957124 1.1288129582 -0.0143408984

x- 0.004

C -0.9588698302 -1.1494162755 0.0030058698
C -1.7386405811 0.0203856977 0.0014211083
C -1.0040630204 1.2380082262 -0.0033469083
C 0.3508182871 1.303034433 -0.0063256447
C 1.082616951 0.1158385836 -0.0047059902
C 0.4058207408 -1.0926194898 -0.0000353396
O -3.0044720727 0.0916492096 0.0039215162
O -1.8089211038 2.3289792955 -0.0045879786
C 2.527830526 0.0860920274 -0.0077123398
O 3.1123490333 1.3008668508 -0.0121011757
O -1.622505803 -2.3532212322 0.007745345
O 3.219872357 -0.9024663464 -0.0067532296
H 0.9951199889 -2.0028108627 0.0011964331
H 0.8533798265 2.259048697 -0.0098875018
H -0.9636884144 -3.05010839 0.0087085232
H -2.6942685374 1.8985974735 -0.0015937224
H 4.0627126522 1.1312651024 -0.0136559651

x+ 0.004

C -0.9475290128 -1.1689485366 0.0031630132
C -1.7341029295 0.0148160847 0.0016313916
C -0.9968447929 1.2437131224 -0.0033573752
C 0.3502010958 1.2994588514 -0.0063867997
C 1.0951183272 0.1068019299 -0.0046544444
C 0.4073923557 -1.1109613451 0.0001407894
O -2.9766030409 0.0713403776 0.0041162996
O -1.7918962934 2.3345175783 -0.0046810529
C 2.5129893659 0.0961026241 -0.0075802201
O 3.0990895657 1.32875212 -0.0123017793
O -1.6371939343 -2.3489981699 0.0078272498
O 3.2603680428 -0.8687077741 -0.0064409711
H 0.9901858189 -2.0251402827 0.0013981048
H 0.8473673144 2.2581808355 -0.0101266208
H -1.0131269598 -3.0761071013 0.0081178343
H -2.6908693134 1.9403784451 -0.0017111741
H 4.0405453907 1.1279242407 -0.0138612451

x- 0.006

C -0.9610798174 -1.1454302175 0.0029705321
C -1.7398790931 0.0214749417 0.0013678432
C -1.0060864708 1.2370577067 -0.003343611
C 0.3504453056 1.3042940354 -0.0062952392
C 1.0802978723 0.11825435 -0.004696348
C 0.4055293964 -1.0886258609 -0.0000623924
O -3.0115618615 0.0952028506 0.003876424
O -1.8134212762 2.328104953 -0.0045736943
C 2.5314962766 0.0837872515 -0.0077031784
O 3.1164082637 1.2945130509 -0.0120529117
O -1.6189845234 -2.3542465385 0.007725161
O 3.2105850802 -0.9107688252 -0.0068666067
H 0.9967446667 -1.9976740652 0.0011660529
H 0.8542162205 2.2597349638 -0.0098094877
H -0.9526204674 -3.044263408 0.0088356224
H -2.6956983981 1.8903060968 -0.00159441
H 4.068699826 1.131401715 -0.0136507563

x+ 0.006

C -0.9442158605 -1.1747186612 0.0032063501
C -1.7332167868 0.0131211908 0.00168734
C -0.9953698666 1.2455732663 -0.0033613174
C 0.3494964468 1.2989153424 -0.006395184
C 1.0990432704 0.1046502935 -0.0046295561

C 0.407882846 -1.1162606649 0.0001942405
O -2.9700541053 0.0649584685 0.0041837831
O -1.7879756159 2.3363227613 -0.0047134546
C 2.5094750143 0.098819898 -0.007521679
O 3.0967187541 1.3364611127 -0.0123413863
O -1.6410439917 -2.3478468063 0.0078515378
O 3.2716840688 -0.8601814149 -0.0063940907
H 0.9893256225 -2.0312859112 0.0014567236
H 0.8452705036 2.2583628089 -0.0101801428
H -1.0268805718 -3.0831546724 0.0079566352
H -2.6906663715 1.9528304343 -0.0017692353
H 4.0356176435 1.1265555544 -0.0139375643

x- 0.008

C -0.9629770652 -1.1417771962 0.0029409269
C -1.7410056729 0.0224569532 0.0013381344
C -1.0081425043 1.236342513 -0.0033551153
C 0.3499259034 1.3057296719 -0.0063328806
C 1.0783110196 0.120739334 -0.0047859162
C 0.405372684 -1.0848043757 -0.0001431499
O -3.0185440725 0.098342545 0.0039462313
O -1.8181747205 2.3272349935 -0.0045572811
C 2.5351025105 0.0815650406 -0.0078639771
O 3.1207940736 1.2883556034 -0.0119141895
O -1.6155284698 -2.355178767 0.0077555086
O 3.2015135979 -0.9190656844 -0.0069512236
H 0.9985976114 -1.9926575216 0.0010617892
H 0.8547754749 2.2606616792 -0.0098300667
H -0.942113416 -3.0386635771 0.0089969914
H -2.6976993173 1.8827338272 -0.0015838768
H 4.0748833632 1.1311079611 -0.0134289048

x+ 0.008

C -0.9408291208 -1.1808061381 0.0032548507
C -1.7325421734 0.0113277814 0.0017544514
C -0.9940889058 1.2475417126 -0.0033699398
C 0.3485686533 1.2984660934 -0.0064188608
C 1.1032272195 0.1025166885 -0.0046221209
C 0.4083907771 -1.1218836719 0.0002415666
O -2.9638842545 0.0581945004 0.0042735067
O -1.7841915054 2.3382720595 -0.0047498665
C 2.50617515 0.1016384741 -0.0074887118
O 3.0947869206 1.3445259359 -0.0123533303
O -1.6449904368 -2.3466450087 0.0078889288

O 3.283656861 -0.8515992871 -0.0063484122
H 0.9886359077 -2.0376645467 0.0015051469
H 0.843045911 2.2586103862 -0.0102581322
H -1.0412141964 -3.0903645322 0.0077919532
H -2.6906521436 1.9659219545 -0.0018239659
H 4.0309963366 1.1250705983 -0.0139840638

Zero Field

C -0.9536892049 -1.1585197174 0.0030740652
C -1.7364257423 0.0179287882 0.001503462
C -1.000213952 1.2402098282 -0.003341031
C 0.3509227311 1.3007326837 -0.0063102807
C 1.0884792837 0.1111492264 -0.0046239172
C 0.4063714387 -1.1014208438 0.0000752855
O -2.9906540731 0.0824731494 0.0039463984
O -1.7998261151 2.3318738103 -0.00463294
C 2.5203549395 0.0910667133 -0.0075582901
O 3.1049463944 1.3145766238 -0.0122620093
O -1.6296569424 -2.3513828597 0.0077454992
O 3.2394520664 -0.885711885 -0.0066067942
H 0.9920286887 -2.0138713203 0.0013241689
H 0.8503978317 2.258368479 -0.0099337208
H -0.9869018815 -3.0625439378 0.0084277197
H -2.6915679526 1.9181527695 -0.0016580918
H 4.0510744895 1.1300414921 -0.0138745237

y- 0.010

C -0.9558118407 -1.1551249044 0.0027652216
C -1.7508527102 0.0117315938 0.0011684206
C -1.0116568493 1.2378245955 -0.0033667734
C 0.3422089451 1.293291099 -0.0062391714
C 1.0849487506 0.105286439 -0.004823662
C 0.4037408272 -1.1033070138 -0.0002525715
O -3.0033164748 0.0436077443 0.0037013037
O -1.7734373043 2.3431133901 -0.0045820287
C 2.5194140732 0.081016509 -0.0078962384
O 3.0918940522 1.2917467016 -0.0118396882
O -1.6148322029 -2.3771920932 0.0076532701
O 3.228043941 -0.9129356615 -0.0071951222
H 0.9904325188 -2.0163398111 0.0009691754
H 0.834937751 2.2551428478 -0.0095687468
H -0.9268630616 -3.0427466798 0.00982889
H -2.6896529789 2.0121159191 -0.0017146271
H 4.0458935634 1.1558923246 -0.0133146517

y+ 0.010

C -0.9536725978 -1.1636950749 0.0032515423
C -1.7226852191 0.0234264314 0.0017941258
C -0.9900031453 1.2428798557 -0.0033875994
C 0.3602263025 1.30647818 -0.0066726327
C 1.0905319157 0.1143014027 -0.0048569077
C 0.409020293 -1.1021387284 0.0001008793
O -2.9792837643 0.1217802596 0.0042500839
O -1.8229264907 2.3220150015 -0.0045808523
C 2.5218730596 0.0994381129 -0.0078359527
O 3.1164756023 1.3392365675 -0.0123201928
O -1.6438559024 -2.3294148784 0.0079115223
O 3.2530281908 -0.8581425046 -0.0057985757
H 0.9930746904 -2.0154043186 0.0013219665
H 0.8680686876 2.2596482896 -0.010676092
H -1.0468378216 -3.0824156524 0.0076583463
H -2.6921194311 1.832172655 -0.0011677702
H 4.0541766305 1.1129574013 -0.0136988909

y- 0.002

C -0.9539302387 -1.1576213856 0.0030472814
C -1.7389604307 0.0167499741 0.0014817372
C -1.0024370254 1.2400042563 -0.0033530477
C 0.3491621595 1.2996504912 -0.0063259826
C 1.0876375959 0.1102653533 -0.0046692497
C 0.4060109488 -1.1014022498 0.000034089
O -2.9926715359 0.0751260955 0.0038665424
O -1.7953020246 2.3333730422 -0.0046289037
C 2.5201270709 0.0889050898 -0.0076445093
O 3.102533669 1.309474909 -0.0121821251
O -1.6267457374 -2.3560558937 0.0077521432
O 3.2368260839 -0.891317654 -0.0066998427
H 0.9921138505 -2.0137029599 0.0012864943
H 0.8476382793 2.2578022001 -0.0099179886
H -0.9751278397 -3.0585982812 0.0086034945
H -2.6921112309 1.9359036457 -0.0016176928
H 4.0503274055 1.1345663668 -0.0137394399

y+ 0.002

C -0.953447794 -1.1593807858 0.0031092408
C -1.7335466041 0.0189217853 0.0015599912
C -0.9980869924 1.2409135058 -0.003344884

C 0.3527742192 1.3021443839 -0.0063703116
C 1.0887658012 0.1120296754 -0.0046630802
C 0.4070700471 -1.1012669948 0.0000786569
O -2.9880497237 0.090246541 0.004067359
O -1.8049464314 2.3293816687 -0.0046237571
C 2.5206673225 0.0929211556 -0.0076046975
O 3.1075001625 1.3191548023 -0.0122809089
O -1.6326796567 -2.3463746556 0.0077810847
O 3.2419531953 -0.880003597 -0.0064556338
H 0.99257116 -2.0136377772 0.0013218488
H 0.8541679573 2.2586364137 -0.0100662366
H -0.9995943845 -3.0666461841 0.0082505471
H -2.692036276 1.9000870352 -0.0016247957
H 4.0520089977 1.1259960276 -0.0138414229

y- 0.004

C -0.9542632218 -1.1568671026 0.0030003688
C -1.7418132645 0.0155662858 0.0014184718
C -1.0046972315 1.2394736633 -0.0033471763
C 0.34737712 1.2981994628 -0.0062537151
C 1.0870447857 0.1091891371 -0.0046074814
C 0.4054909464 -1.1016897012 0.0000357648
O -2.9951420683 0.0674759376 0.0037014268
O -1.7901316279 2.3355799743 -0.0046291048
C 2.5199289629 0.086924545 -0.0075507789
O 3.0998772617 1.3047809062 -0.0121857205
O -1.6237053322 -2.3612310634 0.0076968537
O 3.2343950585 -0.8969199119 -0.0068531827
H 0.9918351304 -2.0140556523 0.0013004055
H 0.8443515714 2.2572616851 -0.0097679655
H -0.9628163586 -3.0546586617 0.0088000387
H -2.6919047794 1.9547238902 -0.0016377999
H 4.0492640473 1.1393696057 -0.0138274049

y+ 0.004

C -0.9533748316 -1.1603762736 0.0031628289
C -1.7307824897 0.0200137864 0.001633776
C -0.9960431617 1.2413976965 -0.0033554548
C 0.3545723826 1.3032876263 -0.0064327149
C 1.0892665475 0.1127288072 -0.0046657769
C 0.4075807425 -1.1013647755 0.0001256013
O -2.9857548323 0.0979898423 0.0040353281
O -1.809528912 2.3274246148 -0.0046228824
C 2.5209351879 0.0946275467 -0.007592401

O 3.1096868908 1.3240041951 -0.0123400987
O -1.6354712624 -2.3420440896 0.0078040128
O 3.2445729419 -0.8745801377 -0.0063003809
H 0.9927921735 -2.0138579998 0.0013745482
H 0.8575363272 2.2589312113 -0.0102041256
H -1.0112893084 -3.0706251841 0.0080350252
H -2.6921184833 1.8832256255 -0.0014785115
H 4.0525110876 1.1223405083 -0.0138857737

y- 0.006

C -0.9547065978 -1.1561648035 0.0029093319
C -1.7448124474 0.0143497824 0.0013179387
C -1.0069133452 1.2389779539 -0.0033546395
C 0.3456607015 1.2967348451 -0.0062779529
C 1.0863595476 0.10805778 -0.0047613755
C 0.4048883942 -1.1020372794 -0.0001201715
O -2.9978521736 0.0594553268 0.0038736328
O -1.7847713639 2.3380819652 -0.004609064
C 2.5197084485 0.0850676898 -0.007804108
O 3.0974669196 1.3003999214 -0.011988572
O -1.6208485057 -2.3661790039 0.0077184404
O 3.2321815586 -0.9021784271 -0.0069578191
H 0.9913409901 -2.0145670222 0.0011129492
H 0.8411959504 2.2567081709 -0.0097385957
H -0.9510944304 -3.0506470526 0.0091965999
H -2.6911481636 1.9727162949 -0.0017368046
H 4.0484355172 1.1443468582 -0.0134867901

y+ 0.006

C -0.9533715079 -1.1614356221 0.0031955259
C -1.7280967503 0.0211084854 0.0016838866
C -0.9940073716 1.2418612517 -0.0033607975
C 0.3564157784 1.3043717993 -0.006485169
C 1.0897311228 0.1133389467 -0.0046837994
C 0.4080779751 -1.1015538236 0.0001451352
O -2.9835617064 0.1057314172 0.0040671856
O -1.814049777 2.3255757608 -0.004614345
C 2.5212392359 0.0963436638 -0.0075995615
O 3.1119726124 1.3289969794 -0.0123809007
O -1.6382981918 -2.3377027139 0.0078210014
O 3.2473259878 -0.8690590241 -0.0061489803
H 0.9929370866 -2.014239449 0.0013919074
H 0.8609537201 2.2591943901 -0.0103221789
H -1.0231902361 -3.0745815852 0.0078771142

H -2.6920959231 1.8662380531 -0.0013854127
H 4.053108945 1.1189344703 -0.0139076114

y- 0.008

C -0.9552150695 -1.1555851332 0.0028386262
C -1.7478158012 0.0130698762 0.0012437619
C -1.009260172 1.2384105437 -0.0033607227
C 0.343921631 1.2950748666 -0.0062624856
C 1.0856729786 0.1067413366 -0.0048008857
C 0.4043205046 -1.1025917544 -0.0001906663
O -3.0005483616 0.051568998 0.0038058966
O -1.7792095686 2.3405515724 -0.0045955192
C 2.5195516499 0.083065412 -0.0078656969
O 3.09475047 1.2959978406 -0.011906756
O -1.6178446469 -2.3715941435 0.0076900073
O 3.2300450111 -0.9075871625 -0.0070742864
H 0.9909082964 -2.0153366783 0.0010347675
H 0.8380206722 2.2559885045 -0.0096593463
H -0.938959982 -3.0466838479 0.0095109831
H -2.6905041782 1.99214101 -0.0017332635
H 4.0472575663 1.1498917592 -0.0133814138

y+ 0.008

C -0.9534575764 -1.1625406215 0.0032209264
C -1.725453134 0.0222183072 0.0017279425
C -0.9920077159 1.2423288734 -0.0033666715
C 0.3582846512 1.305409244 -0.0065435208
C 1.0901584351 0.1138593178 -0.004719577
C 0.4085597337 -1.101821349 0.0001490317
O -2.981443168 0.1135519539 0.0041205974
O -1.8184569881 2.3238141692 -0.0046013861
C 2.5215616561 0.0979893452 -0.007633846
O 3.1142255014 1.3340531647 -0.0124011817
O -1.6410814842 -2.3335109137 0.0078413283
O 3.2501349606 -0.8635746247 -0.0059964678
H 0.9930310223 -2.0147634898 0.0013900682
H 0.8644082887 2.2594343658 -0.010447026
H -1.0350104005 -3.0785142821 0.007749504
H -2.6920248302 1.8493815618 -0.0012982367
H 4.0536620481 1.1158079776 -0.013898485

z- 0.010

C -0.774024778 -1.2737209303 -0.0069480037
C -1.6049232993 -0.1414706176 -0.0841449103
C -0.9717300511 1.1137119455 -0.097994882
C 0.381308388 1.2382104608 -0.0566433653
C 1.1769730379 0.0920629969 -0.0276789901
C 0.580680895 -1.168171673 0.0081703656
O -2.8711526511 -0.2443194682 -0.1188353559
O -1.8202510587 2.1744285787 -0.1424208885
C 2.6145652701 0.1725670987 -0.0124405666
O 3.1084101477 1.4251730522 0.1299076034
O -1.4317435478 -2.4597465554 0.0561694664
O 3.3952119437 -0.7453557663 -0.1246568526
H 1.2009474108 -2.0491465916 0.0923118042
H 0.8329423238 2.2187459382 -0.0255885439
H -2.3641393055 -2.1945439411 0.1518657004
H -2.6955130896 1.757319249 -0.0382667219
H 4.0575293642 1.3073792234 0.2524871409

z+ 0.010

C -0.7738123327 -1.2737314153 0.0130729482
C -1.6045162988 -0.1412342426 0.0870299202
C -0.9715235038 1.114011325 0.0909321711
C 0.3813815316 1.23841279 0.0436254987
C 1.1770541808 0.0922435658 0.0182050793
C 0.5808461155 -1.1682137956 -0.0079972502
O -2.8706758248 -0.2443435452 0.1273493294
O -1.819844638 2.1750065735 0.1324763337
C 2.6146965117 0.1727930551 -0.0028104345
O 3.1076678373 1.4244627884 -0.1544929164
O -1.4318244933 -2.4601296865 -0.0406174921
O 3.3956372171 -0.7445060078 0.112091793
H 1.2009327297 -2.0495729569 -0.0893201053
H 0.8327227921 2.218819197 0.0050621794
H -2.3645247334 -2.1949921116 -0.1338293253
H -2.6955666449 1.7575526576 0.0341897497
H 4.0564405538 1.306544809 -0.2796744788

z- 0.002

C -0.9525451708 -1.159222826 -0.0209231496
C -1.7355908247 0.0167034228 -0.0243877746
C -0.9999014939 1.2397412637 -0.0067639397
C 0.3511214752 1.3005566428 0.0013380799
C 1.0889095509 0.1110160146 -0.0139967549

C 0.4077594815 -1.1015051565 -0.0248879903
O -2.9896063103 0.0815138279 -0.0358903401
O -1.8001283302 2.3302530579 0.0060036988
C 2.5211061494 0.0916226297 -0.0246666908
O 3.1051083052 1.3147464876 0.0090322204
O -1.6273906935 -2.3532562078 -0.0186903277
O 3.2404193415 -0.8839773649 -0.063490423
H 0.9933910244 -2.0137868289 -0.0311675808
H 0.8506767992 2.2578326118 0.0232331288
H -0.9976674352 -3.0565616724 0.1474324671
H -2.6918604322 1.9164093863 0.0120217425
H 4.0512895635 1.1310377115 0.0210966338

z+ 0.002

C -0.9524255264 -1.1590960238 0.0269858627
C -1.735444418 0.0168456104 0.027451914
C -0.9999036201 1.2397201206 0.0001406458
C 0.3510921031 1.300474684 -0.014188478
C 1.0889522366 0.1110407484 0.0042407273
C 0.4078919874 -1.101390247 0.0248675879
O -2.9894203636 0.0818173692 0.0440215513
O -1.8002570493 2.3301399391 -0.0150819385
C 2.5212188226 0.0916986606 0.0093281507
O 3.1050244749 1.3145507867 -0.0343106024
O -1.6272381482 -2.3531355423 0.0341630406
O 3.2406425722 -0.8836867698 0.0513068456
H 0.9935653111 -2.0136195738 0.0340023522
H 0.8505292832 2.2576137068 -0.0435396073
H -0.9981925251 -3.0572704879 -0.1309806271
H -2.6921327673 1.9165367779 -0.0148470818
H 4.0511886269 1.1308832408 -0.0482673428

z- 0.004

C -0.9479595674 -1.1621332121 -0.0492680682
C -1.7329571056 0.0123887174 -0.0517596064
C -0.9986299344 1.2369029008 -0.0098832753
C 0.3517294224 1.2990490389 0.0095001729
C 1.0917153653 0.1104663867 -0.025457933
C 0.4127140018 -1.102205283 -0.053989403
O -2.9865857544 0.077153588 -0.0765762751
O -1.8000812489 2.3259960346 0.0187776881
C 2.5241460556 0.0943186663 -0.0426664259
O 3.105345501 1.3166620556 0.0326938212
O -1.617958212 -2.3612546778 -0.053858628

O 3.2451399206 -0.8775355023 -0.1231066122
H 0.9978366721 -2.0142661306 -0.0700191832
H 0.8497063753 2.2561866157 0.0585798823
H -1.039354086 -3.0348418067 0.3067584355
H -2.6913494005 1.9114555579 0.0273421585
H 4.0516329951 1.1347800506 0.0582262517

z+ 0.004

C -0.9477503233 -1.1618072872 0.0555192491
C -1.7327599552 0.0126662847 0.054890769
C -0.998635036 1.2369148826 0.0032057986
C 0.3516479343 1.2989508413 -0.0222323473
C 1.0917794713 0.110584398 0.016109649
C 0.4129500222 -1.1018777316 0.0541624554
O -2.986317484 0.0775446883 0.0846529099
O -1.8001661415 2.3258660586 -0.0280347306
C 2.5243329243 0.0944774708 0.0273177414
O 3.1051539723 1.3163143226 -0.0572756911
O -1.6176143073 -2.3609961132 0.069484612
O 3.2455454352 -0.8770064562 0.1100690137
H 0.9981588824 -2.0138349944 0.0727331889
H 0.8493995939 2.255802306 -0.078661561
H -1.0405137087 -3.0363199891 -0.2902823888
H -2.6914857556 1.9113902755 -0.0305710233
H 4.0513654757 1.1344540435 -0.0857946447

z- 0.006

C -0.7728553737 -1.2751385474 -0.0141510618
C -1.6046653384 -0.1411405525 0.0119507884
C -0.9731736444 1.1146768852 0.0217618121
C 0.3800281272 1.2383704667 -0.0028090319
C 1.1758373592 0.0927456438 -0.0564753831
C 0.5806477336 -1.1690965667 -0.0549119589
O -2.8702317887 -0.247287899 0.0378900083
O -1.8215571901 2.1744191911 0.0651553326
C 2.6113617873 0.1739104609 -0.1013821379
O 3.1109935245 1.4290971067 0.003693436
O -1.4338769233 -2.4607755871 0.0081320388
O 3.3902697847 -0.7438270392 -0.2278971364
H 1.2038990512 -2.0518494766 -0.0594987941
H 0.832828982 2.2181461019 0.0314395833
H -2.3653530867 -2.1905915309 0.1081364644
H -2.6961136911 1.7513775554 0.1479506064
H 4.0670516866 1.3100867876 0.0363084339

z+ 0.006

C -0.7726901284 -1.2750486047 0.0204420339
C -1.6047326785 -0.1412992413 -0.0082340651
C -0.9733546169 1.1143968648 -0.0277932352
C 0.3799729412 1.2382731646 -0.0098867241
C 1.1760749742 0.0930405505 0.0465224444
C 0.5809713513 -1.1688005353 0.0546469713
O -2.8704255138 -0.2477534777 -0.0280295835
O -1.8218897807 2.1739574364 -0.0733607638
C 2.6118528426 0.1744941968 0.0848197926
O 3.1108514209 1.428985791 -0.0296817388
O -1.4338224017 -2.4608302532 0.0076888061
O 3.391193674 -0.7425711121 0.2133521634
H 1.2043054826 -2.0514821 0.0614521287
H 0.8324877544 2.217896604 -0.0515726383
H -2.3656658617 -2.1909771432 -0.0896230651
H -2.6968572562 1.7506620221 -0.1499326066
H 4.0668187969 1.3101788375 -0.0655169199

z- 0.008

C -0.7736064939 -1.2747380299 -0.0225042107
C -1.6056696603 -0.1404259974 0.0057380904
C -0.9731796409 1.1151030743 0.0215651927
C 0.3800796501 1.2382246657 -0.0031165417
C 1.1754968123 0.0928151068 -0.0676297623
C 0.5797320027 -1.1688823295 -0.0680371203
O -2.8708613786 -0.2463116688 0.0319217822
O -1.8198437673 2.1758866565 0.0726133741
C 2.610719059 0.1745037706 -0.1184673567
O 3.1114067866 1.4250150337 0.024079285
O -1.4336946493 -2.4608964122 0.0038131436
O 3.3878291535 -0.7395261915 -0.2818987479
H 1.2025456466 -2.0520071209 -0.0695761103
H 0.8332755242 2.2173351674 0.0441252786
H -2.3625497351 -2.193802149 0.1317512154
H -2.693227339 1.7560021465 0.1781403459
H 4.0666390292 1.3048272778 0.072775142

z+ 0.008

C -0.7734511314 -1.2745361962 0.0280182754
C -1.6055888757 -0.140566957 -0.0023991527
C -0.9732894269 1.1148913477 -0.0272812355

C 0.3800830706 1.2381823847 -0.0090400128
C 1.1757602744 0.0931088607 0.0578273636
C 0.5801110722 -1.1684770421 0.0673818196
O -2.8710043745 -0.2467316982 -0.0221546965
O -1.8202562131 2.1752710695 -0.0799374545
C 2.6113363613 0.1750356114 0.1020170749
O 3.1112034534 1.424581725 -0.0496635469
O -1.4339389811 -2.4607171594 0.0100645134
O 3.3889403228 -0.7382116334 0.2673321679
H 1.2030027414 -2.0515353868 0.07114348
H 0.8331443895 2.2169985471 -0.0631320973
H -2.3632168238 -2.1934894966 -0.1144018668
H -2.6940598079 1.7547542619 -0.1795203593
H 4.0663149487 1.3045647619 -0.1009612723

Gallic Acid (Radical Cation)

x- 0.010

C -0.9385255906 -1.1927522971 0.0023217677
C -1.6700878412 -0.0103093336 0.0004577146
C -1.0196884826 1.2640018697 -0.0041478028
C 0.3636794319 1.3329150346 -0.0068095413
C 1.0477885466 0.1625644772 -0.004893785
C 0.4071453151 -1.1122502784 -0.0003621196
O -2.9810107377 -0.0162198538 0.0028421125
O -1.7570183307 2.3347110151 -0.0057204665
C 2.5499311508 0.0988474885 -0.0075993114
O 3.0968671029 1.2848593268 -0.0106200568
O -1.709239563 -2.2957612152 0.0066615113
O 3.0933692793 -0.9560137385 -0.0067516197
H 1.0553267366 -1.9823277259 0.0007220927
H 0.8680652998 2.2886399579 -0.0102032369
H -1.2004977454 -3.1155524034 0.008606247
H -3.3004784624 -0.9354586306 0.0061209738
H -2.7040447418 2.1298614333 -0.0032135773
H 4.0699796322 1.2314708735 -0.0121179025

x+ 0.010

C -0.9221799584 -1.2278975263 0.002441756
C -1.6823936196 -0.0221701771 0.0006267166
C -1.0255910902 1.2501970717 -0.0038241555
C 0.3653299518 1.2919600861 -0.0063886504
C 1.0491481358 0.1195628026 -0.0045374729
C 0.4216054816 -1.1492192163 -0.0000956589
O -2.9613764959 -0.0103995105 0.0028320595

O -1.7136796757 2.3396728702 -0.0054295833
C 2.537559026 0.1184352467 -0.0071892682
O 3.0633566984 1.3360751493 -0.0119668529
O -1.6937722499 -2.3012847235 0.0065982058
O 3.2006185872 -0.87352374 -0.0052034608
H 1.0461470689 -2.0316797762 0.001116793
H 0.863488267 2.2485628403 -0.0098316016
H -1.2343518605 -3.1498117008 0.0076327999
H -3.3853827902 -0.8943041735 0.0057315441
H -2.6821655496 2.222196615 -0.003595024
H 4.0252010732 1.2448538622 -0.0136251463

x- 0.002

C -0.9287891091 -1.2081575818 0.0023605509
C -1.6728139998 -0.0128636575 0.0005305542
C -1.0211455091 1.2606331652 -0.0040042098
C 0.3638958009 1.3156847883 -0.0066278284
C 1.0453971309 0.1428626943 -0.0047469806
C 0.4117657827 -1.1296898784 -0.0002527095
O -2.9686650656 -0.015481179 0.0028614012
O -1.7377047468 2.3400355622 -0.0055779071
C 2.5423233988 0.1059995565 -0.007347013
O 3.0776807868 1.3063943627 -0.011336493
O -1.7045148617 -2.296145867 0.0066286375
O 3.1358002788 -0.9232358441 -0.0058220346
H 1.0495974145 -2.0048610956 0.0009171778
H 0.8680383072 2.2703515663 -0.0100402097
H -1.2175164351 -3.1289592884 0.0080585507
H -3.3239003905 -0.9243618814 0.0059425989
H -2.6939865152 2.172014457 -0.0033756447
H 4.0460987321 1.2410061207 -0.012875441

x+ 0.002

C -0.9260856438 -1.2150095641 0.0023859015
C -1.6756432502 -0.0157214002 0.0005634219
C -1.0226460192 1.2573666952 -0.0039453281
C 0.3644517863 1.3074964893 -0.0065497069
C 1.0458403492 0.1347253939 -0.0046805192
C 0.4146567381 -1.136504592 -0.0002059764
O -2.9653817154 -0.0138464435 0.0028573716
O -1.7290332682 2.3403511948 -0.0055308868
C 2.5400242649 0.1100825365 -0.0072884979
O 3.0718545583 1.3164070856 -0.0115505724
O -1.7009267209 -2.2976706108 0.006615961

O 3.1571933421 -0.9067401783 -0.0055927309
H 1.0477979308 -2.0141558645 0.0009789531
H 0.8668092607 2.2626055568 -0.0099700483
H -1.223035768 -3.1357442457 0.0079170223
H -3.3426027345 -0.915232202 0.0058717435
H -2.6896945477 2.1898797701 -0.003458286
H 4.0379824375 1.2429363788 -0.0131248219

x- 0.004

C -0.9303577683 -1.2045992107 0.0023479927
C -1.6715994373 -0.0115391414 0.0005127605
C -1.0204867374 1.2621639703 -0.0040334027
C 0.3634989993 1.3198844085 -0.0066650825
C 1.0454613236 0.1470931168 -0.0047775926
C 0.4105076518 -1.1261406741 -0.00027333
O -2.9707231152 -0.0162651657 0.0028591776
O -1.7423747773 2.3397055049 -0.0056012816
C 2.5437909135 0.1040035662 -0.0073770609
O 3.081221931 1.3012523688 -0.0112313389
O -1.7062403493 -2.2954512292 0.0066335548
O 3.1252094839 -0.9314434393 -0.0059422703
H 1.0508092643 -2.0000314558 0.0008889337
H 0.8684119846 2.2744206308 -0.0100731059
H -1.2146392148 -3.1255812673 0.0081324224
H -3.3154175052 -0.9285725899 0.0059762161
H -2.6963439329 2.1626838586 -0.0033318884
H 4.0508322858 1.2396427486 -0.0127517041

x+ 0.004

C -0.9249444479 -1.2183039444 0.0023983649
C -1.6772219456 -0.0172674729 0.0005790688
C -1.0234466768 1.255642011 -0.0039149633
C 0.3646694959 1.3035501148 -0.0065090057
C 1.046345567 0.130862449 -0.0046457591
C 0.4162567052 -1.1397425662 -0.000181202
O -2.9641084297 -0.0129939449 0.0028524652
O -1.7249906369 2.3403170487 -0.0055058802
C 2.5391499891 0.1121608633 -0.0072600457
O 3.0694869523 1.321294837 -0.0116547869
O -1.6990843396 -2.298522019 0.0066083388
O 3.1678530243 -0.8985297063 -0.0054883754
H 1.0471922377 -2.0185889077 0.0010100801
H 0.8660178117 2.2589701535 -0.0099332876
H -1.22568718 -3.1391635438 0.0078507189

H -3.3527164035 -0.9103094471 0.005835562
H -2.6877179647 2.198315683 -0.0034951369
H 4.0345072414 1.243534392 -0.0132531558

x- 0.006

C -0.9330126145 -1.2007770445 0.0023345759
C -1.6709605532 -0.0112611999 0.0004959266
C -1.0201816802 1.2627664567 -0.0040720218
C 0.3638624503 1.3242771399 -0.0067187881
C 1.0461088863 0.1523700599 -0.0048270267
C 0.4090721445 -1.1214451291 -0.0003149074
O -2.9738242953 -0.0161858192 0.0028601548
O -1.747053216 2.3378392878 -0.0056386667
C 2.5456159912 0.1023510515 -0.0074566251
O 3.0862899353 1.2959124485 -0.0110288242
O -1.7073365701 -2.295687188 0.0066365161
O 3.1144648757 -0.9396500959 -0.0061836241
H 1.051922225 -1.9940908802 0.000816308
H 0.8684571604 2.2792574177 -0.0101210043
H -1.2099271691 -3.122325916 0.0083062943
H -3.3101168142 -0.9308012618 0.0060263867
H -2.6988387997 2.1516468213 -0.0032889643
H 4.0570190437 1.2370298513 -0.0125327096

x+ 0.006

C -0.9239007021 -1.2215805034 0.002410115
C -1.6789519869 -0.0188984139 0.0005996884
C -1.0242969149 1.2538538682 -0.0038943937
C 0.3648480984 1.2996419107 -0.0064982249
C 1.0470525575 0.127065991 -0.0046460338
C 0.4179747962 -1.142917205 -0.0001765046
O -2.9630238338 -0.0121726551 0.0028699167
O -1.721092627 2.3401631381 -0.0054841251
C 2.538415972 0.1143142401 -0.0072984817
O 3.0674934162 1.3262239361 -0.0117240641
O -1.6971946847 -2.2994078497 0.0066151459
O 3.1786819012 -0.890168755 -0.0053758339
H 1.046712145 -2.0229814218 0.0010138336
H 0.8650737766 2.2554453623 -0.0099388285
H -1.228398144 -3.1426593028 0.0077949051
H -3.3634089168 -0.9051384059 0.0058321204
H -2.6858376431 2.206591932 -0.0035192236
H 4.0314137904 1.2438501339 -0.013287011

x- 0.008

C -0.9356260303 -1.1968174522 0.0023246738
C -1.6703837095 -0.0106881272 0.0004799547
C -1.0198447286 1.2635053241 -0.0041136776
C 0.3638347684 1.3286195014 -0.0067805457
C 1.0468625431 0.1574172074 -0.0048820152
C 0.4079766165 -1.1169326695 -0.0003533024
O -2.9771726273 -0.0162973723 0.0028667422
O -1.7519770859 2.3363628768 -0.0056763085
C 2.5476657714 0.1005565381 -0.0075571691
O 3.0913177282 1.2904583764 -0.0108280163
O -1.7084506017 -2.29566356 0.0066524056
O 3.1038318334 -0.9478965824 -0.0064224312
H 1.0534396962 -1.9883164771 0.0007514181
H 0.8683858768 2.2839347921 -0.0101845962
H -1.20547993 -3.1189607019 0.0084538504
H -3.3046732594 -0.9333886822 0.0060890284
H -2.7013932398 2.1408410473 -0.0032413364
H 4.0632473785 1.2344919611 -0.0122856746

x+ 0.008

C -0.9229650733 -1.2248043354 0.0024213161
C -1.6807969398 -0.0206098784 0.0006211188
C -1.025171528 1.25202098 -0.0038759666
C 0.3650085405 1.2958345181 -0.0064939586
C 1.0479592877 0.1234022867 -0.0046541945
C 0.4197818659 -1.1459844409 -0.0001763113
O -2.9621317905 -0.0113711243 0.0028914435
O -1.7173739842 2.3398783735 -0.0054628297
C 2.5378291964 0.1165157748 -0.0073523765
O 3.0658702585 1.3311336576 -0.0117825679
O -1.6952827308 -2.3003436628 0.0066245376
O 3.1895248706 -0.8817826997 -0.0052649841
H 1.04637917 -2.0272591144 0.001010794
H 0.8640142382 2.2520887475 -0.0099532622
H -1.2311353567 -3.1462112176 0.0077435509
H -3.3745809623 -0.8997373327 0.0058365478
H -2.684070366 2.214560352 -0.0035386407
H 4.0287023037 1.2438951161 -0.0133012164

Zero Field

C -0.9273292937 -1.2116468991 0.0023633245
C -1.6740078759 -0.0141660809 0.0005658494

C -1.0219503638 1.259024826 -0.0040157456
C 0.3641915613 1.3116183845 -0.0067124231
C 1.0454595254 0.1388005142 -0.0048617375
C 0.4131880451 -1.1331823968 -0.0003233052
O -2.9668153054 -0.0146691542 0.0029584087
O -1.733469595 2.3402217353 -0.0055657418
C 2.5411384507 0.1080084644 -0.0075840506
O 3.0747603571 1.3112620332 -0.0113159309
O -1.7029683239 -2.2967363594 0.0066686568
O 3.1464324188 -0.9150583763 -0.0056382085
H 1.0489465868 -2.0093845121 0.0008173763
H 0.8672433612 2.2665945791 -0.0101743657
H -1.2206071021 -3.1322590946 0.0080442909
H -3.3326881393 -0.9199796777 0.0060407471
H -2.6919726019 2.1808578488 -0.003364601
H 4.0420092948 1.2419191656 -0.012608544

y- 0.010

C -0.9446789115 -1.1998052404 0.0022234657
C -1.6954248664 -0.0252104106 0.0004657416
C -1.0365042145 1.2453330231 -0.0040586417
C 0.3729985517 1.3047249673 -0.0067454625
C 1.0534658749 0.1464570243 -0.0049189411
C 0.4013970834 -1.1169795154 -0.0004466551
O -2.996270183 -0.0163385449 0.0027809124
O -1.7144378604 2.3283465207 -0.0056695145
C 2.5478609616 0.098320238 -0.0075162778
O 3.0804227026 1.2889469253 -0.0107922536
O -1.6839747926 -2.3299444622 0.0065318273
O 3.1360308008 -0.9423647716 -0.0065304133
H 1.0339059095 -1.9964087353 0.0007066342
H 0.8581602577 2.2715041356 -0.0100712051
H -1.1355679607 -3.1192076162 0.0088106687
H -3.3710567125 -0.9122782449 0.0061782162
H -2.6850430515 2.2278801512 -0.0034088042
H 4.0502774109 1.2582505558 -0.0122462971

y+ 0.010

C -0.9148240228 -1.2139201031 0.0023318938
C -1.6680042805 0.0072795634 0.0005330784
C -1.0187600051 1.2720536131 -0.0037548321
C 0.3295944083 1.2971489254 -0.0062055428
C 1.0436449273 0.0870328073 -0.0043325153
C 0.4511250167 -1.1552911568 -0.0000837164

O -2.9572178318 -0.0066035606 0.0027595392
O -1.7510509773 2.3781160034 -0.0051836872
C 2.5401473404 0.0989857345 -0.0068932782
O 3.0508603909 1.3284019741 -0.0127720754
O -1.6875601827 -2.2627864183 0.0062901131
O 3.1844982569 -0.8921357379 -0.003758069
H 1.0699810272 -2.0437179977 0.0011873833
H 0.8595794417 2.2368219284 -0.0096435348
H -1.251016163 -3.1323249088 0.0073778531
H -3.328726672 -0.9123136109 0.0054638363
H -2.6972196812 2.1824061413 -0.0035367052
H 4.0165100071 1.2420728033 -0.0144867409

y- 0.002

C -0.931055957 -1.2092232567 0.0023637027
C -1.6783414113 -0.0169664322 0.0005403529
C -1.0246663632 1.2555928309 -0.0039939357
C 0.3674064297 1.3105480336 -0.0066205482
C 1.0474012724 0.142345466 -0.0047448561
C 0.4097412664 -1.1292012809 -0.0002497454
O -2.9727063401 -0.0148922497 0.002848522
O -1.7292415607 2.3362505737 -0.0055987162
C 2.5426082592 0.1069910781 -0.0073379587
O 3.0766398995 1.3071204025 -0.0112940559
O -1.7001836758 -2.3038502953 0.0066347646
O 3.1434041689 -0.9203410755 -0.0059391482
H 1.0452070011 -2.0057579289 0.0009302527
H 0.8664966138 2.2680572745 -0.0100207566
H -1.2044675911 -3.1303857029 0.0081019406
H -3.3406776853 -0.9181365839 0.0059590941
H -2.6904471271 2.188186417 -0.0034274921
H 4.0444438007 1.2448887299 -0.0128584167

y+ 0.002

C -0.9234455538 -1.2138010161 0.0023785026
C -1.6704034398 -0.0108464635 0.0005481444
C -1.0193581217 1.2629940674 -0.0039496866
C 0.3596347697 1.3117888727 -0.0065408555
C 1.0434902622 0.1329352595 -0.0046650428
C 0.4177114307 -1.1378087136 -0.0002006908
O -2.9613717778 -0.0145697567 0.0028582189
O -1.7371010936 2.345839804 -0.0054997053
C 2.5394129603 0.1081417196 -0.0072666245
O 3.070863367 1.3154197984 -0.0116348806

O -1.7038941814 -2.2898513351 0.006599389
O 3.1501809543 -0.910158738 -0.0054224081
H 1.0524905738 -2.0145837659 0.0009845117
H 0.8682180589 2.2634691895 -0.0099697778
H -1.2339350976 -3.1336666622 0.0078396728
H -3.3256395133 -0.9216888624 0.0058448228
H -2.692918823 2.1771005411 -0.0034118203
H 4.0376262252 1.2405120613 -0.01319877

y- 0.004

C -0.9348887027 -1.2067391378 0.0023389369
C -1.6826346093 -0.0195203689 0.0005351154
C -1.0276489636 1.2522643682 -0.0040142332
C 0.3698119602 1.3093581673 -0.0066735573
C 1.0492900159 0.1449238687 -0.0048072033
C 0.4069240333 -1.1253885796 -0.0003043034
O -2.9788473548 -0.0149498143 0.0028545436
O -1.7256346742 2.3328940015 -0.0056304374
C 2.5442745646 0.1054818375 -0.0074212331
O 3.0790535016 1.3027509752 -0.0111288709
O -1.6970117331 -2.3103924323 0.0066377418
O 3.1414283341 -0.9254225967 -0.0061206177
H 1.0419837382 -2.0023912101 0.0008653775
H 0.8644787688 2.2696255001 -0.0100652212
H -1.1881837713 -3.1279511455 0.0082608145
H -3.3489155931 -0.916151732 0.006029495
H -2.689329697 2.1954887932 -0.0034220787
H 4.0474111822 1.2473455056 -0.0126412685

y+ 0.004

C -0.9196521558 -1.215552348 0.00237795
C -1.6671780952 -0.0069085853 0.000551578
C -1.0172539461 1.2669596279 -0.0039420515
C 0.353849254 1.3110284055 -0.0065291553
C 1.0417560784 0.1249027502 -0.0046642446
C 0.4236926281 -1.1428389028 -0.000205194
O -2.9566048575 -0.0139617048 0.0028836755
O -1.740883642 2.3527509635 -0.005435855
C 2.5379226396 0.1073271635 -0.00730256
O 3.0659132978 1.3193282778 -0.0118349403
O -1.7033788416 -2.2826437638 0.0065689836
O 3.1551924031 -0.9054480944 -0.0050179213
H 1.0569190043 -2.0206556886 0.0009791313
H 0.8681452473 2.2593590364 -0.009985163

H -1.2453118457 -3.1345275417 0.007708234
H -3.319821785 -0.9225337235 0.005827998
H -2.693951943 2.1750728995 -0.0033853419
H 4.0322075592 1.2395672289 -0.0133021235

y- 0.006

C -0.938315227 -1.2043088385 0.0023115763
C -1.686982416 -0.0216043066 0.0005213215
C -1.030696282 1.2495744671 -0.0040312078
C 0.3713518869 1.3078723895 -0.0067064561
C 1.0508810791 0.1462014219 -0.0048494648
C 0.4047369602 -1.1222523564 -0.0003457426
O -2.9848125421 -0.0153223132 0.0028425559
O -1.7219241689 2.3307140171 -0.0056538147
C 2.5456817189 0.1034376116 -0.0074669388
O 3.0802142287 1.2981652836 -0.0110036563
O -1.6931313553 -2.3169238728 0.0066241139
O 3.1395208539 -0.9309263836 -0.0062734924
H 1.0391680889 -1.9998749279 0.0008207006
H 0.8624505858 2.2704939496 -0.0100825111
H -1.1710213962 -3.1252149799 0.0084044488
H -3.356624719 -0.9146522614 0.0060876617
H -2.688053376 2.205195559 -0.0034192555
H 4.0491170799 1.2506515409 -0.0124868385

y+ 0.006

C -0.9166451665 -1.2161859712 0.0023639157
C -1.6656436316 -0.0022704041 0.0005348894
C -1.0164324744 1.27043861 -0.0038659623
C 0.3460163785 1.3084725137 -0.0063790423
C 1.040677463 0.1137829478 -0.004503054
C 0.4314297783 -1.1478696333 -0.0001300945
O -2.9540303314 -0.0129464855 0.0028035438
O -1.7447051952 2.3611573065 -0.005352582
C 2.5373867392 0.105259995 -0.0070656906
O 3.0608836185 1.3223364181 -0.0122054222
O -1.7003178344 -2.2754439008 0.0064717866
O 3.1626717792 -0.9010719066 -0.0046102856
H 1.0613125806 -2.0280426607 0.0010950591
H 0.8664410141 2.2532860804 -0.0098147907
H -1.2514768204 -3.1340179443 0.0075726965
H -3.3177320439 -0.9219402513 0.0056534025
H -2.6952174059 2.1764159775 -0.0034388304
H 4.0269425524 1.2398653088 -0.013836539

y- 0.008

C -0.9414422043 -1.2019758741 0.0022803025
C -1.6913147567 -0.023409457 0.0005054683
C -1.0338063492 1.2473741966 -0.0040523105
C 0.3722833526 1.3062656016 -0.0067486569
C 1.0522356015 0.1466434526 -0.0049054661
C 0.4029425817 -1.1196003185 -0.0003953754
O -2.9906098964 -0.0159788563 0.0028362818
O -1.7182185687 2.3293730188 -0.0056750267
C 2.546907871 0.1010329551 -0.0075371489
O 3.0806938837 1.2934268366 -0.01087947
O -1.6888256131 -2.3234388793 0.0066115498
O 3.1376835529 -0.9366858018 -0.006399549
H 1.0366444296 -1.997936018 0.0007672558
H 0.8602652622 2.2710356232 -0.0101132368
H -1.153472972 -3.1222803703 0.0085491178
H -3.3638297204 -0.9136321454 0.0061619746
H -2.6866822447 2.2165888695 -0.0034121761
H 4.0501067903 1.2544231668 -0.0123005341

y+ 0.008

C -0.9147902432 -1.2158438077 0.0023483343
C -1.6656668338 0.0026298663 0.0005115321
C -1.0166925947 1.272371048 -0.003777149
C 0.3378367281 1.3039206188 -0.0061864636
C 1.0409955127 0.1007788083 -0.0042988226
C 0.440671869 -1.1522877744 -0.0000352411
O -2.9538309445 -0.0104052627 0.0026922634
O -1.7479249241 2.3699598266 -0.0052364526
C 2.5376603361 0.1020989797 -0.006740811
O 3.0548192811 1.325583924 -0.012713282
O -1.6949447279 -2.2688572408 0.0063227117
O 3.1721766392 -0.8968006672 -0.004043087
H 1.0661422305 -2.0357567222 0.0012363219
H 0.8640623644 2.2455209389 -0.00957567
H -1.253339685 -3.1333140205 0.0073993207
H -3.3201090101 -0.9185473391 0.0054407227
H -2.6961241425 2.1792496173 -0.0034982189
H 4.0206191446 1.2409252068 -0.0145530092

z- 0.010

C -0.9190747787 -1.2136014454 -0.0178892287
C -1.670078751 -0.018623545 -0.0303465864
C -1.0232883653 1.2569242211 -0.0736141391
C 0.3616163995 1.3137494048 -0.0869000503
C 1.0481174257 0.1431510379 -0.071855757
C 0.421056653 -1.1315919323 -0.0574195585
O -2.9622868318 -0.0250572842 -0.0105016796
O -1.7393482536 2.3357117427 -0.101938884
C 2.5425679739 0.12685852 -0.1107029507
O 3.0680046648 1.2510454733 0.3153953095
O -1.6881236891 -2.3059587766 0.0035565328
O 3.1422597615 -0.8198226637 -0.5129590794
H 1.0540906971 -2.0093114607 -0.0669697992
H 0.8612250584 2.2708237731 -0.0723713515
H -1.2495253131 -3.0964944247 0.3434086726
H -3.3193411184 -0.9272761762 0.1058213462
H -2.6902595948 2.1805531236 0.0255075187
H 4.0339490621 1.1801464124 0.3750726846

z+ 0.010

C -0.9191237205 -1.2133812474 0.0228897402
C -1.6700391891 -0.0185557827 0.0315627042
C -1.0230893752 1.2571873654 0.065440528
C 0.3620402824 1.3142122189 0.0734218072
C 1.0484490548 0.1437137137 0.0622501235
C 0.421141922 -1.1311142705 0.0570545363
O -2.9624174958 -0.025048472 0.0165675228
O -1.7389574954 2.3360528056 0.090312454
C 2.5430420404 0.1273289309 0.0958778801
O 3.0670758397 1.2492945852 -0.3374498232
O -1.6880565681 -2.3061999266 0.0103424683
O 3.1438253632 -0.8176150595 0.5006462883
H 1.0542481353 -2.0087603765 0.0691345415
H 0.861455018 2.2712712718 0.0519140891
H -1.2508035535 -3.0978714267 -0.3285279462
H -3.3196935206 -0.9279093134 -0.0936061836
H -2.6903881732 2.1802807962 -0.0325496362
H 4.0328524356 1.1783401874 -0.3999880942

z- 0.002

C -0.9270323536 -1.2117271384 -0.0024524718
C -1.6740052394 -0.0144255575 -0.0059746429
C -1.0219438365 1.2589484758 -0.0177648182

C 0.3640474657 1.3116150986 -0.0220969865
C 1.0455838506 0.138856992 -0.0177270109
C 0.4134651573 -1.133133569 -0.0119969864
O -2.966688305 -0.015108417 0.000143044
O -1.7335624402 2.340067418 -0.0243056217
C 2.5410905252 0.1087216393 -0.0277944177
O 3.0744359783 1.3092979095 0.0531833324
O -1.7021654235 -2.2972397464 0.0046282147
O 3.146124813 -0.911575257 -0.1064704542
H 1.0488028004 -2.0096119923 -0.0136349565
H 0.8672417747 2.2665429806 -0.0213773468
H -1.2214049764 -3.1307553534 0.0748831899
H -3.332343701 -0.9201777876 0.0268496847
H -2.6917334555 2.1810680796 0.0025682625
H 4.0416483659 1.2398622251 0.0646329853

z+ 0.002

C -0.927041549 -1.2116784011 0.0072141529
C -1.6739978093 -0.0144050244 0.0070754819
C -1.0219056506 1.2590041792 0.0098010593
C 0.3641250897 1.3117073537 0.008893903
C 1.0456422629 0.1389659788 0.0082853142
C 0.4134803594 -1.1330353145 0.0115492168
O -2.9667156213 -0.015097053 0.0055933773
O -1.7334894035 2.3401365768 0.013176806
C 2.5411793156 0.1088197603 0.0131496288
O 3.0742325964 1.3089197766 -0.0760605409
O -1.7021550992 -2.2972643015 0.0086618465
O 3.1464319708 -0.9110991508 0.0950477463
H 1.0488381984 -2.0094940261 0.0155671745
H 0.8672816068 2.266628571 0.0013254685
H -1.2215639451 -3.1310880412 -0.0589712933
H -3.3324308218 -0.9202920771 -0.0150145087
H -2.6917563917 2.1810307646 -0.0094134576
H 4.0414058918 1.2394664289 -0.0905883756

z- 0.004

C -0.9260085894 -1.2119930371 -0.0069342135
C -1.6734850225 -0.0149288426 -0.0123882958
C -1.0220888788 1.258723634 -0.0316857493
C 0.3637016199 1.311857642 -0.037766332
C 1.0458595683 0.1393039783 -0.0308034827
C 0.4144442097 -1.1330316204 -0.0235727057
O -2.9660772664 -0.0164039362 -0.0025618038

O -1.7343151176 2.3395569957 -0.0434603603
C 2.5412229215 0.1109828739 -0.0486533125
O 3.073691257 1.3023064689 0.1193203328
O -1.7004582932 -2.298308204 0.0032223384
O 3.1454438143 -0.9003810039 -0.2095325083
H 1.0494562033 -2.0096751402 -0.0278856639
H 0.8665699265 2.266993909 -0.0331159573
H -1.2250573586 -3.1263556364 0.1424813536
H -3.3305170912 -0.9210897999 0.0475761454
H -2.6915710463 2.1809885958 0.0080543702
H 4.0407501435 1.232679123 0.1429988448

z+ 0.004

C -0.9260271965 -1.2118978182 0.0117485903
C -1.6734705871 -0.0148900584 0.0135088655
C -1.0220117357 1.258834679 0.0236849971
C 0.3638578281 1.312041839 0.0245152319
C 1.0459781839 0.1395212677 0.0213444098
C 0.4144748853 -1.1328367115 0.0231602252
O -2.9661319941 -0.0163869674 0.0083333597
O -1.734167902 2.3396963526 0.0322530001
C 2.5414034648 0.1111795818 0.0339766966
O 3.073280446 1.301551999 -0.1420984048
O -1.7004385252 -2.2983622491 0.0101828123
O 3.1460742036 -0.8994238827 0.1979783804
H 1.0495272734 -2.0094408364 0.0298888805
H 0.866652035 2.2671649495 0.0129834848
H -1.2253960023 -3.1270081756 -0.1266409897
H -3.3306904467 -0.9213234738 -0.0357138184
H -2.6916162327 2.1809138019 -0.0149610927
H 4.0402633022 1.2318917028 -0.1688516283

z- 0.006

C -0.9243381055 -1.2124194041 -0.0111310679
C -1.6726143656 -0.0158063302 -0.0186424102
C -1.0223051828 1.2582954869 -0.0455736346
C 0.3632595722 1.3122612775 -0.0535804025
C 1.0463970544 0.1401310811 -0.0440213613
C 0.4160474305 -1.1327887217 -0.0350628689
O -2.965098974 -0.0184686927 -0.0053641701
O -1.7354358184 2.3386536379 -0.0627705918
C 2.5414782586 0.1147213832 -0.0693173671
O 3.0722121961 1.2906028584 0.1843392247
O -1.6975961153 -2.3001455055 0.0023564368

O 3.1445600325 -0.8815918637 -0.3109344246
H 1.0505573843 -2.0096963659 -0.0416413377
H 0.865451917 2.267809741 -0.0452462285
H -1.2311580384 -3.1192340132 0.2097558945
H -3.3276379333 -0.9225324842 0.0677011532
H -2.6911857763 2.1808557639 0.0138513179
H 4.0389674639 1.2205781514 0.2205748383

z+ 0.006

C -0.924364184 -1.2122794475 0.0160451865
C -1.6725915991 -0.0157495253 0.0197942945
C -1.0221906882 1.2584642161 0.0375096822
C 0.3634935254 1.3125407187 0.040271377
C 1.0465746828 0.1404602799 0.0345647519
C 0.4160961498 -1.1324978784 0.0347216578
O -2.9651765034 -0.0184468604 0.0111805747
O -1.7352142538 2.3388677714 0.0513956632
C 2.5417458161 0.1150179567 0.0545961837
O 3.0715965693 1.2895000661 -0.2069427444
O -1.6975580495 -2.3002469253 0.0112439252
O 3.1455056656 -0.8801940082 0.2991124613
H 1.0506679157 -2.0093463553 0.0437554443
H 0.8655769981 2.2680697981 0.0250010153
H -1.2317154496 -3.1201884267 -0.1940355564
H -3.3278683906 -0.9228946541 -0.0557811656
H -2.6912550898 2.1807304114 -0.0208839463
H 4.0382378853 1.2194188628 -0.246255805

z- 0.008

C -0.9220275228 -1.2129806494 -0.015000172
C -1.6714835514 -0.0170214145 -0.0246586659
C -1.0227033407 1.2577171824 -0.0594472114
C 0.3625293255 1.3128737356 -0.0698419964
C 1.0471255527 0.1413558538 -0.0576750541
C 0.4182516252 -1.1323623807 -0.0464668257
O -2.9638113549 -0.02136617 -0.0079943708
O -1.7371278185 2.3374091813 -0.081923791
C 2.5419260773 0.1200047505 -0.0899092967
O 3.0703662572 1.2737777702 0.2493234272
O -1.6935204401 -2.3027155616 0.0020980276
O 3.1435609299 -0.8549910424 -0.4115242691
H 1.0520985578 -2.009623602 -0.0548318693
H 0.8637193125 2.2690193671 -0.0581243938
H -1.2395026947 -3.1092343969 0.2767991226

H -3.3238109322 -0.9246408906 0.0869996836
H -2.6907742383 2.1806891975 0.0198229183
H 4.0367452555 1.2033150697 0.2976477368

z+ 0.008

C -0.9220682503 -1.212801111 0.0199440607
C -1.6714483117 -0.0169599196 0.0258625966
C -1.0225414156 1.2579283562 0.051373353
C 0.3628640753 1.3132399769 0.0564728829
C 1.0473796414 0.1417983242 0.0481661353
C 0.4183143844 -1.1319761465 0.0461335688
O -2.9639140968 -0.0213419922 0.0139729592
O -1.7368130758 2.3376821148 0.0705307346
C 2.5422927049 0.1203841493 0.0751090854
O 3.0695518297 1.2723823273 -0.2716135755
O -1.6934519668 -2.3029012715 0.011611527
O 3.1448152035 -0.853219553 0.3993201742
H 1.0522219143 -2.0091760731 0.0570038121
H 0.8638955533 2.2693704796 0.0377837366
H -1.240374664 -3.1104186383 -0.2616320088
H -3.3240914512 -0.9251318232 -0.0749014199
H -2.6908511776 2.1805004522 -0.0268557356
H 4.0357801031 1.2018663478 -0.3229888866

Caffeic Acid (Neutral)

z- 0.010

C 1.2530201524 0.0670417982 -0.6897109768
C 0.053198156 -0.1394577304 -0.0409613567
C 0.0263526164 -0.237463611 1.323910441
C 1.1939124563 -0.1296539983 2.0617250319
C 2.3854359033 0.0671286066 1.3915076963
C 2.416464262 0.1680495871 0.020522739
O -1.0879171987 -0.2453953727 -0.7668743614
C 1.2305648798 -0.2113356468 3.5193354049
C 0.2169244466 -0.1897122323 4.3555069492
C 0.5075486314 -0.2678046761 5.8071638181
O -0.5963145875 -0.2127681233 6.5343925761
O 1.1971194191 0.1555271251 -2.0639292093
O 1.6063685865 -0.365586883 6.2572763344
H 2.2148994703 -0.2791607033 3.9704307338
H -0.8197745589 -0.1048195985 4.061356206
H -0.3662790839 -0.2593773795 7.476372002
H 2.0651287289 0.3938060118 -2.392598173
H -0.8650698802 -0.1236996041 -1.6942021707

H 3.3565175807 0.3256898687 -0.4956936357
H 3.3015370975 0.1473800275 1.9592552408
H -0.924526078 -0.4047154655 1.8097987101

z+ 0.010

C 1.2691480124 0.051484393 -0.6873547922
C 0.057061794 -0.0716369174 0.0017969939
C 0.0581816764 -0.1207104824 1.3615814849
C 1.2523972174 -0.0484291595 2.0763049752
C 2.4385205957 0.0747554451 1.3797497377
C 2.4511535334 0.1242628773 0.003053272
O -1.0903129032 -0.140288429 -0.6746432547
C 1.2901316175 -0.1007433116 3.5145219593
C 0.2600714985 -0.2325524094 4.3490998062
C 0.4634878864 -0.2709240803 5.7746919631
O -0.6956409809 -0.4218256055 6.4577014063
O 1.1395629019 0.0879562824 -2.0133196306
O 1.496088566 -0.18792764 6.3933139528
H 2.2742574244 -0.0256594841 3.9658973369
H -0.7590866992 -0.3207076144 4.0062035176
H -0.436780279 -0.4403663395 7.3856468228
H 1.9674481702 0.1631628058 -2.500481734
H -0.9290541341 -0.0997116552 -1.6280167709
H 3.3825531614 0.2193069438 -0.5388365994
H 3.3729947881 0.1316087467 1.9213606383
H -0.8970728473 -0.2173823657 1.8563129147

z- 0.002

C 1.2590669295 0.0526287172 -0.6881027658
C 0.0535546329 -0.0800726159 -0.0169889742
C 0.04116323 -0.1359002708 1.3470455155
C 1.2235381151 -0.0613761618 2.0678036435
C 2.4127400382 0.0700993085 1.383846526
C 2.4328957772 0.1273280967 0.0074549333
O -1.0963196796 -0.1527504573 -0.7151117033
C 1.259214424 -0.1161448907 3.5234409767
C 0.2384204758 -0.235720832 4.3476707988
C 0.4865736768 -0.2713072117 5.7937725838
O -0.643469917 -0.3924922729 6.4921772536
O 1.1675943304 0.0994918245 -2.0446143534
O 1.5581472447 -0.2024676903 6.3192321621
H 2.2411268395 -0.0502880268 3.9796121323
H -0.7901093014 -0.3102371156 4.0271677448
H -0.4099722606 -0.4085667083 7.430797616

H 2.0333626742 0.1953452223 -2.4470458471
H -0.8988942676 -0.0952306244 -1.6565354277
H 3.3705618728 0.2310527581 -0.5240613636
H 3.3400045612 0.1292981062 1.9360915689
H -0.9140883961 -0.239017155 1.8409309799

z+ 0.002

C 1.26195835 0.0516168126 -0.6871136026
C 0.0554715988 -0.0748075174 -0.0085072267
C 0.0493985262 -0.1266535739 1.3542246875
C 1.2365353924 -0.0542423427 2.0702925818
C 2.4234137731 0.0717374336 1.3818882523
C 2.4389578546 0.1245669499 0.0044615806
O -1.0950568327 -0.1449002279 -0.6970284674
C 1.2722348484 -0.1073894808 3.5223071312
C 0.2479140473 -0.2365406336 4.3458675972
C 0.4771667957 -0.2714049729 5.786998219
O -0.6636329113 -0.4099610986 6.4759637145
O 1.1546988013 0.0934251684 -2.0338635617
O 1.5340542057 -0.1905645454 6.3458595932
H 2.253783775 -0.0331624798 3.978216141
H -0.7762285781 -0.3216419703 4.015438278
H -0.4257226238 -0.4252269354 7.4120168258
H 2.0082468044 0.1767350843 -2.4664118
H -0.9106926182 -0.0955578806 -1.642859174
H 3.3739886465 0.2232060372 -0.5316982671
H 3.3540636446 0.129332281 1.9289416345
H -0.9054425 -0.2248941077 1.8495898631

z- 0.004

C 1.2575201388 0.0560220355 -0.6886488425
C 0.05294747 -0.0897953383 -0.0221394809
C 0.0372278976 -0.1531971666 1.3422635489
C 1.2166332412 -0.0730447696 2.0663675307
C 2.406618792 0.0697803786 1.3851652597
C 2.4292667195 0.1351212734 0.0096786492
O -1.0956452578 -0.168399937 -0.726163618
C 1.2526684751 -0.1320821547 3.5230783425
C 0.2326063361 -0.2280626895 4.3494523237
C 0.4917414003 -0.2708211018 5.7972496508
O -0.6337653828 -0.3616286882 6.5022598576
O 1.174401613 0.1100922074 -2.0497921818
O 1.5721882001 -0.2300877992 6.3044785299
H 2.2361918904 -0.088713906 3.9784469778

H -0.7997172123 -0.2756731909 4.0352960039
H -0.4009542396 -0.3834619622 7.4417367738
H 2.0447507043 0.2254676298 -2.435922378
H -0.891595934 -0.1008235995 -1.6648849853
H 3.3678863826 0.2484370148 -0.5187190932
H 3.3316729881 0.1324130255 1.9406109743
H -0.9175332226 -0.2678692615 1.8347701567

z+ 0.004

C 1.2635662529 0.0513422317 -0.6868902082
C 0.0562262274 -0.0732051185 -0.0051026951
C 0.052639674 -0.1237646224 1.3569742155
C 1.2418068662 -0.05182485 2.0716224946
C 2.4279630486 0.0725412028 1.3811641475
C 2.4419345884 0.1238970172 0.0035275055
O -1.0940921818 -0.1425276827 -0.6896636929
C 1.2777310077 -0.1045489494 3.5211336943
C 0.2518378627 -0.2361907034 4.3457552214
C 0.4731406236 -0.2713944507 5.7838119148
O -0.6726092443 -0.4155022164 6.4695112609
O 1.1495132452 0.0913213781 -2.0286373133
O 1.5232600501 -0.1876126577 6.3583773557
H 2.2595232799 -0.0283465259 3.976411595
H -0.7705847113 -0.3240456148 4.0113029806
H -0.4312029556 -0.4309686789 7.4039938399
H 1.9967298977 0.1706968141 -2.4754836246
H -0.9158711894 -0.0961515947 -1.6375155992
H 3.375830843 0.2209154249 -0.5345193344
H 3.3599343249 0.1297058036 1.9262295912
H -0.9021665098 -0.2206642071 1.8525806506

z- 0.006

C 1.25571199 0.0616407312 -0.6890032208
C 0.0527931593 -0.1050551025 -0.027887014
C 0.0338330484 -0.1803767468 1.3366828873
C 1.2096458571 -0.0909122565 2.0647794324
C 2.3999307464 0.070228527 1.3868768834
C 2.4249154558 0.1481887379 0.0127178847
O -1.093756712 -0.193313897 -0.7385433175
C 1.2461531004 -0.1575985994 3.5220971582
C 0.2268145295 -0.2146433122 4.3515008617
C 0.4969621402 -0.2704407558 5.8006304299
O -0.6234564037 -0.3128325489 6.5130675678
O 1.1811158882 0.126795183 -2.0545540681

O 1.5857616176 -0.2764971862 6.2887702512
H 2.2313113613 -0.1517545465 3.9760124751
H -0.8089511986 -0.2174616823 4.044263962
H -0.3912622166 -0.3445173462 7.4532702968
H 2.0542953149 0.2712794387 -2.4232541608
H -0.8833492449 -0.1108718694 -1.6740932829
H 3.3639478998 0.2768649495 -0.5120077393
H 3.3223271203 0.1385907682 1.9459676053
H -0.9196324533 -0.313640486 1.8272891076

z+ 0.006

C 1.2653066355 0.0513797657 -0.686826385
C 0.0567872521 -0.0724575257 -0.0022221531
C 0.0552284003 -0.1223884367 1.3591144858
C 1.2462652114 -0.0504179489 2.0730394091
C 2.4319605639 0.0733290639 1.380612972
C 2.4448983911 0.1239229331 0.002960019
O -1.0929010385 -0.1414965074 -0.6835085897
C 1.2825790004 -0.1030099681 3.5194752641
C 0.2551381255 -0.235052053 4.3462312577
C 0.469536864 -0.2712787154 5.7807017711
O -0.6809895031 -0.4183605638 6.4642810271
O 1.1451559908 0.0900608285 -2.0234742456
O 1.5134308619 -0.1871104651 6.3703489445
H 2.2649498423 -0.0268430368 3.9737806122
H -0.7659732744 -0.3233337936 4.0084087298
H -0.4349606711 -0.4346941156 7.3969060979
H 1.9859191989 0.1673177793 -2.4841672551
H -0.9204887099 -0.0973344457 -1.6332629462
H 3.3778124309 0.2201200047 -0.536602397
H 3.3650273081 0.1303379045 1.9240637988
H -0.89957188 -0.2190187039 1.8547235826

z- 0.008

C 1.2539793681 0.06618549 -0.6892534487
C 0.0528811356 -0.1222200613 -0.0340744816
C 0.0304145938 -0.2098266207 1.3306116445
C 1.2022437422 -0.1104366111 2.0632266702
C 2.3928370715 0.0700954102 1.3890045209
C 2.4203854323 0.1607895054 0.0164131189
O -1.0911230052 -0.2205832159 -0.751986178
C 1.239022002 -0.185570334 3.5207913711
C 0.221772415 -0.2008349872 4.3534648956
C 0.5021220395 -0.2698738625 5.803849213

O -0.6110721808 -0.259966157 6.5237175934
O 1.1883035146 0.143269744 -2.059106072
O 1.5968159312 -0.3261016553 6.2729279378
H 2.2243889013 -0.2197457102 3.9731667318
H -0.8152714911 -0.156063391 4.0528509482
H -0.3800002666 -0.3009615184 7.4647427911
H 2.0615410873 0.3270384448 -2.4089275816
H -0.8745873499 -0.119705174 -1.6837841665
H 3.3597163048 0.3054581587 -0.5042366839
H 3.3122456165 0.1447799864 1.9521507195
H -0.9215038622 -0.3620554408 1.8190344561

z+ 0.008

C 1.2671673808 0.0514275318 -0.6869651571
C 0.0570832551 -0.07194502 0.0000905827
C 0.0570915246 -0.1213837006 1.3606674852
C 1.2498121143 -0.0492820402 2.0745951407
C 2.4354739597 0.0740809029 1.3801704628
C 2.4479519109 0.1240561198 0.002802311
O -1.0916234963 -0.1407904504 -0.6784970245
C 1.2867076275 -0.1017325661 3.5172972311
C 0.2578825421 -0.2338033267 4.3473152199
C 0.4663400848 -0.2711334852 5.7776536166
O -0.6886569251 -0.420429356 6.4602880892
O 1.1417951767 0.088926625 -2.0183629615
O 1.5043915452 -0.1873027094 6.3819396513
H 2.2698593554 -0.026020585 3.9703150891
H -0.7621419189 -0.322133679 4.0066718152
H -0.4368479505 -0.4377993068 7.3907513133
H 1.9761007901 0.1648483042 -2.4924832085
H -0.9248395348 -0.0985504188 -1.6300869242
H 3.3800371693 0.2195994046 -0.538032098
H 3.3693804231 0.1309928565 1.9224613203
H -0.8978540342 -0.2179531008 1.8559920453

Zero Field

C 1.2604127009 0.0524783538 -0.6875896984
C 0.0546507757 -0.0779693679 -0.0125466202
C 0.0458693428 -0.1323127105 1.350853332
C 1.2306750781 -0.0584915255 2.0689173541
C 2.4184525702 0.0709514648 1.3827243644
C 2.435830672 0.1265343001 0.0057672608
O -1.0956003168 -0.1497655603 -0.7055260184
C 1.2662568825 -0.1127486282 3.5230283682

C 0.2434367288 -0.2356453972 4.3464770582
C 0.4816361114 -0.2715780019 5.7905739799
O -0.6540740363 -0.3993803997 6.4837247692
O 1.1605975351 0.0971323616 -2.0391179191
O 1.5458613027 -0.1979612739 6.3329871158
H 2.2481345877 -0.0442009466 3.9789992014
H -0.783016682 -0.3136792007 4.0208146375
H -0.4195059295 -0.4153818429 7.4213491281
H 2.0201143016 0.1877705795 -2.4569703663
H -0.9050726423 -0.0960434538 -1.6492336759
H 3.3719636702 0.2282853932 -0.5283672501
H 3.3475303798 0.1295107892 1.9321410557
H -0.9090420327 -0.2338329328 1.8455779232

x- 0.010

C 1.2582628013 0.0193681766 -0.6829578058
C 0.0490522522 -0.0229709782 -0.0040032269
C 0.0338656462 -0.03162987 1.35767898
C 1.2243494567 0.005406047 2.0728617226
C 2.41633879 0.0595117973 1.3835621593
C 2.4375473835 0.0607450851 0.005665098
O -1.1052500628 -0.0499534282 -0.7191199617
C 1.2570813143 -0.015836676 3.5266248563
C 0.248170648 -0.2680157884 4.3417896937
C 0.4693626444 -0.2534740202 5.7846569112
O -0.6322128347 -0.6137710849 6.4828207089
O 1.1515572236 0.0239779464 -2.034784997
O 1.4789216701 0.0330181182 6.3474980176
H 2.2193805751 0.1832886029 3.9873039414
H -0.7451520333 -0.5157011811 3.9981750506
H -0.355527363 -0.6033750372 7.4095457666
H 2.0137283525 0.0458090281 -2.4616889706
H -0.8629388038 -0.0384486141 -1.6532850066
H 3.3798043509 0.0967498833 -0.526122307
H 3.3505078047 0.0945939259 1.926756085
H -0.9217388157 -0.0556199325 1.8616072847

x+ 0.010

C 1.2634219889 0.0494231438 -0.6904536966
C 0.0623490066 -0.1252203527 -0.0148919837
C 0.0661815002 -0.200305634 1.351664995
C 1.2484893059 -0.1068801402 2.0671551542
C 2.4325822802 0.0572735049 1.3794986177
C 2.4398172945 0.1361872991 0.0026264254

O -1.0889526103 -0.2183235911 -0.6779694345
C 1.2822210822 -0.1658082829 3.5231277374
C 0.2535200115 -0.2122472304 4.3440529658
C 0.4796483776 -0.2611772787 5.79393605
O -0.6625638117 -0.2884824158 6.4588317108
O 1.1670383753 0.11140174 -2.042834558
O 1.5535017653 -0.274388885 6.3366638129
H 2.2657422139 -0.1621027559 3.9809583951
H -0.7770170121 -0.2098236993 4.0198589183
H -0.490947943 -0.3183264325 7.4095197796
H 1.9903370204 0.3926775986 -2.4440502245
H -0.9632825486 -0.1128259214 -1.6280660304
H 3.3696706115 0.26517072 -0.5388979229
H 3.3605953491 0.1294833569 1.9308477761
H -0.8872412576 -0.3320327436 1.8430055123

x- 0.002

C 1.2602512463 0.0486065886 -0.686933068
C 0.0534837647 -0.0681338114 -0.0114899838
C 0.0425742653 -0.1153125891 1.3514788699
C 1.2282498305 -0.0472257258 2.0695470667
C 2.4170303291 0.0707419879 1.3830549075
C 2.4360823105 0.1180489093 0.005902089
O -1.0972378032 -0.1333077631 -0.7095940738
C 1.2638598197 -0.0974278923 3.5233812907
C 0.2427776734 -0.2416279041 4.3463736792
C 0.4809329967 -0.2704576504 5.7894761277
O -0.652364079 -0.4319653728 6.4861163266
O 1.1596959576 0.0867658815 -2.0386483157
O 1.5402291827 -0.1668303673 6.3339425422
H 2.2439099132 -0.0084632976 3.9798740067
H -0.7807143237 -0.3455541366 4.0188128278
H -0.4067912069 -0.4433294777 7.4210487899
H 2.0206470928 0.1583393547 -2.4582247046
H -0.8951204811 -0.0890773146 -1.6515005809
H 3.3736817807 0.2097530564 -0.5272334898
H 3.3467450591 0.1255260389 1.9317062412
H -0.9128123283 -0.2053965144 1.8474934513

x+ 0.002

C 1.2607012082 0.0538709623 -0.6880950199
C 0.0556397985 -0.0851826735 -0.0131845442
C 0.0487655795 -0.1437396631 1.3506935693
C 1.23302165 -0.0662800235 2.0686074507

C 2.4201334135 0.0702238243 1.3823598849
C 2.4360945708 0.1307816326 0.0054353175
O -1.0946460911 -0.1612640148 -0.7008060445
C 1.2684993043 -0.1224322771 3.5229142383
C 0.2446944193 -0.2322694552 4.3463909757
C 0.4819317624 -0.2714131007 5.7910870021
O -0.6551692378 -0.3781772832 6.4799836783
O 1.1616723824 0.1026286877 -2.0397268103
O 1.5493001813 -0.2169514841 6.3324809899
H 2.2509679444 -0.0657099324 3.9791232119
H -0.7831749548 -0.2949749391 4.0217307451
H -0.4309972082 -0.3967427114 7.4200016513
H 2.019518893 0.2120092726 -2.4555271934
H -0.9158134865 -0.0992465521 -1.6461889348
H 3.3711230478 0.2388126245 -0.5296581756
H 3.348760688 0.1314399569 1.932431119
H -0.9059128651 -0.2517108505 1.8445308886

x- 0.004

C 1.260064713 0.0430172022 -0.686279116
C 0.0523455641 -0.0579050127 -0.0101984603
C 0.03972995 -0.0967509346 1.3524060852
C 1.2264087627 -0.0352040398 2.0701924933
C 2.4161520154 0.0693788275 1.3832460202
C 2.4364429856 0.1068834302 0.0058599674
O -1.0989750964 -0.1153155216 -0.7130504712
C 1.2617354146 -0.0800638993 3.5239177169
C 0.242860552 -0.248178762 4.3458803586
C 0.4795960057 -0.2682957603 5.788550574
O -0.6497071683 -0.4694382146 6.4875116139
O 1.1584812533 0.0735600137 -2.0380742364
O 1.5317635522 -0.128120409 6.3359585919
H 2.2391518471 0.0324570091 3.9810667767
H -0.7762756244 -0.3823318178 4.0157437807
H -0.3948693422 -0.4754193032 7.4201191673
H 2.0201064192 0.1318263565 -2.4593645308
H -0.8859586235 -0.0799402598 -1.6530836007
H 3.3754292409 0.1867396648 -0.5266398775
H 3.3467144888 0.119956222 1.9308610228
H -0.9160859099 -0.1731827911 1.8499601241

x+ 0.004

C 1.2609493313 0.054866126 -0.688685921
C 0.0568210322 -0.0934156406 -0.0137385799

C 0.0523616183 -0.1565428668 1.3507187473
C 1.2360678375 -0.075135622 2.0682268967
C 2.4223952632 0.0688509927 1.3817799059
C 2.4364226548 0.1346538603 0.0049309672
O -1.0935821553 -0.1739954185 -0.6955512865
C 1.2713247956 -0.1330131691 3.5228583298
C 0.2463785665 -0.2279744891 4.3460943103
C 0.481909497 -0.2706099292 5.7918670128
O -0.6565064309 -0.3559438018 6.475693654
O 1.1624933974 0.1079083336 -2.0402837817
O 1.5517446557 -0.2349942273 6.3327782185
H 2.2544061266 -0.0895230442 3.9792018704
H -0.7826999313 -0.2740226185 4.0221354246
H -0.444327916 -0.3774973263 7.4183781739
H 2.0174524652 0.2419326914 -2.4538745358
H -0.9273299862 -0.1025531681 -1.642497652
H 3.3701454171 0.2491552014 -0.531500404
H 3.3507012281 0.1328800266 1.9323367814
H -0.9020164668 -0.2713539104 1.8437158681

x- 0.006

C 1.2597140251 0.0360939147 -0.6854293747
C 0.0511950505 -0.0466295583 -0.0084911826
C 0.0372763487 -0.0759576769 1.3537898994
C 1.2251315929 -0.021954133 2.0709779559
C 2.4157747439 0.0670860791 1.3833650141
C 2.4368781106 0.0932906646 0.0057430404
O -1.1009590198 -0.0948777878 -0.7157352825
C 1.2598996374 -0.0600547724 3.5246592215
C 0.2438353114 -0.2550710255 4.3449505406
C 0.4773670445 -0.2647761928 5.7874505964
O -0.6457207746 -0.5134948448 6.4873835269
O 1.1567599342 0.0582234207 -2.0372756163
O 1.5192113633 -0.0807994744 6.3389907046
H 2.2334892889 0.0795653169 3.9827755407
H -0.7689271329 -0.4243487591 4.0112368206
H -0.3827164831 -0.5137218433 7.4178619408
H 2.0188074216 0.1032263508 -2.4603946491
H -0.877643081 -0.0682252321 -1.653852032
H 3.3771529465 0.1595450021 -0.5263462916
H 3.3473813204 0.1128856082 1.9297103274
H -0.9187966487 -0.1363330567 1.8532132995

x+ 0.006

C 1.2613043883 0.0549315282 -0.6892688651
C 0.0581525455 -0.1021970564 -0.0141301073
C 0.0563464222 -0.1695964841 1.3509350701
C 1.2396061473 -0.0843328083 2.0678763906
C 2.4251196502 0.0666751557 1.38108351
C 2.4369871852 0.1373231137 0.0042520806
O -1.0924927112 -0.1871044496 -0.689885732
C 1.2745383452 -0.1433592174 3.5228814343
C 0.2484266541 -0.2233696503 4.3456280035
C 0.4815598798 -0.268901354 5.7926044831
O -0.6580828532 -0.3346620173 6.4707382345
O 1.1632876948 0.1118794516 -2.0408851463
O 1.5532405338 -0.2503102288 6.3335853289
H 2.2579926804 -0.1127309738 3.9795300522
H -0.781478255 -0.2534948506 4.021992261
H -0.4586142676 -0.359137114 7.4160953012
H 2.0136560929 0.2768987947 -2.4518250194
H -0.9393872678 -0.1053593026 -1.6381883068
H 3.3693926245 0.2576878054 -0.5336794929
H 3.353246747 0.1334619695 1.9319642153
H -0.8976912363 -0.2906303117 1.8432803046

x- 0.008

C 1.2591202339 0.0280394737 -0.684326116
C 0.0500850465 -0.0348025893 -0.0063883029
C 0.0353198871 -0.0538705014 1.3555911896
C 1.2244688098 -0.0081641118 2.0718800544
C 2.4158759243 0.0637582882 1.3834492986
C 2.4372794317 0.0776254355 0.00564665
O -1.1030980236 -0.072749757 -0.7176848278
C 1.2583749345 -0.0382491823 3.5255791736
C 0.2456929959 -0.2618779882 4.3435558424
C 0.4739930635 -0.2597912033 5.7861474433
O -0.6399745505 -0.5624488314 6.485718345
O 1.1544417484 0.0413379863 -2.0361814418
O 1.5016575699 -0.0261680938 6.3429489673
H 2.2268635569 0.1308479128 3.9849049904
H -0.7584090574 -0.469759888 4.0052713413
H -0.3698242898 -0.55699437 7.4142662872
H 2.0166476057 0.0742204792 -2.4611862103
H -0.8700562064 -0.0541804058 -1.6538458627
H 3.3786581702 0.1289990746 -0.5262343946
H 3.3487025975 0.1043307547 1.9282993702
H -0.9207084479 -0.0964304828 1.8571722026

x+ 0.008

C 1.2618436894 0.0539422226 -0.6898445051
C 0.0598013699 -0.1123327982 -0.0144097971
C 0.0609205966 -0.1840322845 1.3513211797
C 1.243776753 -0.0946581519 2.0675267504
C 2.4284299469 0.0634434974 1.380260766
C 2.4378664877 0.1388579381 0.0034325289
O -1.0911758276 -0.2017121651 -0.6838315349
C 1.2782655651 -0.1543656435 3.5229661021
C 0.2508659026 -0.2177117551 4.3449687396
C 0.480845669 -0.2659921154 5.7932942986
O -0.6601211761 -0.3126972106 6.4650478471
O 1.1642544991 0.1144876147 -2.0415743441
O 1.5538187622 -0.2639469862 6.3349085221
H 2.2619056806 -0.1377094795 3.9800764756
H -0.7795340633 -0.2309300367 4.0212432534
H -0.4742226388 -0.3403805852 7.4130748702
H 2.006745585 0.3212192621 -2.4489925546
H -0.9518680663 -0.1084000576 -1.6332071035
H 3.3688984134 0.2647386196 -0.5361873171
H 3.3564888086 0.1330864821 1.9313448754
H -0.8926949571 -0.311234367 1.8431649472

y- 0.010

C 1.2615896305 0.1013709789 -0.6615176701
C 0.108024509 -0.3351382036 -0.0308972297
C 0.1102312836 -0.5415472789 1.3213215342
C 1.2642732567 -0.3413887208 2.0592174324
C 2.4173973591 0.0503936443 1.4123100535
C 2.4131400553 0.2852807066 0.0555040612
O -1.0091822016 -0.5451338741 -0.7533408382
C 1.2697474074 -0.479285686 3.5122872525
C 0.2651433661 -0.1771940849 4.3094884643
C 0.4219754663 -0.2989935129 5.7625466559
O -0.498440991 0.4006491567 6.4164126375
O 1.1531218126 0.2983074942 -2.0027105427
O 1.2665380047 -0.9396798618 6.3257540239
H 2.1942614313 -0.8044793434 3.977148101
H -0.6568678579 0.2569341068 3.9491168491
H -0.2920866308 0.3864098852 7.360799395
H 1.7392722693 0.9962759521 -2.3106956577
H -0.8802565111 -0.1680083512 -1.6332501846
H 3.3078524687 0.6309111703 -0.4454463025

H 3.3203074665 0.2223066919 1.9816769535
H -0.8109305947 -0.8443188694 1.7988590115

y+ 0.010

C 1.2752969447 0.0134522686 -0.6662514297
C 0.0668441977 0.1884711687 -0.0137821074
C 0.0404100309 0.2833097858 1.3519069934
C 1.2146981736 0.2289883888 2.0811071321
C 2.4159816779 0.1001680674 1.4150245372
C 2.4452748988 -0.0203241224 0.0440222149
O -1.0740278618 0.2561188056 -0.7233547336
C 1.2054619694 0.2469689092 3.5414046098
C 0.2773057547 -0.2919828316 4.3041427235
C 0.4240741389 -0.2614354113 5.7651511482
O -0.3692924986 -1.1447883988 6.3539476539
O 1.2031334539 -0.0915488205 -2.0238089225
O 1.1643935768 0.4592387938 6.3766802422
H 2.0606957683 0.6918430028 4.0385556724
H -0.5609778027 -0.8464402627 3.9059206414
H -0.1768797746 -1.1691270511 7.3013460003
H 1.8408426566 -0.7267605721 -2.3629148975
H -0.891129024 -0.0236166243 -1.6294394285
H 3.3831700193 -0.1606638261 -0.4770226028
H 3.3371516773 0.0430717966 1.9782274437
H -0.9173169771 0.3787289335 1.8437211088

y- 0.002

C 1.2573436956 0.07362571 -0.6834870305
C 0.0639110544 -0.157761324 -0.0144248167
C 0.0613204095 -0.2639540897 1.3463081172
C 1.2413690892 -0.1477974757 2.065863617
C 2.4199104322 0.0661604578 1.3845852887
C 2.4294757548 0.182353333 0.0115512597
O -1.0809705943 -0.2767825944 -0.7103956398
C 1.2762627638 -0.2289324153 3.5189566241
C 0.2467549439 -0.1998084589 4.3426782393
C 0.4753331144 -0.2774178026 5.786474465
O -0.6592189747 -0.1513574861 6.481620014
O 1.1518266673 0.16630136 -2.0324934692
O 1.5319585339 -0.4328635948 6.3268920319
H 2.2589089387 -0.302353033 3.9724761264
H -0.7769444017 -0.0931797854 4.0160000717
H -0.4282444482 -0.1839408271 7.4196558338
H 1.9798790447 0.4352704318 -2.4371838527

H -0.9024124592 -0.1268778576 -1.646163522
H 3.3565263452 0.3599789214 -0.5184341609
H 3.3456257941 0.1561201648 1.9355022893
H -0.8835047038 -0.443111634 1.8386025134

y+ 0.002

C 1.2610254528 0.0319132577 -0.6852583014
C 0.0501005737 0.0026365722 -0.0085875463
C 0.0384488715 0.0001050456 1.3564121881
C 1.225503098 0.0316446568 2.0728660487
C 2.4187793974 0.0767371354 1.3851551982
C 2.4389563494 0.0716062119 0.0073362604
O -1.1029240417 -0.0221146362 -0.700340637
C 1.2557053473 0.0032343775 3.5282419215
C 0.2528004791 -0.2690536883 4.339874725
C 0.4749016966 -0.2670342175 5.7872108323
O -0.6152612759 -0.642192528 6.4618368093
O 1.1647770962 0.0283379121 -2.03852174
O 1.4930404736 0.0262157658 6.344277957
H 2.2136628723 0.2103846311 3.9930575411
H -0.7392675221 -0.5256275685 3.9991685502
H -0.3892033642 -0.6440386983 7.4016905686
H 2.0239173858 -0.0679075331 -2.4559228296
H -0.9089003393 -0.0681751256 -1.6438049776
H 3.379187601 0.0975193409 -0.5286005867
H 3.3497304475 0.1038412233 1.9339273718
H -0.9198695992 -0.0243601349 1.8545646462

y- 0.004

C 1.256526523 0.0827451334 -0.6778460342
C 0.0746447584 -0.2162879092 -0.0165833379
C 0.0760888912 -0.3559075151 1.3418659004
C 1.2506769652 -0.2116918921 2.0638584364
C 2.4214484542 0.0597621992 1.3892509162
C 2.424808048 0.2154664938 0.0204187462
O -1.0641610186 -0.3660456282 -0.7172660668
C 1.2805855995 -0.3107945745 3.5166514773
C 0.2535590071 -0.1874566864 4.3343441465
C 0.4632824164 -0.28423974 5.7801700274
O -0.6373924726 0.0305555321 6.4675685403
O 1.1477872143 0.2077805668 -2.0249669168
O 1.4809954017 -0.6010692281 6.3258626042
H 2.2519168573 -0.4710640801 3.9721534858
H -0.7489226579 0.0342450259 3.9989226629

H -0.4141840873 -0.0012724663 7.4075273263
H 1.9209812913 0.6299115509 -2.4075567095
H -0.899242776 -0.1400631251 -1.6405153147
H 3.3431610453 0.4456722843 -0.5042174206
H 3.3428634726 0.1738785432 1.9429960478
H -0.8603119329 -0.5804524846 1.8319454826

y+ 0.004

C 1.2622053535 0.0244273005 -0.6805845696
C 0.0508617751 0.0627835811 -0.0068670111
C 0.037056782 0.093016036 1.3587575588
C 1.2231283666 0.0960630464 2.0757691232
C 2.4189650388 0.0840585678 1.3905412448
C 2.4402218755 0.0400665702 0.0138052377
O -1.101279103 0.0691799088 -0.7006385555
C 1.2452444413 0.0835967197 3.5324286588
C 0.2616040626 -0.2808387705 4.3306832968
C 0.4629294497 -0.2634048274 5.7817355227
O -0.5622614027 -0.8134076107 6.4341826266
O 1.1698337755 -0.0108005701 -2.0351523646
O 1.4172540269 0.178744171 6.354531234
H 2.176899086 0.3738292709 4.0061018672
H -0.6903496559 -0.6450693657 3.9730910739
H -0.3459909973 -0.8169484645 7.3763916119
H 1.9977766057 -0.2795320849 -2.4404945523
H -0.9085317981 -0.055389647 -1.6375288705
H 3.381019943 0.0135810865 -0.5209023826
H 3.3495053333 0.0864306301 1.9407816425
H -0.9209819584 0.1132864518 1.8579516075

y- 0.006

C 1.2571963172 0.0900856604 -0.672068853
C 0.0858446106 -0.2631261771 -0.0201798853
C 0.089192206 -0.4290298833 1.3361245232
C 1.2574164148 -0.2625534493 2.0621966541
C 2.4214391344 0.0557626362 1.3959165865
C 2.4205520314 0.2428300927 0.0312936924
O -1.0461688609 -0.4367883616 -0.727143239
C 1.2801159656 -0.3768465702 3.5149517094
C 0.2590151861 -0.1813591887 4.3254442325
C 0.4493453119 -0.2908744604 5.7737317884
O -0.5992186483 0.178019626 6.4507700617
O 1.1471491353 0.2422443304 -2.0172827271
O 1.4143337136 -0.7384064648 6.3254021711

H 2.2365293207 -0.604157378 3.973417503
H -0.7171890133 0.1275638636 3.9806776497
H -0.3829721039 0.1503542512 7.3925160189
H 1.8593674482 0.778633546 -2.3754387141
H -0.8942642159 -0.1505281251 -1.636199454
H 3.3305308401 0.5171762444 -0.4864162875
H 3.3374439041 0.1912352871 1.9538999864
H -0.8405476977 -0.6865634796 1.8229705829

y+ 0.006

C 1.2652783683 0.0200883384 -0.6756172648
C 0.0546015223 0.1120664004 -0.0074916174
C 0.0377118333 0.1678132964 1.3583943332
C 1.2209438901 0.1485544908 2.0780054579
C 2.4187705416 0.0908019913 1.3977544423
C 2.4417228106 0.0164702956 0.0227162289
O -1.0947096476 0.1428083998 -0.7052745236
C 1.2332399508 0.1482377427 3.5359526526
C 0.2685250785 -0.2866002058 4.3211079212
C 0.4497102716 -0.261627759 5.7759289142
O -0.5018965374 -0.9471373743 6.4058207565
O 1.1783240741 -0.0416573013 -2.0313462524
O 1.3344575823 0.2937616039 6.3633261377
H 2.1384248983 0.5011977512 4.0182385831
H -0.6434751833 -0.7298877682 3.9480643393
H -0.294598772 -0.9570454884 7.350074412
H 1.9536575809 -0.4570316988 -2.4174561706
H -0.9050042186 -0.0452811582 -1.6325207492
H 3.3819479194 -0.0532165102 -0.5088558124
H 3.3473024867 0.0715413797 1.9511618377
H -0.9198234501 0.219815574 1.8566003738

y- 0.008

C 1.2592612373 0.0957050595 -0.6666934155
C 0.0970180618 -0.3015991304 -0.0251296585
C 0.100371096 -0.4889859526 1.3291432575
C 1.2617828664 -0.3048537622 2.0606392183
C 2.4202184649 0.0521554883 1.4037062727
C 2.4170555369 0.2646839809 0.0430551375
O -1.0276754355 -0.4947610446 -0.7394877065
C 1.2761770627 -0.4315986689 3.5135279815
C 0.2626604537 -0.1788455413 4.3171431084
C 0.4355095632 -0.2957423343 5.7678964681
O -0.5523192724 0.2981093209 6.4334374447

O 1.1496463539 0.2714286683 -2.0100027445
O 1.3423417729 -0.8478158912 6.3255751879
H 2.2169460457 -0.711481699 3.9752410863
H -0.6866605276 0.1980866785 3.9642267034
H -0.3414589548 0.2772190686 7.3766222838
H 1.7969822688 0.8998363427 -2.3422867961
H -0.8875251057 -0.1593356399 -1.6339564226
H 3.3193251112 0.5762807778 -0.466784032
H 3.3300492908 0.2063072716 1.9670151535
H -0.8245948902 -0.7711209925 1.8116954721

y+ 0.008

C 1.2700300515 0.0169736268 -0.6707891644
C 0.0602836799 0.1530462383 -0.0100999501
C 0.0389425094 0.2297620998 1.3558360713
C 1.2180492898 0.1921050038 2.0797188472
C 2.4177755174 0.0967089013 1.4061449113
C 2.4436394923 -0.0023731105 0.0330760637
O -1.0850196587 0.2032886103 -0.7134133123
C 1.2197441106 0.2015404694 3.5389069296
C 0.27330648 -0.2894442112 4.3122876626
C 0.4366436272 -0.2609840364 5.7703849997
O -0.4374954697 -1.0547404515 6.3790318084
O 1.1901883919 -0.0675092794 -2.0276451369
O 1.2502191068 0.3843519781 6.370568527
H 2.0997510658 0.603893604 4.0290120459
H -0.6010939778 -0.7935810404 3.9258581602
H -0.2372712184 -1.0728306225 7.3248004814
H 1.8985147916 -0.6063539519 -2.3905923946
H -0.8984446095 -0.0347344158 -1.630191127
H 3.3828915199 -0.1090011601 -0.4937573264
H 3.343010509 0.0580705525 1.9641359287
H -0.9185542088 0.3054831952 1.8513099745

Caffeic Acid (Radical)

z- 0.010

C 1.2502682431 0.0544623683 -0.7363344892
C 0.0063270512 -0.0835036444 -0.0002377338
C -0.0306840646 -0.1390362224 1.3500384056
C 1.1642023377 -0.0622608206 2.0763246375
C 2.3912365863 0.0755757334 1.3743017673
C 2.4484368044 0.1331831474 0.0326509152
O -1.0753171867 -0.1504920225 -0.7716607922
C 1.2279992814 -0.1171185174 3.5035357341

C 0.2101944442 -0.2369085433 4.3527964501
C 0.5114771939 -0.276936325 5.8056610544
O -0.58652289 -0.3824981737 6.5301078668
O 1.1873813512 0.0936188387 -1.9734356848
O 1.6183625615 -0.220045425 6.2406208213
H 2.2113887717 -0.0556420236 3.9569616053
H -0.8272965545 -0.3064294313 4.0581970174
H -0.3613119091 -0.4022976927 7.4748893501
H -0.7252978108 -0.0824231009 -1.6796162853
H 3.3840862586 0.2390728001 -0.4971157401
H 3.2976995146 0.1348261927 1.9614596936
H -0.980977984 -0.2426281381 1.8526284067

z+ 0.010

C 1.2463360313 0.0552603381 -0.740240442
C -0.0025553815 -0.0824760105 0.0211913871
C -0.0002435977 -0.1357815004 1.3794362274
C 1.2078949718 -0.0598117152 2.0718737135
C 2.4334625013 0.0719128726 1.3548315871
C 2.473046916 0.1277328864 0.0164250709
O -1.0951831505 -0.146734582 -0.6895703952
C 1.2755172503 -0.1083435485 3.4960964346
C 0.2499020229 -0.2339264507 4.3481588702
C 0.4752426069 -0.2678127176 5.7731629616
O -0.6716615209 -0.4083197468 6.473857355
O 1.1693666665 0.1004883213 -1.9485436263
O 1.5216090849 -0.1875495507 6.3653813241
H 2.2650858347 -0.0362550896 3.9339575984
H -0.7744769742 -0.3174586306 4.0202591117
H -0.4020112182 -0.4239461538 7.3990200943
H -0.8482208101 -0.0899616142 -1.6357926995
H 3.3916075646 0.226207964 -0.5443757706
H 3.3518654947 0.1260507643 1.9243833345
H -0.9449322928 -0.2367568362 1.8922608632

z- 0.002

C 1.2449765061 0.0549680121 -0.7365526919
C 0.0039680533 -0.0826881733 0.0126602841
C -0.0107671584 -0.1378413157 1.367823794
C 1.190277289 -0.0615354269 2.0717744082
C 2.412477801 0.0731899205 1.3635437356
C 2.4572594801 0.1304265456 0.0220410204
O -1.0872800631 -0.1482689189 -0.7268058797
C 1.2546810809 -0.1137414908 3.506406046

C 0.2328349029 -0.2362222324 4.3451535258
C 0.4931300534 -0.2722120056 5.7915350871
O -0.6295330644 -0.3959292077 6.4958350487
O 1.1724736479 0.0961756145 -1.9616640253
O 1.572537176 -0.2004495131 6.2976381317
H 2.2396440572 -0.0464510258 3.9546761586
H -0.7975892851 -0.3125161076 4.0316723253
H -0.3964723575 -0.4128216545 7.4349665579
H -0.7841236003 -0.0844823957 -1.6527041006
H 3.3838140458 0.2330093224 -0.5237590745
H 3.3261500216 0.1300851851 1.9396199381
H -0.9568065865 -0.2401761322 1.8779127105

z+ 0.002

C 1.2440617786 0.0551285714 -0.7371939052
C 0.0023144324 -0.0825301905 0.0168365545
C -0.0044106168 -0.1372357959 1.3734607152
C 1.1993934755 -0.0610261647 2.0708250116
C 2.4208885048 0.072570078 1.360028355
C 2.4618341714 0.1295127309 0.0187650841
O -1.0913963648 -0.1477393402 -0.7104223889
C 1.2641319171 -0.1121073683 3.5049754037
C 0.2407009939 -0.2355941152 4.3441359201
C 0.4860309513 -0.2705849113 5.7852770859
O -0.6462503368 -0.4004070873 6.4844578906
O 1.1689559605 0.0978113709 -1.9568433924
O 1.5532123567 -0.1951213781 6.3221477359
H 2.2502579733 -0.0429516784 3.9504612167
H -0.7870984003 -0.3143494697 4.0239992691
H -0.4049030464 -0.4166435969 7.4199640119
H -0.8087392378 -0.0863614853 -1.643713642
H 3.3849356332 0.2307884932 -0.5331984439
H 3.3371147738 0.1285484346 1.9323134513
H -0.9493829196 -0.2391880971 1.8854970668

z- 0.004

C 1.2458918504 0.0540864689 -0.7365711104
C 0.004581025 -0.0827896912 0.0100174098
C -0.0147893006 -0.1379138797 1.3642737696
C 1.1848389401 -0.0617878448 2.0725401191
C 2.4078803432 0.0734482953 1.3656042348
C 2.4551452631 0.1306860885 0.0240550452
O -1.0848539944 -0.1484977315 -0.7363335996
C 1.2490816185 -0.11438915 3.5064520243

C 0.2281211635 -0.2361676685 4.346303417
C 0.4971178961 -0.272594912 5.7950674044
O -0.6200536557 -0.3938360451 6.5029449243
O 1.1750400162 0.096020949 -1.9643987152
O 1.5830397186 -0.2035779978 6.2846700961
H 2.2336035054 -0.0481396657 3.9559850249
H -0.8038297494 -0.3111140141 4.0366919179
H -0.3904474386 -0.4116394953 7.4437639032
H -0.7707419201 -0.0842047423 -1.6581927968
H 3.3836662337 0.2341555624 -0.5182574398
H 3.3199890478 0.1309624096 1.9440907628
H -0.9616285625 -0.2401879357 1.8730666019

z+ 0.004

C 1.2440664889 0.0553845772 -0.7375891249
C 0.0013408583 -0.0824885519 0.0184254408
C -0.0022473935 -0.1369456492 1.3755811874
C 1.2028080169 -0.0607182322 2.0706932473
C 2.4245268982 0.0723823041 1.3586464667
C 2.4642702179 0.1291396103 0.017699811
O -1.0929285554 -0.1475550427 -0.7037129838
C 1.2678846407 -0.1112763894 3.5035438191
C 0.2438006845 -0.2352493692 4.3442973606
C 0.4829561813 -0.2698863166 5.7821667888
O -0.6535165955 -0.4023250582 6.4801704895
O 1.1681907727 0.0983959024 -1.9545696043
O 1.5444696484 -0.1931130904 6.3334933754
H 2.2547176585 -0.0413574061 3.9474362641
H -0.7829211851 -0.3151194346 4.0215582708
H -0.4066302504 -0.4183310892 7.413528559
H -0.8198708607 -0.0872554886 -1.6404258571
H 3.3859424482 0.22971708 -0.5368909052
H 3.3417129539 0.1278931181 1.9295530713
H -0.946920628 -0.2387724738 1.8881673234

z- 0.006

C 1.2470180882 0.0546567899 -0.7363350799
C 0.0052318672 -0.0828990018 0.0070470424
C -0.0195280472 -0.1382389809 1.3601546171
C 1.1785513716 -0.061850522 2.0735835848
C 2.4026955029 0.0740595342 1.3681255666
C 2.4529233681 0.1313763236 0.0266019583
O -1.0820009224 -0.1489326703 -0.7469712128
C 1.2427827412 -0.1151740848 3.5059604515

C 0.2228493041 -0.2365950029 4.3479480141
C 0.5015379987 -0.2740137294 5.7983006789
O -0.609824609 -0.3909686025 6.5109495637
O 1.1785761858 0.0943770395 -1.9671690432
O 1.5940490437 -0.2074040587 6.2708817944
H 2.2268768561 -0.0501289079 3.9567210767
H -0.8107511682 -0.3101413537 4.0428013119
H -0.3822113897 -0.4089640138 7.4531669972
H -0.7565405439 -0.0829289364 -1.6645169715
H 3.3836681054 0.2352559696 -0.5118524997
H 3.3130908682 0.1319472694 1.9492240052
H -0.9673426207 -0.2409140613 1.8671511444

z+ 0.006

C 1.2444003068 0.0556530664 -0.7381935303
C 0.0001948266 -0.0824813364 0.0196687728
C -0.0007495078 -0.1366791497 1.3772823622
C 1.2054632548 -0.0604304822 2.0707826301
C 2.4278640486 0.0722517982 1.3573959424
C 2.4669037762 0.1288235221 0.016968638
O -1.0941096336 -0.1474053742 -0.6979425824
C 1.2710418291 -0.1104797519 3.5016237219
C 0.2463995262 -0.2349019424 4.3449660055
C 0.4801490947 -0.2692597388 5.7791323761
O -0.6601896588 -0.4040041105 6.4768807043
O 1.1680353756 0.0990245992 -1.9524382074
O 1.5363033315 -0.1914916549 6.3444391367
H 2.2587080217 -0.0399113528 3.9437042064
H -0.7794112924 -0.3158060709 4.0200740033
H -0.4068794251 -0.4198400736 7.4078534123
H -0.8302997125 -0.0881921597 -1.6379392819
H 3.3873189565 0.2287472732 -0.5399960157
H 3.3457753321 0.1273091456 1.9273228104
H -0.9452664501 -0.2384072067 1.8901878953

z- 0.008

C 1.2484609206 0.054830766 -0.7362619029
C 0.0057821776 -0.0834493555 0.0036566754
C -0.024771017 -0.1392112207 1.3554299358
C 1.1717618025 -0.0623994392 2.0748407227
C 2.3971916568 0.0749766245 1.3710317604
C 2.4506671642 0.1328360293 0.0294727136
O -1.0787962927 -0.1502414319 -0.7587425328
C 1.2358227988 -0.1167566499 3.5049878861

C 0.2168542107 -0.2366664129 4.3500843369
C 0.5063048917 -0.275656511 5.8018156657
O -0.5988482996 -0.3851648337 6.5199815062
O 1.1825199381 0.094826072 -1.9701222192
O 1.6060451836 -0.2155122418 6.2560409309
H 2.2196000451 -0.0542207047 3.9570594668
H -0.8186971951 -0.3073250014 4.0499818696
H -0.3726703627 -0.4043379773 7.4634887776
H -0.7413426087 -0.0830527484 -1.6716612383
H 3.3837097638 0.2382221281 -0.5048073625
H 3.3056891347 0.1336913663 1.9550342986
H -0.9736319122 -0.2428694577 1.8604617095

z+ 0.008

C 1.245254285 0.0547283389 -0.7390523774
C -0.0010786521 -0.0824098746 0.0205842772
C -0.0001547098 -0.1360913197 1.3785106313
C 1.2070973766 -0.0602245232 2.0711889374
C 2.4307795585 0.0719733412 1.3561903464
C 2.469804436 0.1282025534 0.016597279
O -1.0948751813 -0.1469554048 -0.6933324072
C 1.2735118372 -0.1095197136 3.499137276
C 0.248374535 -0.2344168289 4.3462622369
C 0.4776357582 -0.2684706642 5.7761309549
O -0.6660944075 -0.4061768507 6.4747863893
O 1.1684345381 0.1005055125 -1.9503696699
O 1.5287558671 -0.1894162614 6.354960759
H 2.262081039 -0.0382279944 3.9392164111
H -0.77666215 -0.3165610322 4.0197227175
H -0.4051507899 -0.421917314 7.4030228717
H -0.8395796038 -0.089639512 -1.6364938339
H 3.3891659815 0.2277137502 -0.5424169971
H 3.3490727264 0.1267068393 1.9256780524
H -0.9447204444 -0.2372840417 1.8914491453

Zero Field

C 1.2443641112 0.0548477485 -0.7369127476
C 0.0031552184 -0.0825970688 0.0149302124
C -0.0072181474 -0.1375208031 1.3709073511
C 1.1952554248 -0.0613356538 2.0711691981
C 2.4169251585 0.0728096955 1.3616219266
C 2.459528287 0.1299183257 0.0201937993
O -1.0895265499 -0.1479513802 -0.7180607617
C 1.2597601673 -0.1129513779 3.5059280513

C 0.2370695626 -0.2359230712 4.344392676
C 0.4894086518 -0.2713544853 5.7884428672
O -0.6382780119 -0.3982871978 6.4896571279
O 1.1703020663 0.0972608277 -1.9592128338
O 1.5625596832 -0.1974980052 6.3102547104
H 2.2452883441 -0.044664455 3.9528375945
H -0.791972899 -0.3134895614 4.0273198271
H -0.4017064546 -0.4148177684 7.427127441
H -0.796834063 -0.0855279116 -1.6477454596
H 3.3842317907 0.2319300493 -0.5288839593
H 3.3319778532 0.1292764532 1.9356462755
H -0.952638193 -0.2396053602 1.8821597037

x- 0.010

C 1.2273488346 0.042023249 -0.7284539114
C -0.004900827 -0.0723007905 0.0460145242
C 0.0031178133 -0.1156892276 1.3932722802
C 1.2261974356 -0.0490263193 2.0759934888
C 2.4368532899 0.0621134304 1.3471953064
C 2.4587685861 0.1044961881 0.0011173753
O -1.1047352486 -0.1230145021 -0.6973955937
C 1.2918883463 -0.0873992943 3.509720262
C 0.2567916796 -0.2405768169 4.3327186381
C 0.4668680533 -0.2564409587 5.7789565763
O -0.6806417002 -0.4645189848 6.4606264562
O 1.1057115046 0.0788060273 -1.9475655565
O 1.5031383256 -0.1064728718 6.3429632242
H 2.2722353328 0.0138988291 3.9630951844
H -0.758310938 -0.3668034429 3.9887529583
H -0.4276103474 -0.4747497319 7.3941501534
H -0.7634857041 -0.0712255356 -1.6161904754
H 3.3793731941 0.1856069551 -0.5596794306
H 3.3652744927 0.1102186425 1.9008304994
H -0.9322301232 -0.1964258449 1.9256510402

x+ 0.010

C 1.2613598752 0.0547443518 -0.7471597664
C 0.0113073987 -0.0830222538 -0.0132537867
C -0.0129515375 -0.1392537943 1.3531628953
C 1.1712621489 -0.0622424024 2.0669128782
C 2.4022815815 0.0786645536 1.3728614992
C 2.4617692451 0.1369031349 0.0338510686
O -1.0807503103 -0.1539039328 -0.7269132002
C 1.2347908654 -0.1195309474 3.5048793744

C 0.2257100594 -0.2374122063 4.355489992
C 0.5083906638 -0.2797225949 5.7982430882
O -0.6008414735 -0.3766853271 6.5062977931
O 1.2327990326 0.0914458044 -1.9724648407
O 1.6045241407 -0.2340890133 6.2906137306
H 2.2236779261 -0.0592319019 3.9457602353
H -0.8119901103 -0.3023880461 4.0615753407
H -0.3917894543 -0.3956398595 7.4501726868
H -0.8472207685 -0.0903944104 -1.670156837
H 3.3912712539 0.2465405499 -0.5064360448
H 3.3073570576 0.1412312982 1.9630344107
H -0.9693055943 -0.2434940025 1.8453024827

x- 0.002

C 1.2408199859 0.0549402406 -0.7349565298
C 0.0016773765 -0.0823548924 0.0209232629
C -0.0052881399 -0.1370665407 1.3749811167
C 1.2010433794 -0.0610268957 2.0720780338
C 2.4204878293 0.0716166326 1.3589793533
C 2.4591080605 0.1283083583 0.0168474079
O -1.0919627509 -0.1464416958 -0.7147637586
C 1.2659046609 -0.1113623357 3.5063923584
C 0.2403092309 -0.2356768271 4.3420971629
C 0.4852561383 -0.269376942 5.7864267491
O -0.6471122279 -0.4032177569 6.4849391844
O 1.1574062595 0.0975391611 -1.9566708287
O 1.5528851466 -0.1892105773 6.3155712441
H 2.2508066752 -0.041135004 3.9544985956
H -0.7867850977 -0.3164600662 4.0199568174
H -0.4062153854 -0.4195204659 7.4213476059
H -0.7889528706 -0.0839522952 -1.6419721725
H 3.3828227039 0.2286217025 -0.5342991638
H 3.3379373962 0.1269333304 1.9292523656
H -0.9484963709 -0.2386381305 1.8901441954

x+ 0.002

C 1.2478776054 0.0544162876 -0.7388792668
C 0.0047060859 -0.0827660571 0.0090510901
C -0.0088898405 -0.137760156 1.3670151071
C 1.1897986999 -0.0615154972 2.0702943126
C 2.4135784596 0.0739303207 1.3641256384
C 2.4599686793 0.1312507345 0.0233098875
O -1.0873299537 -0.149282002 -0.720845716
C 1.2539979057 -0.1141959915 3.5055612344

C 0.2341443389 -0.2358651526 4.3466934781
C 0.4933883299 -0.2727466538 5.7904442704
O -0.6298799217 -0.3941603985 6.493886511
O 1.1830609468 0.0966270112 -1.9617869312
O 1.5717319417 -0.2052064503 6.3054251622
H 2.2401338873 -0.0476303862 3.9513197859
H -0.7967451379 -0.3105165504 4.0345034944
H -0.397899658 -0.4113336234 7.4324549319
H -0.805493496 -0.087036471 -1.6531367342
H 3.3856696613 0.2348449317 -0.5237621835
H 3.3263643213 0.1316000382 1.9417218551
H -0.9565308552 -0.240134934 1.8743770726

x- 0.004

C 1.2375731714 0.0521108112 -0.7331998303
C 0.0000307993 -0.0803966716 0.0270534317
C -0.0035574151 -0.132700934 1.3792827317
C 1.2068851604 -0.0585768638 2.0730869535
C 2.4242601936 0.0694638455 1.3562490022
C 2.4590022395 0.123214788 0.0132314124
O -1.0947721945 -0.1415907752 -0.7111983555
C 1.27193336 -0.1062235736 3.5070514723
C 0.2438243663 -0.2365420577 4.3397914365
C 0.4809215897 -0.26647439 5.7844651576
O -0.6553305147 -0.416519509 6.4796011081
O 1.1446618423 0.0942868183 -1.9542740215
O 1.5419396752 -0.1713139525 6.3215393162
H 2.2557786568 -0.0293261154 3.9565631993
H -0.7807317192 -0.3267474459 4.0124717856
H -0.4105793648 -0.4312171996 7.4150772292
H -0.7816538866 -0.0814739322 -1.6361690702
H 3.3819511099 0.2194388018 -0.5401235931
H 3.3442687435 0.1231649036 1.9225828918
H -0.9447538131 -0.2300575479 1.8986907425

x+ 0.004

C 1.2512413993 0.0550880305 -0.7406572371
C 0.0063318452 -0.0828896221 0.0033786665
C -0.010411496 -0.1382206045 1.3632865855
C 1.1845583742 -0.0616149503 2.0694682346
C 2.4102972693 0.0752041077 1.3665723973
C 2.4603195088 0.1328199938 0.0263197739
O -1.0853110534 -0.1506472596 -0.7232010914
C 1.2486001334 -0.1155710001 3.505208505

C 0.2315497684 -0.2362996165 4.3489224566
C 0.4973797947 -0.2748094189 5.7921964572
O -0.6219425261 -0.3896375741 6.4976070402
O 1.1957385583 0.0949644722 -1.9642806163
O 1.5805096738 -0.2127453014 6.3009272187
H 2.2353564801 -0.0506731412 3.9497915142
H -0.8011110497 -0.3082599063 4.0415173853
H -0.3946826284 -0.4068864386 7.437302289
H -0.8145765506 -0.0876866047 -1.658085977
H 3.3870698021 0.2376878692 -0.5187797632
H 3.3209642252 0.1339144437 1.9475353455
H -0.9602295285 -0.2412184789 1.8667438154

x- 0.006

C 1.2341620706 0.0498668469 -0.7315530355
C -0.0015710163 -0.0786041997 0.0332332589
C -0.0014376175 -0.128900971 1.383720749
C 1.213105775 -0.0564278681 2.074024535
C 2.4282540198 0.0674634886 1.3533444959
C 2.4588401957 0.1186183856 0.0094080221
O -1.0977889191 -0.1370931651 -0.7070703273
C 1.2784046062 -0.1016046818 3.5077894356
C 0.2477375405 -0.2373295399 4.3374735428
C 0.4764821555 -0.2636697734 5.7826172204
O -0.6640188391 -0.4285800864 6.473898149
O 1.131728558 0.0911924093 -1.9519673993
O 1.5304389388 -0.154510201 6.3280705462
H 2.2613215285 -0.0187210494 3.9585509178
H -0.7742085797 -0.3363669262 4.0048226359
H -0.41605083 -0.4421262717 7.4086027449
H -0.7750184178 -0.0788015913 -1.6298429252
H 3.3809467262 0.2110484024 -0.5462897325
H 3.350928178 0.1196079509 1.9156153175
H -0.9406040734 -0.2225421586 1.9073248487

x+ 0.006

C 1.2546002048 0.0553217926 -0.742689999
C 0.0080503358 -0.083266079 -0.0022895988
C -0.0114363877 -0.1392823338 1.3597655472
C 1.1797884381 -0.0622828541 2.0686068169
C 2.4074035057 0.0765619709 1.3688390376
C 2.4607205015 0.1348949591 0.029105397
O -1.0835349863 -0.1523694403 -0.7249054004
C 1.2437022114 -0.1176740136 3.5050289144

C 0.2293038925 -0.2365830101 4.3511460366
C 0.501157075 -0.276714746 5.7941645799
O -0.6146453383 -0.3832645696 6.5009351053
O 1.2081703026 0.0948481574 -1.9669089338
O 1.5890300819 -0.2221838975 6.2969213797
H 2.2312231563 -0.0552832224 3.9483212697
H -0.8051667717 -0.3050338374 4.0483841204
H -0.3928640818 -0.4014278397 7.441899402
H -0.8247187093 -0.0890314886 -1.6625378781
H 3.3882936715 0.2419359883 -0.5143528787
H 3.3160341429 0.1366635057 1.9530757268
H -0.9634592449 -0.2433100418 1.8592643555

x- 0.008

C 1.2307535811 0.0466594563 -0.7299767407
C -0.0032045637 -0.0760364309 0.0395413386
C 0.000800659 -0.1235061745 1.3883680849
C 1.2195480961 -0.0533951086 2.0749869366
C 2.4324474842 0.0650795376 1.3503240919
C 2.4587560497 0.1126130396 0.0053707188
O -1.1010949977 -0.1311415046 -0.702482901
C 1.2850755878 -0.0955645253 3.5086670867
C 0.2520358472 -0.2385942585 4.3351274932
C 0.4718354974 -0.2603952168 5.7807884818
O -0.6725716488 -0.444023209 6.4676183246
O 1.118740606 0.0863160484 -1.9497327859
O 1.517719612 -0.1335644902 6.3351900412
H 2.2668780295 -0.0048473868 3.9607031225
H -0.7668577878 -0.3491946546 3.9969585941
H -0.4218330183 -0.4561354399 7.4016681212
H -0.7689609705 -0.0754759951 -1.6231908804
H 3.380074108 0.2001894264 -0.5528020853
H 3.3579211886 0.1154141123 1.9083672178
H -0.9364113599 -0.2118782258 1.9162787394

x+ 0.008

C 1.2580027894 0.0550096676 -0.7448860177
C 0.0096410825 -0.0830842478 -0.0078250402
C -0.0123870484 -0.1390926106 1.3563646169
C 1.1753020296 -0.062137488 2.0677600718
C 2.4046914592 0.0775791396 1.3709315994
C 2.4612317296 0.1357885263 0.031589346
O -1.0820202771 -0.1531107367 -0.7262129196
C 1.2389992132 -0.1184657821 3.5049162948

C 0.2273269576 -0.2370056405 4.3533581867
C 0.5048639949 -0.2782305737 5.7961910938
O -0.607452814 -0.3803047805 6.5038277917
O 1.2205851778 0.093075339 -1.9696577393
O 1.5969798095 -0.2278923994 6.2935011001
H 2.2271794493 -0.0570235961 3.9470103483
H -0.808780363 -0.3038118705 4.055132002
H -0.3917420304 -0.3987073737 7.4461959548
H -0.8354637524 -0.0898048541 -1.66661315
H 3.3898072628 0.2440037971 -0.5101975721
H 3.3114753441 0.1388481474 1.9582221119
H -0.9665880142 -0.2431136634 1.8521649206

y- 0.010

C 1.251592638 0.0415420492 -0.7353535339
C 0.0033159127 -0.0289351935 0.0114270815
C -0.0139306187 -0.0639956938 1.3693977199
C 1.1876478535 -0.045975905 2.0719586716
C 2.4179742632 -0.0310459697 1.3655999021
C 2.4670302102 -0.0066112279 0.0231373641
O -1.092375484 -0.0083981684 -0.7207339549
C 1.2365785057 -0.0132535508 3.5102880888
C 0.2333443202 -0.2584583278 4.3428726695
C 0.4527695221 -0.1489894903 5.7903402937
O -0.5224231051 -0.7231099717 6.4829067379
O 1.1849608958 0.1634610354 -1.9540542161
O 1.3834830349 0.4007885742 6.3089336405
H 2.1942741955 0.2257872489 3.9589527539
H -0.7411329115 -0.5949151984 4.0200480749
H -0.2875066413 -0.717098579 7.421128633
H -0.80068857 -0.0297905834 -1.6519763624
H 3.3976199864 -0.0257003625 -0.5253221273
H 3.3333963703 -0.0667649433 1.9409420944
H -0.9642783778 -0.0960167423 1.8812794689

y+ 0.010

C 1.251592638 0.0415420492 -0.735353534
C 0.0033159127 -0.0289351935 0.0114270815
C -0.0139306187 -0.0639956938 1.3693977199
C 1.1876478535 -0.0459759049 2.0719586716
C 2.4179742632 -0.0310459697 1.3655999021
C 2.4670302103 -0.0066112279 0.0231373641
O -1.092375484 -0.0083981684 -0.7207339549
C 1.2365785056 -0.0132535508 3.5102880888

C 0.2333443202 -0.2584583278 4.3428726695
C 0.4527695221 -0.1489894903 5.7903402937
O -0.5224231051 -0.7231099717 6.4829067379
O 1.1849608958 0.1634610353 -1.9540542161
O 1.3834830349 0.4007885742 6.3089336405
H 2.1942741955 0.225787249 3.9589527539
H -0.7411329115 -0.5949151985 4.0200480749
H -0.2875066413 -0.717098579 7.421128633
H -0.80068857 -0.0297905834 -1.6519763624
H 3.3976199864 -0.0257003625 -0.5253221273
H 3.3333963703 -0.0667649432 1.9409420944
H -0.9642783778 -0.0960167423 1.8812794688

y- 0.002

C 1.2452768489 0.0497732633 -0.736948922
C 0.0025197428 -0.0705304022 0.0147765809
C -0.0090534739 -0.1193953357 1.3711334272
C 1.1939587809 -0.0559923238 2.0714190277
C 2.4179758534 0.0517762192 1.3614494986
C 2.4618384783 0.0996690864 0.0197031113
O -1.0915320835 -0.1173591558 -0.7176730258
C 1.2565013363 -0.0894281283 3.5068891582
C 0.236998905 -0.2414545857 4.3442845319
C 0.4862206173 -0.2448875501 5.7893865758
O -0.6269987952 -0.4722330009 6.4872747034
O 1.1712852046 0.10599711 -1.9589156263
O 1.5459764947 -0.0657224285 6.3135258047
H 2.2379274588 0.017507245 3.9552074209
H -0.7853369224 -0.3781853065 4.0254281368
H -0.3907726073 -0.4847020516 7.4249064336
H -0.7979952139 -0.0730827846 -1.6480873662
H 3.3887719615 0.1751586055 -0.5298815706
H 3.3341275008 0.0896999337 1.9352293499
H -0.956038087 -0.2040894095 1.8826657502

y+ 0.002

C 1.2452768489 0.0497732633 -0.736948922
C 0.0025197428 -0.0705304022 0.0147765809
C -0.0090534739 -0.1193953358 1.3711334272
C 1.1939587809 -0.0559923238 2.0714190277
C 2.4179758534 0.0517762193 1.3614494986
C 2.4618384783 0.0996690864 0.0197031113
O -1.0915320835 -0.1173591559 -0.7176730258
C 1.2565013363 -0.0894281282 3.5068891582

C 0.236998905 -0.2414545857 4.3442845319
C 0.4862206172 -0.2448875501 5.7893865758
O -0.6269987952 -0.4722330009 6.4872747033
O 1.1712852046 0.10599711 -1.9589156263
O 1.5459764947 -0.0657224284 6.3135258047
H 2.2379274588 0.0175072451 3.9552074209
H -0.7853369223 -0.3781853065 4.0254281368
H -0.3907726073 -0.4847020516 7.4249064335
H -0.7979952139 -0.0730827847 -1.6480873662
H 3.3887719615 0.1751586055 -0.5298815706
H 3.3341275008 0.0896999337 1.9352293499
H -0.9560380869 -0.2040894096 1.8826657503

y- 0.004

C 1.246357648 0.0458591046 -0.7368795019
C 0.0021808341 -0.0590848488 0.0144000653
C -0.0104794104 -0.1029914385 1.3711786277
C 1.1927111221 -0.0518700588 2.0715784388
C 2.4186853316 0.0307629459 1.3617306688
C 2.4636738374 0.0707519826 0.0197397598
O -1.0928236003 -0.0878556912 -0.7175820937
C 1.252597462 -0.0676997409 3.507835119
C 0.2368253455 -0.2469129053 4.3439635935
C 0.480580052 -0.219294139 5.7900747073
O -0.6092208437 -0.5419376332 6.4853079442
O 1.1730752407 0.1170283212 -1.9583161255
O 1.5181992187 0.0611760551 6.3150897888
H 2.2289152583 0.0761635822 3.9569864095
H -0.7760008991 -0.439871827 4.0234731114
H -0.373622006 -0.5499211133 7.4231842085
H -0.7990223237 -0.0609088876 -1.6484701221
H 3.3922027052 0.1208032297 -0.5300841366
H 3.3354366176 0.0501613301 1.9355159571
H -0.9586195901 -0.1718392676 1.8830465803

y+ 0.004

C 1.246357648 0.0458591046 -0.7368795019
C 0.0021808341 -0.0590848488 0.0144000653
C -0.0104794104 -0.1029914385 1.3711786277
C 1.1927111221 -0.0518700589 2.0715784388
C 2.4186853316 0.0307629459 1.3617306688
C 2.4636738374 0.0707519826 0.0197397598
O -1.0928236003 -0.0878556912 -0.7175820937
C 1.252597462 -0.0676997409 3.507835119

C 0.2368253455 -0.2469129053 4.3439635935
C 0.480580052 -0.219294139 5.7900747073
O -0.6092208437 -0.5419376332 6.4853079442
O 1.1730752407 0.1170283212 -1.9583161255
O 1.5181992187 0.0611760551 6.3150897888
H 2.2289152583 0.0761635822 3.9569864095
H -0.7760008991 -0.4398718269 4.0234731113
H -0.3736220061 -0.5499211133 7.4231842085
H -0.7990223237 -0.0609088876 -1.6484701221
H 3.3922027052 0.1208032298 -0.5300841366
H 3.3354366176 0.0501613301 1.9355159571
H -0.95861959 -0.1718392677 1.8830465803

y- 0.006

C 1.2477898369 0.0429903621 -0.7365551272
C 0.0022313973 -0.0482626821 0.0136434698
C -0.011813815 -0.0882324261 1.3708327952
C 1.1911511703 -0.0488917268 2.0717082711
C 2.4188197632 0.0097233094 1.362599993
C 2.4650922525 0.043136996 0.0204128434
O -1.0933006337 -0.0592650257 -0.7182324946
C 1.2477676598 -0.0476604221 3.5087171846
C 0.2361268333 -0.2517878421 4.3436148804
C 0.472822573 -0.1945270713 5.7904158517
O -0.5850091238 -0.6078153914 6.4841708944
O 1.1760232307 0.1300412888 -1.9573292791
O 1.4805653864 0.1827939231 6.3145246286
H 2.2181741752 0.1309191711 3.9582081054
H -0.7649968313 -0.4973880937 4.0218624402
H -0.3496261383 -0.6109951352 7.4221817745
H -0.7996740264 -0.0489446753 -1.6493907097
H 3.3947691459 0.0688160491 -0.5291819208
H 3.3356070003 0.0106100953 1.9367118591
H -0.9608678564 -0.1427417032 1.8828575401

y+ 0.006

C 1.2477898369 0.0429903622 -0.7365551272
C 0.0022313973 -0.0482626821 0.0136434698
C -0.0118138149 -0.088232426 1.3708327952
C 1.1911511703 -0.0488917268 2.0717082711
C 2.4188197632 0.0097233095 1.362599993
C 2.4650922524 0.043136996 0.0204128433
O -1.0933006337 -0.0592650257 -0.7182324946
C 1.2477676598 -0.0476604221 3.5087171846

C 0.2361268333 -0.2517878421 4.3436148804
C 0.472822573 -0.1945270713 5.7904158517
O -0.5850091238 -0.6078153915 6.4841708944
O 1.1760232307 0.1300412889 -1.9573292791
O 1.4805653864 0.1827939231 6.3145246286
H 2.2181741752 0.1309191711 3.9582081054
H -0.7649968312 -0.4973880938 4.0218624402
H -0.3496261383 -0.6109951353 7.4221817744
H -0.7996740264 -0.0489446753 -1.6493907097
H 3.3947691459 0.0688160491 -0.5291819208
H 3.3356070003 0.0106100953 1.9367118591
H -0.9608678563 -0.1427417032 1.8828575402

y- 0.008

C 1.2495384128 0.0414699163 -0.7360511634
C 0.0026065978 -0.0381376231 0.0126467844
C -0.0129594782 -0.0751248198 1.3702507568
C 1.1894468159 -0.0468971125 2.0718314846
C 2.4185678109 -0.010981731 1.3639254816
C 2.4661912843 0.0171633362 0.0215831524
O -1.0931198805 -0.0325649774 -0.7192937813
C 1.2423336424 -0.0293611764 3.5095491536
C 0.2349802232 -0.2557135753 4.3432310956
C 0.4633827316 -0.1709865391 5.7904789477
O -0.555617264 -0.6686052032 6.4833829727
O 1.1800165772 0.1454100676 -1.9559318243
O 1.4348817212 0.2966054636 6.3123288269
H 2.2063852752 0.1812356707 3.9588509228
H -0.7530563229 -0.5494712659 4.0207168217
H -0.3204342502 -0.6670687774 7.4214973856
H -0.8002006414 -0.0382996016 -1.6505628053
H 3.3965306252 0.0196337673 -0.5275486706
H 3.3348961004 -0.0285486381 1.9385774343
H -0.9627179807 -0.117238181 1.8823100241

y+ 0.008

C 1.2495384129 0.0414699161 -0.7360511634
C 0.0026065978 -0.038137624 0.0126467843
C -0.0129594782 -0.0751248205 1.3702507568
C 1.1894468159 -0.0468971124 2.0718314846
C 2.4185678108 -0.0109817303 1.3639254816
C 2.4661912843 0.0171633368 0.0215831524
O -1.0931198803 -0.0325649791 -0.7192937814
C 1.2423336423 -0.029361176 3.5095491536

C 0.2349802231 -0.2557135752 4.3432310956
C 0.4633827315 -0.1709865386 5.7904789477
O -0.5556172639 -0.668605203 6.4833829728
O 1.1800165774 0.1454100672 -1.9559318243
O 1.4348817209 0.2966054645 6.3123288269
H 2.206385275 0.1812356715 3.9588509228
H -0.7530563229 -0.5494712662 4.0207168217
H -0.3204342501 -0.667068777 7.4214973856
H -0.8002006413 -0.0382996032 -1.6505628054
H 3.3965306253 0.0196337684 -0.5275486705
H 3.3348961004 -0.0285486368 1.9385774344
H -0.9627179807 -0.1172381823 1.882310024

Caffeic Acid (Radical Cation)

z- 0.010

C 1.2699205642 0.0545469081 -0.6669247974
C 0.0238815706 -0.0897808961 -0.0214600901
C -0.0201101757 -0.1491119453 1.3277851113
C 1.1694787166 -0.0699342974 2.0787173521
C 2.4046475042 0.0720595249 1.3980151923
C 2.45139548 0.1342561463 0.0437232833
O -1.08610186 -0.1650042881 -0.7569596664
C 1.2280151639 -0.1218617228 3.474026006
C 0.1802287511 -0.2414627795 4.3416857203
C 0.5138256403 -0.27786796 5.7973884363
O -0.5583275938 -0.3488087019 6.535176936
O 1.2135865234 0.1062025982 -1.9975671148
O 1.650778493 -0.2448337884 6.1469728022
H 2.2023736131 -0.0619430027 3.950134883
H -0.8578275307 -0.3121500009 4.0424037137
H -0.3495691179 -0.3699456849 7.4875614472
H 2.0868781879 0.2153112088 -2.3879289671
H -0.8819456663 -0.0942309162 -1.6957465214
H 3.392551022 0.2444768825 -0.4791504909
H 3.3137415993 0.13172737 1.9800762841
H -0.9823078852 -0.2579716545 1.80665348

z+ 0.010

C 1.2965048031 0.0149184672 -0.7131968766
C 0.0422964111 -0.006868933 -0.0065276409
C 0.0269380824 -0.0016852426 1.3853904355
C 1.1988503426 0.0186928021 2.0712504794
C 2.4350349611 0.0549230893 1.3523583458

C 2.4941044424 0.047129752 0.0047319178
O -1.0682702317 -0.0262422727 -0.6580819218
C 1.260025652 0.0138635977 3.5283432689
C 0.2732617069 -0.3193677925 4.3389353291
C 0.4695693178 -0.2756931715 5.7949717163
O -0.6356611072 -0.6310953758 6.4552334999
O 1.1654428426 0.007773399 -1.9958302795
O 1.4734136858 0.0332722194 6.3666235618
H 2.2050757088 0.2926138634 3.981583361
H -0.6982443744 -0.6441909989 3.995532917
H -0.4335856318 -0.5789184392 7.3981086084
H 1.9742738515 0.0235807662 -2.5380712291
H -0.9710898705 -0.0255183823 -1.6296159886
H 3.4391208819 0.0700428961 -0.5211314149
H 3.3547992056 0.0851631756 1.9213497489
H -0.93674768 0.0012795804 1.8726251616

z- 0.002

C 1.2772721503 0.0540930749 -0.678100858
C 0.0268236581 -0.0823459144 0.0012148694
C 0.0032630574 -0.1385629272 1.3581895561
C 1.1911496956 -0.0636631212 2.0772373139
C 2.4282728416 0.0723457576 1.3729491537
C 2.4734165526 0.130238681 0.026162497
O -1.0809439925 -0.1512334164 -0.6987262665
C 1.2637127458 -0.113751575 3.4944746565
C 0.224344598 -0.2362945154 4.3276713861
C 0.4932624772 -0.2709800627 5.7886958637
O -0.6207831325 -0.3910397928 6.4812915178
O 1.1808589034 0.0980144547 -1.9831618083
O 1.5898987463 -0.1973228871 6.2438435511
H 2.2433023454 -0.0474980858 3.9545410611
H -0.8060872139 -0.3120856832 4.0094613223
H -0.4215589803 -0.4105669778 7.430697194
H 2.0270668236 0.1914655405 -2.4415680851
H -0.9252538732 -0.0982518878 -1.6520523187
H 3.4102328712 0.2334054413 -0.5047808194
H 3.3408440143 0.1290128328 1.9502601008
H -0.9539812881 -0.2413059359 1.8462831123

z+ 0.002

C 1.2853780261 0.0514079432 -0.6926201096
C 0.0339630344 -0.0745839852 -0.0005630621
C 0.0142136888 -0.12486026 1.3693625064

C 1.1935293939 -0.0545346931 2.0726637066
C 2.4300140948 0.0729660718 1.3618822307
C 2.4816946869 0.124356658 0.0155105444
O -1.0722837028 -0.1396242666 -0.6821441932
C 1.2674843887 -0.101885214 3.5088978828
C 0.23741552 -0.2395657113 4.332603368
C 0.48589788 -0.2711522608 5.7920782335
O -0.6397084395 -0.4167676685 6.473718252
O 1.1728054561 0.0879251122 -1.9883456185
O 1.5643404785 -0.177020626 6.2889927047
H 2.2492198344 -0.0210901795 3.9614910786
H -0.7897629423 -0.3341025699 4.0104600545
H -0.4353313277 -0.4337320191 7.42017363
H 2.0049442695 0.1720886053 -2.4780314258
H -0.938956918 -0.095301313 -1.6424495734
H 3.4206798825 0.219863072 -0.51274296
H 3.3440640452 0.1278492703 1.9374519352
H -0.9444883494 -0.2185629662 1.8561938153

z- 0.004

C 1.2741221548 0.0542166915 -0.6727463158
C 0.0246301524 -0.084102796 -0.0010461214
C -0.0020883737 -0.1413459221 1.3514155805
C 1.1890889642 -0.0656246483 2.0791506277
C 2.4256293362 0.0717422244 1.3791712578
C 2.4685432701 0.1308765588 0.0312296029
O -1.084596538 -0.1539491454 -0.7098333004
C 1.2585856202 -0.1160548477 3.4874534943
C 0.2150735991 -0.2370541008 4.3278358887
C 0.4971092252 -0.2714143444 5.7885149938
O -0.6082408731 -0.384154189 6.4899239588
O 1.1869403489 0.100363301 -1.9832441073
O 1.6031743023 -0.2023217243 6.2202549912
H 2.2362930694 -0.0517915708 3.9526042036
H -0.8167030724 -0.3103409503 4.0124794976
H -0.4088782277 -0.4033982486 7.4404205145
H 2.0400624581 0.1966671874 -2.4256390572
H -0.9171603318 -0.0975616113 -1.6596505882
H 3.4051895384 0.2356809054 -0.4998614269
H 3.3378223241 0.1288216834 1.9569341636
H -0.9594839467 -0.2455814529 1.8392151419

z+ 0.004

C 1.2896058166 0.0387256827 -0.6994005957
C 0.036311065 -0.052252755 -0.0019256132
C 0.0168812247 -0.0824140355 1.3750597127
C 1.1934272337 -0.027616185 2.0719423329
C 2.4307060065 0.0704772619 1.3580514815
C 2.4860682309 0.1002713431 0.0108492935
O -1.0708941605 -0.1035491811 -0.6746082382
C 1.2650561488 -0.0624184762 3.5160573309
C 0.2456317449 -0.2634764983 4.3345078277
C 0.4821684469 -0.2738955777 5.7935608829
O -0.6403065998 -0.4867343124 6.4686144636
O 1.1713349513 0.0581077109 -1.9918442191
O 1.5437990747 -0.1121905967 6.3111877339
H 2.2402786968 0.0774507578 3.9684543724
H -0.7702835158 -0.4313490454 4.006974413
H -0.4352028353 -0.4858342788 7.4142560616
H 1.9980485638 0.1189912038 -2.4961265861
H -0.9468761168 -0.0754327971 -1.6383636616
H 3.4276389462 0.1715721578 -0.516582024
H 3.346259082 0.1187747629 1.9320215438
H -0.9445390049 -0.1435341417 1.8618964875

z- 0.006

C 1.2718862974 0.0543027557 -0.6690606447
C 0.0235261132 -0.0857919419 -0.0056900862
C -0.007795338 -0.1439480972 1.3441059217
C 1.1846969746 -0.0674598419 2.0801249148
C 2.420719846 0.0711168463 1.3856312259
C 2.4630638681 0.1314555219 0.0358916665
O -1.0866021058 -0.1568139797 -0.7234311323
C 1.2507982304 -0.118187764 3.4815426226
C 0.2043946151 -0.238064044 4.3303478453
C 0.5019128199 -0.2721594393 5.7900296693
O -0.5934278344 -0.3764319591 6.5019051191
O 1.1945231002 0.1025955898 -1.9857920389
O 1.6179635915 -0.2091084042 6.1960259392
H 2.2270097627 -0.0555322722 3.9509997852
H -0.8292027107 -0.3095200028 4.0192385564
H -0.3923106196 -0.3955307974 7.4532675535
H 2.0545812044 0.2022071652 -2.4112771433
H -0.9070771996 -0.0963889396 -1.6696356135
H 3.400439966 0.2378630121 -0.493867284
H 3.3322676821 0.1286374927 1.9642295648
H -0.9662552636 -0.2495679003 1.8299965586

z+ 0.006

C 1.2919545647 0.0235031659 -0.7042838139
C 0.0375393755 -0.0187123914 -0.00201892
C 0.0194528703 -0.0245433846 1.381524785
C 1.1944348592 0.0052518062 2.0722174675
C 2.43215126 0.0605842775 1.3554488495
C 2.4892610343 0.0642652947 0.0075788722
O -1.0713366 -0.0471154592 -0.6658936347
C 1.2615356653 -0.0121456872 3.522714578
C 0.2600646915 -0.2988710105 4.334111324
C 0.4774213379 -0.2791344171 5.7932883735
O -0.6333968352 -0.5817486558 6.4590180427
O 1.1678067298 0.0241479505 -1.9935455735
O 1.5106867927 -0.0258121803 6.3336718468
H 2.2203661222 0.2113761692 3.9769390783
H -0.7312187493 -0.5654915327 3.9967377635
H -0.4331861294 -0.5537877397 7.4045699904
H 1.9887874588 0.0533230906 -2.5119775675
H -0.9567180789 -0.0378404894 -1.6327675567
H 3.4329222604 0.1014419775 -0.5196419477
H 3.3498726486 0.0957384358 1.9271276569
H -0.9432882781 -0.04075622 1.8697633857

z- 0.008

C 1.2714630509 0.0520821052 -0.6671624094
C 0.0243767112 -0.0923305059 -0.013007804
C -0.0132093189 -0.149565585 1.3359327607
C 1.178113903 -0.0679584683 2.0801135063
C 2.4135874087 0.074415765 1.3924103365
C 2.4577072812 0.1341859612 0.0404271794
O -1.0855679114 -0.168929237 -0.7399429137
C 1.2399614597 -0.1171117695 3.4773278469
C 0.1919476166 -0.2385381157 4.334927676
C 0.5061734442 -0.2702066185 5.7931401838
O -0.5780956115 -0.364789968 6.5166962719
O 1.2047194116 0.1003502582 -1.9907853586
O 1.6321707494 -0.2131706089 6.1722249877
H 2.2145905359 -0.0523600565 3.9509332118
H -0.8433621921 -0.3125116203 4.0287636852
H -0.3742943457 -0.3823290184 7.4688199417
H 2.0714319315 0.2055559181 -2.3987499857
H -0.893564354 -0.1045233432 -1.6825154504
H 3.3965766398 0.2441139305 -0.4862549475

H 3.3236749471 0.1358230089 1.9728174164
H -0.9732883572 -0.2585290321 1.8184668652

z+ 0.008

C 1.2950266459 0.0127120757 -0.7087696754
C 0.0405726469 -0.0165704702 -0.0043738552
C 0.023369219 -0.0106366171 1.3838748445
C 1.1962680956 0.017600376 2.071766668
C 2.4333896146 0.0610253311 1.3541113019
C 2.4920651338 0.0529352347 0.0062726648
O -1.0688371381 -0.0435648501 -0.6619168408
C 1.2592469408 0.0124269264 3.5263333764
C 0.2687723465 -0.3112800024 4.3360474634
C 0.4720162528 -0.2713299625 5.7940774559
O -0.6331400893 -0.6134586979 6.4556923806
O 1.1673358059 0.0036768846 -1.994764043
O 1.4856270383 0.0262833864 6.3515598947
H 2.2070252928 0.2798203619 3.9803927275
H -0.7071665464 -0.6246103223 3.9942673942
H -0.434648411 -0.5668141122 7.4002051179
H 1.9823106233 0.0244160296 -2.5251955309
H -0.9627793857 -0.0426067693 -1.6312267296
H 3.4366304399 0.0811510441 -0.5199856254
H 3.3519406151 0.0969311265 1.9245758306
H -0.9399121405 -0.0144339731 1.8716381798

Zero Field

C 1.2811736491 0.0540942266 -0.6853218123
C 0.030307662 -0.0805528412 0.0008674421
C 0.0091842265 -0.135823234 1.3639938949
C 1.1926468403 -0.0617812877 2.0746647528
C 2.4295505806 0.0727876229 1.3669666064
C 2.4777787918 0.1296380548 0.0208533783
O -1.0764273113 -0.1487479645 -0.6897385126
C 1.2663635243 -0.1116772737 3.5019098599
C 0.2313699976 -0.2355634445 4.3296073768
C 0.4892870157 -0.270588509 5.7900288914
O -0.6315477069 -0.3974282817 6.4769072346
O 1.1762506017 0.0959671687 -1.985147037
O 1.5771232602 -0.1931391839 6.2670620543
H 2.2476324241 -0.0435781326 3.9577482858
H -0.7980391625 -0.3137432196 4.0095895743
H -0.4298522682 -0.417371616 7.4247857543
H 2.0151971918 0.1868469172 -2.4595949199

H -0.9324221953 -0.0987753788 -1.6466278166
H 3.415161159 0.2312864496 -0.5092594709
H 3.3426985474 0.1290610295 1.9436373743
H -0.948325828 -0.2372391019 1.8516510888

x- 0.010

C 1.276653981 0.0324534641 -0.6775895117
C 0.025130574 -0.0476888448 0.017089265
C 0.0076071563 -0.0757766173 1.3712671714
C 1.2059897524 -0.0219265794 2.0793323727
C 2.440576371 0.0692802695 1.3651411425
C 2.4803317408 0.090856429 0.0164086303
O -1.0918758481 -0.0907152638 -0.6869111626
C 1.273892337 -0.052795062 3.5038717453
C 0.2360779536 -0.243749894 4.3213708899
C 0.4718219715 -0.2550713399 5.7819780794
O -0.6382915788 -0.5401085952 6.4659785508
O 1.1596682374 0.0478122901 -1.975937378
O 1.5218620051 -0.0345705714 6.2843233216
H 2.2469848719 0.0736525223 3.9666944933
H -0.7767051014 -0.4071491262 3.9818862529
H -0.4015156749 -0.5558337582 7.4060162993
H 1.9986834548 0.0961656741 -2.4624419747
H -0.9061574967 -0.0678278088 -1.6365039626
H 3.4184379855 0.1531846672 -0.5208220153
H 3.3622621126 0.1156293945 1.9309900528
H -0.946321805 -0.1321482498 1.8724407378

x+ 0.010

C 1.2865193058 0.0694719002 -0.6957520715
C 0.0371566115 -0.1082721072 -0.0112273928
C 0.018825187 -0.1911377786 1.3639303072
C 1.1886108966 -0.1013237549 2.0711356951
C 2.424258105 0.065935694 1.3644764045
C 2.47686092 0.1524541347 0.0183795538
O -1.0632924357 -0.1910518865 -0.6801299354
C 1.2680340595 -0.1605879738 3.5053990805
C 0.2375824082 -0.2194911742 4.3367453665
C 0.4981816784 -0.2658056922 5.7998670523
O -0.6245276049 -0.3097630105 6.4705908841
O 1.1855761578 0.1368972623 -1.996552087
O 1.5981294845 -0.2617652445 6.2709902844
H 2.2547121854 -0.1426656702 3.9540876829
H -0.7991343547 -0.2287056272 4.0279275168

H -0.4743940958 -0.3376301408 7.4279031643
H 2.0204018633 0.2734468377 -2.4619529037
H -0.9746550898 -0.1117234228 -1.6441787577
H 3.414193052 0.2837919379 -0.5050734733
H 3.3332321849 0.1276516914 1.9472843537
H -0.9411575191 -0.3260529748 1.8407322752

x- 0.002

C 1.2801812026 0.0504311309 -0.6835983333
C 0.0291362167 -0.0746676142 0.0039207076
C 0.0083477836 -0.1246578702 1.3650144373
C 1.194823912 -0.0539936125 2.0755564355
C 2.4313323478 0.073236738 1.3668462101
C 2.4781467645 0.1236655281 0.020321866
O -1.0793541528 -0.1389323196 -0.6898966229
C 1.2675407486 -0.1011775872 3.5018139822
C 0.2317323123 -0.2375087689 4.3280618092
C 0.486702776 -0.2695397217 5.7882611374
O -0.6339699202 -0.4203466596 6.4758467035
O 1.1733703776 0.0870707732 -1.9831150164
O 1.569807218 -0.1705964819 6.2690619442
H 2.2475382078 -0.0229836294 3.9590176657
H -0.7953321144 -0.3301801287 4.0047109551
H -0.4243963399 -0.4391826455 7.4220598272
H 2.0125032526 0.1695709981 -2.4599101195
H -0.9262044331 -0.0947456286 -1.6453162522
H 3.4157124475 0.2185785803 -0.5109750442
H 3.3459336602 0.1281361434 1.9415654455
H -0.9484392673 -0.2185042243 1.8553352622

x+ 0.002

C 1.2821306581 0.0571143208 -0.6870793669
C 0.0314234294 -0.0856199707 -0.0016417232
C 0.0102938146 -0.1455575775 1.3636185854
C 1.1910875338 -0.0686960581 2.0739207299
C 2.4281278072 0.0720105846 1.3667717546
C 2.4775773172 0.13436377 0.0208571499
O -1.0736978171 -0.1569592984 -0.6885629312
C 1.2660562281 -0.1206244199 3.5021469987
C 0.2320597776 -0.2340208211 4.3310141991
C 0.491633048 -0.2712250906 5.7917558023
O -0.6297450046 -0.3786015559 6.4763887581
O 1.1785707882 0.1035941395 -1.9871028637
O 1.5827497818 -0.2104127483 6.2665839501

H 2.2484573689 -0.0607660102 3.9565032703
H -0.7991550434 -0.3003367851 4.0136273026
H -0.4372131278 -0.3991830162 7.4261458537
H 2.0170120129 0.2023146237 -2.4597376353
H -0.9396500527 -0.1016587812 -1.6469494175
H 3.4150456259 0.2416794091 -0.5077338331
H 3.3401473444 0.1293917795 1.9449631279
H -0.9477984905 -0.253133494 1.8490932882

x- 0.004

C 1.2792700738 0.0466384982 -0.6820145651
C 0.0280719253 -0.0687466619 0.0069232624
C 0.0077850933 -0.1136481333 1.3661153008
C 1.197164933 -0.0464595134 2.0764318637
C 2.4332708748 0.0731992733 1.3666378181
C 2.4785569929 0.1172065757 0.0196701254
O -1.082333882 -0.1287756502 -0.6898859855
C 1.2687420714 -0.0906117405 3.5019697424
C 0.2321363459 -0.2389180443 4.3265295945
C 0.483743511 -0.2674476309 5.7866284382
O -0.6359468601 -0.4450107899 6.4746146774
O 1.1703935757 0.0782084038 -1.981259598
O 1.5613295882 -0.1447547014 6.2715169271
H 2.2473748642 -0.0023904175 3.9605983965
H -0.792331054 -0.3461962452 3.9997501652
H -0.4187258549 -0.463128722 7.4191521921
H 2.009681637 0.1525972519 -2.4602982916
H -0.9203630578 -0.0900778356 -1.6438248197
H 3.4162176475 0.2051874298 -0.5130408803
H 3.3494034056 0.1265270415 1.9393777386
H -0.9483288308 -0.1997253879 1.8589908977

x+ 0.004

C 1.2831422279 0.0602522933 -0.688995007
C 0.0326632821 -0.0910424782 -0.0042369075
C 0.01177847 -0.1562095897 1.363268959
C 1.1897962173 -0.0763263219 2.0731560113
C 2.42688021 0.0708489956 1.3664815058
C 2.477376618 0.1391039716 0.0207368251
O -1.0710255593 -0.1654896094 -0.6872269927
C 1.2658558926 -0.1302453277 3.5025845237
C 0.2327447762 -0.2314711609 4.3324485158
C 0.4936580483 -0.2708714592 5.7936343642
O -0.627814252 -0.3602151589 6.4758238095

O 1.1808134411 0.1117771318 -1.9892434016
O 1.5877616312 -0.2259215277 6.2664505299
H 2.2493669483 -0.0797915517 3.9555698007
H -0.800200557 -0.2845367839 4.017659764
H -0.4447687384 -0.3820306775 7.42743323
H 2.0186964853 0.2190252826 -2.459910477
H -0.947369794 -0.1044375653 -1.6470780448
H 3.4147898919 0.2523642031 -0.5065929535
H 3.3378559679 0.1292961485 1.9461478494
H -0.9468882073 -0.2704058144 1.8464710957

x- 0.006

C 1.2783838677 0.0424554799 -0.6804985204
C 0.0270473272 -0.0623975698 0.0100897591
C 0.0074733696 -0.1020439817 1.3674868604
C 1.1998065948 -0.0387108185 2.077347757
C 2.4354513224 0.0726036622 1.3662855144
C 2.4790568737 0.1097744264 0.018800326
O -1.085422534 -0.1175889027 -0.6894257054
C 1.2702034288 -0.0792551581 3.5023358378
C 0.2329174059 -0.2402271884 4.3249258726
C 0.480351799 -0.2643712044 5.7850502637
O -0.6375136213 -0.4728219309 6.4726646875
O 1.1671574418 0.068827893 -1.9794582398
O 1.5509828334 -0.1139974194 6.2748018588
H 2.2472952492 0.0199401025 3.9624004849
H -0.788467907 -0.3635934166 3.9943756501
H -0.4131805099 -0.4902814095 7.4156002859
H 2.0064876673 0.1349551791 -2.4608402163
H -0.9150758931 -0.0842962109 -1.6418906425
H 3.4168353997 0.1901628546 -0.51538042
H 3.3532695334 0.1240454129 1.9368950369
H -0.9479466486 -0.1795067997 1.8630165493

x+ 0.006

C 1.2842231468 0.0632958027 -0.6910783929
C 0.0340182382 -0.0964952746 -0.0066934935
C 0.013638906 -0.1670980987 1.3632116985
C 1.1888980247 -0.0841518125 2.072430109
C 2.4258112365 0.0694278745 1.3659979406
C 2.4772139952 0.1435636708 0.0202831527
O -1.068403718 -0.1738189416 -0.6853886342
C 1.2660904703 -0.1398796981 3.5032754917
C 0.2338901081 -0.2284008339 4.33389131

C 0.4954481144 -0.2698874248 5.7956147856
O -0.6262494385 -0.3429564482 6.4746626224
O 1.1827420814 0.1199084699 -1.9915342741
O 1.591960388 -0.2393157325 6.2671644711
H 2.250692905 -0.0991447045 3.954830687
H -0.8005519349 -0.2680245185 4.0214124611
H -0.4534033664 -0.3662799579 7.4281631135
H 2.019863536 0.2361241174 -2.4603571104
H -0.9557391903 -0.1069131888 -1.6466854186
H 3.414609283 0.2626695131 -0.5057594417
H 3.3359239395 0.1289015762 1.9469396579
H -0.945563725 -0.28785139 1.8442022642

x- 0.008

C 1.2775312488 0.0377354237 -0.6790392692
C 0.0260816812 -0.0553642829 0.0135103519
C 0.0074114887 -0.0893358223 1.369263408
C 1.2027296672 -0.0304234753 2.0783101625
C 2.4378705093 0.0713906999 1.3657578864
C 2.4796587202 0.1010321999 0.0176664953
O -1.088587955 -0.1049296285 -0.6883710697
C 1.2719752463 -0.0665625509 3.5030085626
C 0.2343129706 -0.2419575699 4.3232096002
C 0.4764506256 -0.2604051164 5.7834935133
O -0.6385397927 -0.504323102 6.4697367264
O 1.1635316523 0.0585990601 -1.9777030199
O 1.5380854906 -0.0777564201 6.2791431629
H 2.2472580586 0.0454943461 3.9644061759
H -0.7831965463 -0.3841863935 3.9883831672
H -0.4077406826 -0.5209441764 7.4111834028
H 2.0027584613 0.1159996596 -2.4616070075
H -0.9103247778 -0.0769152466 -1.6393886463
H 3.4176092084 0.1728510535 -0.5179935107
H 3.3575408633 0.1205437755 1.9340678488
H -0.9473031379 -0.1568694334 1.8675450591

x+ 0.008

C 1.2853467511 0.0663387742 -0.6933229015
C 0.0354977244 -0.1021685754 -0.009025745
C 0.0159566711 -0.1786034194 1.3634278964
C 1.1884730314 -0.092405712 2.0717538136
C 2.4249434059 0.0677777117 1.3653299559
C 2.4770564492 0.1479463045 0.0195097985
O -1.0658399135 -0.1822384417 -0.6830424578

C 1.2667882823 -0.1498764567 3.5042066155
C 0.2354728212 -0.2245164356 4.3353206415
C 0.4969540888 -0.2682155838 5.7976907826
O -0.6251117279 -0.3263259118 6.4729421881
O 1.1843550206 0.1282155618 -1.9939657104
O 1.5954127176 -0.2510810275 6.2686500474
H 2.2524470159 -0.1197662545 3.9543398839
H -0.8002397898 -0.2497773724 4.0248449439
H -0.4631837336 -0.3515952107 7.4283453133
H 2.020484613 0.2540788119 -2.4610379282
H -0.9648110345 -0.1092737225 -1.6457431718
H 3.4144264442 0.2730086097 -0.5052575508
H 3.3343826501 0.1283110209 1.9473300891
H -0.9436984876 -0.3061596708 1.8422864957

y- 0.010

C 1.2625013587 0.1676574655 -0.6534598278
C 0.0675926954 -0.3034785299 -0.0119620641
C 0.0657401876 -0.5425663816 1.3384357374
C 1.2145628266 -0.3394081161 2.0633250298
C 2.4144439897 0.0636113313 1.3952166806
C 2.4370669039 0.3341158409 0.0731361881
O -1.0040497782 -0.5031891921 -0.7268207826
C 1.2630861704 -0.4847291075 3.4964274036
C 0.2446570884 -0.2164571444 4.2970278867
C 0.4316038698 -0.3154646671 5.7658835151
O -0.450607714 0.4193559278 6.4056295402
O 1.1254531111 0.3842756383 -1.9311893405
O 1.2809717777 -0.9813787177 6.2763588218
H 2.213516281 -0.741858329 3.9508554104
H -0.7079471756 0.1552850479 3.9427166148
H -0.2614707438 0.4411237986 7.3563342662
H 1.8790716511 0.8151781885 -2.3640709855
H -0.9087729837 -0.1942910133 -1.6421198159
H 3.336157915 0.6807822754 -0.4185794586
H 3.3114951065 0.1895961666 1.986693777
H -0.8499595376 -0.8744874821 1.8047444031

y+ 0.010

C 1.2828156015 -0.0542795229 -0.6633203256
C 0.0271830484 0.1337874748 0.0052997872
C -0.0068896677 0.2541521413 1.3692512651
C 1.1667632409 0.2056032163 2.0854646389
C 2.4146717111 0.0898325284 1.3941850346

C 2.4743811434 -0.0601648049 0.054382983
O -1.0689534985 0.1923800075 -0.6979126224
C 1.2055830978 0.2324214948 3.5220024161
C 0.241998519 -0.2412263402 4.2984136003
C 0.4362835544 -0.2391376311 5.7710864669
O -0.3463844952 -1.1181538355 6.3506824545
O 1.1813827392 -0.1869487921 -1.957313314
O 1.2129537728 0.4795069765 6.3245219892
H 2.1149997062 0.5776673779 4.0010964694
H -0.6576462062 -0.7067767073 3.9173145418
H -0.1553085583 -1.1922908058 7.2987617723
H 1.9979741285 -0.4453566089 -2.4107506871
H -0.9326440705 -0.0267501169 -1.6332508406
H 3.4170856522 -0.192819149 -0.4591677808
H 3.3239512308 0.0826268917 1.9800775533
H -0.9650876498 0.3695992054 1.8537575978

y- 0.002

C 1.276950319 0.0881745982 -0.6816250705
C 0.03688006 -0.141955666 -0.0003740595
C 0.0217351639 -0.2499688925 1.3604326366
C 1.2008247649 -0.139945788 2.071614441
C 2.4298788558 0.0678691273 1.3680275468
C 2.4710567828 0.1877013159 0.025630994
O -1.0650435717 -0.2481714569 -0.6930471158
C 1.2746167828 -0.2168112347 3.4989411801
C 0.2336567443 -0.2169881946 4.3266868739
C 0.4847669701 -0.2814953 5.7871420768
O -0.6365016616 -0.1722376515 6.4763703466
O 1.1646585934 0.1813513703 -1.9779383379
O 1.5678024037 -0.416128411 6.2626837458
H 2.2590641574 -0.2499929937 3.9519280277
H -0.7964976286 -0.1493146863 4.0061596332
H -0.4372446714 -0.1918643785 7.4247426397
H 1.9916755688 0.3611228736 -2.4482928099
H -0.9292540558 -0.1297616491 -1.6452642921
H 3.4010585436 0.3571011521 -0.5001153934
H 3.3415552479 0.1398527989 1.9453623285
H -0.9265263692 -0.4248639336 1.8455176085

y+ 0.002

C 1.282859361 0.021502084 -0.6842386887
C 0.0261712653 -0.0214130748 0.0036083758
C 0.0014289926 -0.0262423065 1.368415081
C 1.1864189351 0.0134683196 2.0777007748
C 2.4282998859 0.0782783295 1.3689623476
C 2.480683204 0.0745312095 0.021618839
O -1.0820037442 -0.0529701612 -0.686349692
C 1.2559420888 -0.011711124 3.5064900162
C 0.235628341 -0.2512846003 4.3257731443
C 0.4843500231 -0.2612607729 5.7883535966
O -0.5975434458 -0.6085897551 6.4601760174
O 1.1807821818 0.0136506432 -1.985062659
O 1.5345797795 0.0130473605 6.2775195277
H 2.2239150436 0.1502423085 3.9671714875
H -0.7713867796 -0.4643342834 3.9954487043
H -0.3989892892 -0.6312880283 7.4087023633
H 2.0239425036 0.0166254706 -2.460683268
H -0.9349382198 -0.0713673408 -1.6439826122
H 3.4224455825 0.1111369625 -0.5091548272
H 3.3422822376 0.1196179788 1.9456009129
H -0.9597549471 -0.0579662193 1.8585135588

y- 0.004

C 1.2726336357 0.11514684 -0.6755023064
C 0.0444254063 -0.1930853253 -0.0021984605
C 0.0342713684 -0.343879242 1.3563841748
C 1.2066159191 -0.204435372 2.0688740601
C 2.4277706483 0.0650208767 1.3723815724
C 2.4626635582 0.2352749133 0.0348830184
O -1.0504632718 -0.3303788838 -0.6987783344
C 1.276503655 -0.304517576 3.4977206328
C 0.238362191 -0.2086698619 4.3199841475
C 0.4741586356 -0.2927679323 5.7820391399
O -0.611349521 0.0196366188 6.4648639096
O 1.1524678474 0.2491925514 -1.9673446378
O 1.5179101302 -0.6053441316 6.2629371318
H 2.2555285196 -0.4178874764 3.9497424942
H -0.776332464 -0.0287935772 3.9925604044
H -0.4157542381 0.0065925291 7.4141155771
H 1.9631383893 0.5069548074 -2.4304443787
H -0.924813338 -0.1525252304 -1.6434926973
H 3.3846363011 0.4610478866 -0.4838041797
H 3.336817399 0.1518034047 1.951984543
H -0.904077714 -0.5747128192 1.8376771887

y+ 0.004

C 1.2831963956 -0.0036656588 -0.6803947244
C 0.0245942779 0.0267033721 0.0055352856
C -0.0026248487 0.0615959438 1.3711528635
C 1.1811695051 0.0736258875 2.0800928805
C 2.4259099518 0.0816117438 1.3734285833
C 2.4806475657 0.0305514765 0.0268421854
O -1.0822369616 0.0245727312 -0.6858278344
C 1.2439415026 0.0676572867 3.5111705575
C 0.2399821329 -0.2558757154 4.3192001327
C 0.4738047189 -0.252133604 5.7846311224
O -0.5445344549 -0.7787295123 6.43603393
O 1.1816618137 -0.0508781913 -1.9805332851
O 1.4634732171 0.1777531207 6.2893291008
H 2.1955875601 0.2979641126 3.9768882525
H -0.7375321866 -0.5648002996 3.9752875253
H -0.3494109596 -0.8101788365 7.3851090877
H 2.023048528 -0.1243906125 -2.4538452266
H -0.9354383365 -0.0526854634 -1.6408227525
H 3.4241503198 0.0141865115 -0.501839937
H 3.3397126649 0.1092107457 1.9512727201
H -0.9639894062 0.0815779617 1.861872533

y- 0.006

C 1.2687795584 0.1363003759 -0.6683832682
C 0.0521964375 -0.235443389 -0.0047682002
C 0.0458286704 -0.4208016298 1.3513610157
C 1.2105723217 -0.2568906326 2.0666657918
C 2.4241824475 0.0640392194 1.3788858585
C 2.4539546993 0.2741866239 0.0465537257
O -1.0350409233 -0.3973646515 -0.7065813338
C 1.2742232969 -0.3757562834 3.4971398348
C 0.2421963312 -0.2073869301 4.312142954
C 0.4605919135 -0.3026565449 5.7763686784
O -0.5673996647 0.17776256 6.4477941463
O 1.1417534403 0.3028208588 -1.9555039148
O 1.4467676384 -0.7590613459 6.2656986596
H 2.2441246235 -0.5506535201 3.9493956227
H -0.7515693815 0.0554538702 3.9756883886
H -0.3747305426 0.174710561 7.3977842516
H 1.9341986518 0.6263166576 -2.4096476265
H -0.919639128 -0.1698645026 -1.6423400676
H 3.3679919128 0.5466746375 -0.4637243907

H 3.329769023 0.1648439917 1.9617994149
H -0.8836383263 -0.6935569262 1.828253459

y+ 0.006

C 1.2830849306 -0.0239484274 -0.6751814475
C 0.0245571965 0.0673455217 0.0064568894
C -0.0048082659 0.1354008476 1.3720926292
C 1.176347002 0.1243598208 2.0821444035
C 2.4227221983 0.0844934075 1.3794803956
C 2.4791641337 -0.0053782964 0.0346713067
O -1.0794391888 0.0889351558 -0.6877863242
C 1.2313127217 0.1327975066 3.5153752433
C 0.2426947651 -0.2539478938 4.3119471957
C 0.4611723934 -0.245430535 5.7801550653
O -0.4818034571 -0.9160456985 6.4083365858
O 1.1814359796 -0.104137608 -1.9736990161
O 1.3807630855 0.3054198203 6.3016002985
H 2.1669787898 0.413507832 3.9859081543
H -0.7056194242 -0.6318421147 3.9543663025
H -0.2890867099 -0.9602109745 7.3575305856
H 2.0171066494 -0.2453584716 -2.4422090536
H -0.9349393752 -0.0403025303 -1.6378190185
H 3.423043609 -0.0663888666 -0.4900552118
H 3.3356020839 0.0995379752 1.9593601519
H -0.9651761174 0.1948665293 1.8619078645

y- 0.008

C 1.265430986 0.1534262678 -0.6609420848
C 0.0599317848 -0.2715329022 -0.008020354
C 0.0562939423 -0.4858552194 1.3453648228
C 1.213183368 -0.3012529971 2.0648540437
C 2.4197005177 0.0635187995 1.3866166734
C 2.4454226594 0.3063991915 0.0594503362
O -1.0195522356 -0.4537100926 -0.7159560911
C 1.2695759089 -0.4349051442 3.4967644332
C 0.2444166185 -0.2108963407 4.3043720604
C 0.4460965497 -0.310239951 5.7709422447
O -0.5124365344 0.3092392988 6.4273633609
O 1.132796443 0.3469782491 -1.9433400015
O 1.3657865231 -0.8821861904 6.2706509574
H 2.2295861109 -0.6562476893 3.9498585125
H -0.7281489537 0.1134296614 3.9587437921
H -0.3220451621 0.3181706653 7.377872316
H 1.9059683737 0.7278303014 -2.3871907291

H -0.9143139395 -0.1829850884 -1.641777422
H 3.3518536985 0.6184492416 -0.4417430438
H 3.3212878559 0.1772219719 1.9735081414
H -0.865721515 -0.7911790329 1.8171910315

y+ 0.008

C 1.2830241307 -0.0403630868 -0.6694622517
C 0.0255500224 0.1025499274 0.0060964907
C -0.0062621668 0.1985125411 1.3712075973
C 1.1712607995 0.1675084146 2.0838603957
C 2.4186913624 0.0869643864 1.3866104872
C 2.4769357016 -0.0351210009 0.0441191993
O -1.074639355 0.1440665015 -0.6923138722
C 1.2180804341 0.1867532032 3.51897021
C 0.243070527 -0.2484975841 4.3050790482
C 0.4485866027 -0.2411633044 5.7756631911
O -0.4145928231 -1.0268743229 6.3800330856
O 1.1814322354 -0.1483478018 -1.9659104969
O 1.2964231892 0.4034913202 6.3131825829
H 2.1395486623 0.5047358938 3.9938625936
H -0.6791298922 -0.6768031741 3.9352670818
H -0.2227175063 -1.085676535 7.3287889526
H 2.0086489418 -0.3508653536 -2.4275421217
H -0.9337017971 -0.0320127459 -1.6356869887
H 3.4205334089 -0.1343297859 -0.4752703689
H 3.3299315348 0.0903013546 1.9693683466
H -0.9655610122 0.2888441527 1.8586598378

Caffeic Acid (Anion)

z- 0.010

C 1.2480314048 0.0536804553 -0.7586825309
C 0.0323155268 -0.0796389795 -0.0259392565
C -0.0192354455 -0.1353956888 1.326261165
C 1.1644008696 -0.0613693837 2.0763819062
C 2.3503416862 0.0698934967 1.3890850963
C 2.4046301816 0.1276456444 0.0068796332
O -1.0587654161 -0.1440993579 -0.8342448008
C 1.2016202837 -0.1180146815 3.5241013609
C 0.207925903 -0.2391246342 4.3901962737
C 0.5174725146 -0.2752545964 5.8231881171
O -0.5785374055 -0.3910302111 6.576875768
O 1.1506095952 0.0920513629 -2.0440713387
O 1.6135071198 -0.2120707385 6.3000236724
H 2.1895732442 -0.0528530185 3.9702372446

H -0.8332708207 -0.3131394666 4.1126082758
H -0.3044895474 -0.4048993466 7.5060615501
H -0.6127272979 -0.0698987893 -1.7108677241
H 3.3570456593 0.2328814477 -0.4976924774
H 3.2682677598 0.1298614769 1.9616660771
H -0.9770648156 -0.2367069915 1.8197029881

z+ 0.010

C 1.2402760305 0.0572824805 -0.7412277821
C -0.0021865765 -0.0830108575 0.0234648385
C -0.0109530539 -0.1387463125 1.3548951938
C 1.2134753357 -0.0626987938 2.1032747788
C 2.4223219279 0.0707735007 1.3561494346
C 2.4580490496 0.1287585276 0.0180628519
O -1.095875907 -0.1459561708 -0.738754174
C 1.2756291139 -0.1100295723 3.4663522802
C 0.2347658502 -0.2373289258 4.3905578182
C 0.4619254343 -0.267476588 5.7524271986
O -0.6930888632 -0.4043012797 6.5199162053
O 1.1590152456 0.1036601601 -1.9561424893
O 1.5060831847 -0.1946120852 6.4139463177
H 2.2690083179 -0.0401157899 3.8993009987
H -0.7888583807 -0.3208383795 4.061242347
H -0.3244161084 -0.4123077694 7.4077741232
H -0.7725119224 -0.0821212529 -1.6597131847
H 3.3781499296 0.2286822555 -0.5401371407
H 3.3491361537 0.1257947817 1.9158675855
H -0.9582937615 -0.242889929 1.8645137988

z- 0.002

C 1.2432526723 0.0544781034 -0.7477098486
C 0.0211647258 -0.0805172646 -0.0011367905
C -0.0124681121 -0.1363597905 1.3433771735
C 1.1867025736 -0.0619458858 2.084728782
C 2.3739092503 0.0690003579 1.381465946
C 2.4195719427 0.1270086489 0.0105528201
O -1.0715258169 -0.1439432932 -0.7913472096
C 1.2286944287 -0.1154348061 3.5062520638
C 0.221233398 -0.2385280423 4.3793745001
C 0.4989336653 -0.2714078937 5.791853754
O -0.6179482058 -0.3981234626 6.5415268317
O 1.1416781416 0.0951869063 -2.0046234566
O 1.5733916252 -0.2006897549 6.3345974661
H 2.2177188357 -0.0471346337 3.9497081088

H -0.8127976747 -0.3162277652 4.0807912944
H -0.3186080826 -0.4083964591 7.4592017292
H -0.662277211 -0.0731210303 -1.6835788463
H 3.3602297246 0.2298312125 -0.5134707952
H 3.2971322407 0.1271265036 1.9466475692
H -0.9663371214 -0.2382836506 1.843559908

z+ 0.002

C 1.2429545462 0.0557783745 -0.7430162944
C 0.0138652293 -0.0813638228 0.0082234073
C -0.012300969 -0.1375034369 1.3479220464
C 1.1943078113 -0.062533232 2.0908112439
C 2.3869894841 0.0692390965 1.3766279626
C 2.4312481424 0.1276123016 0.0158551167
O -1.0788597729 -0.1444845775 -0.7740675825
C 1.2397926002 -0.1143020932 3.4929287741
C 0.2237959833 -0.2384337512 4.3786927727
C 0.4891390514 -0.2701854184 5.7749238304
O -0.6367410759 -0.3999750676 6.5315083461
O 1.1475422723 0.097035456 -1.9850503164
O 1.5546836418 -0.1976900447 6.3516140276
H 2.2297415576 -0.045302463 3.9344407045
H -0.8072609101 -0.3175473429 4.0716727439
H -0.3150493238 -0.4082464835 7.4400055438
H -0.6948195825 -0.0748667116 -1.6750991502
H 3.3659633644 0.2293179034 -0.5178594601
H 3.3110946314 0.1263114174 1.9408745315
H -0.9644356814 -0.2403421041 1.8507627521

z- 0.004

C 1.2439039231 0.0545294082 -0.7502613756
C 0.0242133158 -0.0802514635 -0.0065555289
C -0.0132633989 -0.1361495552 1.3400910031
C 1.1822414747 -0.0616507839 2.0822331222
C 2.3680317446 0.0692159075 1.3834310381
C 2.4150089821 0.1270824441 0.0086740979
O -1.0682228509 -0.1437284911 -0.8009353713
C 1.2229459979 -0.1159460541 3.5117361994
C 0.2190695877 -0.2388771559 4.3810393629
C 0.5033991648 -0.2724742023 5.7999323358
O -0.6088245313 -0.3968824724 6.5486712567
O 1.1413566348 0.0930420323 -2.0144483672
O 1.5826703895 -0.2024755072 6.3266694857
H 2.2115221911 -0.0479910414 3.9561097691

H -0.81649384 -0.316062539 4.0868099557
H -0.3179707905 -0.4077890054 7.4699475136
H -0.6489289151 -0.0710433386 -1.6893848045
H 3.3585645614 0.2301235929 -0.5106896916
H 3.2903764818 0.1277248572 1.9497601697
H -0.9679491226 -0.2378786322 1.8389408291

z+ 0.004

C 1.2427952276 0.05555412 -0.741372988
C 0.0099002289 -0.0817485312 0.0124878503
C -0.0124975596 -0.1376730233 1.3496877477
C 1.1982112926 -0.0627423454 2.0941568767
C 2.3947951606 0.0694210556 1.3730555377
C 2.4379648564 0.1277910714 0.0182012444
O -1.083095408 -0.1449560295 -0.765302999
C 1.2462547671 -0.1134949184 3.4856874734
C 0.2247791953 -0.2379403045 4.3799460838
C 0.4833182212 -0.2692455741 5.7670729488
O -0.6478814548 -0.4009241364 6.5277655991
O 1.1517461283 0.0996400412 -1.9759696603
O 1.5447053626 -0.1972289488 6.361983216
H 2.2367931235 -0.0444824609 3.9259013618
H -0.8047771056 -0.3175742876 4.0685565411
H -0.3134287042 -0.4089121999 7.4308533253
H -0.7128610705 -0.0777351455 -1.6707849688
H 3.3693041561 0.2294225245 -0.5210112815
H 3.3192436562 0.1260904206 1.9368381676
H -0.9636190738 -0.2407433279 1.854018924

z- 0.006

C 1.2449155909 0.0539879449 -0.7529839271
C 0.0269995137 -0.0799723911 -0.0124591168
C -0.0146989334 -0.1356931778 1.3361572837
C 1.1770656928 -0.0614911636 2.0799854348
C 2.3622197301 0.0692802101 1.3852500663
C 2.4110153475 0.1270575441 0.007364381
O -1.0651105745 -0.1437800546 -0.8110955851
C 1.2165664779 -0.1165475373 3.5164750712
C 0.2160769473 -0.2388798906 4.3834049993
C 0.5078723282 -0.2732247501 5.8078145487
O -0.5993352683 -0.3952462143 6.5569395542
O 1.1427144432 0.0931072667 -2.0243139552
O 1.5924305609 -0.2053084889 6.3182539109
H 2.2048094252 -0.0493803086 3.9616334734

H -0.8212043049 -0.3150979487 4.0940605422
H -0.315404116 -0.4072607367 7.481268265
H -0.6358371021 -0.0711145485 -1.6954896515
H 3.3574493845 0.2308998509 -0.5072437028
H 3.2833886204 0.1283023662 1.9531896338
H -0.9702827636 -0.237119972 1.833559774

z+ 0.006

C 1.2423473051 0.0563504457 -0.7403244441
C 0.0057775848 -0.0822308352 0.0163933893
C -0.0124375864 -0.1382123875 1.3512851462
C 1.2026810754 -0.0628439082 2.0975657112
C 2.4035513324 0.0698636242 1.3684928314
C 2.4450229816 0.1282069239 0.0196955717
O -1.0872978464 -0.1453170559 -0.7568684256
C 1.2542959605 -0.1125056045 3.4785441615
C 0.2266658585 -0.2378324312 4.3825144032
C 0.4767341001 -0.2687396656 5.7603801716
O -0.6609182015 -0.4019308677 6.524984746
O 1.155477769 0.100570288 -1.9677475079
O 1.5332853595 -0.1962975783 6.375709299
H 2.2455636412 -0.0431669885 3.9169544641
H -0.801167048 -0.3185536181 4.0660917023
H -0.3138387393 -0.4094127913 7.4226044872
H -0.7329263113 -0.07881402 -1.66757453
H 3.3727373066 0.2291774837 -0.5255799629
H 3.3284913833 0.1259521456 1.9314737101
H -0.962394925 -0.2417451591 1.8571760757

z- 0.008

C 1.2462854152 0.0537952588 -0.7557874203
C 0.0297129345 -0.0797767056 -0.0189240771
C -0.0166745682 -0.1354872033 1.3315369813
C 1.1711418263 -0.0613840666 2.0780623069
C 2.3563829898 0.0695482732 1.3871182029
C 2.4076003097 0.127279261 0.0067862133
O -1.0619626174 -0.1438794931 -0.8222151435
C 1.2094898483 -0.1172249059 3.5205810465
C 0.2123547916 -0.2390183806 4.386496592
C 0.5125359045 -0.2742090805 5.8155671929
O -0.5892990153 -0.3933143634 6.5663733489
O 1.1458531157 0.0924805912 -2.034172497
O 1.6026929497 -0.2084219375 6.3094270699
H 2.1975226763 -0.0509436425 3.9663187009

H -0.8268014564 -0.3142393381 4.1027023245
H -0.310926327 -0.4062476201 7.4933118944
H -0.6240109488 -0.0704491825 -1.7027381307
H 3.3569751288 0.2317754998 -0.5029305117
H 3.2760802626 0.1290354793 1.9571349794
H -0.9733022201 -0.2368004435 1.8271219267

z+ 0.008

C 1.2415008811 0.0567966134 -0.7402593544
C 0.0016747731 -0.0826563985 0.0201410016
C -0.0119050536 -0.1385203 1.3530442937
C 1.2078996244 -0.0628146619 2.1006794941
C 2.4129556199 0.0703242218 1.3627530025
C 2.4518581544 0.1285168491 0.0196510095
O -1.0917384919 -0.1456941481 -0.7477561116
C 1.2642222197 -0.1113143876 3.4720010054
C 0.2298865704 -0.2375510276 4.386042541
C 0.4694158896 -0.2681425206 5.7553482211
O -0.6762063055 -0.4030756341 6.5223618246
O 1.1580045892 0.1021050146 -1.9610787974
O 1.5203088778 -0.195590368 6.393007297
H 2.256387921 -0.0417222113 3.9081155401
H -0.7959369372 -0.3194889561 4.0634788258
H -0.3174844232 -0.4105971815 7.4147909121
H -0.7530894662 -0.0805567449 -1.6636318599
H 3.3757555576 0.228987929 -0.5320743125
H 3.3386959463 0.1258918315 1.9243519783
H -0.9605549469 -0.2423799191 1.8608044889

Zero Field

C 1.24305326 0.0550458129 -0.7452245691
C 0.0177160687 -0.0809023349 0.0037848462
C -0.0122956468 -0.1368839605 1.345941138
C 1.1905840618 -0.0622260486 2.0876572481
C 2.3800620788 0.0690469276 1.3793324911
C 2.4250751884 0.1272420836 0.0131625007
O -1.0751853377 -0.1441838248 -0.7824865693
C 1.2340872193 -0.1148758776 3.4998824133
C 0.2226446916 -0.2384228905 4.3785216593
C 0.4942674654 -0.2706607892 5.7832231145
O -0.6270098324 -0.3991756753 6.5358502181
O 1.1441858725 0.0960873386 -1.9947094229
O 1.5642153188 -0.1990238559 6.3425294841
H 2.2235254664 -0.0461970938 3.9425529732

H -0.8098805222 -0.3168045811 4.0756650817
H -0.3169824128 -0.4084681164 7.4491846975
H -0.6779083396 -0.0740254475 -1.6790317686
H 3.3629298417 0.2295070671 -0.5153745757
H 3.3038549149 0.1266602307 1.9438646983
H -0.9652873567 -0.2392199645 1.8474473415

x- 0.010

C 1.2220564243 0.0568038871 -0.7347152903
C 0.0110821568 -0.0805808879 0.0357975221
C 0.0042954558 -0.1393128609 1.3747839569
C 1.2223960887 -0.0648412437 2.092698546
C 2.4022282342 0.0641040946 1.3580041847
C 2.4223673381 0.1233875445 -0.0074468819
O -1.0864191684 -0.1386605097 -0.759783513
C 1.2721894134 -0.1117469784 3.5000003273
C 0.2420483611 -0.2372262836 4.3670836815
C 0.4719574475 -0.2611279343 5.7729371329
O -0.6826644467 -0.4118996624 6.5088525395
O 1.0671970744 0.1022854697 -1.9807638289
O 1.5082709494 -0.1682048232 6.3767307466
H 2.2593489616 -0.0374255828 3.9478432013
H -0.7805138916 -0.3304970988 4.0364519838
H -0.3551966824 -0.4218630007 7.4168161662
H -0.6359506088 -0.0650984716 -1.6445331466
H 3.3538610279 0.2205863445 -0.5473208685
H 3.3395451019 0.1176693297 1.8997535002
H -0.9364482373 -0.243833332 1.8985810401

x+ 0.010

C 1.2622776038 0.050859434 -0.7562158662
C 0.0246901766 -0.080602728 -0.0240779456
C -0.0211860362 -0.1331550232 1.3219782963
C 1.1687069294 -0.0590008661 2.0825936883
C 2.3656223239 0.0733005846 1.3966986918
C 2.4284967037 0.128534269 0.0277983976
O -1.0704834927 -0.1473655148 -0.7909458386
C 1.2067258815 -0.1158104381 3.5012288731
C 0.2113842002 -0.2400189402 4.3885386477
C 0.5136118805 -0.2780831979 5.7938464406
O -0.5846771458 -0.3910941977 6.551116757
O 1.2140329419 0.086233082 -2.0081302427
O 1.6082844157 -0.2219507374 6.3207663568
H 2.1988733667 -0.0493658026 3.9384798587

H -0.8292237655 -0.3107660741 4.1099664776
H -0.3039990449 -0.4011383403 7.4734096912
H -0.7366333701 -0.078989235 -1.7042335666
H 3.3712192483 0.2362783556 -0.4945588945
H 3.279180275 0.1360638304 1.9795558888
H -0.9852520919 -0.2314104602 1.8039552887

x- 0.002

C 1.2389391291 0.055323008 -0.7431535334
C 0.0162952494 -0.0808882066 0.0098843544
C -0.0094505418 -0.1373532897 1.3513799449
C 1.1962475486 -0.0628305558 2.0886637768
C 2.3839826981 0.067983892 1.3752749936
C 2.4244230591 0.1265377443 0.0094004767
O -1.0769799364 -0.1433835785 -0.7790189223
C 1.2409816062 -0.1143157193 3.4998578752
C 0.2259309947 -0.2377532828 4.3763344335
C 0.4898302275 -0.2683974185 5.7812738763
O -0.6372447599 -0.401528958 6.5314488846
O 1.1291712895 0.0983168869 -1.9920642744
O 1.5538176475 -0.1937219491 6.3485390651
H 2.2299132324 -0.044868098 3.9435600957
H -0.8047349188 -0.3184042699 4.0680804805
H -0.3227580682 -0.4113278433 7.443398962
H -0.667899413 -0.0732652185 -1.6726771543
H 3.3610450171 0.2279034733 -0.5211525596
H 3.310239099 0.1247451346 1.9355888579
H -0.9600981601 -0.2402537514 1.8571513669

x+ 0.002

C 1.2470371628 0.0545368339 -0.7473225223
C 0.0190644962 -0.08089387 -0.0022122008
C -0.0146805981 -0.1362986815 1.3406730859
C 1.1853310547 -0.0616073479 2.086580715
C 2.3765185923 0.0700301437 1.3832019079
C 2.4256329554 0.1277610738 0.0165700015
O -1.0734398384 -0.1448788487 -0.78543141
C 1.2276776902 -0.1153000951 3.5000303615
C 0.219810506 -0.2389309621 4.3806834006
C 0.4985545111 -0.2725912578 5.7854351995
O -0.6173174258 -0.3971405325 6.5398266919
O 1.15848891 0.0939775932 -1.997388437
O 1.5740284331 -0.2040271986 6.3372542141
H 2.2176830033 -0.0472785476 3.9414362724

H -0.8145203423 -0.3153211611 4.0832079137
H -0.3125703715 -0.4062046997 7.4547638048
H -0.688001499 -0.0748696831 -1.6849269069
H 3.3644980953 0.2309849543 -0.5104989055
H 3.2979083986 0.1285413009 1.9518906302
H -0.9700527336 -0.2379710141 1.8379971834

x- 0.004

C 1.2348250492 0.0563951239 -0.7411107022
C 0.0150301384 -0.0809337304 0.0158696904
C -0.0066049971 -0.1382741158 1.3566900742
C 1.2019325221 -0.0634859693 2.089629067
C 2.387878777 0.0671571999 1.371303543
C 2.4237947879 0.1261554651 0.0056276365
O -1.0786821758 -0.1423350728 -0.7754069942
C 1.2478500869 -0.114033927 3.499773368
C 0.2293484126 -0.2380756485 4.3741915987
C 0.4858088651 -0.2674085604 5.7792324506
O -0.6474268128 -0.4034174234 6.5268683559
O 1.1144162379 0.0986631039 -1.9894237993
O 1.5435720586 -0.1876330903 6.3547119743
H 2.2363213527 -0.0434874143 3.9444742187
H -0.799484862 -0.3214310298 4.0607318801
H -0.3292194876 -0.4125421917 7.4376786356
H -0.6586766863 -0.0702061193 -1.6661926315
H 3.3592666752 0.2263146517 -0.5269163736
H 3.3166337355 0.1230261248 1.9274065245
H -0.9549326774 -0.2419293763 1.8666324832

x+ 0.004

C 1.2509325218 0.0533176392 -0.7494511758
C 0.0203958626 -0.080790911 -0.0077966755
C -0.0167363466 -0.1353656566 1.3358341571
C 1.1806762045 -0.0609700678 2.0856075779
C 2.3733965093 0.0708073051 1.3867540782
C 2.4262992299 0.1279439804 0.019693429
O -1.0724095491 -0.1455954321 -0.7875846169
C 1.2219421023 -0.1154857735 3.5002665369
C 0.2173085575 -0.2389679883 4.3827259563
C 0.5023905052 -0.2737590303 5.7875092673
O -0.6085613633 -0.3955427044 6.5431786057
O 1.172528763 0.0929767547 -2.0000039523
O 1.5830808661 -0.2089786362 6.3324584415
H 2.2124687253 -0.0481207941 3.9406321276

H -0.81866237 -0.3135460634 4.0901487552
H -0.308947905 -0.4050815317 7.4597029869
H -0.6989798642 -0.0769283607 -1.6903915484
H 3.3661860895 0.232398423 -0.5059045462
H 3.2926578357 0.1303399595 1.959164794
H -0.9743153745 -0.2361331115 1.8292268015

x- 0.006

C 1.2307267128 0.0564041214 -0.738942356
C 0.0137310739 -0.0808593446 0.0224485128
C -0.0030651701 -0.1386171397 1.3626693772
C 1.2086200468 -0.0639435394 2.0906637627
C 2.3926195886 0.0661826541 1.3669917613
C 2.423441226 0.1253077478 0.0014618694
O -1.0811439141 -0.1413183649 -0.7703798608
C 1.2556871888 -0.1133672932 3.499803438
C 0.233241347 -0.2376355648 4.3717219044
C 0.481081602 -0.2653035941 5.7770841016
O -0.6588571717 -0.4060179049 6.5211281619
O 1.0989200896 0.1004404408 -1.9865116234
O 1.5321136413 -0.1817939511 6.3615473292
H 2.2436728798 -0.0418146683 3.9456571833
H -0.7935782744 -0.3237702725 4.05252351
H -0.337151164 -0.4155082258 7.4308220451
H -0.6512658235 -0.0691756536 -1.6591598892
H 3.3575779972 0.2246301313 -0.533432228
H 3.3241406905 0.1213016524 1.9184122463
H -0.9488615667 -0.2426232307 1.8772617543

x+ 0.006

C 1.2548004299 0.0523764698 -0.7516221483
C 0.0217887202 -0.0807204966 -0.013329785
C -0.0185227454 -0.1345900395 1.3310743367
C 1.1763296806 -0.0603340674 2.0846119873
C 2.3705282435 0.0716466871 1.3902309406
C 2.4270133683 0.1281746086 0.0226345679
O -1.0715060845 -0.1462025141 -0.789252507
C 1.216485436 -0.1156882032 3.5005291826
C 0.2150502364 -0.2392794286 4.38472671
C 0.50625046 -0.2752059973 5.7895935857
O -0.6001487535 -0.3939667428 6.5461612264
O 1.1864764131 0.0911652669 -2.002640888
O 1.59188017 -0.2134918054 6.3280598151
H 2.2075555619 -0.0487904049 3.9398305975

H -0.8225329904 -0.312332622 4.0970146436
H -0.3063192885 -0.4036514355 7.4644509973
H -0.7108261744 -0.0780524582 -1.6954833225
H 3.3678875921 0.2337548852 -0.5016852898
H 3.2877537214 0.1322123253 1.9662721991
H -0.9782929967 -0.2345060275 1.820594151

x- 0.008

C 1.2264536665 0.0566577141 -0.7368437751
C 0.0124165484 -0.0807498755 0.0290252241
C 0.000499004 -0.1390172581 1.3686252601
C 1.215337216 -0.0644166017 2.0916803974
C 2.3973093359 0.0651650256 1.3625773832
C 2.4229215411 0.1244172877 -0.0028744
O -1.0836681895 -0.1400829344 -0.7653202423
C 1.2637152921 -0.1126227242 3.4998748303
C 0.2374457988 -0.2374114179 4.3694056529
C 0.4765407635 -0.2632871679 5.775008682
O -0.6704976425 -0.4088113649 6.5152531489
O 1.0832686126 0.1014733426 -1.9836767743
O 1.5204578521 -0.1752470896 6.3688644499
H 2.2512683965 -0.0397840123 3.9467552332
H -0.7872966165 -0.32688167 4.0445341442
H -0.3456884798 -0.4185022401 7.4240039764
H -0.6434640554 -0.0672322677 -1.6519768874
H 3.3557600606 0.2227013928 -0.5401721323
H 3.3316668018 0.1195012059 1.9092536319
H -0.9427949063 -0.2433513444 1.8877731966

x+ 0.008

C 1.2586135367 0.0513624321 -0.7538407912
C 0.0232085166 -0.0806506667 -0.0186948212
C -0.0199621677 -0.133810393 1.3265224581
C 1.172427534 -0.059710099 2.0836221647
C 2.3680168104 0.0724493803 1.3935390662
C 2.4277892106 0.1283289321 0.0253270381
O -1.070894783 -0.1467782902 -0.790284579
C 1.2114707405 -0.115842437 3.5008507105
C 0.2130861487 -0.2396063251 4.3866352184
C 0.5099449215 -0.2765890807 5.7916776683
O -0.592299918 -0.3925070065 6.5486825992
O 1.2001964313 0.0892854181 -2.0052871406
O 1.6002325717 -0.2177615928 6.3241236115
H 2.203083927 -0.0493056329 3.9391285748

H -0.8260423116 -0.3113371328 4.1035937176
H -0.3047582054 -0.4023677235 7.4688724746
H -0.7235429225 -0.0790199267 -1.7000952754
H 3.3695896007 0.2351068459 -0.49792398
H 3.2833559903 0.1341146401 1.9730177849
H -0.9818646317 -0.2328433418 1.8123045005

y- 0.010

C 1.2496320232 -0.0066429147 -0.7423796732
C 0.0203013667 -0.1001334765 0.0073876916
C -0.0137682952 -0.096756568 1.3499429074
C 1.1882936028 -0.0012385697 2.0917646766
C 2.3763067468 0.150787156 1.3811038745
C 2.4242243533 0.1608873587 0.0151495072
O -1.0707272973 -0.2068137832 -0.7788243614
C 1.2354534151 -0.1021791369 3.4984947273
C 0.220735359 -0.2333577084 4.376895335
C 0.4922774077 -0.3827390493 5.7709686472
O -0.6260646156 -0.3265683782 6.5387153037
O 1.1617710602 -0.0823429004 -1.9903677527
O 1.5592997731 -0.5660093713 6.3150129711
H 2.2284665432 -0.0817355575 3.9379521231
H -0.8150910269 -0.1642235338 4.0827883295
H -0.3077688235 -0.3101616082 7.4488844095
H -0.6788035471 -0.1197087835 -1.6754763708
H 3.3537851561 0.3173651246 -0.5146288203
H 3.2927953224 0.2817584793 1.9452467374
H -0.9694675241 -0.1576687792 1.8531407374

y+ 0.010

C 1.2422376746 0.1187251131 -0.740180995
C 0.0197104167 -0.0613104957 0.0018129286
C -0.0087948654 -0.177008486 1.341202158
C 1.1928972543 -0.1237166797 2.0847102582
C 2.3846956964 -0.0121122045 1.3788558912
C 2.4280755667 0.0957285988 0.0144608559
O -1.0786192238 -0.0841200513 -0.7800199262
C 1.2300530797 -0.1295555056 3.5003716183
C 0.2186781833 -0.2434440798 4.3784908507
C 0.4786395272 -0.1615024372 5.785331262
O -0.6006101602 -0.4713633147 6.5383662685
O 1.1418893656 0.2772756811 -1.9823409238
O 1.5077134326 0.1608317327 6.3367802823
H 2.2150379521 -0.0140783023 3.9431145402

H -0.7952803927 -0.4588169101 4.0783561232
H -0.2875530466 -0.5004268575 7.4502805431
H -0.6887261448 -0.0344999587 -1.679036356
H 3.3693294577 0.1426162686 -0.5162618232
H 3.3118367593 -0.0288649072 1.9407223772
H -0.9595595328 -0.3218392038 1.8367550668

y- 0.002

C 1.2438126905 0.0429393173 -0.7452842203
C 0.0178632343 -0.0849132708 0.0043452747
C -0.0125799136 -0.1294582343 1.3467876308
C 1.1902200484 -0.0504723543 2.0883192521
C 2.3793146272 0.0850699543 1.3795447981
C 2.4246437939 0.1339020837 0.0132103562
O -1.0742543549 -0.1565632989 -0.7822196398
C 1.2347053522 -0.1125326684 3.4997258408
C 0.2228704616 -0.237179227 4.3783358571
C 0.4952957174 -0.292693295 5.7817626009
O -0.6290814766 -0.3842608713 6.5359465343
O 1.1460921902 0.0614116261 -1.9951966008
O 1.5680791692 -0.2718875936 6.33997872
H 2.2249909463 -0.0536883976 3.9418521533
H -0.811682512 -0.2864925141 4.0763095596
H -0.3186978563 -0.388788312 7.4491494701
H -0.6769160966 -0.0827514316 -1.6785080967
H 3.3611056842 0.247388057 -0.5154833442
H 3.3019606991 0.1572553069 1.9442601383
H -0.9660914044 -0.2237668765 1.8489347155

y+ 0.002

C 1.2424503912 0.0671820546 -0.7448821762
C 0.0177045994 -0.0769535036 0.0032077428
C -0.0117686782 -0.1443341453 1.3450306469
C 1.1909636346 -0.0739859432 2.0869662325
C 2.3809070018 0.0531308485 1.3791568045
C 2.4254588176 0.120766653 0.0131365326
O -1.0757858741 -0.1320988835 -0.7825601643
C 1.2334072116 -0.1173177789 3.5000556652
C 0.2223085942 -0.2394915872 4.3786680436
C 0.492584845 -0.2488726658 5.7845107223
O -0.6239050729 -0.4136581605 6.5360379238
O 1.1424337456 0.1310513755 -1.9936403466
O 1.5579131858 -0.1272087725 6.343971142
H 2.2220208501 -0.0390534348 3.9429076512

H -0.8076321535 -0.3462091996 4.0756149746
H -0.3142063496 -0.4278639414 7.4494129542
H -0.678798423 -0.065821498 -1.6792895958
H 3.3643242991 0.2118930302 -0.515737839
H 3.305615867 0.0962002496 1.9435129676
H -0.9643454918 -0.2548366971 1.845691118

y- 0.004

C 1.2448669142 0.0310967713 -0.7450252464
C 0.0182174922 -0.0888749025 0.004991772
C -0.0129212834 -0.1218572316 1.3476040842
C 1.1897952025 -0.0386325406 2.0890849532
C 2.3785342332 0.1013054999 1.3798556598
C 2.4243663356 0.1410192513 0.0135074197
O -1.0733789011 -0.1695248971 -0.7817503581
C 1.2351169892 -0.110333542 3.4994741253
C 0.2227158465 -0.2361188023 4.3780790866
C 0.495615298 -0.3152060082 5.7797050613
O -0.6300343188 -0.368123302 6.5363624881
O 1.1489583983 0.0266048102 -1.9950006047
O 1.5695703644 -0.3468337423 6.3357636335
H 2.2261897372 -0.0615919865 3.941067034
H -0.8132055648 -0.2556187474 4.0773173345
H -0.3183879915 -0.3682627314 7.4491111943
H -0.6766522792 -0.0922828545 -1.6779946587
H 3.3593286647 0.2658164976 -0.5152478922
H 3.2998749307 0.1881974843 1.9446158444
H -0.9669190679 -0.2082610265 1.8502500692

y+ 0.004

C 1.2421151038 0.0793439846 -0.744232367
C 0.0179185316 -0.0730933356 0.0027337223
C -0.0112006511 -0.152069992 1.3441214056
C 1.1913733857 -0.0858567513 2.0863567228
C 2.3817641306 0.0371338379 1.3790417948
C 2.4260037874 0.1141414084 0.0132730435
O -1.076543304 -0.1198292048 -0.7823325721
C 1.2326355075 -0.1197609247 3.5002031894
C 0.2216847222 -0.2402203566 4.3787508223
C 0.4901485359 -0.2268562821 5.785324708
O -0.6196023974 -0.429099788 6.5363024498
O 1.141508475 0.166206552 -1.9919247134
O 1.5490093769 -0.0543761298 6.3441219697
H 2.2203648455 -0.0319420295 3.9432272567

H -0.8050539025 -0.3748966795 4.0758366966
H -0.3096598445 -0.4475797645 7.4495306269
H -0.6805765296 -0.0573317692 -1.6794868069
H 3.3657914221 0.1939499441 -0.5158656392
H 3.3072951631 0.0654752737 1.943004752
H -0.9633253582 -0.270819993 1.8437839381

y- 0.006

C 1.2461926435 0.0190355813 -0.7444792942
C 0.0187519153 -0.092879475 0.0056623476
C -0.0132549561 -0.1142304703 1.3483510717
C 1.1892791951 -0.0267299993 2.0899026449
C 2.3777150392 0.1176341759 1.3802444138
C 2.4241795676 0.1480298816 0.0139518018
O -1.0724326065 -0.1822312251 -0.7811541841
C 1.2352977229 -0.1080732946 3.4991831163
C 0.2222318573 -0.2352063437 4.3777757252
C 0.4951788345 -0.3377306962 5.7772520066
O -0.6296782693 -0.3523653115 6.5371319491
O 1.1525284863 -0.0085399874 -1.9941777003
O 1.5685511789 -0.4213967597 6.3300512806
H 2.2270802137 -0.0691060228 3.9401544776
H -0.8143537912 -0.2249147286 4.078767462
H -0.3162133873 -0.3478321932 7.449210417
H -0.6766632151 -0.1015071739 -1.6773780012
H 3.3574795911 0.2839187975 -0.5149680348
H 3.2975618254 0.2192602785 1.9449712905
H -0.9677808452 -0.1926170335 1.8513182101

y+ 0.006

C 1.2419430939 0.0918360678 -0.7432530399
C 0.018296247 -0.0690643006 0.0023751358
C -0.0105446197 -0.1597515083 1.3432312557
C 1.1918299975 -0.0978522256 2.085785745
C 2.382673701 0.0209693414 1.3789357894
C 2.4266019594 0.1076295537 0.0134873192
O -1.077239199 -0.1077567566 -0.781836948
C 1.2318355687 -0.1224230452 3.5003290245
C 0.2208776676 -0.2409849347 4.3787395422
C 0.4869328764 -0.204925469 5.7857736628
O -0.61414481 -0.4446666454 6.5367303875
O 1.1410177316 0.2018714667 -1.9895405653
O 1.5374556738 0.0185065384 6.3430559612
H 2.2186709537 -0.0252728432 3.943383297

H -0.8020918617 -0.4030932105 4.0763010583
H -0.3036359029 -0.4668202996 7.4496991999
H -0.6825931091 -0.0493793999 -1.6794497759
H 3.3670927264 0.1761360982 -0.5160603169
H 3.3088985085 0.034374375 1.9423396353
H -0.962226203 -0.2868148027 1.8417446321

y- 0.008

C 1.2477898925 0.0064472032 -0.7436096204
C 0.0194475749 -0.0965979534 0.0064497592
C -0.0135486195 -0.1058167051 1.3491252194
C 1.1887631293 -0.014240825 2.0907941553
C 2.3769659548 0.1340953765 1.3806686196
C 2.4241382432 0.1545993921 0.0145022839
O -1.0715446348 -0.1946353362 -0.7801955004
C 1.2353875374 -0.1053156796 3.4988606509
C 0.2215579743 -0.2342593258 4.3773871404
C 0.4940728014 -0.3601871651 5.7743480369
O -0.6283027744 -0.3387894315 6.5379243781
O 1.1568138603 -0.0448516876 -1.9926602021
O 1.565102779 -0.4941091759 6.3231404555
H 2.2278141841 -0.0757598617 3.9391161379
H -0.8149947656 -0.194483313 4.080606656
H -0.3126293028 -0.3286266435 7.4491499972
H -0.6773716539 -0.1106806298 -1.676558425
H 3.3556443726 0.301018124 -0.5147460851
H 3.2951960355 0.2503756652 1.9451952286
H -0.9686515883 -0.1756640279 1.852272114

y+ 0.008

C 1.2419810407 0.1049499857 -0.7419172333
C 0.0188947263 -0.0651518521 0.0020777099
C -0.009727069 -0.168079695 1.342270721
C 1.1923611293 -0.1104873027 2.0852423539
C 2.3836684859 0.0045566015 1.3788657181
C 2.4272981925 0.101490314 0.0138754483
O -1.0779487992 -0.0958192484 -0.7810380446
C 1.2309991069 -0.1256938541 3.5003839702
C 0.2198983439 -0.2421254532 4.3786507776
C 0.483090649 -0.1831617012 5.785770136
O -0.6078552161 -0.4586103318 6.5373944895
O 1.1411427704 0.2388681461 -1.9863671665
O 1.5236518487 0.0901315391 6.3406455585
H 2.2169099644 -0.0192639078 3.9433505821

H -0.7987848107 -0.4312001807 4.0771353776
H -0.2963114751 -0.4843426995 7.4499237522
H -0.6853698009 -0.0416811305 -1.6792832824
H 3.3682702869 0.1590168326 -0.5162084106
H 3.3104326422 0.0029535561 1.9415690209
H -0.9609510164 -0.3038316179 1.8394295216

Optimized Structures of Gallic Acid and Caffeic acid and their radicals in different electric field along C-O direction at 6-311++G(3df,2p) basis set

B3LYP Caffeic Acid (Neutral) -0.010 a.u.

C 1.2614275288 0.0495546367 -0.7238373737
C 0.0410199894 -0.1011661243 -0.0646472201
C 0.0091353733 -0.1684598151 1.316701601
C 1.1901142044 -0.0864804379 2.0697731834
C 2.4024404753 0.0616549887 1.3838369467
C 2.4381731696 0.1293140902 -0.001847076
O -1.1247002349 -0.1816798168 -0.7842126779
C 1.2312762889 -0.1427477001 3.5295640979
C 0.2151861102 -0.2340658162 4.3897995208
C 0.5117496206 -0.2684231534 5.8505915765
O -0.6171940853 -0.343093604 6.5719681065
O 1.2152353523 0.1109929453 -2.1160820897
O 1.6200175349 -0.2327225063 6.3155255337
H 2.2213068237 -0.0975210793 3.971784472
H -0.8250138836 -0.2805988051 4.0961636079
H -0.3858736908 -0.3585162021 7.5149352026
H 2.1033584817 0.2953802421 -2.4304016924
H -0.900148832 -0.0860641714 -1.7149418136
H 3.3854251227 0.2451019463 -0.5189653001
H 3.3226442668 0.1269970231 1.947653158
H -0.9504686159 -0.2837846405 1.8012222363

B3LYP Caffeic Acid (Neutral) -0.002 a.u.

C 1.2637766636 0.0535623215 -0.7196637166
C 0.0444841951 -0.0787816869 -0.0411439335
C 0.0321584338 -0.134674571 1.338497242
C 1.225132545 -0.0605640238 2.0736566864
C 2.4304626275 0.0714575075 1.3761077537
C 2.4504033843 0.128166624 -0.0113886383
O -1.1258282474 -0.1523943908 -0.7326122804
C 1.2669004696 -0.1140387507 3.529361304
C 0.2409605167 -0.2379855929 4.3800677395
C 0.488064061 -0.2725371075 5.8320719211
O -0.6695272897 -0.3994785942 6.5261045678
O 1.1784113742 0.1007116739 -2.0897490879

O 1.5637871083 -0.2003606922 6.3747898998
H 2.2543405925 -0.0438672069 3.9739116276
H -0.7886430451 -0.3164277864 4.0608455548
H -0.437451131 -0.4146417453 7.4656666723
H 2.054550834 0.1962204035 -2.4727828084
H -0.932281692 -0.0959978756 -1.6752651846
H 3.3899431672 0.2311224579 -0.5419653433
H 3.3595880406 0.1308477136 1.9263384493
H -0.9241216081 -0.2366666775 1.8317355747

B3LYP Caffeic Acid (Neutral) -0.004 a.u.

C 1.2628604866 0.0529424454 -0.7203870556
C 0.0435307284 -0.081360411 -0.0461515474
C 0.0269555734 -0.1385075769 1.3340669571
C 1.2172810561 -0.0637414054 2.0726463451
C 2.4240815155 0.0700776354 1.3777850186
C 2.4473489623 0.1280936596 -0.009468826
O -1.1263015587 -0.1558538181 -0.7435682241
C 1.2587882617 -0.1174643696 3.5300177015
C 0.2352656421 -0.2386252736 4.381634747
C 0.4933259061 -0.2723453681 5.8362867321
O -0.6573139661 -0.3922378567 6.5359656499
O 1.1865079908 0.1018748826 -2.0960920373
O 1.5768570188 -0.2039255865 6.3606455016
H 2.246326258 -0.0491788387 3.9745202871
H -0.7964519111 -0.3144462168 4.0679041535
H -0.4262753108 -0.4068639194 7.4765119112
H 2.0678585103 0.2079921517 -2.4631790721
H -0.9254018053 -0.0938401482 -1.6838155466
H 3.3886533842 0.2326118009 -0.5372810111
H 3.351330222 0.1301351139 1.9309005991
H -0.9301159643 -0.2416649005 1.8256417164

B3LYP Caffeic Acid (Neutral) -0.006 a.u.

C 1.2620526514 0.0525051612 -0.7213545774
C 0.0425143619 -0.0853836828 -0.0516706718
C 0.0213420664 -0.1447588972 1.3290013034
C 1.2088543095 -0.0685556831 2.0716960173
C 2.4172883871 0.0684553257 1.3795862468
C 2.4442081623 0.1287168306 -0.007304675
O -1.1264373603 -0.1613568375 -0.7556849436
C 1.250211923 -0.1229546856 3.5302784522
C 0.2291357001 -0.2381955291 4.38381848
C 0.4990938404 -0.2719127072 5.840859402
O -0.644637062 -0.3811060321 6.546887393
O 1.1952097206 0.1041783153 -2.1025871897

O 1.590655313 -0.2107559326 6.3462015684
H 2.2383042414 -0.0593304015 3.9742683977
H -0.8050727379 -0.3080265388 4.0760570908
H -0.414244444 -0.3958460295 7.488365456
H 2.0811007611 0.2249985066 -2.4531151302
H -0.9178309331 -0.0920354275 -1.6932566135
H 3.3873968345 0.2359052212 -0.5319776596
H 3.3424874535 0.129662786 1.9358521897
H -0.9365221886 -0.2505317624 1.8186634633

B3LYP Caffeic Acid (Neutral) -0.008 a.u.

C 1.2614942023 0.0516760578 -0.7225110187
C 0.0415662938 -0.0913418801 -0.0578146509
C 0.0152898258 -0.1538062875 1.3232571074
C 1.1997001152 -0.0753611502 2.0707694383
C 2.4100069784 0.0661752489 1.3815996973
C 2.4410753681 0.1294641797 -0.0047642057
O -1.1260348644 -0.169404418 -0.7691659757
C 1.2409851197 -0.130664664 3.5301446225
C 0.2224454958 -0.2369897441 4.3865607527
C 0.5052831053 -0.2710376524 5.845623509
O -0.6312168919 -0.3656328117 6.558935758
O 1.2047602582 0.1072051191 -2.1092522261
O 1.6051453051 -0.2205123018 6.3311410077
H 2.229899885 -0.0740862116 3.973362227
H -0.8145775817 -0.2979036937 4.0854784491
H -0.4006671023 -0.380736094 7.5012023976
H 2.0938319917 0.250088947 -2.4424165375
H -0.9095471073 -0.0894338581 -1.7036587596
H 3.3862523184 0.240298878 -0.5259108646
H 3.3328684977 0.1290658525 1.9414256883
H -0.9434502129 -0.2633915157 1.8105775841

B3LYP Gallic Acid (Neutral) -0.010 a.u.

C -0.9536690508 -1.1590007796 0.0021231493
C -1.6932228027 0.0177789691 0.0002623774
C -1.04647878 1.2486625022 -0.0040828109
C 0.3410913489 1.3033270934 -0.0065997747
C 1.0711469411 0.1173310076 -0.004766924
C 0.4249172389 -1.1190495413 -0.0004158571
O -3.0761705682 -0.0071803538 0.0027387284
O -1.7831725756 2.4035341727 -0.0058455939
C 2.5686744085 0.0817256136 -0.0072850089
O 3.1210501217 1.3036092964 -0.0109846236
O -1.6996182906 -2.322568372 0.0065600594
O 3.1950268167 -0.944155675 -0.0066390829

H 1.0253746295 -2.0200394722 0.0009355378
H 0.8412713464 2.2599958908 -0.0098828795
H -1.1036236451 -3.0780586172 0.0084818964
H -3.3330266959 -0.9363626207 0.006199855
H -2.7143596434 2.1596522799 -0.0030098794
H 4.0863502007 1.2020236061 -0.0124951688

B3LYP Gallic Acid (Neutral) -0.002 a.u.

C -0.9526340312 -1.1720785363 0.0022902417
C -1.6925529298 0.0080698104 0.0004855384
C -1.0418941063 1.2403321463 -0.0038856803
C 0.3446754899 1.290643868 -0.0064788588
C 1.0758510926 0.1039982469 -0.0046799625
C 0.427728741 -1.1332054503 -0.0002815472
O -3.0589800633 0.0046569587 0.0028840759
O -1.7627220859 2.3944207623 -0.0056416434
C 2.559520946 0.0906398164 -0.0073498886
O 3.1046272985 1.3274943348 -0.0114243413
O -1.7002724416 -2.3248885451 0.0066428573
O 3.2337040737 -0.9101956776 -0.0061470515
H 1.0188508379 -2.0393477673 0.0010562705
H 0.8393250486 2.2494287903 -0.0098686631
H -1.1230996899 -3.0938594147 0.0080408225
H -3.3641228822 -0.9102802079 0.0058475991
H -2.7015608263 2.1747774938 -0.0033424129
H 4.0651165282 1.2106183712 -0.0128533558

B3LYP Gallic Acid (Neutral) -0.004 a.u.

C -0.9529711439 -1.1687712737 0.0022545243
C -1.6926115893 0.0105000832 0.0004414809
C -1.042933182 1.242281113 -0.0039305338
C 0.3438776972 1.2936132502 -0.0065176669
C 1.0744661498 0.1071427434 -0.0047173025
C 0.4269711658 -1.1297384261 -0.0003222614
O -3.0631460141 0.0018851562 0.0028651335
O -1.7674285715 2.396686302 -0.0056858109
C 2.5616340118 0.0883983336 -0.0073684942
O 3.1082102844 1.3215981243 -0.0113102192
O -1.7000314299 -2.3243359438 0.0066313587
O 3.2239826379 -0.9186618095 -0.0062523049
H 1.0202282818 -2.0346824092 0.0010149103
H 0.8399693599 2.2518116931 -0.0098879452
H -1.1179394129 -3.0898147616 0.0081466354
H -3.3562072364 -0.9167947093 0.0059307063
H -2.7044067257 2.1711663582 -0.0032704137
H 4.0698967171 1.208941176 -0.0127277965

B3LYP Gallic Acid (Neutral) -0.006 a.u.

C -0.9532543089 -1.1654950513 0.0022153443
C -1.6927427135 0.0129273396 0.000390994
C -1.0440391968 1.2443204173 -0.0039782114
C 0.3430165954 1.2967136753 -0.0065525469
C 1.0732280217 0.1104067683 -0.0047468686
C 0.4262498036 -1.1262309024 -0.0003595131
O -3.0673927602 -0.0010122688 0.0028372481
O -1.7723970063 2.3989638475 -0.005733898
C 2.5638583084 0.0861675744 -0.0073692136
O 3.1121304913 1.3156649382 -0.0111979569
O -1.6998465487 -2.3237659682 0.0066150998
O 3.2143109484 -0.9271413014 -0.006367266
H 1.0217669545 -2.0299220153 0.0009789682
H 0.8405144823 2.2543623004 -0.0098997313
H -1.1129847934 -3.0858382672 0.0082549025
H -3.3483893585 -0.9233129752 0.0060179089
H -2.7074836136 2.167451521 -0.0031917791
H 4.0750156943 1.2069653676 -0.0126194807

B3LYP Gallic Acid (Neutral) -0.008 a.u.

C -0.9534856562 -1.1622426302 0.0021715648
C -1.6929446916 0.0153507749 0.0003305597
C -1.0452241122 1.2464465108 -0.004028293
C 0.34208655 1.2999571512 -0.0065769904
C 1.0721197996 0.1138082609 -0.0047596123
C 0.4255682247 -1.1226690232 -0.0003886884
O -3.0717371432 -0.0040308801 0.0027921543
O -1.7776480416 2.401247909 -0.0057874459
C 2.5662147799 0.0839426795 -0.0073349675
O 3.1164186992 1.3096590862 -0.0110910992
O -1.699714119 -2.3231766895 0.0065897943
O 3.2046628865 -0.9356509531 -0.0065005293
H 1.0234880208 -2.0250411487 0.0009548775
H 0.8409411655 2.2570997322 -0.0098938076
H -1.1082177371 -3.0819202717 0.0083678223
H -3.3406698124 -0.9298344595 0.0061046501
H -2.7108074443 2.1636091463 -0.003105914
H 4.0805096315 1.204669805 -0.0125500754

B3LYP Caffeic Acid (Radical) -0.010 a.u.

C 1.2591787139 0.0545812515 -0.770716898
C 0.0042327218 -0.0812537214 -0.02632271
C -0.037497104 -0.1362649002 1.3385229319
C 1.1655118852 -0.06020889 2.0789709824

C 2.4028984231 0.0764193575 1.3697042451
C 2.4598120976 0.1324454259 0.0098141038
O -1.0966128779 -0.1486318146 -0.7961759192
C 1.2315702092 -0.1136817022 3.5101694249
C 0.2092475451 -0.2393210417 4.3858955193
C 0.512925836 -0.2785659033 5.8463619771
O -0.6067824637 -0.3902575543 6.5683147563
O 1.2002004576 0.0929202538 -2.0254112002
O 1.6285821483 -0.2174563887 6.2906633591
H 2.2196689402 -0.0468040856 3.9533218326
H -0.8286729544 -0.3142355747 4.0910693095
H -0.3814396135 -0.4097119087 7.5133914243
H -0.7435186526 -0.0824060718 -1.7049018215
H 3.4008808465 0.236667021 -0.5134384403
H 3.3117438172 0.1359572292 1.9540747266
H -0.9902779756 -0.2376719818 1.8384653963

B3LYP Caffeic Acid (Radical) -0.002 a.u.

C 1.2535049642 0.055493705 -0.7697511544
C 0.0006458446 -0.0812089536 -0.0111474647
C -0.0176962644 -0.1365609918 1.3581779585
C 1.192584707 -0.0605741911 2.0745208272
C 2.4249008242 0.0742772719 1.3569524267
C 2.4691349943 0.1310487176 -0.0012677032
O -1.1084258418 -0.1478053323 -0.7472026971
C 1.261831727 -0.1119030482 3.5118035102
C 0.2354044048 -0.2373255411 4.3763415616
C 0.4951631943 -0.2732256109 5.8292497129
O -0.6538972604 -0.4019506911 6.5290003092
O 1.1827486356 0.0974593275 -2.0110947478
O 1.5801336336 -0.1998401991 6.3504538105
H 2.2520671161 -0.0419382651 3.9488860006
H -0.7959082461 -0.3157514118 4.0633546931
H -0.422529685 -0.4190658143 7.4691058951
H -0.8036825326 -0.0854913756 -1.6741640324
H 3.4004312979 0.2332593397 -0.5409062936
H 3.3403101308 0.1316740941 1.9315871743
H -0.9650696444 -0.2380520297 1.8678732133

B3LYP Caffeic Acid (Radical) -0.004 a.u.

C 1.2543720243 0.0549771464 -0.7697184259
C 0.001466998 -0.0812209543 -0.0139036504
C -0.0217084729 -0.1365499418 1.3543650673
C 1.1870678703 -0.0606775694 2.0754868036
C 2.4202344205 0.0746137323 1.3595392743
C 2.4668353966 0.1313014089 0.0009300753

O -1.1061298405 -0.1479264569 -0.7573401889
C 1.2557339341 -0.1125001036 3.5120006583
C 0.2300938755 -0.2377105775 4.3776739496
C 0.499069751 -0.2741567691 5.8332281004
O -0.6437719215 -0.3996408836 6.5366272159
O 1.1856485281 0.0967789142 -2.0141226561
O 1.5910926957 -0.2029796912 6.3368825117
H 2.2454107074 -0.0433077787 3.9505480558
H -0.8026224619 -0.3151276147 4.0683168323
H -0.4155158772 -0.4172671772 7.4782576297
H -0.7900193816 -0.0848814723 -1.6801871724
H 3.4001893305 0.2341877491 -0.5352458363
H 3.3342872668 0.1325732725 1.9361549429
H -0.9700828433 -0.2379662331 1.862279813

B3LYP Caffeic Acid (Radical) -0.006 a.u.

C 1.2555371198 0.0553139163 -0.7697628982
C 0.002352072 -0.0811809924 -0.0173029463
C -0.0263493146 -0.1365238476 1.3498589441
C 1.1807162138 -0.0604995877 2.0765775327
C 2.4150203129 0.0751489991 1.3625609989
C 2.464531122 0.1316637224 0.0035819069
O -1.1032918189 -0.1480623667 -0.768935824
C 1.2486957231 -0.1128931813 3.5117731198
C 0.2239894573 -0.2383027715 4.3796324054
C 0.5032779903 -0.2754873874 5.8372369286
O -0.6326093515 -0.3972286253 6.5457271898
O 1.1894722357 0.0948176803 -2.0174159606
O 1.6027289708 -0.2063978581 6.3224740335
H 2.2378067638 -0.0443305922 3.951817664
H -0.8102751207 -0.31500163 4.0745524889
H -0.4061613431 -0.4151546168 7.4886569214
H -0.775584077 -0.0835011147 -1.6874548802
H 3.4002005882 0.2347016122 -0.5287735719
H 3.3275433428 0.1334479415 1.9414476028
H -0.9759488867 -0.2380103 1.8555213444

B3LYP Caffeic Acid (Radical) -0.008 a.u.

C 1.2571164768 0.0551281207 -0.7701082179
C 0.0032533589 -0.0811546866 -0.0214070873
C -0.0315725275 -0.1363841456 1.3446336632
C 1.1735875279 -0.0603610132 2.0777687446
C 2.4093280637 0.0756672776 1.3659029851
C 2.4622240832 0.1319547081 0.0065052377
O -1.1001606456 -0.1482115064 -0.7817963142
C 1.2407718482 -0.1132704729 3.5111788612

C 0.2171558104 -0.2387418952 4.3823840779
C 0.5079023625 -0.2767998578 5.8416686521
O -0.6204237277 -0.3946077447 6.5561679116
O 1.1942296163 0.0935082704 -2.0211659492
O 1.6151156909 -0.2104678077 6.3073223346
H 2.2294025794 -0.0454914503 3.9526748813
H -0.8188295269 -0.3145499625 4.0820477109
H -0.3950679764 -0.4130792893 7.5002655031
H -0.7602906631 -0.0826440654 -1.6956881029
H 3.4004413608 0.2353971657 -0.5216060765
H 3.3201235392 0.1344490289 1.9473807304
H -0.9826552509 -0.2378216738 1.8476434545

B3LYP Gallic Acid (Radical) -0.010 a.u.

C -0.9500243657 -1.2062215822 0.0031960193
C -1.7539559983 0.0018766905 0.0014324274
C -1.0211931757 1.2684541601 -0.0034176969
C 0.3515568454 1.3303738204 -0.0064535099
C 1.0659701263 0.1266689083 -0.0047918236
C 0.4164400012 -1.1239042705 0.0000055141
O -3.0058070922 0.0326931049 0.0039164315
O -1.7991045362 2.3600392319 -0.0047466855
C 2.5663050192 0.0832918548 -0.0080812037
O 3.1206349185 1.3008262556 -0.0116986577
O -1.6344320068 -2.3739832607 0.008027211
O 3.1785165053 -0.9508766682 -0.0073055028
H 1.0391204097 -2.0103403319 0.0011282653
H 0.8674183064 2.2784310964 -0.0100296267
H -1.0043593687 -3.1041250826 0.0092965492
H -2.7089747651 2.0059153031 -0.001821054
H 4.0869811765 1.20400377 -0.0133616569

B3LYP Gallic Acid (Radical) -0.002 a.u.

C -0.9486269717 -1.2162941804 0.003223642
C -1.7526517621 -0.0022806698 0.0015643397
C -1.0194788605 1.2655249922 -0.0033669064
C 0.3551364816 1.3196086692 -0.006403246
C 1.0675964617 0.1149981385 -0.0046715783
C 0.420291293 -1.1367093233 0.0000950994
O -2.9948512268 0.0249434759 0.0040545832
O -1.7790357886 2.3605442882 -0.0047394003
C 2.556157952 0.0910399987 -0.0078202819
O 3.1060213103 1.3218104488 -0.0121610016
O -1.6420286134 -2.3694235306 0.0078869985
O 3.2137210511 -0.9196585139 -0.0066309705
H 1.0345367472 -2.0279186862 0.0012428419

H 0.8675423782 2.2688248184 -0.0100455559
H -1.0348923013 -3.1179576992 0.0088506539
H -2.7015391752 2.0388566032 -0.0019362245
H 4.0671930245 1.2072141705 -0.0138479933

B3LYP Gallic Acid (Radical) -0.004 a.u.

C -0.9490411951 -1.2137042465 0.0032135117
C -1.7528475105 -0.0011699015 0.0015225675
C -1.0197822766 1.266171537 -0.0033773367
C 0.354363676 1.3221163081 -0.0064077417
C 1.0669451932 0.1177491838 -0.004693633
C 0.4192807464 -1.1335075664 0.0000744727
O -2.9973941304 0.0271196355 0.0040114105
O -1.7837725743 2.3604146167 -0.0047394702
C 2.5585754674 0.0890205567 -0.0078652949
O 3.1092023979 1.3165399734 -0.0120524859
O -1.640062954 -2.3705687902 0.0079165684
O 3.2048577633 -0.9275031824 -0.0067986345
H 1.0354721369 -2.0235931372 0.0012197907
H 0.8676921029 2.2709790253 -0.0100268333
H -1.0268941697 -3.1143462275 0.0089626542
H -2.7031726786 2.0305702742 -0.0019128893
H 4.0716700053 1.2068349409 -0.0137516561

B3LYP Gallic Acid (Radical) -0.006 a.u.

C -0.9494101949 -1.2111562919 0.0032052792
C -1.7531321891 -0.0001059486 0.0014831079
C -1.0201664276 1.2668827725 -0.0033890108
C 0.3535073411 1.3247587791 -0.0064128274
C 1.0664527749 0.1206226793 -0.0047150937
C 0.4182984475 -1.1302951323 0.0000558077
O -3.0000642555 0.0291591996 0.0039701929
O -1.7887229822 2.3602791802 -0.0047424039
C 2.5610950654 0.0870367842 -0.0079138443
O 3.1127077627 1.3112547439 -0.0119355829
O -1.6381363923 -2.3717142443 0.0079486
O 3.1960159235 -0.9353620887 -0.0069824965
H 1.0365523853 -2.0192062339 0.0011968961
H 0.867722492 2.2733093909 -0.0100101787
H -1.0191181945 -3.1108236194 0.0090771002
H -2.7049806734 2.0222903635 -0.0018917702
H 4.0764711171 1.2061926659 -0.0136487755

B3LYP Gallic Acid (Radical) -0.008 a.u.

C -0.9497359163 -1.2086388021 0.0031975067
C -1.75349724 0.0009119157 0.0014449383

C -1.0206377716 1.2676477304 -0.0034008852
C 0.3525622981 1.3275326744 -0.0064173697
C 1.0661155143 0.1236226322 -0.0047356333
C 0.417345909 -1.1270636375 0.0000386537
O -3.0028657975 0.0310560263 0.0039319941
O -1.7938886978 2.3601325258 -0.004746288
C 2.563708519 0.0850988667 -0.0079638606
O 3.116549904 1.3059472571 -0.0118184816
O -1.6362405581 -2.3728564925 0.0079809039
O 3.1871733703 -0.9432223439 -0.0071708121
H 1.0377794907 -2.0147464446 0.001174734
H 0.8676196335 2.275814675 -0.0099940215
H -1.0115448786 -3.1073796059 0.0091905394
H -2.7069626036 2.0140155014 -0.0018720943
H 4.0816108247 1.2052505215 -0.0135448237

B3LYP Caffeic Acid (Neutral) Zero field

C 1.2649426796 0.0535005171 -0.7191477218
C 0.0453252641 -0.0771983356 -0.0367574951
C 0.0366732381 -0.1318818228 1.3423259677
C 1.2320397008 -0.0581800234 2.0747450155
C 2.4362813208 0.072338429 1.374615639
C 2.4535330515 0.1276969255 -0.0129182478
O -1.1250240286 -0.1501706336 -0.7229371714
C 1.2742132765 -0.1112150375 3.5283189403
C 0.246084259 -0.2373545991 4.3790808048
C 0.4831700406 -0.2724687018 5.8279255484
O -0.6808918755 -0.4050476565 6.5174747165
O 1.1714243575 0.0987945616 -2.0835920184
O 1.5514430693 -0.1973972433 6.3882913638
H 2.2616522117 -0.0394666083 3.9727584891
H -0.7816154059 -0.3180710824 4.0550376362
H -0.44652805 -0.4205632406 7.4557827059
H 2.0416079432 0.1901196713 -2.4819198985
H -0.9386655273 -0.0972740412 -1.6677771896
H 3.3914804386 0.2290806305 -0.5459663072
H 3.3669823901 0.1312306105 1.9224315892
H -0.919017354 -0.2328003192 1.8368116336

B3LYP Caffeic Acid (Neutral) 0.010 a.u.

C 1.2728817279 0.052995373 -0.7209004986
C 0.045595684 -0.0720223255 -0.0235351956
C 0.0481606348 -0.1223115561 1.3523128022
C 1.2530840671 -0.0495054638 2.0817449529
C 2.4576647931 0.0764624596 1.3682140141

C 2.4698927039 0.1264588938 -0.0161699325
O -1.119279866 -0.1419686244 -0.6929501046
C 1.3007970422 -0.1007372578 3.5174232618
C 0.2645818079 -0.2341028174 4.3842806567
C 0.4648473305 -0.2722472617 5.8109479925
O -0.7281044564 -0.4238662155 6.4942494891
O 1.1505890793 0.0910325132 -2.0561476919
O 1.5005641179 -0.190307775 6.4527015609
H 2.2909404123 -0.0247210283 3.956680475
H -0.7564210908 -0.3227053721 4.0434125115
H -0.465992478 -0.4421990209 7.4224891571
H 1.9904950836 0.1686670171 -2.5245308937
H -0.9641409246 -0.1016313085 -1.6472295786
H 3.4026569279 0.2222078928 -0.5572538034
H 3.3929506262 0.1339706608 1.9096816866
H -0.9066522228 -0.2197967831 1.8491631385

B3LYP Caffeic Acid (Neutral) 0.002 a.u.

C 1.2663146225 0.053135087 -0.7188393373
C 0.045937951 -0.0752913371 -0.0329172736
C 0.0402926495 -0.1284166635 1.3455770552
C 1.237895512 -0.0553502129 2.075943689
C 2.4414807194 0.0732334874 1.3732967162
C 2.4567209383 0.1268165751 -0.0141210732
O -1.1241280951 -0.1472701273 -0.7145507397
C 1.2806218279 -0.107781286 3.5269223808
C 0.2506249594 -0.2371860291 4.3786725854
C 0.4787554696 -0.2724242081 5.8238910029
O -0.6912461492 -0.4117062411 6.5101193316
O 1.1654440248 0.0963652856 -2.0776872754
O 1.5397418601 -0.193533368 6.4013577209
H 2.2680624868 -0.0334526602 3.9710795974
H -0.7752258398 -0.3214621885 4.0504313863
H -0.4533377951 -0.4272241034 7.4469063413
H 2.0297171204 0.1829702718 -2.4908409898
H -0.9443960156 -0.0979254132 -1.6614540284
H 3.3933248219 0.2262654294 -0.5492989803
H 3.3735274807 0.1315573969 1.9190815174
H -0.9150175494 -0.2276476948 1.8410143733

B3LYP Caffeic Acid (Neutral) 0.004 a.u.

C 1.267755989 0.0531668053 -0.7188261107
C 0.0463339467 -0.0743229547 -0.029679826
C 0.0433840091 -0.1266584168 1.3481898114
C 1.2430343373 -0.0536617186 2.0772215479
C 2.4462421439 0.0741199701 1.3720193373

C 2.4598791861 0.1267530865 -0.0150410541
O -1.1230004131 -0.1459083271 -0.7073107759
C 1.2865467908 -0.1058336174 3.5251047264
C 0.2547253047 -0.2361855015 4.3789659682
C 0.4747134952 -0.2723339753 5.8202226244
O -0.701173876 -0.4152762476 6.504060678
O 1.1602794833 0.0949677721 -2.0719330217
O 1.5289156113 -0.1925352756 6.4142025916
H 2.274412889 -0.0311180669 3.9685135152
H -0.7696688144 -0.3214043146 4.0469702493
H -0.4590144261 -0.4315479987 7.4391621127
H 2.0184526331 0.1787175595 -2.4994750429
H -0.9497647779 -0.0991878958 -1.6561631886
H 3.3952364665 0.2251818177 -0.552078478
H 3.3794120341 0.1321884855 1.9161516633
H -0.9115910125 -0.2254491861 1.8443066723

B3LYP Caffeic Acid (Neutral) 0.006 a.u.

C 1.2693317694 0.0531526024 -0.7191243942
C 0.0464292118 -0.0735606038 -0.0270129545
C 0.0457850822 -0.1251779338 1.3502415137
C 1.2473409657 -0.0521824341 2.0786471463
C 2.4505558805 0.0749573989 1.3707998555
C 2.4631189995 0.1267096824 -0.0156563706
O -1.1217574059 -0.1447632432 -0.7012476637
C 1.2919294101 -0.1040631192 3.522937494
C 0.2584746343 -0.2351538597 4.3799877041
C 0.4710019614 -0.2722012774 5.8168365513
O -0.7106058282 -0.4182991206 6.4991600253
O 1.1560281284 0.0935790469 -2.0663400532
O 1.518781265 -0.1919684078 6.4269957541
H 2.2804276398 -0.0291279199 3.9652526561
H -0.7646588941 -0.3211521114 4.0446452015
H -0.4631615055 -0.4354502161 7.4323186742
H 2.0079905944 0.1752562208 -2.507978488
H -0.9549442406 -0.100295543 -1.6520023229
H 3.3974038529 0.2242199443 -0.5543067905
H 3.3846455771 0.1328254371 1.913654121
H -0.9090060981 -0.223632543 1.8467763402

B3LYP Caffeic Acid (Neutral) 0.008 a.u.

C 1.2710380501 0.0530657823 -0.7197556912
C 0.0462242919 -0.0727709983 -0.0249249451
C 0.0473962072 -0.1236581948 1.351659277
C 1.2507224363 -0.0507331791 2.0801342519
C 2.4543741221 0.075754934 1.3695357265

C 2.4664577566 0.1265848975 -0.016050613
O -1.1205025283 -0.1434486508 -0.69636441
C 1.2966853312 -0.1022787616 3.5203650976
C 0.2617776394 -0.234407027 4.3816913419
C 0.4676728638 -0.2720941519 5.8137233705
O -0.7195015403 -0.4212835901 6.4957651328
O 1.152749819 0.0921966153 -2.0610417715
O 1.5092595665 -0.191271641 6.4398039234
H 2.2859335738 -0.0268609139 3.9612797216
H -0.7602185958 -0.3215888409 4.043450882
H -0.4655730901 -0.4391732013 7.4266791389
H 1.9986015585 0.1717928093 -2.5163050223
H -0.9596920601 -0.1011086866 -1.6489187776
H 3.3998672352 0.2231635378 -0.5560396221
H 3.3891744647 0.1334261998 1.9114735986
H -0.9073361017 -0.2216349385 1.8484233903

B3LYP Gallic Acid (Neutral) Zero field

C -0.9522419751 -1.175419272 0.0023229757
C -1.6925686124 0.0056393041 0.0005251241
C -1.0409190229 1.2384782726 -0.0038449819
C 0.3454090838 1.2878056329 -0.0064421159
C 1.0773906039 0.1009716811 -0.004642706
C 0.428519632 -1.1366342271 -0.0002415641
O -3.0548945661 0.0072942569 0.0028999025
O -1.7582743423 2.3921760551 -0.0056015798
C 2.5575244348 0.0928839527 -0.0073273887
O 3.101377338 1.3333552589 -0.0115336489
O -1.7005751842 -2.3254220354 0.0066530506
O 3.2434877186 -0.9017568874 -0.0060483666
H 1.0176215362 -2.043927983 0.0010973663
H 0.8385832593 2.2472129818 -0.0098505362
H -1.1284736778 -3.0979708449 0.0079385215
H -3.3721298451 -0.9037841147 0.0057738246
H -2.6989464833 2.178298106 -0.0034069394
H 4.0606711027 1.2120248625 -0.0129769379

B3LYP Gallic Acid (Neutral) 0.010 a.u.

C -0.9493485317 -1.1928384391 0.0024824591
C -1.6938867925 -0.006398211 0.0006945132
C -1.0367769414 1.230893724 -0.0036940707
C 0.3480237895 1.2753721817 -0.0063025821
C 1.0878495326 0.0873518227 -0.0044720138
C 0.4327154609 -1.1534114669 -0.0000342525
O -3.0353229164 0.0179379745 0.002974406

O -1.7395152018 2.3815726674 -0.0054647692
C 2.5488951073 0.1039924085 -0.007201369
O 3.0898031153 1.3631654076 -0.0119645606
O -1.7031798431 -2.3276869808 0.0067584228
O 3.2939313507 -0.8598506677 -0.0056978303
H 1.0130915807 -2.0659774246 0.0013269113
H 0.8336966853 2.2382317881 -0.0098185167
H -1.1592772471 -3.1196285169 0.0073698945
H -3.4130061276 -0.8722223942 0.0055294544
H -2.6889904973 2.1953210662 -0.0036734446
H 4.0428584764 1.2154000606 -0.013518652

B3LYP Gallic Acid (Neutral) 0.002 a.u.

C -0.9517957799 -1.1788054623 0.0023547215
C -1.6926764301 0.0032052291 0.0005625662
C -1.0399988362 1.2367227002 -0.0038082877
C 0.3460807577 1.285080213 -0.0064096846
C 1.0791110025 0.0980493285 -0.0046083879
C 0.4293380152 -1.1400249593 -0.000202661
O -3.0508745841 0.0097786356 0.0029165822
O -1.7540585112 2.3899539813 -0.0055653888
C 2.555648545 0.0951055131 -0.0073073698
O 3.0984445883 1.3392205642 -0.0116358444
O -1.7009276669 -2.325936415 0.0066659043
O 3.2533697619 -0.8933402363 -0.0059550107
H 1.0164916999 -2.0484556968 0.0011379545
H 0.8377385261 2.245152478 -0.0098378355
H -1.1340739864 -3.1021630226 0.007834829
H -3.3802504617 -0.8973114543 0.0057093858
H -2.696546348 2.1817825635 -0.0034658656
H 4.0565407079 1.2132110402 -0.0130916076

B3LYP Gallic Acid (Neutral) 0.004 a.u.

C -0.9512774365 -1.1822430321 0.0023860669
C -1.692856463 0.0007795186 0.0005973044
C -1.0391061116 1.2350854724 -0.003774124
C 0.3467039183 1.2824711937 -0.0063765626
C 1.0810272272 0.095218303 -0.0045704152
C 0.4301838088 -1.1433987344 -0.0001608237
O -3.046897735 0.0120972134 0.0029298921
O -1.7500560698 2.3877795101 -0.0055327178
C 2.5538359694 0.0973249696 -0.0072787944
O 3.0957584538 1.3451569498 -0.0117347043
O -1.7013458185 -2.3264327497 0.006679824
O 3.2633415652 -0.8849379443 -0.0058733616
H 1.015476668 -2.0529405295 0.0011830654

H 0.836849257 2.2432293109 -0.0098239919
H -1.1399417788 -3.1064529403 0.0077278714
H -3.3884337302 -0.890889172 0.0056493393
H -2.6943370436 2.1852372466 -0.0035223623
H 4.0526363194 1.2141404143 -0.0132115058

B3LYP Gallic Acid (Neutral) 0.006 a.u.

C -0.9506937675 -1.1857409528 0.0024187716
C -1.6931302425 -0.0016263983 0.0006255834
C -1.0382398114 1.233586022 -0.0037335528
C 0.3472717288 1.2799747271 -0.0063154271
C 1.0831551548 0.0924678257 -0.0044931699
C 0.4310399293 -1.1467645372 -0.0000957383
O -3.0429579529 0.014247137 0.0029182006
O -1.7462503681 2.385668507 -0.0055001717
C 2.5520786262 0.0995225416 -0.0071822301
O 3.0932942326 1.3512077119 -0.0118635027
O -1.7018473757 -2.3268937087 0.0066835617
O 3.2734164377 -0.8765760274 -0.0058215438
H 1.0145450589 -2.0574094001 0.0012587178
H 0.8359232503 2.2414435144 -0.0097720746
H -1.1460868761 -3.1108144625 0.0076079939
H -3.3966012562 -0.8845447004 0.0055626199
H -2.6922863776 2.188634363 -0.0035874939
H 4.0489306094 1.2148428375 -0.013416544

B3LYP Gallic Acid (Neutral) 0.008 a.u.

C -0.9500414387 -1.1892922041 0.0024563992
C -1.6935236119 -0.0039954217 0.0006422948
C -1.0374192889 1.2322564443 -0.0036722096
C 0.3477553211 1.2776081551 -0.0061837025
C 1.085509912 0.0898165723 -0.0043210978
C 0.4318888666 -1.1501035263 0.0000247698
O -3.0390885208 0.0161783142 0.002848992
O -1.7427104005 2.3836458775 -0.0054621532
C 2.5503773445 0.101690843 -0.0069296047
O 3.09117156 1.3573815655 -0.0120776081
O -1.7024522903 -2.327303792 0.0066605994
O 3.2836359292 -0.8682594624 -0.0058262145
H 1.0136839166 -2.0618450938 0.0014050608
H 0.8349480769 2.239810959 -0.0096259593
H -1.1525323326 -3.1152370111 0.0074575403
H -3.4047191392 -0.8783658168 0.005401199
H -2.69046427 2.1919956806 -0.0036783054
H 4.0455413661 1.2152429167 -0.0138260003

B3LYP Caffeic Acid (Radical) Zero field

C 1.253007645 0.0559668079 -0.7700519263
C -0.0002284189 -0.0811273944 -0.0088966136
C -0.014331523 -0.1363865913 1.3613874605
C 1.1973283988 -0.0603607772 2.0737544223
C 2.4291583194 0.0739624394 1.3546957936
C 2.4715302467 0.1306891052 -0.0030557145
O -1.1103304608 -0.1475308 -0.7383538197
C 1.267145843 -0.1111817916 3.5111560604
C 0.2400373668 -0.2371823729 4.3755722817
C 0.4917301395 -0.2726183487 5.8254624758
O -0.663141069 -0.4042987155 6.5225637374
O 1.1804956162 0.0979963503 -2.0082913224
O 1.5699013538 -0.1966587543 6.363457951
H 2.2580173799 -0.0402500099 3.946688357
H -0.7900372067 -0.3169253512 4.0595189139
H -0.427844803 -0.4206414865 7.4610180312
H -0.8166085543 -0.0860305041 -1.6692220744
H 3.4010102197 0.2321176938 -0.5458344328
H 3.3457518897 0.1307778826 1.9276726582
H -0.9609403827 -0.2377983814 1.8725307606

B3LYP Caffeic Acid (Radical) 0.010 a.u.

C 1.2563699804 0.0565816184 -0.7760961344
C -0.0057989768 -0.0812156399 -0.0065099082
C -0.0079644912 -0.1354154872 1.3685405805
C 1.2082507887 -0.0595549859 2.0720715434
C 2.443912777 0.0729905095 1.3453064266
C 2.4854847089 0.1292052589 -0.0083137302
O -1.1148060908 -0.1468948229 -0.7115833744
C 1.2831596197 -0.1074402638 3.5018127387
C 0.2545843328 -0.2349854955 4.3824023578
C 0.4785458589 -0.268793603 5.8107416966
O -0.6996817583 -0.4126480597 6.5113059086
O 1.1820990363 0.1033514358 -1.9994907366
O 1.5292707845 -0.1887635753 6.4228586142
H 2.2786012202 -0.033634876 3.9270478697
H -0.771693941 -0.3197592606 4.0573618996
H -0.4282156129 -0.428646694 7.4370802989
H -0.8687868577 -0.0909858496 -1.6591839518
H 3.4092276249 0.2279296935 -0.561400781
H 3.3627223261 0.1274887601 1.9159437294
H -0.9536293297 -0.2362896626 1.8818779525

B3LYP Caffeic Acid (Radical) 0.002 a.u.

C 1.2528644246 0.0565270783 -0.7705646413

C -0.0011703693 -0.0811650462 -0.0073556075
C -0.0116325051 -0.1363327268 1.3639311534
C 1.2012454819 -0.0601451579 2.0730872483
C 2.4329641783 0.0737474299 1.3525933144
C 2.4739915532 0.1304430035 -0.0046754746
O -1.1120203819 -0.1475290714 -0.7305445682
C 1.2716888291 -0.1104261246 3.5100943459
C 0.2440675048 -0.2365761619 4.3756157327
C 0.4884267085 -0.2716420517 5.8220083206
O -0.6716572997 -0.4063332737 6.5176033694
O 1.1795331782 0.098595083 -2.0059700041
O 1.5603318743 -0.1945233867 6.3758912634
H 2.2632723354 -0.0389048189 3.9439608337
H -0.7849184929 -0.3171910347 4.0568244417
H -0.4312793253 -0.4225853206 7.4540808841
H -0.8287559002 -0.0867603607 -1.6650528147
H 3.4018641754 0.2311423029 -0.5502023857
H 3.3504828398 0.1300103439 1.924297296
H -0.9576468089 -0.2378317058 1.8761502926

B3LYP Caffeic Acid (Radical) 0.004 a.u.

C 1.2530851645 0.0570747396 -0.7713824348
C -0.0022174888 -0.0811707617 -0.0062665976
C -0.0096212424 -0.1361742544 1.3659547375
C 1.2043597433 -0.0598795773 2.0726376684
C 2.4363981308 0.0735579866 1.35070326
C 2.476618584 0.1301447155 -0.0059212954
O -1.1133163083 -0.1474278243 -0.7239466323
C 1.2755716372 -0.109612358 3.508578234
C 0.2475172355 -0.2361808724 4.3762249611
C 0.4855169698 -0.2709284824 5.8186897426
O -0.6795428152 -0.408279352 6.5138456646
O 1.1791253662 0.0991529261 -2.0038590421
O 1.5514559649 -0.1924691998 6.3879711983
H 2.2679725837 -0.0373796586 3.9406154932
H -0.7805464843 -0.317888877 4.0551775048
H -0.4330807603 -0.4242505244 7.4481447252
H -0.840141124 -0.0874404885 -1.6619279663
H 3.4031062303 0.2300673387 -0.553916617
H 3.3546466813 0.1292605049 1.9214985388
H -0.9552560682 -0.2376569806 1.8789518571

B3LYP Caffeic Acid (Radical) 0.006 a.u.

C 1.253869787 0.0565013219 -0.7724742636
C -0.0032841465 -0.0811367912 -0.0057722356
C -0.0085265979 -0.1357628482 1.3672779172

C 1.2063543424 -0.059730952 2.072379206
C 2.4391875783 0.0733041007 1.3489776962
C 2.4793795167 0.1296772999 -0.0068153797
O -1.1141367653 -0.1471141373 -0.7189363375
C 1.2785616365 -0.1088071406 3.5066707642
C 0.2501854158 -0.2357652246 4.3775799869
C 0.483042659 -0.2701082293 5.8156776562
O -0.6864973864 -0.4101035932 6.5116853222
O 1.1794365453 0.1006006232 -2.0019616454
O 1.5435942744 -0.1908432519 6.3994160404
H 2.2718014454 -0.0359104155 3.9367723642
H -0.7771143818 -0.3186094094 4.054911102
H -0.4325686236 -0.4259724158 7.4434159869
H -0.8501426751 -0.0887745769 -1.660218475
H 3.4047426936 0.2292484558 -0.5567906317
H 3.3578148315 0.1286809609 1.9193806472
H -0.9540481494 -0.2368547765 1.8805972786

B3LYP Caffeic Acid (Radical) 0.008 a.u.

C 1.2549046741 0.0563989407 -0.7739984462
C -0.004488167 -0.0811640261 -0.005819479
C -0.0078890211 -0.13556579 1.3681910723
C 1.2077825267 -0.059645879 2.0721790455
C 2.4417801899 0.0731320042 1.3471891363
C 2.4823153453 0.1294277247 -0.0076406879
O -1.1146971319 -0.1470146919 -0.7146312913
C 1.2811637712 -0.1081415957 3.5043958825
C 0.2525944172 -0.2353304721 4.3795643643
C 0.4806483403 -0.2694323426 5.8129971495
O -0.6932676052 -0.4114166819 6.5107064844
O 1.1804326303 0.1020828992 -2.0004968054
O 1.5361149848 -0.1897720875 6.411045563
H 2.2754408491 -0.0348177037 3.9322240299
H -0.7741197944 -0.3190683624 4.055507469
H -0.4311952286 -0.42733141 7.439658096
H -0.859857166 -0.0900284672 -1.6591144214
H 3.4067334892 0.2286354619 -0.5593497604
H 3.3606392627 0.1281103723 1.917477302
H -0.9533843667 -0.2365388928 1.8816882968

B3LYP Gallic Acid (Radical) Zero field

C -0.9482973497 -1.2190777515 0.0032510505
C -1.7528096218 -0.0034833792 0.0016593467
C -1.0192450868 1.265109146 -0.003398312
C 0.3558850922 1.3170885508 -0.0065712324
C 1.0685028606 0.1122377998 -0.0048735902

C 0.42120721 -1.1399710191 -0.0000031247
O -2.9925207952 0.0221500399 0.0042944985
O -1.7740846034 2.3608624585 -0.0047346345
C 2.554103815 0.0930026954 -0.0081705543
O 3.1029451398 1.3271950313 -0.0120849891
O -1.6440230955 -2.3684101384 0.0079780474
O 3.2226696338 -0.9118064905 -0.0063766567
H 1.0335695182 -2.0322952486 0.0011056891
H 0.8674794086 2.2666363174 -0.0103060964
H -1.0434696516 -3.121957176 0.0088269298
H -2.6996377438 2.0476357843 -0.0018665601
H 4.0628172696 1.2082063799 -0.0134348116

B3LYP Gallic Acid (Radical) 0.010 a.u.

C -0.9448101701 -1.233562085 0.0033182966
C -1.7539279269 -0.009791509 0.0018871777
C -1.0190831575 1.2636175503 -0.0033529811
C 0.3581822781 1.3074237822 -0.0064636992
C 1.0752382049 0.1008768596 -0.0046276963
C 0.4268049261 -1.1561625593 0.0001938189
O -2.9821205445 0.0089635076 0.0044663653
O -1.7549856188 2.3614192509 -0.0048025362
C 2.5433425887 0.1038870674 -0.0077500393
O 3.0936323493 1.3545133866 -0.012547738
O -1.6547248383 -2.3625497697 0.0077987418
O 3.2680275838 -0.8731527136 -0.005917503
H 1.0319132118 -2.0530206052 0.001306424
H 0.8649389621 2.2593360196 -0.0103013164
H -1.0887692001 -3.142101973 0.0082829098
H -2.6952540359 2.088799364 -0.0020880883
H 4.0466873875 1.2046274264 -0.0141071362

B3LYP Gallic Acid (Radical) 0.002 a.u.

C -0.94770034 -1.2217663647 0.0032532316
C -1.7527790717 -0.0046621896 0.0016602449
C -1.0190920662 1.2645885133 -0.0033814381
C 0.3564924713 1.3148598396 -0.006521685
C 1.0694689273 0.109723035 -0.0048030593
C 0.4223479571 -1.1431843219 0.0000424096
O -2.9901551338 0.0197492079 0.0043336371
O -1.7697254953 2.3608883315 -0.0047432901
C 2.5516652705 0.0951682598 -0.0080384137
O 3.1003668348 1.3326020729 -0.0121885615
O -1.6460574165 -2.3670983321 0.0079352141
O 3.2315685085 -0.9039283228 -0.0063031112
H 1.0329453506 -2.0365652097 0.0011639949

H 0.8670360965 2.2648693261 -0.0102543161
H -1.0519509461 -3.1256094754 0.0087214113
H -2.6982264869 2.0557048209 -0.0019499131
H 4.0588875399 1.2077838093 -0.0136313552

B3LYP Gallic Acid (Radical) 0.004 a.u.

C -0.9470831165 -1.2245161898 0.0032509532
C -1.7528179202 -0.0058886158 0.0016468402
C -1.0190434245 1.2641285347 -0.0033543865
C 0.3569903605 1.3127605852 -0.0064268806
C 1.0706075871 0.1073240534 -0.0046744827
C 0.4234701163 -1.1464025062 0.0001197151
O -2.9879382467 0.0172975917 0.0043291155
O -1.7657425399 2.3609011517 -0.0047532531
C 2.5494044619 0.0973693822 -0.0078062556
O 3.098292001 1.3379368962 -0.0123462338
O -1.6481738762 -2.3658348997 0.0078620376
O 3.2406551579 -0.8960362337 -0.0062515853
H 1.0324363792 -2.0407690795 0.0012633401
H 0.8664689561 2.2632590147 -0.0101393264
H -1.06068795 -3.1293872268 0.0085907082
H -2.6972242414 2.0638497881 -0.0020582436
H 4.0554782956 1.2071307536 -0.0139570622

B3LYP Gallic Acid (Radical) 0.006 a.u.

C -0.9463713585 -1.227461946 0.0032619881
C -1.7530751627 -0.0072010165 0.0016797285
C -1.0190971139 1.2638121332 -0.0033541144
C 0.3573999564 1.3107245716 -0.0064461935
C 1.0719943255 0.1049966831 -0.0046898
C 0.4246255291 -1.1496721171 0.0001237582
O -2.9857892461 0.0145457899 0.004440466
O -1.7619597582 2.3609023643 -0.0047597106
C 2.5472735036 0.0996197737 -0.0078244813
O 3.0966717006 1.3434124728 -0.0123890832
O -1.6502929554 -2.3645912848 0.0078617812
O 3.2499240606 -0.8880509758 -0.0061302167
H 1.0320341766 -2.0449940438 0.0012628519
H 0.8657772273 2.2617394194 -0.0101885576
H -1.0699689535 -3.1334826701 0.0085054699
H -2.6965235241 2.0724759344 -0.002093791
H 4.0524695927 1.206347912 -0.0139650953

B3LYP Gallic Acid (Radical) 0.008 a.u.

C -0.9456398563 -1.2304147145 0.003302355
C -1.7534113985 -0.0084455009 0.0018084727

C -1.0190221293 1.2636637931 -0.0033539776
C 0.3578572641 1.3091252809 -0.0064558013
C 1.0735210856 0.1029627591 -0.0046440761
C 0.4257067108 -1.1528637177 0.0001742036
O -2.9840551349 0.0119398074 0.0044182993
O -1.7585008135 2.361299156 -0.0047875751
C 2.5453564052 0.1016704776 -0.0077674057
O 3.0949530852 1.3488381172 -0.012476975
O -1.6525198499 -2.3637187622 0.0078338424
O 3.2587660437 -0.8808546008 -0.0060192152
H 1.0320007347 -2.0489578523 0.001300773
H 0.8654888805 2.2605849352 -0.0102541011
H -1.0790020178 -3.1377797786 0.0083561059
H -2.6958828486 2.0804480827 -0.0020764454
H 4.049475839 1.2056255178 -0.0140634794

CBS-QB3 Caffeic Acid (Neutral) -0.010 a.u.

C 1.2685144171 0.0228975155 -0.7286583468
C 0.0427044397 -0.1293722765 -0.0697194894
C 0.0098949959 -0.2002155916 1.3144483355
C 1.1938905558 -0.1149410353 2.069192665
C 2.4106250761 0.0334450378 1.38399302
C 2.4479708175 0.1002240754 -0.0050843597
O -1.1180315502 -0.2018489219 -0.7990507782
C 1.2311501563 -0.1585867344 3.5320313873
C 0.2103824609 -0.2383973504 4.3928330914
C 0.5091764978 -0.2494788489 5.8561055313
O -0.6215818643 -0.3152667099 6.5771302383
O 1.2142374391 0.0882497042 -2.125162023
O 1.6202657433 -0.2026405448 6.3190368111
H 2.2203531375 -0.1079664792 3.9806920531
H -0.8320892894 -0.2890134606 4.1000589616
H -0.3849331571 -0.3156264871 7.5197160477
H 2.034874143 0.4918871417 -2.4206248389
H -0.8682614445 -0.059504995 -1.7191965943
H 3.3976212429 0.2099831621 -0.5231500451
H 3.3308062843 0.1006086082 1.951382091
H -0.9524591014 -0.3107638091 1.798610242

CBS-QB3 Caffeic Acid (Neutral) -0.002 a.u.

C 1.2648639961 0.0538121005 -0.7241846715
C 0.0405629549 -0.0794475204 -0.0449567209
C 0.0283669786 -0.1358162076 1.3372586597
C 1.224859168 -0.0613107924 2.0742443839
C 2.4335798999 0.0713819154 1.3769462602
C 2.4537468034 0.1286999211 -0.0143647166

O -1.1268553513 -0.1525277053 -0.743769836
C 1.2639980287 -0.1150641274 3.5327315733
C 0.234778489 -0.2385099264 4.3840840646
C 0.4876020061 -0.2724463622 5.838106049
O -0.6694064767 -0.3991406476 6.534493624
O 1.1698183185 0.1005976664 -2.0965961886
O 1.5679060882 -0.1997520366 6.3760556413
H 2.2511119409 -0.0456178006 3.9834249557
H -0.7975686166 -0.3166610047 4.0665002045
H -0.427306172 -0.4133442594 7.4724554901
H 2.0473383668 0.1972706069 -2.4785710636
H -0.9112537106 -0.0932898859 -1.6827724116
H 3.3954250841 0.2322222367 -0.5455357984
H 3.363847183 0.1308799589 1.9291932905
H -0.9303039789 -0.2382641295 1.8298412105

CBS-QB3 Caffeic Acid (Neutral) -0.004 a.u.

C 1.2639816899 0.0518266545 -0.7249825446
C 0.0395835907 -0.0834260635 -0.049873675
C 0.023252917 -0.1411311123 1.3328646584
C 1.2172008895 -0.0657138502 2.0731795179
C 2.4273281774 0.0689199089 1.3784683703
C 2.4507666527 0.1274004347 -0.0125862795
O -1.1271778092 -0.1572632616 -0.7547548686
C 1.2561799997 -0.1191675284 3.5332263042
C 0.2293645257 -0.2391279513 4.3857390743
C 0.4929290467 -0.2713613276 5.8422548303
O -0.6574396346 -0.3909377044 6.5439514101
O 1.1778175438 0.0999979759 -2.1029587002
O 1.5807926534 -0.2017449757 6.3621795744
H 2.243488389 -0.0515674365 3.9836345321
H -0.8051230639 -0.3145942834 4.0737180093
H -0.4171647536 -0.4040270974 7.4830815196
H 2.0593986318 0.2180952186 -2.4683735537
H -0.903928838 -0.0894964299 -1.6908799087
H 3.3942727153 0.2321848344 -0.5409755794
H 3.3556711301 0.1293097431 1.9336214348
H -0.9360834535 -0.2445037479 1.8240498743

CBS-QB3 Caffeic Acid (Neutral) -0.006 a.u.

C 1.2633665401 0.0493066822 -0.7260128811
C 0.038753772 -0.0898731455 -0.055451895
C 0.017843672 -0.1501180781 1.3277514743
C 1.2089596522 -0.0727928689 2.0721009171
C 2.4207279234 0.0654521441 1.380130828
C 2.4478559842 0.1261883122 -0.01048926

O -1.1269209878 -0.1650529271 -0.7671062815
C 1.2478470292 -0.1260700014 3.5333120223
C 0.2234053406 -0.2388240318 4.3879593928
C 0.4987023976 -0.2695094133 5.8467516866
O -0.6449942601 -0.3773839729 6.5545830103
O 1.1866275156 0.1002827539 -2.1095305403
O 1.5944722226 -0.2067287661 6.3478833355
H 2.2357531018 -0.063147202 3.9830651547
H -0.8136406038 -0.3080782769 4.082139599
H -0.4059988822 -0.3896591585 7.4948014091
H 2.0702986138 0.2495811826 -2.4573951525
H -0.8958422239 -0.0847965818 -1.6998844189
H 3.3932620936 0.2334437672 -0.535758493
H 3.3468621186 0.1273885182 1.9386094669
H -0.9422300195 -0.2559369359 1.8171246258

CBS-QB3 Caffeic Acid (Neutral) -0.008 a.u.

C 1.2638763319 0.0416577041 -0.7273417295
C 0.038674695 -0.1012182281 -0.0618075231
C 0.0124537598 -0.1644294599 1.3218602662
C 1.2004444274 -0.0847130561 2.0709412229
C 2.4143159241 0.0568999841 1.3819181717
C 2.4459256226 0.1191800377 -0.0081589665
O -1.1254241197 -0.1758796882 -0.7811490712
C 1.2389809923 -0.1353685641 3.5330372647
C 0.2170339419 -0.2393444973 4.3905731069
C 0.504542497 -0.2642527293 5.8514978638
O -0.6321300371 -0.3594364031 6.5660613938
O 1.1973828516 0.0957819255 -2.1166608614
O 1.6080165435 -0.2059981948 6.3334139007
H 2.2274105129 -0.0755142143 3.9821202332
H -0.8225480166 -0.3037502604 4.0913981657
H -0.3939882531 -0.3680956304 7.5073485413
H 2.073459048 0.3171920242 -2.4441992639
H -0.8860949585 -0.0756755789 -1.7095539246
H 3.3935409934 0.2273705285 -0.5299899216
H 3.337911231 0.1207653936 1.9442194905
H -0.9486729875 -0.2714990926 1.8090556406

CBS-QB3 Gallic Acid (Neutral) -0.010 a.u.

C -0.9550666722 -1.1612130581 0.0020494772
C -1.6942986479 0.0198754697 0.0001818918
C -1.0480071812 1.255106971 -0.004118021
C 0.3434642825 1.3082020354 -0.0066077063
C 1.07348194 0.1185930265 -0.0047608615

C 0.426942467 -1.1216154614 -0.0004497869
O -3.0810655317 -0.0040812765 0.0026625116
O -1.7906760624 2.4075992475 -0.0058292319
C 2.5727480401 0.0812624633 -0.0071829366
O 3.1226656211 1.3060123219 -0.0111104455
O -1.7112345594 -2.3214471838 0.0064512677
O 3.2000170638 -0.9465467004 -0.006453747
H 1.0320491922 -2.0218256408 0.000897357
H 0.84680144 2.2651994186 -0.0098442305
H -1.1138261496 -3.076947137 0.0085921561
H -3.3239027426 -0.93832024 0.0062929815
H -2.7168872431 2.1407369616 -0.0028609122
H 4.0883557433 1.2006337824 -0.0126157635

CBS-QB3 Gallic Acid (Neutral) -0.002 a.u.

C -0.9537968205 -1.1741660323 0.0022868511
C -1.6934451666 0.0099530471 0.0004730197
C -1.0436955215 1.2465662072 -0.0038998162
C 0.346657501 1.2957577608 -0.0064890745
C 1.0782079174 0.1057846897 -0.0046812387
C 0.4300178517 -1.1352300609 -0.0002855499
O -3.0638636758 0.0073754755 0.0028719044
O -1.7705287426 2.3986262535 -0.0056344478
C 2.5639033988 0.0900010072 -0.0073346545
O 3.1072152833 1.3294788033 -0.0114564577
O -1.7113495536 -2.3239289336 0.00662754
O 3.2384077262 -0.9128333366 -0.0061225612
H 1.026200686 -2.0404935505 0.0010355566
H 0.8436383123 2.2554187993 -0.0098743382
H -1.1324346412 -3.0927134553 0.0080969882
H -3.3561238527 -0.9129764427 0.0058327191
H -2.7053471402 2.1575360815 -0.0032717817
H 4.0678974379 1.2070686868 -0.0128806586

CBS-QB3 Gallic Acid (Neutral) -0.004 a.u.

C -0.9541947345 -1.1708928614 0.0022380016
C -1.693550739 0.0124485282 0.0004175336
C -1.044659264 1.2485815775 -0.0039494196
C 0.3459632085 1.2986767718 -0.0065314081
C 1.0768312595 0.1087955067 -0.0047221877
C 0.4291927181 -1.1319047738 -0.0003347528
O -3.0680432644 0.0046931459 0.0028442622
O -1.7751561622 2.4008794315 -0.0056765148
C 2.5659362871 0.0877984671 -0.0073462438
O 3.1105462762 1.3236749516 -0.011360517
O -1.7112471207 -2.3233470677 0.0065993693

O 3.2287535877 -0.9212694273 -0.0061884501
H 1.0274263311 -2.0359858609 0.0009865
H 0.8445969428 2.2576157076 -0.0098907123
H -1.1275158426 -3.088709315 0.0082136742
H -3.3479205938 -0.919331292 0.0059387757
H -2.7078868382 2.1535242802 -0.0031821459
H 4.0724889482 1.2059772299 -0.0127617644

CBS-QB3 Gallic Acid (Neutral) -0.006 a.u.

C -0.9545392633 -1.1676496508 0.0021831932
C -1.6937271603 0.0149339463 0.0003527975
C -1.0456927956 1.2506771516 -0.0040025568
C 0.345202616 1.3017177841 -0.0065689367
C 1.0755917755 0.1119243321 -0.0047540457
C 0.4284029807 -1.1285377052 -0.0003809495
O -3.0722962917 0.0018934809 0.0028048689
O -1.7800417142 2.4031302153 -0.0057224846
C 2.5680860757 0.0856065538 -0.0073346842
O 3.1142103532 1.3178440174 -0.0112681733
O -1.7111985846 -2.322742107 0.0065634138
O 3.2191585543 -0.9296957168 -0.0062625617
H 1.0287978884 -2.0313895734 0.000943443
H 0.845451371 2.2599704257 -0.0098970016
H -1.1227872506 -3.0847547639 0.0083342649
H -3.3398181118 -0.9256688531 0.0060527507
H -2.7106453367 2.1493961343 -0.0030843178
H 4.0774058939 1.2045693286 -0.0126650201

CBS-QB3 Gallic Acid (Neutral) -0.008 a.u.

C -0.9548292329 -1.1644286891 0.0021203079
C -1.6939725577 0.0174067288 0.0002742765
C -1.0468088655 1.2528502092 -0.0040586117
C 0.344369543 1.3048944999 -0.0065940577
C 1.0744736199 0.1151904589 -0.0047666126
C 0.4276542285 -1.1251139866 -0.0004192738
O -3.0766350049 -0.0010245047 0.0027438999
O -1.7852104757 2.4053699302 -0.0057733912
C 2.5703598886 0.0834284272 -0.0072797839
O 3.1182449138 1.3119557322 -0.011185224
O -1.7111997918 -2.3221090408 0.0065135988
O 3.2095875322 -0.9381250721 -0.0063516115
H 1.0303427491 -2.0266738043 0.0009134636
H 0.8461857315 2.2625005002 -0.0098810262
H -1.1182308364 -3.0808357592 0.0084614721
H -3.3318160624 -0.9319921321 0.0061703893

H -2.7136434148 2.1451300968 -0.0029773134
H 4.0826890354 1.2028014056 -0.0126165022

CBS-QB3 Caffeic Acid (Radical) -0.010 a.u.

C 1.2585217167 0.0558355553 -0.7763870557
C -0.0005828148 -0.0816329888 -0.0310456182
C -0.0431983133 -0.1379956641 1.337776822
C 1.1622472088 -0.0618110484 2.0789153859
C 2.4030182116 0.0753313414 1.3688435432
C 2.4611977729 0.1326727288 0.0053911548
O -1.0952772652 -0.1476865537 -0.811547843
C 1.227814517 -0.1152816124 3.514157749
C 0.2041818761 -0.2401473598 4.3918760448
C 0.5146817093 -0.2773775603 5.8534850903
O -0.6051370393 -0.392202294 6.5771769273
O 1.1916913308 0.0940972193 -2.032399172
O 1.6338391625 -0.2115278543 6.2942861295
H 2.2168071278 -0.048526953 3.9605198194
H -0.8369794743 -0.3153668328 4.100723495
H -0.3718521118 -0.409536153 7.5211285672
H -0.7166992098 -0.0779282833 -1.7127389246
H 3.4027133134 0.2371786396 -0.5210769286
H 3.3129145172 0.1343794421 1.9553915277
H -0.9982502356 -0.2399547685 1.8372962861

CBS-QB3 Caffeic Acid (Radical) -0.002 a.u.

C 1.2536349983 0.0561562001 -0.7751551817
C -0.0027878882 -0.0815542185 -0.016248123
C -0.0225338396 -0.1376764847 1.3568597901
C 1.1898723836 -0.0614665567 2.0748872088
C 2.4253363453 0.074008244 1.3566530824
C 2.4706699159 0.1316247025 -0.0052631964
O -1.1080971 -0.147438759 -0.7612504575
C 1.2574553655 -0.1130372242 3.5158344988
C 0.2289075979 -0.2381361761 4.381738484
C 0.4959961751 -0.2730917322 5.8362314302
O -0.65206044 -0.4016349859 6.5392968599
O 1.1767230572 0.0983846705 -2.0189217519
O 1.5857355502 -0.1990603241 6.352087482
H 2.2479229133 -0.0434447411 3.9577880921
H -0.8055021513 -0.3166284411 4.0716482162
H -0.4102144978 -0.4176363662 7.4776788739
H -0.7813798173 -0.0828359431 -1.6828822305
H 3.4025435465 0.2343366896 -0.5476596575
H 3.3420804187 0.1313422849 1.9330517182
H -0.9726505333 -0.2396918387 1.8653978618

CBS-QB3 Caffeic Acid (Radical) -0.004 a.u.

C 1.254325576 0.0557613337 -0.7751718711
C -0.0022774218 -0.0816174366 -0.0188923795
C -0.0267435221 -0.1378511278 1.3532149698
C 1.1842400878 -0.0617416873 2.0757491719
C 2.4205881316 0.074197245 1.3590840367
C 2.4683287984 0.1318521031 -0.0031990268
O -1.1055956607 -0.1475079973 -0.7716545949
C 1.2515030567 -0.1137503872 3.5159809087
C 0.2238867585 -0.2385751248 4.383203629
C 0.5000811425 -0.2738510922 5.8402052559
O -0.6419591317 -0.3994327654 6.546619548
O 1.1790323625 0.0979492066 -2.0217954341
O 1.5966677478 -0.2016471967 6.338862516
H 2.24151993 -0.0448681594 3.9590945759
H -0.8119682639 -0.3161360705 4.0769323113
H -0.4038695148 -0.4158190628 7.486700188
H -0.7665213647 -0.0819302123 -1.6886534462
H 3.402230894 0.2352684332 -0.5422191803
H 3.3359129342 0.1320404163 1.9375434058
H -0.9777305402 -0.2398214175 1.8601684159

CBS-QB3 Caffeic Acid (Radical) -0.006 a.u.

C 1.2552823024 0.0561876675 -0.7752900447
C -0.0017285671 -0.0816165705 -0.0221994703
C -0.0315877103 -0.1380233066 1.3488483752
C 1.1777663415 -0.0617631085 2.0767459715
C 2.4152774684 0.0745889349 1.3619714797
C 2.4659479435 0.13220012 -0.000664263
O -1.102490001 -0.1475559151 -0.7835531471
C 1.2446161312 -0.1143070435 3.5157410861
C 0.2181373108 -0.2392354025 4.3853242653
C 0.5045105025 -0.2750651354 5.8442176199
O -0.630849994 -0.3972085316 6.555341819
O 1.1822112239 0.0961340833 -2.024905952
O 1.6082599483 -0.2043196504 6.3248216645
H 2.2342091915 -0.0460152877 3.9599757869
H -0.8193118708 -0.3161183922 4.083532806
H -0.3952211641 -0.4136594429 7.4968675515
H -0.7508671802 -0.0801344245 -1.6956247753
H 3.4021406548 0.2358009383 -0.5359357642
H 3.3290038787 0.1327304092 1.9427888196
H -0.9836544102 -0.2401009419 1.8537691713

CBS-QB3 Caffeic Acid (Radical) -0.008 a.u.

C 1.2566974672 0.0560314086 -0.7757129036

C -0.0011935894 -0.0816251643 -0.026220904
C -0.0370828882 -0.1380401127 1.3437272218
C 1.1704457926 -0.0618152504 2.0778136499
C 2.409455737 0.0749354139 1.3651950174
C 2.4635987588 0.1324354127 0.002184087
O -1.0991108855 -0.1476071799 -0.7967878734
C 1.2367549492 -0.1148250717 3.5151136793
C 0.2115928706 -0.2397126556 4.3881954221
C 0.5093906477 -0.2761648211 5.8486760627
O -0.6186149534 -0.3948270919 6.5654903741
O 1.1864392824 0.0950936157 -2.0284340192
O 1.6206587446 -0.2076084201 6.3100089636
H 2.226017846 -0.0472681711 3.9604174661
H -0.8276268479 -0.3157738323 4.0914023202
H -0.3846624916 -0.4116582243 7.5083171447
H -0.7342824445 -0.0789880581 -1.7036045371
H 3.4023168103 0.2364864487 -0.5289226881
H 3.3213640711 0.1335174174 1.9487237849
H -0.990506877 -0.2400666635 1.8461907318

CBS-QB3 Gallic Acid (Radical) -0.010 a.u.

C -0.9530183949 -1.2074771773 0.0031860047
C -1.7552958673 0.0036549479 0.0014311057
C -1.0220757767 1.273037341 -0.0034309006
C 0.3549926759 1.3353975467 -0.0064798552
C 1.0685268634 0.1283998025 -0.0048052684
C 0.4174866849 -1.124742284 -0.0000219458
O -3.0102903441 0.0390997104 0.0039443595
O -1.8082640049 2.3612548767 -0.0047274254
C 2.5705369935 0.0820623419 -0.0080426079
O 3.1229326806 1.3022637718 -0.0117959189
O -1.6433359776 -2.3744957716 0.0080170544
O 3.1834568485 -0.9540529209 -0.007143628
H 1.0433920668 -2.0114155071 0.0010919117
H 0.8738080251 2.283827504 -0.010044759
H -1.0060257885 -3.0996388581 0.009271155
H -2.7114058418 1.984418737 -0.0017383144
H 4.089671157 1.2015289392 -0.0134159674

CBS-QB3 Gallic Acid (Radical) -0.002 a.u.

C -0.9513527708 -1.2175926678 0.0032362816
C -1.7540291935 -0.0009962431 0.0015646653
C -1.0208300566 1.2695306079 -0.0033850708
C 0.3578365215 1.3245425054 -0.0064343146
C 1.0701627338 0.1170105628 -0.0046890622
C 0.4214536707 -1.1374277355 0.0000854407

O -2.9997521988 0.0296664895 0.0040633173
O -1.7876716356 2.3624284838 -0.0047385411
C 2.5604533183 0.0897537884 -0.0078276027
O 3.108948345 1.322986898 -0.0121306113
O -1.6502909902 -2.3701833355 0.007919075
O 3.2182197333 -0.9230770682 -0.006671209
H 1.0395366291 -2.0285723919 0.0012187162
H 0.8723061859 2.2747263094 -0.0100793281
H -1.0352121744 -3.1134631127 0.0088596051
H -2.704986291 2.0209685882 -0.0018800773
H 4.0703001733 1.2028213213 -0.0138162843

CBS-QB3 Gallic Acid (Radical) -0.004 a.u.

C -0.9518445848 -1.2149995987 0.0032215781
C -1.7542068848 0.0002343489 0.0015243943
C -1.021007141 1.2703195378 -0.0033948506
C 0.3572643463 1.3270877063 -0.0064394756
C 1.0695262404 0.1196950743 -0.0047111831
C 0.4204156418 -1.134265736 0.0000606203
O -3.0022147296 0.032286268 0.0040236317
O -1.7925282416 2.3621308418 -0.0047343164
C 2.5628524414 0.0877528602 -0.0078650199
O 3.1119649594 1.3177826824 -0.0120525261
O -1.6484961373 -2.3712716604 0.0079386535
O 3.2094588423 -0.9308912727 -0.0067893428
H 1.040317857 -2.0243466474 0.0011917724
H 0.8728792128 2.2767728401 -0.0100589918
H -1.027599126 -3.109887741 0.0089642034
H -2.706368353 2.0117511852 -0.001847573
H 4.0746776567 1.2029723113 -0.0137365745

CBS-QB3 Gallic Acid (Radical) -0.006 a.u.

C -0.9522876351 -1.2124479741 0.0032074527
C -1.7544755887 0.0014183093 0.0014856187
C -1.0212694048 1.2711763962 -0.0034052343
C 0.3566020117 1.3297565406 -0.0064446569
C 1.0690375386 0.1224950662 -0.0047333956
C 0.41940463 -1.1310938811 0.0000364191
O -3.0047892435 0.0347500191 0.0039887869
O -1.7975938377 2.3618319859 -0.0047316888
C 2.5653493123 0.085789747 -0.0079046852
O 3.1152996734 1.3125787681 -0.0119716549
O -1.6467424685 -2.3723567956 0.0079595303
O 3.2007429889 -0.938685422 -0.0069132194
H 1.0412261921 -2.0200702951 0.0011643127
H 0.8733315546 2.2789798875 -0.0100397135

H -1.0201942294 -3.1063877981 0.009068516
H -2.7079126245 2.0025602445 -0.00181767
H 4.0793631307 1.2028282016 -0.0136537177

CBS-QB3 Gallic Acid (Radical) -0.008 a.u.

C -0.9526694288 -1.2099868919 0.003198997
C -1.7548523736 0.0025543224 0.001467232
C -1.0216243735 1.2720694611 -0.0034201032
C 0.3558512514 1.332483267 -0.006475594
C 1.0687244721 0.1253478568 -0.0047842086
C 0.4184385562 -1.1279742516 -0.0000001129
O -3.0074778539 0.0369267196 0.003972787
O -1.8027248921 2.361590152 -0.0047279301
C 2.5678403644 0.0839466047 -0.0079987983
O 3.1189015701 1.3075274933 -0.0118806719
O -1.6450386369 -2.3734266618 0.0079937748
O 3.1921771147 -0.9462879466 -0.0070067104
H 1.0422258713 -2.0158369958 0.0011183903
H 0.8736407704 2.2812920671 -0.0100630279
H -1.0131162231 -3.103053429 0.0091689248
H -2.7094971619 1.9936000579 -0.0017645027
H 4.0842929733 1.2023511747 -0.0135034458

CBS-QB3 Caffeic Acid (Neutral) Zero field

C 1.2661276259 0.0539002558 -0.7236604142
C 0.0415392417 -0.0777818989 -0.040656518
C 0.0329662133 -0.1329282622 1.3410106138
C 1.2317694224 -0.0588104257 2.075346409
C 2.439373145 0.0724110451 1.3755697253
C 2.456874016 0.1283976338 -0.0158365286
O -1.1260369392 -0.1503273542 -0.7340996198
C 1.271129141 -0.1122425652 3.5318409531
C 0.2396984328 -0.2378128222 4.3830001796
C 0.4825985252 -0.2726081705 5.8340780312
O -0.6807575905 -0.4044594737 6.5262426023
O 1.1630056401 0.0988391516 -2.0904867999
O 1.555547986 -0.1974626165 6.3894517381
H 2.2581848191 -0.0414095545 3.9826301171
H -0.7907198231 -0.3180161754 4.060443911
H -0.4357168174 -0.4191192929 7.4627906172
H 2.0345261479 0.19070978 -2.4880195963
H -0.9180514455 -0.0949883541 -1.6755836354
H 3.3969493376 0.2303863185 -0.5494624373
H 3.3713006203 0.131416081 1.9252918594
H -0.9251966985 -0.2344213 1.8346927925

CBS-QB3 Caffeic Acid (Neutral) 0.010 a.u.

C 1.2746654112 0.0537445845 -0.7252860712
C 0.0430276648 -0.0724824632 -0.0282904555
C 0.0450029303 -0.1231122352 1.3504097101
C 1.2525274785 -0.0497435763 2.0821159935
C 2.4602639193 0.0769502581 1.3700195122
C 2.4730698902 0.1276296923 -0.0186459481
O -1.1199239916 -0.1425725324 -0.7042819787
C 1.296081728 -0.1016824572 3.5219986456
C 0.2568748607 -0.2336493595 4.3874435815
C 0.4637921025 -0.2726910124 5.8180456482
O -0.7270052522 -0.4225406931 6.50515476
O 1.1433709263 0.0914381656 -2.0635804893
O 1.5044268927 -0.1933793566 6.4531042166
H 2.2855770017 -0.0274865449 3.9685638346
H -0.7667736662 -0.3205636788 4.0477703346
H -0.4506084224 -0.440632404 7.4304387814
H 1.9840134636 0.168504972 -2.5323373566
H -0.9455935636 -0.1010603254 -1.6564224231
H 3.4080094863 0.2240530759 -0.5598845492
H 3.3970930229 0.1346165656 1.9128868542
H -0.9127808829 -0.2216686751 1.845361399

CBS-QB3 Caffeic Acid (Neutral) 0.002 a.u.

C 1.2675588758 0.0539230997 -0.7233867411
C 0.0423400934 -0.0763217187 -0.0369558303
C 0.0368353661 -0.1303261661 1.3441595358
C 1.2377322962 -0.0564954186 2.0765530607
C 2.4445910833 0.0734288317 1.3743455175
C 2.4600186492 0.1281385197 -0.0169605181
O -1.125040659 -0.1483643916 -0.7256651073
C 1.2774946428 -0.1096061343 3.5305937534
C 0.2440942236 -0.2369470589 4.3825472142
C 0.4779784427 -0.2726394011 5.8302489237
O -0.6912877686 -0.4092710238 6.5192877574
O 1.1571703715 0.097120097 -2.084588591
O 1.5438673202 -0.1957984097 6.402488082
H 2.2646632207 -0.0376773887 3.9811920743
H -0.784568136 -0.3188924537 4.0555241383
H -0.4421440338 -0.4245841391 7.4541503252
H 2.0225694579 0.1847758694 -2.497260124
H -0.9243897524 -0.0965542412 -1.6695053664
H 3.3986830276 0.2287226309 -0.5527087454
H 3.3779375776 0.1320297357 1.9219387766
H -0.9209932988 -0.2309888387 1.8385858645

CBS-QB3 Caffeic Acid (Neutral) 0.004 a.u.

C 1.2691317151 0.0538937751 -0.7233660342
C 0.0429207613 -0.0750708878 -0.0338605717
C 0.039956976 -0.1280327288 1.3466865614
C 1.2427759423 -0.054407153 2.0778335701
C 2.4492714433 0.0744070285 1.3732344048
C 2.4631933866 0.1279235264 -0.0177855885
O -1.1239117551 -0.1466293926 -0.7184804875
C 1.2831157209 -0.107217974 3.5289868973
C 0.247963211 -0.236086489 4.3827115568
C 0.4738246192 -0.2726841179 5.8266999713
O -0.7010446196 -0.4134832443 6.5136250715
O 1.1522663509 0.0954790338 -2.0789440667
O 1.5329598745 -0.1946080184 6.4152333524
H 2.2705871365 -0.0344071272 3.9790752732
H -0.7791532783 -0.3195648264 4.0518031439
H -0.4468189733 -0.4294635363 7.4465759143
H 2.0115138771 0.1795906577 -2.5062396609
H -0.9302353408 -0.0979152978 -1.664548522
H 3.4006465395 0.2272413778 -0.5553371617
H 3.3838197213 0.1326811645 1.9190765065
H -0.9176723085 -0.2279737703 1.8416038695

CBS-QB3 Caffeic Acid (Neutral) 0.006 a.u.

C 1.2708507068 0.0538429782 -0.7236439042
C 0.0432414763 -0.0740216744 -0.0313764942
C 0.0423459318 -0.1260652082 1.3485744982
C 1.2469099362 -0.0525754409 2.0791985669
C 2.4534207925 0.0753285635 1.3721916688
C 2.4664067706 0.1277650204 -0.0183177121
O -1.1226629422 -0.1450891919 -0.7125594266
C 1.2880336429 -0.1051011138 3.527019888
C 0.2513466184 -0.2352490161 4.383562676
C 0.4701234871 -0.2727175635 5.8234577077
O -0.7101636396 -0.4170919963 6.5093346075
O 1.1483405683 0.0939761066 -2.0735504287
O 1.5227953918 -0.1938437756 6.4277988645
H 2.275991701 -0.0316141121 3.9762782951
H -0.7744252323 -0.3200613499 4.0493028581
H -0.4497362007 -0.4337467108 7.4400765009
H 2.001400861 0.1751268637 -2.5150471461
H -0.935688224 -0.099100804 -1.6607490448
H 3.4028426779 0.2259709277 -0.5573691474
H 3.3889473462 0.1333476174 1.9166630514
H -0.91521067 -0.2254081198 1.843738121

CBS-QB3 Caffeic Acid (Neutral) 0.008 a.u.

C 1.272682292 0.0537828915 -0.7242489875
C 0.0433015731 -0.0731986631 -0.0295161185
C 0.0440275964 -0.1244700446 1.3498324256
C 1.2501532757 -0.0510422095 2.0806203119
C 2.4570763592 0.0761790879 1.3711395749
C 2.4696860834 0.1276792318 -0.0185987005
O -1.1213339335 -0.1438161606 -0.7078079366
C 1.2923324699 -0.1032786109 3.5247045432
C 0.2542910359 -0.2343653732 4.3851109288
C 0.4667731215 -0.2726644781 5.8205807075
O -0.7187384102 -0.4200370637 6.5064451399
O 1.1453690438 0.09261733 -2.0684403256
O 1.513344804 -0.1935650986 6.4403007255
H 2.2809733169 -0.0294003019 3.9727816056
H -0.7703412474 -0.3202298484 4.0479698205
H -0.4510166536 -0.4374692018 7.4346650998
H 1.9922416201 0.1715522871 -2.5236812511
H -0.9407648769 -0.100166822 -1.6580077662
H 3.4052807875 0.2249381864 -0.5588735144
H 3.3933589049 0.1340073215 1.9146226174
H -0.9135861627 -0.22338046 1.8449850998

CBS-QB3 Gallic Acid (Neutral) Zero field

C -0.9533473416 -1.1774789391 0.0023310634
C -1.6934134269 0.0074485834 0.0005221669
C -1.0427956093 1.2446370871 -0.0038547005
C 0.3472888089 1.2929539672 -0.0064480184
C 1.0797344117 0.1028811959 -0.0046391661
C 0.4308730921 -1.1385245794 -0.0002372263
O -3.0597515763 0.0099379253 0.0028947538
O -1.7661467053 2.396375853 -0.0055961642
C 2.5619904087 0.0922034567 -0.0073151456
O 3.1042025764 1.3352789233 -0.0115499119
O -1.711511761 -2.3244906224 0.0066523938
O 3.2481500759 -0.9043885297 -0.0060610003
H 1.025102742 -2.0449346786 0.0010851171
H 0.8425872601 2.2533709084 -0.0098572076
H -1.1375632216 -3.0967799645 0.0079834577
H -3.3644358739 -0.9066043954 0.0057385784
H -2.7030190227 2.1614495261 -0.00335324
H 4.0636161629 1.2078892826 -0.0130017502

CBS-QB3 Gallic Acid (Neutral) 0.010 a.u.

C -0.9501532048 -1.1946156511 0.0025332026
C -1.6945432034 -0.0049222835 0.0006948226

C -1.03902249 1.2367062552 -0.0036391497
C 0.3494206192 1.2806493956 -0.0061306953
C 1.0900728745 0.0898645644 -0.004239463
C 0.4353528751 -1.1545258499 0.0001128469
O -3.0400934436 0.0201670175 0.002867894
O -1.7478515056 2.3856872817 -0.0054428957
C 2.5537085308 0.1030528135 -0.0068447321
O 3.093725776 1.3651763447 -0.0121349084
O -1.7133081254 -2.3268169722 0.0067333613
O 3.2985534735 -0.8621238392 -0.0059430662
H 1.020970801 -2.066351218 0.0014919049
H 0.8363758647 2.2451239767 -0.0096071049
H -1.1667329375 -3.1179983705 0.0073231174
H -3.4067533478 -0.8756362818 0.0052579097
H -2.6945008853 2.1802862397 -0.0037463536
H 4.0463393285 1.2075015772 -0.0139926904

CBS-QB3 Gallic Acid (Neutral) 0.004 a.u.

C -0.9522693785 -1.1842159583 0.0024110617
C -1.6936054091 0.0024256476 0.0006106111
C -1.0411735129 1.2410647852 -0.0037809415
C 0.3483425325 1.2876873 -0.0063872177
C 1.0832989834 0.0973871817 -0.0045738455
C 0.4326558817 -1.1450071968 -0.0001524316
O -3.0517052612 0.0146028669 0.0029460505
O -1.7581246958 2.3919188358 -0.0055320558
C 2.5584411189 0.0966156635 -0.0072924604
O 3.0991646366 1.3469679413 -0.0117080755
O -1.7120088751 -2.3255235716 0.0067087242
O 3.2679801943 -0.8874247842 -0.0059448496
H 1.0232131048 -2.0536382417 0.001173754
H 0.8402176515 2.2496947329 -0.0098478944
H -1.1484708 -3.1050812094 0.007756582
H -3.3813423959 -0.8939251888 0.0055977716
H -2.6990246375 2.1690987205 -0.0034939461
H 4.0559718622 1.2085774752 -0.013196837

CBS-QB3 Gallic Acid (Neutral) 0.006 a.u.

C -0.9516311629 -1.1876392159 0.002449107
C -1.6938199402 -0.0000616275 0.0006483946
C -1.0404221123 1.2394560028 -0.0037472042
C 0.3487764079 1.28522719 -0.0063514919
C 1.0853562451 0.094786018 -0.0045298626
C 0.4335693483 -1.1482082272 -0.0001032621
O -3.0477833185 0.0166652687 0.0029617603
O -1.7544700362 2.3897715081 -0.0055051696

C 2.5568040309 0.0987968361 -0.0072558351
O 3.0970697039 1.3529012352 -0.0117890779
O -1.7123539314 -2.3260092351 0.0067355712
O 3.2780506469 -0.8789648689 -0.0059039642
H 1.022408309 -2.0579181284 0.0012287944
H 0.8389649261 2.248050154 -0.0098345126
H -1.1542803093 -3.1093433146 0.0076357011
H -3.3898683127 -0.887695376 0.005533315
H -2.6973412294 2.1728959216 -0.0035610659
H 4.0525317349 1.2085148593 -0.0133171974

CBS-QB3 Gallic Acid (Neutral) 0.008 a.u.

C -0.9509230105 -1.191109852 0.002487903
C -1.6941152594 -0.002517658 0.0006787283
C -1.0396950301 1.2379910888 -0.0037069411
C 0.3491493766 1.2828764492 -0.0062865372
C 1.0876079682 0.0922727277 -0.0044450944
C 0.4344796145 -1.1513896959 -0.0000304209
O -3.0438985149 0.0185401536 0.0029510199
O -1.7510212793 2.3876888261 -0.0054780931
C 2.5552279847 0.1009491712 -0.0071482897
O 3.0952025397 1.3589595113 -0.0119042033
O -1.712779006 -2.3264516302 0.0067514468
O 3.2882180266 -0.8705340091 -0.0058907084
H 1.0216745735 -2.0621612141 0.0013153989
H 0.8376911016 2.2465222539 -0.0097812005
H -1.160361812 -3.1136603086 0.0075001829
H -3.3983540445 -0.8815643642 0.0054432623
H -2.6958115938 2.1766259402 -0.00363674
H 4.0492693648 1.2081876102 -0.0135257133

CBS-QB3 Gallic Acid (Neutral) 0.002 a.u.

C -0.9528409333 -1.1808345376 0.0023729525
C -1.6934673245 0.0049330394 0.0005677203
C -1.041959158 1.2428014727 -0.0038137247
C 0.347850432 1.2902597534 -0.006410336
C 1.0814298149 0.1000823577 -0.004598509
C 0.4317530459 -1.1417821015 -0.0001899023
O -3.0556900882 0.0123564239 0.0029170942
O -1.762012916 2.3941232666 -0.0055613048
C 2.560172255 0.0944007878 -0.007293105
O 3.1015288154 1.3411130615 -0.011639109
O -1.7117311952 -2.3250168719 0.0066781755
O 3.2580137948 -0.8959086316 -0.0060031868
H 1.0241055688 -2.0493164899 0.0011351394
H 0.841438558 2.2514627936 -0.0098434793

H -1.1429126267 -3.1008996281 0.0078676977
H -3.372855999 -0.9002335661 0.005655162
H -2.7009122556 2.1652881087 -0.0034287759
H 4.0596512116 1.2083957614 -0.0131185088

CBS-QB3 Caffeic Acid (Radical) Zero field

C 1.2533244858 0.0565634322 -0.775407723
C -0.0034175668 -0.0814451102 -0.0141561825
C -0.0190559435 -0.1373762007 1.3598617461
C 1.1946556232 -0.0611136019 2.0741751825
C 2.4296077825 0.0738470321 1.3545478126
C 2.4730962853 0.1313418188 -0.0069473605
O -1.1101978212 -0.1472652671 -0.7521700578
C 1.2625616808 -0.1122595716 3.5152424021
C 0.2332483467 -0.237898262 4.3808796044
C 0.492422138 -0.2726512749 5.8324733535
O -0.6612516767 -0.4037948812 6.5331765455
O 1.1751664188 0.0987206325 -2.016295011
O 1.5755918158 -0.1965017233 6.3647324895
H 2.2535776885 -0.0418515842 3.9559069905
H -0.7999056223 -0.3175199718 4.0676021453
H -0.4147395406 -0.4191745782 7.4696795648
H -0.7952886581 -0.0836689759 -1.6781332867
H 3.4032061239 0.2332664491 -0.5523363944
H 3.3475603155 0.1306466207 1.9292630008
H -0.9685098756 -0.2393459827 1.8696781783

CBS-QB3 Caffeic Acid (Radical) 0.010 a.u.

C 1.2578644335 0.0569921404 -0.7811833914
C -0.0074395654 -0.0812055791 -0.0129407109
C -0.0121012666 -0.1354533372 1.3653842152
C 1.2054212221 -0.0594208031 2.0726176731
C 2.4442285857 0.0734956181 1.346513016
C 2.4872945256 0.1299129194 -0.0108986762
O -1.1155773451 -0.1467318189 -0.724934389
C 1.2766212275 -0.1080299069 3.5062126574
C 0.2458258537 -0.235419733 4.3866974314
C 0.4789665503 -0.2695453796 5.8179201607
O -0.6964141198 -0.4122636091 6.5242490567
O 1.1813248544 0.1024685159 -2.0079223136
O 1.5352352341 -0.1903046471 6.4221520037
H 2.2718225171 -0.0350190888 3.9378524284
H -0.7834096761 -0.3198003007 4.064120365
H -0.4092751177 -0.4273807011 7.4464940382
H -0.8538911755 -0.089814107 -1.6697019348
H 3.412044916 0.2287247972 -0.5658461825

H 3.3644690738 0.1280762938 1.9188223802
H -0.9613587274 -0.2367622733 1.8761651722

CBS-QB3 Caffeic Acid (Radical) 0.002 a.u.

C 1.2533832591 0.0570125494 -0.775827266
C -0.0040112911 -0.0814025655 -0.0127376616
C -0.0161594348 -0.1370943286 1.3621938393
C 1.1986388578 -0.0607028011 2.0735798576
C 2.4334677627 0.0737708296 1.3526617181
C 2.475612083 0.1310949295 -0.008322034
O -1.1120819516 -0.1472759963 -0.7441379927
C 1.2668733117 -0.1113743723 3.5142192029
C 0.2369513214 -0.237271999 4.3806840747
C 0.4889552724 -0.2718633846 5.828959635
O -0.6696548959 -0.4058224803 6.5286054327
O 1.1749125702 0.0989976594 -2.0140208302
O 1.5659640677 -0.1947539737 6.3768470833
H 2.2584964408 -0.0403994653 3.9535120368
H -0.7950480979 -0.3177543536 4.0644726467
H -0.4172191799 -0.4211537717 7.4628949905
H -0.8087806705 -0.0846693244 -1.6742462639
H 3.4041344919 0.2322188878 -0.5564058369
H 3.3524031855 0.1300555089 1.9260180833
H -0.9651851025 -0.2390925481 1.8728222845

CBS-QB3 Caffeic Acid (Radical) 0.004 a.u.

C 1.2538324713 0.0574305711 -0.7766130155
C -0.0047748501 -0.0813385834 -0.0118447273
C -0.0140365065 -0.1367289031 1.3639412597
C 1.2017423842 -0.0602639624 2.0731551549
C 2.4368906227 0.0737146349 1.3509878934
C 2.4782898094 0.1308155553 -0.0093614134
O -1.1135774266 -0.1472175723 -0.7373677
C 1.270434889 -0.1104658768 3.5127540853
C 0.2400471421 -0.2368003355 4.3811139949
C 0.4859600361 -0.2712917414 5.8256661394
O -0.6773563707 -0.407729093 6.525272799
O 1.1753524844 0.099327009 -2.0120342718
O 1.5571589443 -0.1931489503 6.38856182
H 2.2627997771 -0.0388703532 3.9504629364
H -0.7910058994 -0.318281278 4.0625581967
H -0.4180180614 -0.422879781 7.4571197693
H -0.8213314008 -0.085683617 -1.6713637879
H 3.4054914187 0.2311277314 -0.5597729583
H 3.3565756124 0.1294818691 1.9234121015
H -0.9628230761 -0.2386783236 1.8751247236

CBS-QB3 Caffeic Acid (Radical) 0.006 a.u.

C 1.2548348512 0.0568447046 -0.7776760102
C -0.0055317327 -0.0812566366 -0.0115890914
C -0.0127408349 -0.1361502588 1.3649593646
C 1.2038158503 -0.0599446344 2.0729140624
C 2.4397405432 0.073586716 1.3494816349
C 2.4811231187 0.1303769569 -0.0100626776
O -1.1145760484 -0.1469463069 -0.7322334999
C 1.2731607951 -0.1095681617 3.5109142058
C 0.2424450875 -0.2362785784 4.3822687667
C 0.4833569614 -0.2705766145 5.8227471335
O -0.6841218194 -0.4095495253 6.5235655652
O 1.1764678368 0.1005001742 -2.0102223997
O 1.5491810642 -0.1919243541 6.3998646724
H 2.266312218 -0.037396096 3.9468962103
H -0.7878048623 -0.3187888827 4.0619278703
H -0.4166456697 -0.4247006814 7.4525917195
H -0.8329570181 -0.0873160088 -1.6700362554
H 3.4072705222 0.2302706086 -0.5623057074
H 3.3598439925 0.1290471507 1.9214682465
H -0.9615228559 -0.2377105712 1.8762991894

CBS-QB3 Caffeic Acid (Radical) 0.008 a.u.

C 1.2561301218 0.0568414581 -0.7791492762
C -0.0064229545 -0.0812258888 -0.0119439959
C -0.0120639248 -0.1357878761 1.3654572358
C 1.2050920849 -0.0596721338 2.0727293616
C 2.4422099801 0.0735381584 1.3480250347
C 2.4840906097 0.1301358266 -0.0105710648
O -1.1152911154 -0.146843873 -0.7279752338
C 1.2752206455 -0.1088021502 3.5087310226
C 0.2443649618 -0.2358267384 4.3840916863
C 0.4810054777 -0.2700620331 5.8201382963
O -0.6904721948 -0.4109535895 6.5231225117
O 1.1785353744 0.1014865726 -2.0088598972
O 1.5418971252 -0.1910458692 6.4109414709
H 2.2693294132 -0.0362108135 3.9426954552
H -0.7852929722 -0.319232853 4.0624199894
H -0.4138071651 -0.42607184 7.4489801332
H -0.8438117699 -0.0886270526 -1.669318277
H 3.4094057414 0.2295101732 -0.5643481933
H 3.3625249654 0.1285858041 1.9199372693
H -0.9609924046 -0.2372162817 1.8766694715

CBS-QB3 Gallic Acid (Radical) Zero field

C -0.9509519081 -1.2204231753 0.0032723383
C -1.7540644638 -0.0022679654 0.0016587671
C -1.0206930438 1.269120304 -0.003414107
C 0.3584008678 1.3221208515 -0.0065821788
C 1.0709515799 0.1144402554 -0.0048609745
C 0.4223322411 -1.1405631407 0.0000067747
O -2.9973588371 0.0265462271 0.0042782193
O -1.7829009387 2.3629875307 -0.0047464891
C 2.5583926737 0.0916652469 -0.0081436267
O 3.1063262719 1.3282030617 -0.0120243519
O -1.6521215904 -2.3694348655 0.0080125845
O 3.2270022152 -0.9152271038 -0.0065039022
H 1.0387744294 -2.0327043032 0.0010992524
H 0.8718652218 2.2727637369 -0.0103170429
H -1.0434837483 -3.1177793312 0.0088345608
H -2.7037297187 2.0305768325 -0.0018373115
H 4.0663507481 1.2030988384 -0.0134375125

CBS-QB3 Gallic Acid (Radical) 0.010 a.u.

C -0.9470004606 -1.2347631557 0.0033479874
C -1.7554467502 -0.0092138732 0.0018682998
C -1.0212329139 1.2668864341 -0.0033605796
C 0.3595559028 1.3119934248 -0.0064572044
C 1.0774081412 0.1032731835 -0.0046129235
C 0.4280752406 -1.1565151347 0.0002195973
O -2.9872190759 0.0107795455 0.0044482307
O -1.7630178399 2.3643126382 -0.0048144828
C 2.5478053418 0.1024418627 -0.0077224311
O 3.0976306503 1.3554033655 -0.0124476336
O -1.6619538826 -2.3636138749 0.0078664768
O 3.2721329532 -0.8761685637 -0.0061196159
H 1.0374799222 -2.0531111302 0.0013258131
H 0.8670831171 2.2656734866 -0.0102978476
H -1.0863600539 -3.1371543584 0.008261745
H -2.7001003181 2.0765886113 -0.0021067128
H 4.0502520257 1.1963105385 -0.0141037188

CBS-QB3 Gallic Acid (Radical) 0.002 a.u.

C -0.9502512976 -1.2232129606 0.0032874738
C -1.7541468779 -0.0035915561 0.0016976986
C -1.0206457903 1.2685538129 -0.0034194681
C 0.3588493915 1.3197961437 -0.0066297682
C 1.0719326218 0.1119547031 -0.0049154998
C 0.4235078114 -1.1437622724 -0.0000096627
O -2.9949645186 0.0235013435 0.0044107913
O -1.7782937043 2.3631851091 -0.0047506598

C 2.5559697952 0.0937816665 -0.0082325242
O 3.1038313503 1.3337269105 -0.0120212023
O -1.6539812508 -2.3681732058 0.0080374448
O 3.2358233249 -0.9072572673 -0.0063812762
H 1.0382741754 -2.0369260626 0.0010738367
H 0.871065148 2.2710246652 -0.0104069123
H -1.051769006 -3.1214983283 0.0087681093
H -2.7024701866 2.0398130804 -0.0018614623
H 4.0623610137 1.2022072181 -0.0133519186

CBS-QB3 Gallic Acid (Radical) 0.004 a.u.

C -0.949523002 -1.2259451165 0.0032887552
C -1.7542850234 -0.0049397685 0.0017037858
C -1.0206913192 1.2679319693 -0.0034037942
C 0.3591637994 1.3176118449 -0.0065963836
C 1.0730532559 0.1095670414 -0.0048721531
C 0.4246972265 -1.1469775443 0.0000232868
O -2.9928444968 0.0204055663 0.0044769663
O -1.7738791273 2.3634102498 -0.0047539706
C 2.553623097 0.0959959856 -0.0081419056
O 3.1015775373 1.3392082238 -0.0121160441
O -1.6559507054 -2.3668260695 0.0080038757
O 3.2448081219 -0.8993240057 -0.0062852543
H 1.0378697714 -2.0411230738 0.0011185079
H 0.8701198573 2.269464942 -0.0103831149
H -1.0600595763 -3.1250246099 0.0086649946
H -2.7012096014 2.0487456916 -0.0019377796
H 4.058622185 1.2009416735 -0.0134947723

CBS-QB3 Gallic Acid (Radical) 0.006 a.u.

C -0.9487928821 -1.2287286451 0.0032806991
C -1.7544949547 -0.0063392335 0.0016755438
C -1.0208558297 1.2673881615 -0.0033663716
C 0.3593479159 1.3155522189 -0.0064676974
C 1.0743193928 0.1073057541 -0.0047092951
C 0.425834509 -1.1501623576 0.0001179445
O -2.9908539307 0.0173109609 0.004455068
O -1.7699581205 2.3636119669 -0.0047620299
C 2.5515590018 0.098191396 -0.0078512438
O 3.0999126321 1.3444953327 -0.0123074937
O -1.6579649607 -2.3655933681 0.0079110749
O 3.2539932001 -0.8914118461 -0.0062591946
H 1.0375509734 -2.0452109036 0.0012428422
H 0.8690584466 2.268033815 -0.0102245253
H -1.0685175934 -3.1286980378 0.0085276001
H -2.7005423248 2.0578739324 -0.0020777462

H 4.0554965248 1.1995038534 -0.0138901748

CBS-QB3 Gallic Acid (Radical) 0.008 a.u.

C -0.9479453788 -1.2317384456 0.0032895206
C -1.7548862439 -0.0078106359 0.0016923605
C -1.0211217166 1.2670426542 -0.0033553965
C 0.359445724 1.31359456 -0.0064453815
C 1.0758033526 0.1051518544 -0.0046777629
C 0.4270046956 -1.1533869035 0.000146104
O -2.9888469435 0.0139751803 0.0045389995
O -1.7663432789 2.3637818004 -0.0047724651
C 2.5495704666 0.1004342326 -0.0077957482
O 3.0988057812 1.3499622974 -0.0123691918
O -1.659991947 -2.3643997824 0.0078929535
O 3.2633840948 -0.8833431911 -0.0061991774
H 1.0373702553 -2.0492956963 0.0012718224
H 0.8678766765 2.2667296232 -0.0102191464
H -1.0775607671 -3.1327552689 0.0084377296
H -2.7003110018 2.0674300592 -0.0021561402
H 4.0528382309 1.1977506621 -0.0139840803

LC-BLYP Caffeic Acid (Neutral) -0.010 a.u.

C 1.2530201524 0.0670417982 -0.6897109768
C 0.053198156 -0.1394577304 -0.0409613567
C 0.0263526164 -0.237463611 1.323910441
C 1.1939124563 -0.1296539983 2.0617250319
C 2.3854359033 0.0671286066 1.3915076963
C 2.416464262 0.1680495871 0.020522739
O -1.0879171987 -0.2453953727 -0.7668743614
C 1.2305648798 -0.2113356468 3.5193354049
C 0.2169244466 -0.1897122323 4.3555069492
C 0.5075486314 -0.2678046761 5.8071638181
O -0.5963145875 -0.2127681233 6.5343925761
O 1.1971194191 0.1555271251 -2.0639292093
O 1.6063685865 -0.365586883 6.2572763344
H 2.2148994703 -0.2791607033 3.9704307338
H -0.8197745589 -0.1048195985 4.061356206
H -0.3662790839 -0.2593773795 7.476372002
H 2.0651287289 0.3938060118 -2.392598173
H -0.8650698802 -0.1236996041 -1.6942021707
H 3.3565175807 0.3256898687 -0.4956936357
H 3.3015370975 0.1473800275 1.9592552408
H -0.924526078 -0.4047154655 1.8097987101

LC-BLYP Caffeic Acid (Neutral) -0.002 a.u.

C 1.2590669295 0.0526287172 -0.6881027658

C 0.0535546329 -0.0800726159 -0.0169889742
C 0.04116323 -0.1359002708 1.3470455155
C 1.2235381151 -0.0613761618 2.0678036435
C 2.4127400382 0.0700993085 1.383846526
C 2.4328957772 0.1273280967 0.0074549333
O -1.0963196796 -0.1527504573 -0.7151117033
C 1.259214424 -0.1161448907 3.5234409767
C 0.2384204758 -0.235720832 4.3476707988
C 0.4865736768 -0.2713072117 5.7937725838
O -0.643469917 -0.3924922729 6.4921772536
O 1.1675943304 0.0994918245 -2.0446143534
O 1.5581472447 -0.2024676903 6.3192321621
H 2.2411268395 -0.0502880268 3.9796121323
H -0.7901093014 -0.3102371156 4.0271677448
H -0.4099722606 -0.4085667083 7.430797616
H 2.0333626742 0.1953452223 -2.4470458471
H -0.8988942676 -0.0952306244 -1.6565354277
H 3.3705618728 0.2310527581 -0.5240613636
H 3.3400045612 0.1292981062 1.9360915689
H -0.9140883961 -0.239017155 1.8409309799

LC-BLYP Caffeic Acid (Neutral) -0.004 a.u.

C 1.2575201388 0.0560220355 -0.6886488425
C 0.05294747 -0.0897953383 -0.0221394809
C 0.0372278976 -0.1531971666 1.3422635489
C 1.2166332412 -0.0730447696 2.0663675307
C 2.406618792 0.0697803786 1.3851652597
C 2.4292667195 0.1351212734 0.0096786492
O -1.0956452578 -0.168399937 -0.726163618
C 1.2526684751 -0.1320821547 3.5230783425
C 0.2326063361 -0.2280626895 4.3494523237
C 0.4917414003 -0.2708211018 5.7972496508
O -0.6337653828 -0.3616286882 6.5022598576
O 1.174401613 0.1100922074 -2.0497921818
O 1.5721882001 -0.2300877992 6.3044785299
H 2.2361918904 -0.088713906 3.9784469778
H -0.7997172123 -0.2756731909 4.0352960039
H -0.4009542396 -0.3834619622 7.4417367738
H 2.0447507043 0.2254676298 -2.435922378
H -0.891595934 -0.1008235995 -1.6648849853
H 3.3678863826 0.2484370148 -0.5187190932
H 3.3316729881 0.1324130255 1.9406109743
H -0.9175332226 -0.2678692615 1.8347701567

LC-BLYP Caffeic Acid (Neutral) -0.006 a.u.

C 1.25571199 0.0616407312 -0.6890032208

C 0.0527931593 -0.1050551025 -0.027887014
C 0.0338330484 -0.1803767468 1.3366828873
C 1.2096458571 -0.0909122565 2.0647794324
C 2.3999307464 0.070228527 1.3868768834
C 2.4249154558 0.1481887379 0.0127178847
O -1.093756712 -0.193313897 -0.7385433175
C 1.2461531004 -0.1575985994 3.5220971582
C 0.2268145295 -0.2146433122 4.3515008617
C 0.4969621402 -0.2704407558 5.8006304299
O -0.6234564037 -0.3128325489 6.5130675678
O 1.1811158882 0.126795183 -2.0545540681
O 1.5857616176 -0.2764971862 6.2887702512
H 2.2313113613 -0.1517545465 3.9760124751
H -0.8089511986 -0.2174616823 4.044263962
H -0.3912622166 -0.3445173462 7.4532702968
H 2.0542953149 0.2712794387 -2.4232541608
H -0.8833492449 -0.1108718694 -1.6740932829
H 3.3639478998 0.2768649495 -0.5120077393
H 3.3223271203 0.1385907682 1.9459676053
H -0.9196324533 -0.313640486 1.8272891076

LC-BLYP Caffeic Acid (Neutral) -0.008 a.u.

C 1.2539793681 0.06618549 -0.6892534487
C 0.0528811356 -0.1222200613 -0.0340744816
C 0.0304145938 -0.2098266207 1.3306116445
C 1.2022437422 -0.1104366111 2.0632266702
C 2.3928370715 0.0700954102 1.3890045209
C 2.4203854323 0.1607895054 0.0164131189
O -1.0911230052 -0.2205832159 -0.751986178
C 1.239022002 -0.185570334 3.5207913711
C 0.221772415 -0.2008349872 4.3534648956
C 0.5021220395 -0.2698738625 5.803849213
O -0.6110721808 -0.259966157 6.5237175934
O 1.1883035146 0.143269744 -2.059106072
O 1.5968159312 -0.3261016553 6.2729279378
H 2.2243889013 -0.2197457102 3.9731667318
H -0.8152714911 -0.156063391 4.0528509482
H -0.3800002666 -0.3009615184 7.4647427911
H 2.0615410873 0.3270384448 -2.4089275816
H -0.8745873499 -0.119705174 -1.6837841665
H 3.3597163048 0.3054581587 -0.5042366839
H 3.3122456165 0.1447799864 1.9521507195
H -0.9215038622 -0.3620554408 1.8190344561

LC-BLYP Gallic Acid (Neutral) -0.010 a.u.

C -0.9442993342 -1.1425110732 0.0020197783

C -1.6714249843 0.0235205663 0.0001991428
C -1.0335866321 1.2401570759 -0.0041590457
C 0.3402499848 1.2933746176 -0.0067108056
C 1.0538735592 0.1175716864 -0.0048858422
C 0.4199053217 -1.1066690796 -0.0005360855
O -3.0377434478 -0.0063513096 0.0027937994
O -1.774955043 2.3732880527 -0.0058168001
C 2.5410933448 0.0846297597 -0.0074030152
O 3.092602187 1.2867999916 -0.0108334101
O -1.6885387869 -2.2886056774 0.0064807576
O 3.158370364 -0.933888322 -0.0063774063
H 1.0248945092 -2.004409946 0.0007807023
H 0.8471045968 2.2466495479 -0.0100166237
H -1.1106693067 -3.0568416921 0.0083346273
H -3.2991291432 -0.9340271412 0.0064104249
H -2.7046120549 2.1267356648 -0.0028727192
H 4.0584258654 1.1918022781 -0.012113479

LC-BLYP Gallic Acid (Neutral) -0.002 a.u.

C -0.942994 -1.155173 0.002198
C -1.670193 0.013545 0.000413
C -1.029064 1.23129 -0.003938
C 0.343908 1.280847 -0.00651
C 1.058581 0.104764 -0.004696
C 0.423377 -1.119932 -0.000345
O -3.022444 0.005483 0.002865
O -1.75525 2.364692 -0.005621
C 2.534676 0.093843 -0.007302
O 3.077489 1.309107 -0.011308
O -1.688631 -2.291862 0.006536
O 3.19799 -0.900429 -0.005999
H 1.01862 -2.022999 0.000968
H 0.843598 2.237002 -0.009892
H -1.130319 -3.073309 0.007909
H -3.333149 -0.907439 0.005967
H -2.693024 2.14187 -0.003242
H 4.03839 1.199924 -0.012711

LC-BLYP Gallic Acid (Neutral) -0.004 a.u.

C -0.9433734359 -1.1519912988 0.0021569224
C -1.6703907339 0.0160305501 0.0003654439
C -1.0301203645 1.2334027554 -0.0039871464
C 0.3430617313 1.2838444045 -0.0065556657
C 1.0572092995 0.1078369928 -0.0047406221
C 0.4224742589 -1.1166754239 -0.0003910125
O -3.026170923 0.0026983422 0.0028491618

O -1.7598668101 2.3668296332 -0.0056644408
C 2.536136311 0.0915383332 -0.0073271389
O 3.0808995823 1.3035894731 -0.0111936368
O -1.6885395501 -2.2910722428 0.0065215473
O 3.1880308357 -0.9088343619 -0.0060916785
H 1.0200072693 -2.0184678316 0.0009216964
H 0.8445778921 2.2392356126 -0.0099183115
H -1.1251411234 -3.0691189205 0.0080144879
H -3.3245735957 -0.9140985824 0.0060666107
H -2.6956712616 2.1382315395 -0.0031639108
H 4.0430116181 1.1982460253 -0.0125683063

LC-BLYP Gallic Acid (Neutral) -0.006 a.u.

C -0.9437143793 -1.148824781 0.0021139181
C -1.670659935 0.018521748 0.0003140856
C -1.0312227896 1.2355867916 -0.0040403464
C 0.3421705876 1.2869298174 -0.0066043454
C 1.0559726518 0.1109930517 -0.0047873988
C 0.4215943101 -1.1133836272 -0.0004381113
O -3.0299551091 -0.0002064184 0.0028319206
O -1.764684666 2.3689783932 -0.0057118256
C 2.5376859004 0.0892364061 -0.0073527408
O 3.0845482588 1.2980401196 -0.0110754875
O -1.6884965488 -2.2902650265 0.0065077345
O 3.1781121222 -0.9172108104 -0.0061869082
H 1.0215116016 -2.0138651648 0.0008750118
H 0.8454923465 2.2415848446 -0.0099482913
H -1.1201523757 -3.0649809406 0.0081206014
H -3.3160398219 -0.9207546938 0.006174271
H -2.6984826935 2.1345055216 -0.003077506
H 4.04788154 1.1963397689 -0.0124205816

LC-BLYP Gallic Acid (Neutral) -0.008 a.u.

C -0.9440215227 -1.1456665822 0.0020682887
C -1.671003694 0.0210184111 0.000258734
C -1.032376489 1.237839075 -0.0040976198
C 0.3412337921 1.29010569 -0.0066560391
C 1.054863073 0.1142365604 -0.0048358005
C 0.4207378371 -1.110050135 -0.0004864286
O -3.0338086715 -0.00322474 0.0028134674
O -1.7697113295 2.3711326525 -0.0057626878
C 2.5393347553 0.0869344617 -0.0073781881
O 3.0884454435 1.2924474493 -0.0109548933
O -1.6884977096 -2.2894423735 0.0064942222

O 3.1682272321 -0.9255611299 -0.0062829032
H 1.0231387272 -2.0091821693 0.0008280213
H 0.8463364558 2.2440545057 -0.0099810436
H -1.1153339639 -3.0608900854 0.0082273255
H -3.3075558509 -0.927399503 0.0062892395
H -2.7014616326 2.1306777116 -0.0029810274
H 4.0530145476 1.1941952011 -0.0122686672

LC-BLYP Caffeic Acid (Radical) -0.010 a.u.

C 1.2502682431 0.0544623683 -0.7363344892
C 0.0063270512 -0.0835036444 -0.0002377338
C -0.0306840646 -0.1390362224 1.3500384056
C 1.1642023377 -0.0622608206 2.0763246375
C 2.3912365863 0.0755757334 1.3743017673
C 2.4484368044 0.1331831474 0.0326509152
O -1.0753171867 -0.1504920225 -0.7716607922
C 1.2279992814 -0.1171185174 3.5035357341
C 0.2101944442 -0.2369085433 4.3527964501
C 0.5114771939 -0.276936325 5.8056610544
O -0.58652289 -0.3824981737 6.5301078668
O 1.1873813512 0.0936188387 -1.9734356848
O 1.6183625615 -0.220045425 6.2406208213
H 2.2113887717 -0.0556420236 3.9569616053
H -0.8272965545 -0.3064294313 4.0581970174
H -0.3613119091 -0.4022976927 7.4748893501
H -0.7252978108 -0.0824231009 -1.6796162853
H 3.3840862586 0.2390728001 -0.4971157401
H 3.2976995146 0.1348261927 1.9614596936
H -0.980977984 -0.2426281381 1.8526284067

LC-BLYP Caffeic Acid (Radical) -0.002 a.u.

C 1.2449765061 0.0549680121 -0.7365526919
C 0.0039680533 -0.0826881733 0.0126602841
C -0.0107671584 -0.1378413157 1.367823794
C 1.190277289 -0.0615354269 2.0717744082
C 2.412477801 0.0731899205 1.3635437356
C 2.4572594801 0.1304265456 0.0220410204
O -1.0872800631 -0.1482689189 -0.7268058797
C 1.2546810809 -0.1137414908 3.506406046
C 0.2328349029 -0.2362222324 4.3451535258
C 0.4931300534 -0.2722120056 5.7915350871
O -0.6295330644 -0.3959292077 6.4958350487
O 1.1724736479 0.0961756145 -1.9616640253
O 1.572537176 -0.2004495131 6.2976381317
H 2.2396440572 -0.0464510258 3.9546761586
H -0.7975892851 -0.3125161076 4.0316723253

H -0.3964723575 -0.4128216545 7.4349665579
H -0.7841236003 -0.0844823957 -1.6527041006
H 3.3838140458 0.2330093224 -0.5237590745
H 3.3261500216 0.1300851851 1.9396199381
H -0.9568065865 -0.2401761322 1.8779127105

LC-BLYP Caffeic Acid (Radical) -0.004 a.u.

C 1.2458918504 0.0540864689 -0.736571104
C 0.004581025 -0.0827896912 0.0100174098
C -0.0147893006 -0.1379138797 1.3642737696
C 1.1848389401 -0.0617878448 2.0725401191
C 2.4078803432 0.0734482953 1.3656042348
C 2.4551452631 0.1306860885 0.0240550452
O -1.0848539944 -0.1484977315 -0.7363335996
C 1.2490816185 -0.11438915 3.5064520243
C 0.2281211635 -0.2361676685 4.346303417
C 0.4971178961 -0.272594912 5.7950674044
O -0.6200536557 -0.3938360451 6.5029449243
O 1.1750400162 0.096020949 -1.9643987152
O 1.5830397186 -0.2035779978 6.2846700961
H 2.2336035054 -0.0481396657 3.9559850249
H -0.8038297494 -0.3111140141 4.0366919179
H -0.3904474386 -0.4116394953 7.4437639032
H -0.7707419201 -0.0842047423 -1.6581927968
H 3.3836662337 0.2341555624 -0.5182574398
H 3.3199890478 0.1309624096 1.9440907628
H -0.9616285625 -0.2401879357 1.8730666019

LC-BLYP Caffeic Acid (Radical) -0.006 a.u.

C 1.2470180882 0.0546567899 -0.7363350799
C 0.0052318672 -0.0828990018 0.0070470424
C -0.0195280472 -0.1382389809 1.3601546171
C 1.1785513716 -0.061850522 2.0735835848
C 2.4026955029 0.0740595342 1.3681255666
C 2.4529233681 0.1313763236 0.0266019583
O -1.0820009224 -0.1489326703 -0.7469712128
C 1.2427827412 -0.1151740848 3.5059604515
C 0.2228493041 -0.2365950029 4.3479480141
C 0.5015379987 -0.2740137294 5.7983006789
O -0.609824609 -0.3909686025 6.5109495637
O 1.1785761858 0.0943770395 -1.9671690432
O 1.5940490437 -0.2074040587 6.2708817944
H 2.2268768561 -0.0501289079 3.9567210767
H -0.8107511682 -0.3101413537 4.0428013119
H -0.3822113897 -0.4089640138 7.4531669972
H -0.7565405439 -0.0829289364 -1.6645169715

H 3.3836681054 0.2352559696 -0.5118524997
H 3.3130908682 0.1319472694 1.9492240052
H -0.9673426207 -0.2409140613 1.8671511444

LC-BLYP Caffeic Acid (Radical) -0.008 a.u.

C 1.2484609206 0.054830766 -0.7362619029
C 0.0057821776 -0.0834493555 0.0036566754
C -0.024771017 -0.1392112207 1.3554299358
C 1.1717618025 -0.0623994392 2.0748407227
C 2.3971916568 0.0749766245 1.3710317604
C 2.4506671642 0.1328360293 0.0294727136
O -1.0787962927 -0.1502414319 -0.7587425328
C 1.2358227988 -0.1167566499 3.5049878861
C 0.2168542107 -0.2366664129 4.3500843369
C 0.5063048917 -0.275656511 5.8018156657
O -0.5988482996 -0.3851648337 6.5199815062
O 1.1825199381 0.094826072 -1.9701222192
O 1.6060451836 -0.2155122418 6.2560409309
H 2.2196000451 -0.0542207047 3.9570594668
H -0.8186971951 -0.3073250014 4.0499818696
H -0.3726703627 -0.4043379773 7.4634887776
H -0.7413426087 -0.0830527484 -1.6716612383
H 3.3837097638 0.2382221281 -0.5048073625
H 3.3056891347 0.1336913663 1.9550342986
H -0.9736319122 -0.2428694577 1.8604617095

LC-BLYP Gallic Acid (Radical) -0.010 a.u.

C -0.9375246767 -1.1953215858 0.0031379567
C -1.7291355106 0.0065417479 0.0013884811
C -1.0077569867 1.2625598589 -0.0034246076
C 0.351826471 1.3219908564 -0.0063917847
C 1.0510429742 0.1274058153 -0.0046833925
C 0.4129691803 -1.1146252412 0.0000471043
O -2.9647093355 0.0383147809 0.0038073082
O -1.7894212152 2.3334596098 -0.0047138875
C 2.5413275205 0.0865030526 -0.0078693846
O 3.0939318085 1.2852467698 -0.0117440755
O -1.6213135738 -2.3459029911 0.007832762
O 3.1443221263 -0.9395921557 -0.0071079889
H 1.0404594363 -1.9972895421 0.0011533034
H 0.8730992761 2.2670285689 -0.009953619
H -1.007713898 -3.0882401068 0.009123968
H -2.6973105667 1.9780911583 -0.0017689072
H 4.0609989701 1.1969524039 -0.0135382363

LC-BLYP Gallic Acid (Radical) -0.002 a.u.

C -0.9359505577 -1.2053004404 0.0031713275
C -1.7280854976 0.0021305776 0.0015232805
C -1.006170687 1.2596225748 -0.0033947997
C 0.3553222822 1.3114470414 -0.0063940788
C 1.0533207794 0.1162457591 -0.0046289482
C 0.4173239359 -1.127013187 0.0000955225
O -2.9545519294 0.0300192994 0.0040037061
O -1.77008206 2.3346291565 -0.0047108419
C 2.5329011093 0.0950140743 -0.0077226747
O 3.080283256 1.3053734219 -0.0120988293
O -1.6286275244 -2.3419954662 0.0077583093
O 3.1803655676 -0.9083514315 -0.0064998359
H 1.0357067264 -2.0147404033 0.0012173023
H 0.871741234 2.258250018 -0.0100364524
H -1.0393191291 -3.1028084496 0.00873184
H -2.6910100309 2.0117201999 -0.0018729034
H 4.0419245255 1.1988802551 -0.013846924

LC-BLYP Gallic Acid (Radical) -0.004 a.u.

C -0.9364160832 -1.2027421487 0.0031619226
C -1.7282477685 0.0032930995 0.0014900863
C -1.0064909204 1.2602667513 -0.0034020674
C 0.3545542257 1.3139077375 -0.0063965952
C 1.0525489855 0.1188783786 -0.0046457894
C 0.4162139693 -1.1239200248 0.0000800227
O -2.9569283501 0.0322460035 0.0039522205
O -1.7746516679 2.3343634042 -0.0047090373
C 2.5348655529 0.0928415715 -0.0077598411
O 3.0833051814 1.3003743417 -0.0120142077
O -1.6267476822 -2.3429743284 0.0077755752
O 3.1713469813 -0.9161879805 -0.0066361915
H 1.03669856 -2.0104625527 0.0011989718
H 0.8722205511 2.2602210488 -0.0100191835
H -1.0310824871 -3.0990398376 0.0088286339
H -2.6923865525 2.0033405342 -0.0018410676
H 4.0462895048 1.1987170017 -0.0137684525

LC-BLYP Gallic Acid (Radical) -0.006 a.u.

C -0.9368288814 -1.2002337446 0.0031532904
C -1.7284781947 0.0044163842 0.0014562688
C -1.0068579701 1.260978633 -0.0034095358
C 0.3537187647 1.3164864643 -0.0063965948
C 1.0519148888 0.1216151658 -0.0046598839
C 0.4151174826 -1.1208284715 0.0000671764
O -2.95940598 0.0343696143 0.0039017642
O -1.7793969894 2.3340806014 -0.0047093436

C 2.5369211651 0.0906995521 -0.0077956286
O 3.0865828076 1.2953575605 -0.0119256561
O -1.6249044437 -2.3439502236 0.007793795
O 3.1623369732 -0.924008478 -0.0067857816
H 1.0378210795 -2.0061318453 0.0011827452
H 0.8726149806 2.2623395763 -0.0099989438
H -1.0230858999 -3.095361258 0.0089267979
H -2.6938942337 1.9949396362 -0.001813822
H 4.0509164508 1.1983538329 -0.0136916478

LC-BLYP Gallic Acid (Radical) -0.008 a.u.

C -0.9371963908 -1.1977630179 0.0031453442
C -1.7287738445 0.0054996766 0.00142236
C -1.0072777069 1.2617458824 -0.0034170741
C 0.3528113499 1.3191812979 -0.0063948676
C 1.0514136629 0.124457232 -0.004672248
C 0.4140351147 -1.117731976 0.0000563049
O -2.961995724 0.0363929202 0.0038533706
O -1.7843194428 2.3337795099 -0.0047111004
C 2.5390727697 0.0885867345 -0.0078317496
O 3.0901219092 1.2903168392 -0.011835379
O -1.6230940475 -2.3449259487 0.0078128303
O 3.1533296779 -0.9318106621 -0.0069437253
H 1.0390741126 -2.0017423718 0.0011676063
H 0.8729124675 2.2646076595 -0.0099768842
H -1.0153022558 -3.0917631064 0.0090253563
H -2.6955347382 1.9865210404 -0.0017900037
H 4.0558150862 1.1977712904 -0.0136151405

LC-BLYP Caffeic Acid (Neutral) Zero field

C 1.2604127009 0.0524783538 -0.6875896984
C 0.0546507757 -0.0779693679 -0.0125466202
C 0.0458693428 -0.1323127105 1.350853332
C 1.2306750781 -0.0584915255 2.0689173541
C 2.4184525702 0.0709514648 1.3827243644
C 2.435830672 0.1265343001 0.0057672608
O -1.0956003168 -0.1497655603 -0.7055260184
C 1.2662568825 -0.1127486282 3.5230283682
C 0.2434367288 -0.2356453972 4.3464770582
C 0.4816361114 -0.2715780019 5.7905739799
O -0.6540740363 -0.3993803997 6.4837247692
O 1.1605975351 0.0971323616 -2.0391179191
O 1.5458613027 -0.1979612739 6.3329871158
H 2.2481345877 -0.0442009466 3.9789992014
H -0.783016682 -0.3136792007 4.0208146375

H -0.4195059295 -0.4153818429 7.4213491281
H 2.0201143016 0.1877705795 -2.4569703663
H -0.9050726423 -0.0960434538 -1.6492336759
H 3.3719636702 0.2282853932 -0.5283672501
H 3.3475303798 0.1295107892 1.9321410557
H -0.9090420327 -0.2338329328 1.8455779232

LC-BLYP Caffeic Acid (Neutral) 0.010 a.u.

C 1.2691480124 0.051484393 -0.6873547922
C 0.057061794 -0.0716369174 0.0017969939
C 0.0581816764 -0.1207104824 1.3615814849
C 1.2523972174 -0.0484291595 2.0763049752
C 2.4385205957 0.0747554451 1.3797497377
C 2.4511535334 0.1242628773 0.003053272
O -1.0903129032 -0.140288429 -0.6746432547
C 1.2901316175 -0.1007433116 3.5145219593
C 0.2600714985 -0.2325524094 4.3490998062
C 0.4634878864 -0.2709240803 5.7746919631
O -0.6956409809 -0.4218256055 6.4577014063
O 1.1395629019 0.0879562824 -2.0133196306
O 1.496088566 -0.18792764 6.3933139528
H 2.2742574244 -0.0256594841 3.9658973369
H -0.7590866992 -0.3207076144 4.0062035176
H -0.436780279 -0.4403663395 7.3856468228
H 1.9674481702 0.1631628058 -2.500481734
H -0.9290541341 -0.0997116552 -1.6280167709
H 3.3825531614 0.2193069438 -0.5388365994
H 3.3729947881 0.1316087467 1.9213606383
H -0.8970728473 -0.2173823657 1.8563129147

LC-BLYP Caffeic Acid (Neutral) 0.002 a.u.

C 1.26195835 0.0516168126 -0.6871136026
C 0.0554715988 -0.0748075174 -0.0085072267
C 0.0493985262 -0.1266535739 1.3542246875
C 1.2365353924 -0.0542423427 2.0702925818
C 2.4234137731 0.0717374336 1.3818882523
C 2.4389578546 0.1245669499 0.0044615806
O -1.0950568327 -0.1449002279 -0.6970284674
C 1.2722348484 -0.1073894808 3.5223071312
C 0.2479140473 -0.2365406336 4.3458675972
C 0.4771667957 -0.2714049729 5.786998219
O -0.6636329113 -0.4099610986 6.4759637145
O 1.1546988013 0.0934251684 -2.0338635617
O 1.5340542057 -0.1905645454 6.3458595932
H 2.253783775 -0.0331624798 3.978216141
H -0.7762285781 -0.3216419703 4.015438278

H -0.4257226238 -0.4252269354 7.4120168258
H 2.0082468044 0.1767350843 -2.4664118
H -0.9106926182 -0.0955578806 -1.642859174
H 3.3739886465 0.2232060372 -0.5316982671
H 3.3540636446 0.129332281 1.9289416345
H -0.9054425 -0.2248941077 1.8495898631

LC-BLYP Caffeic Acid (Neutral) 0.004 a.u.

C 1.2635662529 0.0513422317 -0.6868902082
C 0.0562262274 -0.0732051185 -0.0051026951
C 0.052639674 -0.1237646224 1.3569742155
C 1.2418068662 -0.05182485 2.0716224946
C 2.4279630486 0.0725412028 1.3811641475
C 2.4419345884 0.1238970172 0.0035275055
O -1.0940921818 -0.1425276827 -0.6896636929
C 1.2777310077 -0.1045489494 3.5211336943
C 0.2518378627 -0.2361907034 4.3457552214
C 0.4731406236 -0.2713944507 5.7838119148
O -0.6726092443 -0.4155022164 6.4695112609
O 1.1495132452 0.0913213781 -2.0286373133
O 1.5232600501 -0.1876126577 6.3583773557
H 2.2595232799 -0.0283465259 3.976411595
H -0.7705847113 -0.3240456148 4.0113029806
H -0.4312029556 -0.4309686789 7.4039938399
H 1.9967298977 0.1706968141 -2.4754836246
H -0.9158711894 -0.0961515947 -1.6375155992
H 3.375830843 0.2209154249 -0.5345193344
H 3.3599343249 0.1297058036 1.9262295912
H -0.9021665098 -0.2206642071 1.8525806506

LC-BLYP Caffeic Acid (Neutral) 0.006 a.u.

C 1.2653066355 0.0513797657 -0.686826385
C 0.0567872521 -0.0724575257 -0.0022221531
C 0.0552284003 -0.1223884367 1.3591144858
C 1.2462652114 -0.0504179489 2.0730394091
C 2.4319605639 0.0733290639 1.380612972
C 2.4448983911 0.1239229331 0.002960019
O -1.0929010385 -0.1414965074 -0.6835085897
C 1.2825790004 -0.1030099681 3.5194752641
C 0.2551381255 -0.235052053 4.3462312577
C 0.469536864 -0.2712787154 5.7807017711
O -0.6809895031 -0.4183605638 6.4642810271
O 1.1451559908 0.0900608285 -2.0234742456
O 1.5134308619 -0.1871104651 6.3703489445
H 2.2649498423 -0.0268430368 3.9737806122
H -0.7659732744 -0.3233337936 4.0084087298

H -0.4349606711 -0.4346941156 7.3969060979
H 1.9859191989 0.1673177793 -2.4841672551
H -0.9204887099 -0.0973344457 -1.6332629462
H 3.3778124309 0.2201200047 -0.536602397
H 3.3650273081 0.1303379045 1.9240637988
H -0.89957188 -0.2190187039 1.8547235826

LC-BLYP Caffeic Acid (Neutral) 0.008 a.u.

C 1.2671673808 0.0514275318 -0.6869651571
C 0.0570832551 -0.07194502 0.0000905827
C 0.0570915246 -0.1213837006 1.3606674852
C 1.2498121143 -0.0492820402 2.0745951407
C 2.4354739597 0.0740809029 1.3801704628
C 2.4479519109 0.1240561198 0.002802311
O -1.0916234963 -0.1407904504 -0.6784970245
C 1.2867076275 -0.1017325661 3.5172972311
C 0.2578825421 -0.2338033267 4.3473152199
C 0.4663400848 -0.2711334852 5.7776536166
O -0.6886569251 -0.420429356 6.4602880892
O 1.1417951767 0.088926625 -2.0183629615
O 1.5043915452 -0.1873027094 6.3819396513
H 2.2698593554 -0.026020585 3.9703150891
H -0.7621419189 -0.322133679 4.0066718152
H -0.4368479505 -0.4377993068 7.3907513133
H 1.9761007901 0.1648483042 -2.4924832085
H -0.9248395348 -0.0985504188 -1.6300869242
H 3.3800371693 0.2195994046 -0.538032098
H 3.3693804231 0.1309928565 1.9224613203
H -0.8978540342 -0.2179531008 1.8559920453

LC-BLYP Gallic Acid (Neutral) Zero field

C -0.9425689036 -1.1583751222 0.0022362189
C -1.6700658504 0.011065172 0.0004575719
C -1.0280493776 1.22925432 -0.0038924016
C 0.3447081456 1.277936365 -0.0064676475
C 1.0600977975 0.1017716766 -0.0046525344
C 0.4243008292 -1.1231587184 -0.0003002421
O -3.0187617453 0.0081369214 0.0028806848
O -1.7508270708 2.3625705989 -0.0055800614
C 2.5332931073 0.0961522815 -0.0072771279
O 3.0743094117 1.3146066717 -0.0114187473
O -1.6887776535 -2.2926327792 0.0065515926
O 3.2079987558 -0.8919911645 -0.0059090597
H 1.0173434861 -2.0274684264 0.0010141541
H 0.8425550776 2.2348811908 -0.0098678283
H -1.1357067912 -3.0775564628 0.0078040694

H -3.3417566506 -0.9007862264 0.0058742704
H -2.6905368491 2.1454385934 -0.0033111618
H 4.0340052816 1.2013801088 -0.0128477501

LC-BLYP Gallic Acid (Neutral) 0.010 a.u.

C -0.9394871461 -1.1749857647 0.0023985575
C -1.6703970723 -0.0011876263 0.0006281601
C -1.0234556773 1.2205078242 -0.0037202539
C 0.347901317 1.264763173 -0.0062928872
C 1.0702392632 0.087993318 -0.0044582733
C 0.4291545701 -1.1390554191 -0.0000917301
O -3.0005633303 0.0189813815 0.0029223391
O -1.7314684186 2.3525646966 -0.0054335896
C 2.5271330905 0.107823203 -0.0071553321
O 3.0617047141 1.3422258937 -0.0118456117
O -1.6905104131 -2.2961194732 0.0066334033
O 3.2589702375 -0.8493894341 -0.0056059683
H 1.0124784696 -2.0491037564 0.0012307941
H 0.8364018567 2.2259679821 -0.0097816953
H -1.166580052 -3.0998415959 0.0073509417
H -3.3847369687 -0.868258537 0.0055377295
H -2.6804739909 2.1629465443 -0.0035792967
H 4.0152505508 1.2053925901 -0.0134432871

LC-BLYP Gallic Acid (Neutral) 0.002 a.u.

C -0.9421149834 -1.1616184288 0.0022907958
C -1.6700527802 0.0085283438 0.0004512641
C -1.0272052488 1.2272909156 -0.0037536595
C 0.3453194413 1.2751043329 -0.0061208183
C 1.0617323131 0.0989365608 -0.0042217648
C 0.4252405124 -1.1262098666 -0.0000287231
O -3.0151316462 0.0106065928 0.0026462515
O -1.7468111462 2.3603118434 -0.0055100804
C 2.5321570274 0.0984950138 -0.0065814694
O 3.0718954963 1.3197525893 -0.0118836895
O -1.6889349602 -2.293252884 0.0064352994
O 3.2182137212 -0.8834906669 -0.006024484
H 1.0160987348 -2.0317980843 0.0013560595
H 0.841149092 2.2329552755 -0.0094221273
H -1.1413677045 -3.0818118732 0.0076044461
H -3.3506294823 -0.8941075488 0.0054481378
H -2.6884664768 2.1489050986 -0.0034951464
H 4.0304690901 1.2026277861 -0.0138962917

LC-BLYP Gallic Acid (Neutral) 0.004 a.u.

C -0.9415516187 -1.164859682 0.0023049535

C -1.6700270777 0.0061350035 0.0005337479
C -1.0261305084 1.2254390265 -0.0038135228
C 0.3461591147 1.2724037219 -0.0063899451
C 1.0635998247 0.0960397797 -0.004570402
C 0.426202873 -1.1295391667 -0.0002153812
O -3.0114972584 0.0129960796 0.0029021589
O -1.7425415072 2.3584261374 -0.0055109529
C 2.5307088339 0.1007659212 -0.0072273097
O 3.068624802 1.3255800253 -0.0116122663
O -1.6892352595 -2.2941214525 0.0065800608
O 3.228140744 -0.8750701681 -0.0057627288
H 1.0151136915 -2.0362310007 0.0011004886
H 0.8402703172 2.2309996139 -0.0098250149
H -1.147133053 -3.0862333947 0.0076191735
H -3.3590116626 -0.8875799925 0.0057148285
H -2.6860354627 2.1524504242 -0.0034314171
H 4.0259042071 1.203624124 -0.0131024709

LC-BLYP Gallic Acid (Neutral) 0.006 a.u.

C -0.9409452172 -1.1681740514 0.0023369439
C -1.6700885629 0.0036822732 0.0005676153
C -1.0252125652 1.2236772858 -0.0037793396
C 0.3468086804 1.2697619205 -0.0063553486
C 1.0656133237 0.0932801548 -0.0045320153
C 0.4271783518 -1.1327161519 -0.0001742151
O -3.0078689417 0.0151879367 0.0029107242
O -1.7386692455 2.3564125599 -0.0054818022
C 2.5294880085 0.1031029559 -0.0072036854
O 3.066091942 1.3310971905 -0.0116981949
O -1.6895785045 -2.2948234747 0.0065958507
O 3.2383248307 -0.8665426109 -0.0057003378
H 1.0141508808 -2.0405519766 0.0011428951
H 0.8390536915 2.2292088337 -0.0098080461
H -1.1532884708 -3.090688977 0.0075295345
H -3.3676252525 -0.8810447284 0.005647949
H -2.6840192865 2.1559229648 -0.0034838737
H 4.0221473373 1.204432895 -0.013220654

LC-BLYP Gallic Acid (Neutral) 0.008 a.u.

C -0.9402612899 -1.1715448198 0.002368049
C -1.6702104534 0.0012410259 0.0005988024
C -1.0243204138 1.2220282504 -0.0037483881
C 0.3473936706 1.2672136193 -0.0063227908
C 1.067819431 0.0905970251 -0.0044943858
C 0.4281638575 -1.1358863984 -0.0001329572

O -3.0042287727 0.0171936594 0.0029169007
O -1.734975692 2.3544540375 -0.0054563339
C 2.52829903 0.1054534137 -0.0071793459
O 3.0637763021 1.3366405742 -0.0117750225
O -1.6900005871 -2.2954913824 0.0066135377
O 3.2485921137 -0.8579851635 -0.0056501177
H 1.0132747307 -2.044840608 0.0011863455
H 0.8377683619 2.2275303465 -0.0097931932
H -1.1597550133 -3.0952205465 0.0074413288
H -3.3762032893 -0.8745919966 0.0055888044
H -2.6821608643 2.1594066123 -0.0035330856
H 4.0185898783 1.2050273509 -0.0133341477

LC-BLYP Caffeic Acid (Radical) Zero field

C 1.2443641112 0.0548477485 -0.7369127476
C 0.0031552184 -0.0825970688 0.0149302124
C -0.0072181474 -0.1375208031 1.3709073511
C 1.1952554248 -0.0613356538 2.0711691981
C 2.4169251585 0.0728096955 1.3616219266
C 2.459528287 0.1299183257 0.0201937993
O -1.0895265499 -0.1479513802 -0.7180607617
C 1.2597601673 -0.1129513779 3.5059280513
C 0.2370695626 -0.2359230712 4.344392676
C 0.4894086518 -0.2713544853 5.7884428672
O -0.6382780119 -0.3982871978 6.4896571279
O 1.1703020663 0.0972608277 -1.9592128338
O 1.5625596832 -0.1974980052 6.3102547104
H 2.2452883441 -0.044664455 3.9528375945
H -0.791972899 -0.3134895614 4.0273198271
H -0.4017064546 -0.4148177684 7.427127441
H -0.796834063 -0.0855279116 -1.6477454596
H 3.3842317907 0.2319300493 -0.5288839593
H 3.3319778532 0.1292764532 1.9356462755
H -0.952638193 -0.2396053602 1.8821597037

LC-BLYP Caffeic Acid (Radical) 0.010 a.u.

C 1.2463360313 0.0552603381 -0.740240442
C -0.0025553815 -0.0824760105 0.0211913871
C -0.0002435977 -0.1357815004 1.3794362274
C 1.2078949718 -0.0598117152 2.0718737135
C 2.4334625013 0.0719128726 1.3548315871
C 2.473046916 0.1277328864 0.0164250709
O -1.0951831505 -0.146734582 -0.6895703952
C 1.2755172503 -0.1083435485 3.4960964346
C 0.2499020229 -0.2339264507 4.3481588702
C 0.4752426069 -0.2678127176 5.7731629616

O -0.6716615209 -0.4083197468 6.473857355
O 1.1693666665 0.1004883213 -1.9485436263
O 1.5216090849 -0.1875495507 6.3653813241
H 2.2650858347 -0.0362550896 3.9339575984
H -0.7744769742 -0.3174586306 4.0202591117
H -0.4020112182 -0.4239461538 7.3990200943
H -0.8482208101 -0.0899616142 -1.6357926995
H 3.3916075646 0.226207964 -0.5443757706
H 3.3518654947 0.1260507643 1.9243833345
H -0.9449322928 -0.2367568362 1.8922608632

LC-BLYP Caffeic Acid (Radical) 0.002 a.u.

C 1.2440617786 0.0551285714 -0.7371939052
C 0.0023144324 -0.0825301905 0.0168365545
C -0.0044106168 -0.1372357959 1.3734607152
C 1.1993934755 -0.0610261647 2.0708250116
C 2.4208885048 0.072570078 1.360028355
C 2.4618341714 0.1295127309 0.0187650841
O -1.0913963648 -0.1477393402 -0.7104223889
C 1.2641319171 -0.1121073683 3.5049754037
C 0.2407009939 -0.2355941152 4.3441359201
C 0.4860309513 -0.2705849113 5.7852770859
O -0.6462503368 -0.4004070873 6.4844578906
O 1.1689559605 0.0978113709 -1.9568433924
O 1.5532123567 -0.1951213781 6.3221477359
H 2.2502579733 -0.0429516784 3.9504612167
H -0.7870984003 -0.3143494697 4.0239992691
H -0.4049030464 -0.4166435969 7.4199640119
H -0.8087392378 -0.0863614853 -1.643713642
H 3.3849356332 0.2307884932 -0.5331984439
H 3.3371147738 0.1285484346 1.9323134513
H -0.9493829196 -0.2391880971 1.8854970668

LC-BLYP Caffeic Acid (Radical) 0.004 a.u.

C 1.2440664889 0.0553845772 -0.7375891249
C 0.0013408583 -0.0824885519 0.0184254408
C -0.0022473935 -0.1369456492 1.3755811874
C 1.2028080169 -0.0607182322 2.0706932473
C 2.4245268982 0.0723823041 1.3586464667
C 2.4642702179 0.1291396103 0.017699811
O -1.0929285554 -0.1475550427 -0.7037129838
C 1.2678846407 -0.1112763894 3.5035438191
C 0.2438006845 -0.2352493692 4.3442973606
C 0.4829561813 -0.2698863166 5.7821667888
O -0.6535165955 -0.4023250582 6.4801704895
O 1.1681907727 0.0983959024 -1.9545696043

O 1.5444696484 -0.1931130904 6.3334933754
H 2.2547176585 -0.0413574061 3.9474362641
H -0.7829211851 -0.3151194346 4.0215582708
H -0.4066302504 -0.4183310892 7.413528559
H -0.8198708607 -0.0872554886 -1.6404258571
H 3.3859424482 0.22971708 -0.5368909052
H 3.3417129539 0.1278931181 1.9295530713
H -0.946920628 -0.2387724738 1.8881673234

LC-BLYP Caffeic Acid (Radical) 0.006 a.u.

C 1.2444003068 0.0556530664 -0.7381935303
C 0.0001948266 -0.0824813364 0.0196687728
C -0.0007495078 -0.1366791497 1.3772823622
C 1.2054632548 -0.0604304822 2.0707826301
C 2.4278640486 0.0722517982 1.3573959424
C 2.4669037762 0.1288235221 0.016968638
O -1.0941096336 -0.1474053742 -0.6979425824
C 1.2710418291 -0.1104797519 3.5016237219
C 0.2463995262 -0.2349019424 4.3449660055
C 0.4801490947 -0.2692597388 5.7791323761
O -0.6601896588 -0.4040041105 6.4768807043
O 1.1680353756 0.0990245992 -1.9524382074
O 1.5363033315 -0.1914916549 6.3444391367
H 2.2587080217 -0.0399113528 3.9437042064
H -0.7794112924 -0.3158060709 4.0200740033
H -0.4068794251 -0.4198400736 7.4078534123
H -0.8302997125 -0.0881921597 -1.6379392819
H 3.3873189565 0.2287472732 -0.5399960157
H 3.3457753321 0.1273091456 1.9273228104
H -0.9452664501 -0.2384072067 1.8901878953

LC-BLYP Caffeic Acid (Radical) 0.008 a.u.

C 1.245254285 0.0547283389 -0.7390523774
C -0.0010786521 -0.0824098746 0.0205842772
C -0.0001547098 -0.1360913197 1.3785106313
C 1.2070973766 -0.0602245232 2.0711889374
C 2.4307795585 0.0719733412 1.3561903464
C 2.469804436 0.1282025534 0.016597279
O -1.0948751813 -0.1469554048 -0.6933324072
C 1.2735118372 -0.1095197136 3.499137276
C 0.248374535 -0.2344168289 4.3462622369
C 0.4776357582 -0.2684706642 5.7761309549
O -0.6660944075 -0.4061768507 6.4747863893
O 1.1684345381 0.1005055125 -1.9503696699
O 1.5287558671 -0.1894162614 6.354960759
H 2.262081039 -0.0382279944 3.9392164111

H -0.77666215 -0.3165610322 4.0197227175
H -0.4051507899 -0.421917314 7.4030228717
H -0.8395796038 -0.089639512 -1.6364938339
H 3.3891659815 0.2277137502 -0.5424169971
H 3.3490727264 0.1267068393 1.9256780524
H -0.9447204444 -0.2372840417 1.8914491453

LC-BLYP Gallic Acid (Radical) Zero field

C -0.935420728 -1.2079259816 0.0031815602
C -1.7279982316 0.0009288345 0.0015559347
C -1.0058907439 1.2590604727 -0.0033875545
C 0.35602737 1.3091050018 -0.0063882655
C 1.0542388876 0.1137152289 -0.0046080576
C 0.4184493634 -1.1301175347 0.0001144897
O -2.9522651021 0.0276801007 0.0040550371
O -1.7656828123 2.3348801648 -0.0047147385
C 2.5310193695 0.0972226265 -0.0076817137
O 3.0775112761 1.3103694229 -0.0121815562
O -1.6305481775 -2.3410085303 0.007741139
O 3.1894031945 -0.9004940515 -0.0063750481
H 1.0348466846 -2.0189756722 0.001238617
H 0.8711870871 2.2564243794 -0.0100496579
H -1.0478367048 -3.1066833091 0.0086349554
H -2.6897596155 2.020082578 -0.0019094648
H 4.0378108826 1.1988592691 -0.0139306763

LC-BLYP Gallic Acid (Radical) 0.010 a.u.

C -0.9313042359 -1.2225942532 0.0032506285
C -1.7287188595 -0.005680612 0.0017427196
C -1.0046971955 1.2578340038 -0.0033646504
C 0.3587790794 1.2992993515 -0.0063530692
C 1.0614230281 0.1025582618 -0.0044846183
C 0.4243557129 -1.1462055773 0.0002418842
O -2.9416760509 0.0140494038 0.0043525821
O -1.7459098951 2.336027335 -0.0047692244
C 2.5220730591 0.1090654191 -0.0074794187
O 3.0669327835 1.3362622397 -0.0125364288
O -1.6408510575 -2.3358333155 0.007672809
O 3.2351665716 -0.8605878117 -0.0058928891
H 1.0325390323 -2.0399096794 0.001363048
H 0.8676427842 2.2494907964 -0.0101226199
H -1.0957995234 -3.1280303489 0.0081403904
H -2.6850687472 2.0616276326 -0.0021301477
H 4.020205514 1.1957501544 -0.0143359955

LC-BLYP Gallic Acid (Radical) 0.002 a.u.

C -0.9348108878 -1.2106379909 0.0031927976
C -1.7279917933 -0.0003130091 0.0015889409
C -1.0056421297 1.2585928263 -0.003380614
C 0.3566739528 1.3068823322 -0.0063798694
C 1.0553150509 0.111284706 -0.0045833957
C 0.4195932903 -1.1332450642 0.0001369622
O -2.950053967 0.025213048 0.0041067543
O -1.7614432243 2.3351206667 -0.0047210078
C 2.5292007066 0.0994781294 -0.0076365777
O 3.0749813013 1.3153901927 -0.0122626561
O -1.6325135106 -2.3400080875 0.007724082
O 3.198472987 -0.8925997392 -0.0062608593
H 1.0341185368 -2.0231819007 0.0012630011
H 0.870565849 2.2547428253 -0.0100599477
H -1.0566816276 -3.1106831704 0.0085367915
H -2.6886250335 2.028436186 -0.0019500832
H 4.0339324988 1.1986510494 -0.0140193188

LC-BLYP Gallic Acid (Radical) 0.004 a.u.

C -0.9341059016 -1.2134499986 0.0032051761
C -1.7280649568 -0.0015955336 0.0016232351
C -1.0054126339 1.2582275296 -0.0033742251
C 0.3572661527 1.3047833342 -0.0063700735
C 1.056560469 0.108953628 -0.0045562476
C 0.4207570342 -1.1364066689 0.0001623291
O -2.9479034527 0.0226075822 0.0041600234
O -1.757351117 2.3353558809 -0.0047295023
C 2.5274168565 0.1017897585 -0.007589785
O 3.0726791983 1.3204671438 -0.012341848
O -1.6345250317 -2.3389917138 0.0077076093
O 3.2075819842 -0.8846546669 -0.0061551701
H 1.033521589 -2.0273702443 0.0012896064
H 0.8698853746 2.2532066616 -0.0100694653
H -1.0658840135 -3.1148182095 0.0084368829
H -2.6875935205 2.0367814905 -0.0019936365
H 4.0302639692 1.1982370263 -0.0141099089

LC-BLYP Gallic Acid (Radical) 0.006 a.u.

C -0.9332938976 -1.2163709167 0.0032190675
C -1.7282115463 -0.0029180901 0.0016600906
C -1.0051876926 1.2579713237 -0.0033692628
C 0.3578095814 1.3028154028 -0.006361601
C 1.0579850721 0.1067226335 -0.0045299695
C 0.4219393337 -1.1396120954 0.0001887558
O -2.9457988806 0.019868866 0.004217472
O -1.753398607 2.3355879027 -0.0047405418

C 2.5256432692 0.1041592446 -0.0075473445
O 3.0705833288 1.3256243737 -0.0124143355
O -1.6365835935 -2.337959053 0.0076937476
O 3.2167300145 -0.8766618364 -0.0060596433
H 1.0330566186 -2.0315482477 0.0013159007
H 0.8691590121 2.2518185704 -0.0100820194
H -1.0754566884 -3.1190876099 0.0083373822
H -2.6866558682 2.0451044352 -0.0020387533
H 4.0267725438 1.1976080967 -0.0141939454

LC-BLYP Gallic Acid (Radical) 0.008 a.u.

C -0.9323643057 -1.2194124812 0.0032342572
C -1.7284283558 -0.0042795806 0.001700186
C -1.0049529435 1.2578348048 -0.0033660936
C 0.3583113776 1.3009854918 -0.0063564996
C 1.0596007534 0.1045909672 -0.0045067382
C 0.4231388127 -1.14287345 0.0002149835
O -2.9437271567 0.0170119334 0.0042819126
O -1.7495837634 2.335814247 -0.004753575
C 2.5238652544 0.1065840531 -0.007511813
O 3.0686715914 1.3308816037 -0.0124798234
O -1.6386913603 -2.3369081592 0.0076824156
O 3.2259205781 -0.8686355154 -0.005970347
H 1.0327269939 -2.0357245609 0.0013400996
H 0.8684052418 2.2505798149 -0.0101005916
H -1.0854162077 -3.1234895866 0.008238193
H -2.6858112828 2.0533889089 -0.0020835779
H 4.0234267724 1.1967745089 -0.0142679882

LC- ω PBE Caffeic Acid (Neutral) -0.010 a.u.

C 1.2527800412 0.0753268722 -0.7041299718
C 0.0499574767 -0.1594411882 -0.0550732428
C 0.0256478387 -0.2729991509 1.316585678
C 1.1952387431 -0.1517978591 2.0602129153
C 2.390065523 0.0712633398 1.389370738
C 2.4198446009 0.1878950691 0.0138413589
O -1.0982688441 -0.2803075211 -0.779238743
C 1.2319520405 -0.2468816991 3.5234243703
C 0.2160931846 -0.1697344776 4.3659748136
C 0.5052609596 -0.2691148114 5.824857428
O -0.6016537806 -0.148239204 6.5533811714
O 1.2022738513 0.1776601476 -2.0836677519
O 1.6015953271 -0.4338063765 6.2762567499
H 2.2142805714 -0.3694594099 3.9714585009
H -0.8147631768 -0.0207921488 4.0698321367
H -0.3641268572 -0.2110767823 7.4904310007

H 2.0678373995 0.4512926134 -2.3872203895
H -0.8726714472 -0.1377330896 -1.7015530031
H 3.3597969405 0.3662191169 -0.5002371028
H 3.3067768339 0.1607189946 1.9584270914
H -0.9228062262 -0.4653204353 1.8016502518

LC- ω PBE Caffeic Acid (Neutral) -0.002 a.u.

C 1.2602141095 0.0531697697 -0.7044794457
C 0.0477098417 -0.0797071392 -0.0308669501
C 0.0358163943 -0.1354796822 1.3410322549
C 1.222271943 -0.0609131207 2.0666062637
C 2.4181607414 0.0708585312 1.3799199815
C 2.4392968441 0.1280103111 -0.0021045151
O -1.1111036205 -0.1531375628 -0.7259158597
C 1.2588742988 -0.115733913 3.5285764986
C 0.2336778033 -0.2366996998 4.3595886533
C 0.4865297297 -0.2719996425 5.8130111198
O -0.6514978049 -0.3949762646 6.5134268132
O 1.1751098539 0.1003902532 -2.0668503076
O 1.5634801575 -0.2023967685 6.3398790412
H 2.2433865142 -0.0488621328 3.9830519859
H -0.7968315985 -0.3122236667 4.0394166977
H -0.4070610018 -0.4101293556 7.4475891082
H 2.0490295466 0.1955698371 -2.4481440471
H -0.907757571 -0.0953999602 -1.6644408462
H 3.3797064344 0.2316115338 -0.5328199014
H 3.347317648 0.1301404786 1.932864097
H -0.9212192637 -0.2384198061 1.8352433579

LC- ω PBE Caffeic Acid (Neutral) -0.004 a.u.

C 1.2575742802 0.0651173604 -0.7042530077
C 0.0484617451 -0.1037696089 -0.0362004976
C 0.0347289503 -0.1799271937 1.3354498325
C 1.2172302259 -0.0894607383 2.0647063081
C 2.4118301566 0.0735262107 1.3815661182
C 2.4338426232 0.1526786558 0.0011430039
O -1.1081307307 -0.1944347044 -0.7375153502
C 1.2547042732 -0.1576194578 3.5273462242
C 0.2278442158 -0.2119303671 4.3615382135
C 0.4910420769 -0.2719247498 5.8159899777
O -0.6448011052 -0.3145156183 6.52403523
O 1.179774109 0.1303192403 -2.0708220672
O 1.5782655603 -0.2816887927 6.3233168253
H 2.2424629074 -0.1558081496 3.9796243485

H -0.8078626139 -0.2100330028 4.048469265
H -0.4008882562 -0.3497226406 7.4584688806
H 2.0561931743 0.259546758 -2.4350933382
H -0.8994693148 -0.1158219658 -1.6727883657
H 3.3734538661 0.2825428178 -0.5257971679
H 3.3382391414 0.1424481562 1.9378589732
H -0.919384285 -0.3158502094 1.827540594

LC- ω PBE Caffeic Acid (Neutral) -0.006 a.u.

C 1.255003229 0.0732229377 -0.7038532975
C 0.0489248617 -0.1239938571 -0.0417083723
C 0.0328592565 -0.2160641951 1.3298148385
C 1.2112700253 -0.1127280127 2.0630924535
C 2.4050655864 0.0755481622 1.3837427992
C 2.4283757938 0.1715532338 0.0050369946
O -1.1051650436 -0.2284035218 -0.7498113655
C 1.2489458968 -0.1927134947 3.5261152586
C 0.2239257478 -0.1928402175 4.3628685306
C 0.4953220253 -0.2720537375 5.818769703
O -0.6334135766 -0.2481698864 6.5335727232
O 1.1851473922 0.1528920526 -2.0746132503
O 1.5874040083 -0.3471474423 6.3073786555
H 2.2362209065 -0.2438872836 3.9766411281
H -0.8117952166 -0.1282597385 4.055604339
H -0.3920120799 -0.2979768644 7.4687482001
H 2.0626688013 0.317205474 -2.4209137485
H -0.8911189237 -0.1303623799 -1.6815165803
H 3.3674083362 0.3224675505 -0.517984984
H 3.3285490719 0.1527033812 1.9436914026
H -0.9184750988 -0.3773201607 1.8199085717

LC- ω PBE Caffeic Acid (Neutral) -0.008 a.u.

C 1.2532712216 0.0766189662 -0.7038379101
C 0.0491410748 -0.1407408183 -0.0478881388
C 0.0295059911 -0.2441021101 1.3236878435
C 1.2037271319 -0.1313713411 2.0616879954
C 2.3976993239 0.0753845047 1.3863196574
C 2.4236186631 0.1828748807 0.0091992077
O -1.1022595947 -0.2546286573 -0.7635151221
C 1.2411856416 -0.220029382 3.5248912053
C 0.220070293 -0.1801577757 4.3643872762
C 0.5001236726 -0.2715902414 5.8217620412
O -0.6187209204 -0.1976175625 6.5433783478
O 1.1925564444 0.1674573258 -2.0789389124

O 1.5950522655 -0.3942001219 6.2917596218
H 2.226461461 -0.3093528528 3.9740318701
H -0.8138117443 -0.0706329532 4.0627278542
H -0.3794593629 -0.2556675468 7.4794340412
H 2.0685761771 0.3731925573 -2.4057573385
H -0.8824419251 -0.1370107856 -1.6911353904
H 3.3628585524 0.3488023583 -0.5095990373
H 3.3180269482 0.1589490909 1.9504471146
H -0.9200703148 -0.4225055353 1.8115417734

LC- ω PBE Gallic Acid (Neutral) -0.010 a.u.

C -0.950400203 -1.1491175793 0.002047241
C -1.6841228628 0.021837541 0.0001703878
C -1.0422505152 1.2456436229 -0.0041210646
C 0.3383770911 1.2996961687 -0.0065435976
C 1.0578711866 0.1195787755 -0.0046546662
C 0.4211935341 -1.1101376338 -0.0003895757
O -3.0571103238 -0.0069967723 0.002633445
O -1.781217204 2.3879388836 -0.0058573443
C 2.55390762 0.0832154222 -0.0069865558
O 3.1077479781 1.2922099685 -0.0109864417
O -1.6916973912 -2.3038491118 0.0064349132
O 3.1725302085 -0.9411172692 -0.0066171054
H 1.0269330842 -2.0094378792 0.0009787365
H 0.8429938186 2.2558427476 -0.0097736182
H -1.0973595605 -3.0575207142 0.0083081855
H -3.3082792073 -0.9357363236 0.0062845356
H -2.7077495952 2.134873903 -0.0029508705
H 4.0701933419 1.1843012505 -0.0126826046

LC- ω PBE Gallic Acid (Neutral) -0.002 a.u.

C -0.9493963934 -1.1619329919 0.0022320975
C -1.6830235824 0.0119856533 0.0004153947
C -1.0375957049 1.2368454127 -0.0039027294
C 0.3422926598 1.286862518 -0.0064015648
C 1.0624135021 0.1062473303 -0.0045532203
C 0.4243807345 -1.1238901591 -0.0002492927
O -3.0415329592 0.0053362563 0.0027888778
O -1.7610153555 2.3792566572 -0.0056420124
C 2.5469002552 0.0924009324 -0.0070623748
O 3.0916930377 1.315047391 -0.0114552451
O -1.6921932364 -2.3070945892 0.0065317328
O 3.2120477114 -0.9073438212 -0.0061290767
H 1.0203002528 -2.0286816808 0.0010912899

H 0.8403246132 2.2457224662 -0.009738745
H -1.116259149 -3.0738169552 0.007884447
H -3.3416412461 -0.9091415816 0.0058513151
H -2.6955749257 2.1501359384 -0.0033046473
H 4.0494407858 1.193286223 -0.0130622462

LC- ω PBE Gallic Acid (Neutral) -0.004 a.u.

C -0.9497061354 -1.158701464 0.0021897387
C -1.6831778779 0.014453523 0.0003630507
C -1.0386720401 1.2389397945 -0.0039550529
C 0.3413868292 1.2899332589 -0.0064451005
C 1.0610701144 0.1094427191 -0.0045922025
C 0.4235400891 -1.120516247 -0.0002917605
O -3.0453323446 0.0024344415 0.0027634378
O -1.7657390894 2.3814272862 -0.0056920604
C 2.5485088607 0.0900843075 -0.0070717356
O 3.0952817016 1.3093758452 -0.0113293028
O -1.6919987499 -2.3063132042 0.0065141237
O 3.2020856654 -0.9158576455 -0.0062427121
H 1.0217671521 -2.0239924227 0.0010515916
H 0.8411230112 2.2480596444 -0.0097608474
H -1.1112405839 -3.0696447249 0.00799023
H -3.3331879775 -0.9158085795 0.0059623051
H -2.6983437857 2.1464514465 -0.0032271651
H 4.0541961607 1.1914570208 -0.0129325377

LC- ω PBE Gallic Acid (Neutral) -0.006 a.u.

C -0.9499720934 -1.1554923774 0.0021457362
C -1.6834114052 0.0169167007 0.000307478
C -1.0398024143 1.2411053366 -0.0040104213
C 0.3404324529 1.2930934726 -0.006490722
C 1.0598729883 0.1127263317 -0.0046316773
C 0.4227287847 -1.117103107 -0.0003344312
O -3.0491851198 -0.0005934806 0.0027371382
O -1.7706735014 2.3836005606 -0.005744889
C 2.5501999922 0.0877853951 -0.0070805232
O 3.0991470803 1.3036942605 -0.0112012185
O -1.6918554876 -2.3055096202 0.00649638
O 3.1921868576 -0.9243161957 -0.006356729
H 1.0233555141 -2.0192294466 0.0010128464
H 0.8418357986 2.2505219121 -0.0097852886
H -1.1064319945 -3.0655411832 0.0080960472
H -3.3248037368 -0.9224679326 0.0060774789
H -2.7012915281 2.1426883291 -0.0031408338

H 4.0592288125 1.1893460444 -0.0128023708

LC- ω PBE Gallic Acid (Neutral) -0.008 a.u.

C -0.9502030215 -1.152300047 0.0020976816
C -1.6837257896 0.0193784443 0.0002429891
C -1.040993796 1.2433416396 -0.0040652837
C 0.339429938 1.296346433 -0.006523065
C 1.0588095279 0.1161029341 -0.0046521743
C 0.4219461796 -1.1136458813 -0.0003670728
O -3.0531086713 -0.0037403781 0.0026930844
O -1.7758324792 2.3857725505 -0.0057985766
C 2.5520004594 0.0854943245 -0.0070508975
O 3.1033031657 1.2979725731 -0.0110910879
O -1.691756642 -2.3046885616 0.0064689499
O 3.1823368808 -0.9327408998 -0.0064769143
H 1.025075491 -2.014381337 0.0009886925
H 0.8424620623 2.2531139925 -0.0097883798
H -1.101813846 -3.0615048454 0.0082006464
H -3.3165022021 -0.9291129958 0.0061858129
H -2.7044294089 2.1388383024 -0.0030492646
H 4.064563152 1.1869787522 -0.0127211402

LC- ω PBE Caffeic Acid (Radical) -0.010 a.u.

C 1.2530318106 0.0554648224 -0.7534545743
C 0.0023454077 -0.0834722958 -0.0139358231
C -0.0380778644 -0.1397343416 1.3442545929
C 1.1611858016 -0.0624998968 2.0753650364
C 2.3947189779 0.0764228496 1.3712398978
C 2.4551912306 0.1346867724 0.0228482905
O -1.0837902818 -0.1508935373 -0.7892411824
C 1.2264856221 -0.1177412686 3.508352305
C 0.2043037318 -0.2378977244 4.3661798966
C 0.5119938108 -0.278233168 5.8257408645
O -0.5931375078 -0.3820940317 6.5532948663
O 1.192411203 0.094858341 -1.9961464566
O 1.6251813464 -0.2231403904 6.2605472855
H 2.212755338 -0.056350232 3.959499793
H -0.8351655675 -0.3068926048 4.0720942256
H -0.3550944656 -0.4013273573 7.4927221191
H -0.7195320468 -0.081903097 -1.6911030766
H 3.3949150505 0.2411642253 -0.5033656036
H 3.3021651048 0.1359510285 1.9603257388
H -0.990234702 -0.2438490936 1.8465548048

LC- ω PBE Caffeic Acid (Radical) -0.002 a.u.

C 1.2470898047 0.0554469826 -0.7535321675
C -0.0001291173 -0.0826653952 -0.0000726881
C -0.0170832078 -0.1384164227 1.3630044375
C 1.1891050184 -0.0618181541 2.070782559
C 2.417274664 0.0737563438 1.3600642034
C 2.4640028327 0.1315726236 0.0115829957
O -1.0967809689 -0.1486153857 -0.7423599371
C 1.2551381523 -0.1141003076 3.5114773511
C 0.2284320458 -0.2368124757 4.3575696084
C 0.4928635518 -0.2725627943 5.8110997309
O -0.6382103702 -0.3968630128 6.516969995
O 1.1760075751 0.0980337435 -1.9841877124
O 1.5776626648 -0.2019854758 6.3190663439
H 2.2428060156 -0.0467311281 3.9578590494
H -0.8038876517 -0.3128384839 4.0439934424
H -0.3939532606 -0.4132852295 7.4514797016
H -0.7805028476 -0.0842266026 -1.6628942069
H 3.3940903414 0.234766289 -0.5314769928
H 3.3323521878 0.1308840529 1.9375590504
H -0.9646254303 -0.2410201672 1.8737882363

LC- ω PBE Caffeic Acid (Radical) -0.004 a.u.

C 1.2480940768 0.0551306504 -0.753461931
C 0.0005275262 -0.0827555621 -0.0028463067
C -0.0213508527 -0.1386244059 1.3593105554
C 1.1832593814 -0.0620648823 2.0716347734
C 2.4123739027 0.0741666672 1.362230563
C 2.461874586 0.132084057 0.0137671073
O -1.0941625012 -0.1488970636 -0.7522618847
C 1.2491677319 -0.1149778869 3.5114933852
C 0.2234226831 -0.237207417 4.3589287183
C 0.4970469979 -0.2737084233 5.814576284
O -0.6284439973 -0.3940799801 6.5243726202
O 1.1789548834 0.0975152852 -1.9869039902
O 1.5885214013 -0.205529932 6.3056789855
H 2.2363943754 -0.0487300446 3.9590943711
H -0.8104147058 -0.3118465542 4.0493135307
H -0.3870156574 -0.4108912818 7.460339719
H -0.7667017747 -0.0836488022 -1.6686168803
H 3.394047587 0.2360970591 -0.5256364868
H 3.3258092293 0.1318536452 1.9422111583
H -0.9697528731 -0.2413661282 1.8685487082

LC- ω PBE Caffeic Acid (Radical) -0.006 a.u.

C 1.2493545551 0.0556075778 -0.7533025517

C 0.00118957 -0.082858302 -0.0060163404
C -0.0262728112 -0.1389218631 1.3550134642
C 1.1766432297 -0.0621263939 2.0726860571
C 2.40697521 0.0747865872 1.36480752
C 2.4596784004 0.1327591023 0.0164204805
O -1.0910900073 -0.1492747976 -0.7632933908
C 1.2424811642 -0.1157430322 3.5109549121
C 0.2178412818 -0.2376269566 4.3607613138
C 0.5015784791 -0.2751110912 5.8179997773
O -0.6177862065 -0.3911354945 6.5327987289
O 1.1826807357 0.0958526268 -1.9897215569
O 1.5998532507 -0.2095027146 6.2916845926
H 2.2293328303 -0.0506626261 3.9596773945
H -0.8176568221 -0.3108873766 4.0556928625
H -0.3781510958 -0.4082722162 7.4700393104
H -0.7520648427 -0.082391083 -1.6751805277
H 3.3941703381 0.2371832237 -0.5190082863
H 3.3186269014 0.1328704911 1.9474862966
H -0.9757321612 -0.2420266614 1.8622729432

LC- ω PBE Caffeic Acid (Radical) -0.008 a.u.

C 1.251023588 0.0556959434 -0.7533300931
C 0.0017522482 -0.0833507147 -0.009717998
C -0.0318614136 -0.139780113 1.3499700809
C 1.1692987181 -0.062612972 2.0738967593
C 2.4010731072 0.0756713675 1.3678092523
C 2.4574382141 0.1340943741 0.0194511791
O -1.0876098776 -0.1504174299 -0.7756587042
C 1.2348925681 -0.1172105207 3.509885354
C 0.2113842523 -0.2376693993 4.3631492804
C 0.5065464339 -0.2767051749 5.8217054947
O -0.6060594229 -0.3856704684 6.5425299199
O 1.1871456832 0.0959613603 -1.9927822824
O 1.612282562 -0.2172420222 6.2764279224
H 2.2214565208 -0.0544795937 3.9598277727
H -0.8260928966 -0.3081554312 4.0633572809
H -0.3674851677 -0.4040239526 7.4808915098
H -0.7361693694 -0.0823145632 -1.6826740848
H 3.3944151739 0.2399117037 -0.51153182
H 3.3106989012 0.134579715 1.9535545991
H -0.9824778234 -0.2437631084 1.855011577

LC- ω PBE Gallic Acid (Radical) -0.010 a.u.

C -0.9442338613 -1.2001955201 0.0031671653
C -1.7421542227 0.0063772198 0.0014022672
C -1.0153562316 1.2682212234 -0.00342285

C 0.3513104043 1.3297387002 -0.0064157584
C 1.0553115233 0.1296659139 -0.0047154299
C 0.4144112029 -1.1172830438 0.000039584
O -2.9835080608 0.0383313231 0.0038610098
O -1.7999938751 2.3447653899 -0.0047116999
C 2.554194325 0.0848104549 -0.0079257902
O 3.1089098657 1.2906009577 -0.0117573678
O -1.6274431461 -2.3581501273 0.0079080533
O 3.1586743845 -0.9470430182 -0.0071551699
H 1.0426301659 -2.0015504903 0.0011531326
H 0.871316985 2.2770998317 -0.0099784539
H -0.999381397 -3.0866003818 0.0091176708
H -2.7020386813 1.9761195738 -0.0017752158
H 4.0724426194 1.1882149931 -0.0134961471

LC- ω PBE Gallic Acid (Radical) -0.002 a.u.

C -0.9429335763 -1.2102013215 0.0031999927
C -1.7411557814 0.0019873098 0.0015436934
C -1.0137046431 1.2652102926 -0.0033919454
C 0.3549400911 1.3189008887 -0.0064102626
C 1.0573005399 0.1180507284 -0.0046471251
C 0.4186135307 -1.1300931771 0.0000957827
O -2.973443049 0.0301701276 0.0040404226
O -1.780148853 2.3460989194 -0.0047153112
C 2.5452883672 0.0933608755 -0.0077572254
O 3.0948817448 1.3110569753 -0.0121322885
O -1.6352125518 -2.3542682336 0.0078186101
O 3.1947156345 -0.9154726621 -0.0065380416
H 1.0378108749 -2.019453113 0.0012202006
H 0.8705886021 2.2678970587 -0.0100516567
H -1.0301757925 -3.1010129719 0.008722124
H -2.6954385522 2.0101024083 -0.0018701692
H 4.0531654143 1.1907888946 -0.0138318002

LC- ω PBE Gallic Acid (Radical) -0.004 a.u.

C -0.9433230983 -1.2076272613 0.0031918008
C -1.7412717125 0.0031527553 0.0015132992
C -1.0140144351 1.265852758 -0.0034020497
C 0.3541510965 1.321420768 -0.0064269217
C 1.0565959756 0.1207795675 -0.0046823578
C 0.4175392035 -1.126908195 0.0000705788
O -2.9757681331 0.0323589321 0.0040041962
O -1.7847804626 2.345797538 -0.0047107391
C 2.5473044015 0.0911992062 -0.0078269628
O 3.0979155913 1.3060325599 -0.0120339081
O -1.6332122881 -2.3552307606 0.007846485

O 3.1856775194 -0.9233471401 -0.0066625474
H 1.038797557 -2.0150854172 0.0011908327
H 0.8709260685 2.2699566663 -0.0100550066
H -1.0221353659 -3.0972550791 0.0088235547
H -2.6967994087 2.001596416 -0.001831989
H 4.0574894911 1.1904296861 -0.0137132651

LC- ω PBE Gallic Acid (Radical) -0.006 a.u.

C -0.9436681994 -1.2051216959 0.0031832914
C -1.7414960616 0.0042693498 0.0014767416
C -1.0143969992 1.2665925665 -0.0034092166
C 0.3532850795 1.3240750586 -0.0064258231
C 1.0560354516 0.1236290585 -0.0046959801
C 0.4164817984 -1.12371537 0.0000579196
O -2.9782220449 0.0344608991 0.003955158
O -1.7896703063 2.3454693523 -0.0047098413
C 2.5494971442 0.0890444592 -0.0078610825
O 3.1013030861 1.3009237556 -0.0119419688
O -1.6312610335 -2.3562051865 0.0078669272
O 3.1766811696 -0.9312563218 -0.006819241
H 1.0399416258 -2.0106441813 0.0011766588
H 0.8711695517 2.2721822483 -0.0100326263
H -1.0143665652 -3.0936334254 0.0089214745
H -2.6984118552 1.993116845 -0.001809407
H 4.0621901583 1.189935588 -0.0136379843

LC- ω PBE Gallic Acid (Radical) -0.008 a.u.

C -0.943970027 -1.2026469543 0.0031756701
C -1.7417892923 0.0053447866 0.0014399804
C -1.0148415156 1.2673840026 -0.0034165591
C 0.3523401224 1.3268470366 -0.0064224649
C 1.0556081119 0.1265892584 -0.0047072548
C 0.4154384337 -1.1205095502 0.0000476993
O -2.9807977245 0.0364522626 0.0039066627
O -1.7947390756 2.345125744 -0.0047109953
C 2.5517899832 0.0869149457 -0.0078956569
O 3.1049621083 1.2957831929 -0.0118450852
O -1.629338838 -2.3571777169 0.0078887027
O 3.1676826717 -0.9391539181 -0.0069907113
H 1.0412175924 -2.0061355126 0.0011634659
H 0.8713047157 2.2745608983 -0.0100076648
H -1.0067861877 -3.0900824991 0.0090223873
H -2.7001562043 1.9846244581 -0.0017910669
H 4.0671671257 1.1892025653 -0.0135621091

LC- ω PBE Caffeic Acid (Neutral) Zero field

C 1.2615133847 0.0530635245 -0.7038618643
C 0.0487920606 -0.0775964654 -0.0263303251
C 0.0404791954 -0.1319474343 1.3449300148
C 1.2294021342 -0.0581224799 2.0677249324
C 2.423895667 0.07163482 1.3787618452
C 2.4422621074 0.1272152648 -0.0037461236
O -1.1104030347 -0.1501117773 -0.7162307532
C 1.2660510317 -0.1124640959 3.5280809119
C 0.2388689043 -0.2369284661 4.3583540053
C 0.4816064005 -0.2726611486 5.8094698123
O -0.6624053715 -0.4017741385 6.5047154888
O 1.1678758741 0.0981580081 -2.0612356625
O 1.551012029 -0.1975159883 6.3536127965
H 2.2504627418 -0.0428441391 3.9824662867
H -0.7895619848 -0.3160829378 4.0331044466
H -0.4164732394 -0.416248311 7.4378436059
H 2.0358736658 0.1882691633 -2.4579681871
H -0.9139567079 -0.096168432 -1.6570358634
H 3.3811210294 0.2288584247 -0.5370274078
H 3.3548743417 0.1302277816 1.9288801903
H -0.9161792293 -0.2332891727 1.8400758503

LC- ω PBE Caffeic Acid (Neutral) 0.010 a.u.

C 1.2702322774 0.0519080635 -0.703760552
C 0.0508533826 -0.0711035003 -0.0123838032
C 0.052218193 -0.1199845675 1.3553678032
C 1.2506669063 -0.0477965905 2.0748555478
C 2.4438556902 0.075408366 1.3756207747
C 2.4577449746 0.1246756979 -0.0064818006
O -1.104903295 -0.140248808 -0.6860394186
C 1.2898756685 -0.1000309307 3.5190586476
C 0.2560477059 -0.2338958955 4.3612253388
C 0.4637757078 -0.2717013336 5.7935960945
O -0.7041337094 -0.4253208282 6.4792249233
O 1.1461522583 0.0887244266 -2.0352514523
O 1.5012302083 -0.1867119614 6.4144369987
H 2.2766476388 -0.0233848546 3.9687833108
H -0.7653177315 -0.3239104797 4.0194016015
H -0.4336796594 -0.4418963607 7.4027884612
H 1.9839860021 0.1632874908 -2.5015279367
H -0.9373450237 -0.099774082 -1.6363180441
H 3.3918905018 0.2193553643 -0.5472206669
H 3.3800984681 0.1321604662 1.9183652068
H -0.9047851648 -0.2160876826 1.8508429654

LC- ω PBE Caffeic Acid (Neutral) 0.002 a.u.

C 1.26306797 0.0512727915 -0.7034986614
C 0.0494350607 -0.0729569847 -0.022284382
C 0.0438018782 -0.1234212727 1.3484449487
C 1.235140176 -0.0520169233 2.0691206754
C 2.4289772066 0.0722550942 1.3778061144
C 2.4455671071 0.1235546024 -0.0051467347
O -1.1100773393 -0.142646977 -0.7075448693
C 1.2719151158 -0.1044385656 3.5274061388
C 0.2437051505 -0.2394606704 4.3576861032
C 0.4770656094 -0.2723424672 5.8059381002
O -0.6716450836 -0.4175008379 6.4967320957
O 1.1619956463 0.0924039042 -2.056019002
O 1.5385977415 -0.1853336221 6.3668392552
H 2.2556246106 -0.0249207673 3.9819086835
H -0.7819476345 -0.3307069895 4.0274618405
H -0.4226731425 -0.4298359425 7.4284357242
H 2.0244174783 0.1735391016 -2.4676208644
H -0.9197977972 -0.0942682939 -1.6504883825
H 3.3833995205 0.2203931535 -0.5405969098
H 3.3615491683 0.1292887764 1.9256497163
H -0.9130074425 -0.2191851097 1.8443544099

LC- ω PBE Caffeic Acid (Neutral) 0.004 a.u.

C 1.2646417126 0.0513267487 -0.7032620225
C 0.0501754449 -0.0718935934 -0.0189168314
C 0.0470483289 -0.1215642292 1.3511324777
C 1.2404484602 -0.0502503812 2.0703725685
C 2.4335300097 0.0731250987 1.3770384475
C 2.4485249736 0.1234920165 -0.0060924625
O -1.1089855613 -0.1411891555 -0.7003041792
C 1.2775382869 -0.1025366126 3.5260936822
C 0.247678413 -0.238439128 4.3576129075
C 0.4730536341 -0.2722694525 5.8027044102
O -0.6808739726 -0.4213773657 6.4903947304
O 1.156530739 0.0910554004 -2.0507088791
O 1.5278982992 -0.1840516088 6.379399333
H 2.261644181 -0.0226216874 3.9799258678
H -0.7764750545 -0.3306006196 4.0235587883
H -0.4283042927 -0.4343423857 7.4205501779
H 2.0128643134 0.1688166151 -2.4766679665
H -0.924784498 -0.0954591893 -1.6452161881
H 3.3851731083 0.219317858 -0.543334387
H 3.367406142 0.1299189054 1.9229354527
H -0.9096216677 -0.2167852337 1.8473680725

LC- ω PBE Caffeic Acid (Neutral) 0.006 a.u.

C 1.2663531904 0.0514215736 -0.7032220145
C 0.0507028467 -0.0713182331 -0.016136252
C 0.0495935559 -0.1204770646 1.3532157391
C 1.244846513 -0.0490160375 2.071726522
C 2.4375402602 0.073942401 1.3764395669
C 2.451512536 0.1236665014 -0.0066366517
O -1.1077324109 -0.1404462411 -0.6942616357
C 1.2824229883 -0.1012597849 3.5243110549
C 0.2510795409 -0.2371375788 4.3581326952
C 0.4695110494 -0.2721436116 5.7995818173
O -0.6893659101 -0.4237440913 6.4852858478
O 1.1520258534 0.0899616575 -2.0454886103
O 1.5180988756 -0.1840672575 6.3914780226
H 2.2671836051 -0.0218148884 3.9771293627
H -0.7718699133 -0.3292516627 4.0208657426
H -0.4321300643 -0.4376502871 7.4136158766
H 2.0021743754 0.1659477327 -2.4853203854
H -0.9293620559 -0.096795398 -1.6410454683
H 3.3871364715 0.2188274004 -0.5453765657
H 3.3724655784 0.130643638 1.920828731
H -0.9070758859 -0.2156167679 1.8494606049

LC- ω PBE Caffeic Acid (Neutral) 0.008 a.u.

C 1.2682249069 0.0516871541 -0.7033781924
C 0.0509490766 -0.0711625908 -0.0139459116
C 0.0513269941 -0.1201639949 1.3546256804
C 1.2482714794 -0.0483357589 2.0732029079
C 2.4409546571 0.0747121809 1.3759904204
C 2.4545555555 0.1241873038 -0.006782549
O -1.1063335682 -0.1403187889 -0.6895267721
C 1.286530865 -0.100620884 3.5219788949
C 0.2538467064 -0.2354865872 4.3593206514
C 0.4664421984 -0.2719437332 5.7965478602
O -0.6971217457 -0.424701808 6.4815599319
O 1.1485220318 0.0893626626 -2.0403456488
O 1.509252514 -0.1853007327 6.4031064545
H 2.2722051481 -0.0225796658 3.9734329356
H -0.7682140685 -0.3265041105 4.0194957818
H -0.4339474029 -0.4399135017 7.407706732
H 1.9924846439 0.1643392072 -2.4936203949
H -0.9334481997 -0.0983529608 -1.6380845108
H 3.3893542351 0.219098199 -0.5466446065
H 3.3766786496 0.1314430801 1.9193067298
H -0.9054236772 -0.2157726703 1.8506376054

LC- ω PBE Gallic Acid (Neutral) Zero field

C -0.9490283337 -1.1651845768 0.0022689415
C -1.6829425897 0.0095221875 0.0004672378
C -1.0365600207 1.2348279336 -0.0038636248
C 0.343152761 1.2838807707 -0.0063887162
C 1.0639168938 0.1031355632 -0.0045509919
C 0.425246547 -1.1272378297 -0.0002290109
O -3.03777238 0.0080933951 0.0028344451
O -1.7564901937 2.3771116806 -0.0055985897
C 2.5453287252 0.0947466959 -0.0071118814
O 3.0883527208 1.3207579692 -0.0115478581
O -1.6924528675 -2.3078573647 0.0065596087
O 3.2220727278 -0.8987512739 -0.0059976349
H 1.0189566608 -2.0333045318 0.0011034713
H 0.8394687559 2.2434957571 -0.009756939
H -1.1215101268 -3.0780632354 0.0077876962
H -3.3501228624 -0.9024975658 0.0057843895
H -2.6929723515 2.1537619109 -0.0033625383
H 4.0449169337 1.1947875145 -0.0131040049

LC- ω PBE Gallic Acid (Neutral) 0.010 a.u.

C -0.9461297199 -1.1819688851 0.0024380361
C -1.6833934928 -0.0026518063 0.0006508464
C -1.0319029942 1.2262665501 -0.0036822179
C 0.3465841046 1.2705361105 -0.0062163536
C 1.074073974 0.0890060008 -0.0043618638
C 0.4299113377 -1.1435191981 -0.0000184329
O -3.0194139131 0.0193464308 0.0029035673
O -1.7370076767 2.3670882337 -0.0054334935
C 2.5383686722 0.1065698033 -0.0070115676
O 3.0753526079 1.3492095249 -0.0120416093
O -1.6948389659 -2.3112343612 0.0066555812
O 3.2730471538 -0.8556399934 -0.0056158004
H 1.0139616264 -2.0554227808 0.001323801
H 0.8341250888 2.2342774407 -0.0096836415
H -1.1516771324 -3.1003869121 0.007280617
H -3.3925291738 -0.8702693965 0.0054250423
H -2.6827476691 2.1714889435 -0.0036347732
H 4.0257771728 1.1985292949 -0.0136837376

LC- ω PBE Gallic Acid (Neutral) 0.002 a.u.

C -0.9485943726 -1.1684495384 0.0023037071
C -1.6829193038 0.0070646458 0.0005135843
C -1.0355751254 1.2328928544 -0.0038267999
C 0.34394806 1.2810114247 -0.006371145
C 1.0655704702 0.1001352137 -0.0045402453
C 0.426137069 -1.130538216 -0.0002041881

O -3.0340621189 0.0106988833 0.0028709471
O -1.7521999264 2.374995562 -0.0055595873
C 2.5438136031 0.0971067969 -0.0071437095
O 3.0853088883 1.3264339303 -0.0116366543
O -1.6927862367 -2.3085854312 0.006584171
O 3.232142117 -0.8901294467 -0.0058848674
H 1.0177495802 -2.0378289769 0.0011224161
H 0.838524897 2.2414064056 -0.0097668306
H -1.1269871368 -3.0823591787 0.0076954547
H -3.3586119765 -0.8959053492 0.0057181945
H -2.6905763403 2.1573070188 -0.0034169662
H 4.0406788526 1.1959684015 -0.013163481

LC- ω PBE Gallic Acid (Neutral) 0.004 a.u.

C -0.9480929224 -1.171735309 0.0023347883
C -1.6829493109 0.0046250452 0.0005532768
C -1.0346317648 1.2310548662 -0.0037933578
C 0.3446842788 1.2782535985 -0.0063513936
C 1.0673810027 0.0972384184 -0.0045243575
C 0.4270475487 -1.1338090994 -0.0001771517
O -3.0303984819 0.0131360543 0.0028975023
O -1.748127998 2.3729338481 -0.0055248077
C 2.542362309 0.099470211 -0.0071624037
O 3.0825170574 1.3320792498 -0.0117197316
O -1.6931959925 -2.3092899593 0.0066044501
O 3.242240314 -0.8815102559 -0.0057893657
H 1.0166839074 -2.0422665398 0.0011450731
H 0.8375231261 2.2394424289 -0.009771387
H -1.1327049084 -3.0867169356 0.0076115528
H -3.3670846389 -0.8893914931 0.0056591567
H -2.6883718053 2.1608174191 -0.0034660316
H 4.0366792789 1.1968934528 -0.0132318122

LC- ω PBE Gallic Acid (Neutral) 0.006 a.u.

C -0.9475267334 -1.175070183 0.0023665549
C -1.6830389258 0.0021921436 0.0005892066
C -1.0337213145 1.2293248913 -0.0037599742
C 0.3453649617 1.2755931899 -0.0063228007
C 1.0693738915 0.0944271709 -0.0044945802
C 0.4279802653 -1.1370558211 -0.0001409923
O -3.0267550344 0.0154053798 0.0029135397
O -1.7442539598 2.370914356 -0.0054938967
C 2.5409953079 0.1018295981 -0.0071559964
O 3.0799565791 1.3377052369 -0.0118044721
O -1.693670066 -2.3099659101 0.00662331
O 3.2524024104 -0.8729032458 -0.0057141944

H 1.0157181223 -2.0466552191 0.0011806561
H 0.8364462494 2.2376040519 -0.0097637564
H -1.1386928726 -3.0911559029 0.0075200336
H -3.375576827 -0.8829302647 0.0055986167
H -2.6863446697 2.1643202169 -0.0035181331
H 4.0329036157 1.1976453113 -0.0133291209

LC- ω PBE Gallic Acid (Neutral) 0.008 a.u.

C -0.946880614 -1.1784826441 0.0024031263
C -1.6831972021 -0.000243967 0.0006240846
C -1.0328172094 1.2277270213 -0.0037226026
C 0.345996447 1.2730189407 -0.006280318
C 1.0716118283 0.0916845046 -0.0044432373
C 0.4289403223 -1.1402747106 -0.0000877285
O -3.0231075817 0.0174802456 0.0029203063
O -1.7405669491 2.3689520852 -0.0054628494
C 2.5396848167 0.1041936222 -0.007109849
O 3.0776129466 1.3433973683 -0.0119163815
O -1.6942072865 -2.3106157404 0.006645009
O 3.2627027767 -0.8642653483 -0.0056455191
H 1.0147870969 -2.0510445318 0.0012422949
H 0.8352867639 2.2358941861 -0.0097390374
H -1.1450041958 -3.0957191346 0.0073970535
H -3.3841075989 -0.87653841 0.0055201087
H -2.6844968866 2.1678767652 -0.0035733054
H 4.0293235256 1.1981847474 -0.0134771549

LC- ω PBE Caffeic Acid (Radical) Zero field

C 1.2463798212 0.0558352502 -0.7537586403
C -0.0009143814 -0.0825506588 0.0022850998
C -0.013469029 -0.1381973806 1.3661489962
C 1.1942287424 -0.0616094548 2.0701579299
C 2.4217767418 0.0733869866 1.3581445778
C 2.466193859 0.1311364767 0.0096655156
O -1.0992085255 -0.148301508 -0.7333506242
C 1.2604630355 -0.1133745833 3.5110149577
C 0.232932256 -0.2367760975 4.3567338332
C 0.4890943575 -0.2721145041 5.8077657639
O -0.6472733109 -0.3993160279 6.5105519756
O 1.1739588426 0.0987365329 -1.981761171
O 1.5673900336 -0.1984773145 6.3317955978
H 2.2486236001 -0.0449357721 3.9561542583
H -0.797984248 -0.3142009201 4.0395551968
H -0.3993806058 -0.4147848077 7.44342007
H -0.793523229 -0.0847647086 -1.6577496201
H 3.3944109163 0.2335585043 -0.5366781231

H 3.3382937827 0.1299472363 1.9335068479
H -0.960340659 -0.2406782489 1.8781705584

LC- ω PBE Caffeic Acid (Radical) 0.010 a.u.

C 1.2484563726 0.0558395411 -0.7575268934
C -0.0065296208 -0.0823316335 0.0078914437
C -0.0063383833 -0.1362329818 1.374255821
C 1.207030008 -0.0600884437 2.0701548229
C 2.4381610405 0.0723135963 1.3515171525
C 2.4793541212 0.1287789725 0.0055298222
O -1.1052715685 -0.1471670723 -0.7046313523
C 1.2764645553 -0.1087489399 3.5013761617
C 0.2467801018 -0.2346708805 4.360621443
C 0.4752584521 -0.2684949779 5.7928728727
O -0.681122381 -0.4097626021 6.4949330835
O 1.1736649075 0.1028896015 -1.9719740257
O 1.5262155241 -0.1881560107 6.3880068386
H 2.2688790509 -0.0364995373 3.9372583419
H -0.7797551859 -0.3181361108 4.0332468912
H -0.4009954511 -0.4241079895 7.4158485889
H -0.8455638737 -0.0897475399 -1.6457011719
H 3.4013740217 0.2277918148 -0.5523500353
H 3.3581190319 0.1265356595 1.9224098827
H -0.9525287234 -0.2374854657 1.8880333121

LC- ω PBE Caffeic Acid (Radical) 0.002 a.u.

C 1.2460213964 0.0561218216 -0.7540681681
C -0.0017678243 -0.0824688629 0.0042278081
C -0.01055035 -0.1378659575 1.3687474469
C 1.1985498347 -0.0612686437 2.0697293314
C 2.425855066 0.0730897715 1.3565250815
C 2.4684645035 0.1306308062 0.0081389602
O -1.1012258997 -0.1480538204 -0.7254761363
C 1.2650410137 -0.1124248591 3.5100804292
C 0.2368063041 -0.2363914293 4.3563770763
C 0.4856565946 -0.2712598522 5.8045704687
O -0.6554323515 -0.4018306002 6.5051878533
O 1.1725776958 0.0992232063 -1.9794671803
O 1.5578080832 -0.1956060643 6.3439125172
H 2.2537933702 -0.0430084999 3.9538300184
H -0.7928805126 -0.3151389319 4.036144048
H -0.4030543064 -0.41691705 7.4362153583
H -0.8056862801 -0.0854686489 -1.6535417287
H 3.3950244085 0.2322111281 -0.5411631822
H 3.3435919387 0.1291096432 1.9301122586
H -0.9569406845 -0.2401641567 1.8816907394

LC- ω PBE Caffeic Acid (Radical) 0.004 a.u.

C 1.2460120994 0.0564140056 -0.7545718848
C -0.0027536219 -0.0824070041 0.0057661045
C -0.0083209566 -0.1375087202 1.3708466834
C 1.202068352 -0.0609056517 2.0694982188
C 2.4295545731 0.0728464101 1.3551272326
C 2.4708794202 0.1301411055 0.0069756847
O -1.1028705156 -0.1478265076 -0.7186503367
C 1.2689233143 -0.1114581468 3.508679693
C 0.2401286287 -0.2359951156 4.3565277941
C 0.4825775512 -0.2705020805 5.8015071108
O -0.6628349139 -0.4041819234 6.5008648381
O 1.1718756904 0.0997093483 -1.9773444008
O 1.5488873336 -0.1930736328 6.3555239641
H 2.2583931202 -0.0411422456 3.9508348299
H -0.7885052206 -0.3160318684 4.0337572656
H -0.4051459789 -0.4189356075 7.4298465785
H -0.8170607526 -0.086211866 -1.6501939686
H 3.3959740366 0.2308784556 -0.5449976094
H 3.348273003 0.1283309074 1.9273433939
H -0.9544031626 -0.2396208625 1.8844318084

LC- ω PBE Caffeic Acid (Radical) 0.006 a.u.

C 1.2463597812 0.0565785044 -0.7552469043
C -0.0038749709 -0.0823674606 0.0069231215
C -0.0067987165 -0.1371187888 1.3724972325
C 1.2047706065 -0.0605486534 2.0694734119
C 2.4328881299 0.0726248009 1.3538863116
C 2.4734684497 0.1296356394 0.0061425711
O -1.1041648497 -0.1476137822 -0.712774334
C 1.2721533094 -0.1104607535 3.5067856048
C 0.2429221862 -0.2355185713 4.3571932784
C 0.479788049 -0.2697465137 5.7985085181
O -0.6695923754 -0.4064394511 6.4975739063
O 1.1718495852 0.1003548892 -1.9753854053
O 1.540575114 -0.1908249041 6.3666899558
H 2.2624635578 -0.0393404658 3.9471347762
H -0.7848227736 -0.3167996038 4.0323373396
H -0.4056091479 -0.4209672846 7.4242365698
H -0.8276429055 -0.0870831179 -1.6476250419
H 3.3973036089 0.2295734774 -0.5481777447
H 3.3523488215 0.1275947428 1.9251341448
H -0.9527334599 -0.2390137033 1.8864656881

LC- ω PBE Caffeic Acid (Radical) 0.008 a.u.

C 1.2472406408 0.0558028389 -0.7562069543
C -0.0051034908 -0.082287117 0.0076415714
C -0.0062205899 -0.1365200836 1.3735750395
C 1.206354102 -0.0602963138 2.0697293856
C 2.4356837573 0.0724178286 1.3527206214
C 2.4762575816 0.1291033467 0.005698533
O -1.1049606222 -0.1473034775 -0.7082070286
C 1.2746216602 -0.109574102 3.5043320342
C 0.2450896451 -0.2351031017 4.3585617535
C 0.4774210863 -0.2690982126 5.7956259944
O -0.6755576748 -0.4082736274 6.495623078
O 1.172431019 0.1018550311 -1.9735375707
O 1.5331042601 -0.1893264429 6.3774157127
H 2.2658893618 -0.0378268241 3.9426322759
H -0.7819506232 -0.317523222 4.0322181602
H -0.4040947361 -0.4226733793 7.4196026205
H -0.83693374 -0.0886934061 -1.6462148646
H 3.3990704094 0.2286852602 -0.5505522026
H 3.3555323589 0.1270952538 1.9235440654
H -0.9522224056 -0.2379412494 1.887570775

LC- ω PBE Gallic Acid (Radical) Zero field

C -0.9424736066 -1.212819776 0.003210104
C -1.741091795 0.0007878603 0.0015823199
C -1.0134270024 1.2646141251 -0.0033854855
C 0.3556655829 1.3164803317 -0.0064074847
C 1.0581509761 0.1154092366 -0.0046276241
C 0.4197052158 -1.1332924138 0.0001139064
O -2.9712016553 0.0278374414 0.0040910888
O -1.7756197723 2.3464003942 -0.0047203876
C 2.5432857153 0.0955746544 -0.0077174972
O 3.0920317247 1.3161420016 -0.012223585
O -1.6372420763 -2.3532826449 0.0077976147
O 3.2037574936 -0.9075289918 -0.006395278
H 1.0369318887 -2.0237960628 0.0012382027
H 0.8701653189 2.2659658718 -0.010069517
H -1.0384405209 -3.104835591 0.0086213994
H -2.6941094753 2.018591053 -0.001897853
H 4.049003988 1.1908755101 -0.0139149238

LC- ω PBE Gallic Acid (Radical) 0.010 a.u.

C -0.9388312782 -1.2272704683 0.0032855674
C -1.7419667764 -0.0057933005 0.00182361
C -1.0124170761 1.2630906292 -0.0033813991
C 0.3584462567 1.3062496098 -0.006448161
C 1.0649750852 0.1037085878 -0.0045873053

C 0.4254388678 -1.1497407317 0.0001974783
O -2.9611247376 0.0142953265 0.0044499318
O -1.7553312096 2.347853162 -0.0047822614
C 2.5339391701 0.1072819142 -0.0076630797
O 3.0812110689 1.3423339123 -0.0125296845
O -1.6480708677 -2.3481463727 0.0077517764
O 3.2494895403 -0.8674795665 -0.005818217
H 1.0345495696 -2.0451515463 0.0012921178
H 0.867162381 2.2584946748 -0.0102565631
H -1.0845075591 -3.1257567689 0.0081441372
H -2.6891524027 2.0609067111 -0.0020467131
H 4.0312819678 1.1882472271 -0.0141362345

LC- ω PBE Gallic Acid (Radical) 0.002 a.u.

C -0.9419355418 -1.215516016 0.0032216465
C -1.7411104821 -0.0004519093 0.0016228887
C -1.0131875348 1.2641051922 -0.0033798221
C 0.3563278705 1.3141768477 -0.0064043396
C 1.0591587966 0.1128684784 -0.0046072981
C 0.4208166278 -1.136508736 0.0001340351
O -2.9690423059 0.0253804247 0.0041434637
O -1.7712608977 2.3466894717 -0.0047279467
C 2.5413519567 0.0978271128 -0.0076793825
O 3.0894331546 1.3212453246 -0.0123092633
O -1.6393137166 -2.3522822595 0.0077784519
O 3.2128320814 -0.8995548285 -0.0062644661
H 1.0361868514 -2.0281037045 0.001257013
H 0.8696663459 2.264177793 -0.0100883663
H -1.0470025807 -3.1087753887 0.0085215172
H -2.6929116154 2.0270863504 -0.0019281889
H 4.0450829901 1.190758847 -0.0139949425

LC- ω PBE Gallic Acid (Radical) 0.004 a.u.

C -0.9413047052 -1.2183033861 0.0032352438
C -1.7412104764 -0.0017332138 0.001667912
C -1.0129779094 1.263689709 -0.0033753369
C 0.356928957 1.3119947479 -0.0064018606
C 1.060336346 0.1104296784 -0.0045860405
C 0.4219490949 -1.1397522495 0.0001567284
O -2.966953656 0.022785725 0.0041973915
O -1.7670625179 2.3469744254 -0.0047386451
C 2.5394606339 0.1001291333 -0.0076431865
O 3.0870787731 1.3263978337 -0.0123891429
O -1.6414297504 -2.3512671265 0.0077604523
O 3.2219470584 -0.8915374332 -0.0061437672
H 1.0355770469 -2.0323852511 0.0012768377

H 0.8690970341 2.2625343955 -0.010109948
H -1.0558904947 -3.1128463256 0.0084203184
H -2.6918365706 2.0355961372 -0.0019597922
H 4.0413831362 1.1904162005 -0.0140721641

LC- ω PBE Gallic Acid (Radical) 0.006 a.u.

C -0.9406039025 -1.2211673662 0.0032488567
C -1.7413652948 -0.0030457325 0.0017084512
C -1.012782629 1.2633643892 -0.0033746363
C 0.3574908569 1.3099339019 -0.0064087165
C 1.0616811267 0.1080734188 -0.0045782463
C 0.4230943922 -1.1430370596 0.000172764
O -2.9649553434 0.0200718169 0.0042759756
O -1.7629639531 2.347272684 -0.0047512722
C 2.5375938835 0.1024649102 -0.0076327285
O 3.0848668007 1.3316291477 -0.0124498251
O -1.6435847541 -2.3502435482 0.0077531219
O 3.2310706981 -0.8835277252 -0.0060283476
H 1.0350853104 -2.0366609313 0.0012883056
H 0.8684971921 2.2610282572 -0.0101440386
H -1.0650384786 -3.1169941698 0.0083274223
H -2.6907894187 2.0440553633 -0.0019966454
H 4.0377955137 1.1899056436 -0.0141154407

LC- ω PBE Gallic Acid (Radical) 0.008 a.u.

C -0.9397746312 -1.2241592611 0.0032664142
C -1.7416252071 -0.0044009708 0.0017661197
C -1.0126009999 1.2631649281 -0.0033760162
C 0.357990848 1.3080214469 -0.0064236154
C 1.0632285318 0.1058393135 -0.0045762936
C 0.424260824 -1.1463623807 0.0001878156
O -2.9630139486 0.0172443796 0.0043515721
O -1.7590768766 2.3475648212 -0.0047654382
C 2.535760461 0.1048500532 -0.0076368239
O 3.0829424139 1.3369292835 -0.0125022302
O -1.6458013868 -2.3492095815 0.0077468379
O 3.2402606328 -0.8754988844 -0.0059161627
H 1.0347498791 -2.0409103344 0.001294114
H 0.8678419359 2.2596864997 -0.0101938932
H -1.0745858187 -3.1213167411 0.0082341064
H -2.6899296054 2.0525134966 -0.002020879
H 4.0344649477 1.1891669318 -0.0141406273

M06-2X Caffeic Acid (Neutral) -0.010 a.u.

C 1.257400439 0.0638635894 -0.7129281874
C 0.0458233289 -0.1332757986 -0.0552425632

C 0.0199032028 -0.2258712052 1.3222234195
C 1.1994025575 -0.1219042836 2.0658805817
C 2.4026355673 0.0665554014 1.3865077574
C 2.4323719994 0.1616216646 0.0035302142
O -1.1084088825 -0.2360331055 -0.7763781036
C 1.2380387289 -0.1986287482 3.5293156851
C 0.2115461787 -0.1968530351 4.3724425596
C 0.5051894175 -0.2680232398 5.8364938527
O -0.6145743784 -0.2395350142 6.557980498
O 1.1999401146 0.147083847 -2.0953509212
O 1.6097486891 -0.3393663585 6.2890650739
H 2.2262029295 -0.2449652683 3.977995852
H -0.8268484998 -0.1353774121 4.0737042256
H -0.3838869576 -0.281891421 7.4985285918
H 2.0741138318 0.3803020308 -2.4107672318
H -0.8841174813 -0.1164457329 -1.7026555655
H 3.3725927194 0.3121003957 -0.5168665544
H 3.3214066153 0.1443833842 1.95196836
H -0.93336912 -0.38406769 1.8091364556

M06-2X Caffeic Acid (Neutral) -0.002 a.u.

C 1.2625186571 0.0480759222 -0.7108064733
C 0.0452216821 -0.0712068204 -0.0318972064
C 0.0336833144 -0.1199387139 1.3451518619
C 1.2274964148 -0.051198838 2.0711575929
C 2.4292666573 0.069449393 1.378805772
C 2.4484195932 0.117887214 -0.0084336232
O -1.1169592274 -0.1370570596 -0.7248775818
C 1.2650062274 -0.100366701 3.5320766892
C 0.2350447141 -0.2491377887 4.3632260407
C 0.484727414 -0.2716748148 5.8204381612
O -0.6565479063 -0.4268687655 6.5143472185
O 1.1711508653 0.0899076053 -2.074481218
O 1.5568574005 -0.1668078594 6.3494218094
H 2.2464476048 -0.005028142 3.9877206898
H -0.7903771794 -0.3574623137 4.0387972352
H -0.4242393236 -0.4324720643 7.4520312926
H 2.045436074 0.1724140468 -2.4606385228
H -0.9190012795 -0.0809988247 -1.665127863
H 3.3862259115 0.2116980831 -0.5435998628
H 3.3581205019 0.1250329856 1.9305504446
H -0.9233871161 -0.2105745438 1.8407215432

M06-2X Caffeic Acid (Neutral) -0.004 a.u.

C 1.2611020411 0.0526877142 -0.7115050666
C 0.0447316619 -0.0805118485 -0.0370920794

C 0.0297351128 -0.1377225326 1.34023558
C 1.2206239533 -0.0635625709 2.0698310767
C 2.4230463183 0.0688747082 1.3802480982
C 2.4447364968 0.1266121487 -0.0063268609
O -1.1164008135 -0.1520492387 -0.7361074713
C 1.2584656295 -0.1169373018 3.5320194972
C 0.228778075 -0.2425846013 4.3652703025
C 0.4900647764 -0.2716234703 5.8246400128
O -0.6474567954 -0.3943271442 6.5250874783
O 1.1779005843 0.1028135867 -2.0800083755
O 1.5721843903 -0.1954665435 6.3348531415
H 2.2422461915 -0.0424903049 3.9864060928
H -0.8012986133 -0.3247244587 4.0469754531
H -0.4154336084 -0.4055746996 7.463573632
H 2.0572242205 0.198995805 -2.450377137
H -0.9114714311 -0.0867939252 -1.6737059763
H 3.3835696676 0.2308860792 -0.5383449127
H 3.3498965179 0.1277309334 1.9348854435
H -0.9271333756 -0.2405603354 1.8340260712

M06-2X Caffeic Acid (Neutral) -0.006 a.u.

C 1.2596657651 0.0584552096 -0.711812412
C 0.0458053595 -0.1062401621 -0.0432724724
C 0.0277692307 -0.1804518627 1.3339397641
C 1.2145884706 -0.0918699158 2.0680214164
C 2.4164685116 0.0674193197 1.3821845355
C 2.4402076717 0.1435390035 -0.0030593887
O -1.1128923282 -0.1928298958 -0.7494755773
C 1.2529009483 -0.1551753957 3.5308641589
C 0.2219095695 -0.2228940388 4.3675741501
C 0.494984287 -0.2706982029 5.828384346
O -0.6393991869 -0.316066949 6.5370967125
O 1.1845610445 0.1237567799 -2.0848956169
O 1.5878765528 -0.2675797826 6.3180612987
H 2.240379534 -0.1353627374 3.9828669774
H -0.813996184 -0.2389318438 4.056645813
H -0.4069557574 -0.3423642771 7.4760011679
H 2.0611241254 0.2892608516 -2.4359346084
H -0.9021979369 -0.102760115 -1.6831849368
H 3.3789709712 0.2697419965 -0.5310166893
H 3.3405508582 0.135058961 1.9403267821
H -0.9272105068 -0.3103349432 1.8252685794

M06-2X Caffeic Acid (Neutral) -0.008 a.u.

C 1.2586042296 0.060734228 -0.7124788989
C 0.0455331782 -0.1173170698 -0.0491259276

C 0.0234467061 -0.1992216169 1.3283158633
C 1.2068220814 -0.1043377494 2.0669563701
C 2.4096367634 0.0669662773 1.3841759227
C 2.4365367482 0.1509568632 -0.0000892583
O -1.1112653233 -0.2104504699 -0.7624560951
C 1.2453228759 -0.172999216 3.5303001288
C 0.2162179053 -0.2128187376 4.3700151524
C 0.5002194048 -0.269778738 5.8325066056
O -0.6272852815 -0.2840601609 6.5477581252
O 1.1923800032 0.1335008341 -2.0903472131
O 1.5999095266 -0.2971394072 6.3035047882
H 2.2336716812 -0.179905473 3.9808121695
H -0.8218952618 -0.1976485558 4.0653427403
H -0.3953163303 -0.3165767369 7.487465385
H 2.0696433344 0.3267435183 -2.4242706037
H -0.893516772 -0.1080799539 -1.6927822733
H 3.3762966382 0.2871746183 -0.5244707132
H 3.3312163139 0.1387291575 1.9458688554
H -0.9310674216 -0.3407996116 1.8175828767

M06-2X Gallic Acid (Neutral) -0.010 a.u.

C -0.9517023247 -1.1564829278 0.0018599551
C -1.6867566338 0.0196989078 0.0000415169
C -1.0428535839 1.2477795067 -0.0041879001
C 0.3428435112 1.3023098613 -0.0066484271
C 1.0641082242 0.1165619402 -0.0048113501
C 0.4249598143 -1.118305724 -0.0005746593
O -3.0622255892 -0.0051301587 0.0025780588
O -1.7821119877 2.3920627573 -0.0058339076
C 2.5627153399 0.0821398921 -0.0072162412
O 3.1085749296 1.2975115874 -0.0112826111
O -1.6991904673 -2.3098049912 0.0062766621
O 3.1822039219 -0.940271307 -0.0058165541
H 1.0270143933 -2.0192467768 0.0007349542
H 0.8470185518 2.25802133 -0.0099295456
H -1.1068327481 -3.0662988712 0.0085782111
H -3.3187074647 -0.9329599145 0.0065900711
H -2.7101974817 2.1424466427 -0.0025547616
H 4.0727005949 1.2011932458 -0.0125094716

M06-2X Gallic Acid (Neutral) -0.002 a.u.

C -0.9504238523 -1.1690453915 0.0020914627
C -1.6858148519 0.0100010267 0.0003112535
C -1.0386145082 1.2393823829 -0.0039060842
C 0.346240059 1.2901572482 -0.0063869154
C 1.0682457791 0.103960019 -0.0045780316

C 0.4281258764 -1.1315950568 -0.0003326029
O -3.0461648003 0.0062241862 0.0026638867
O -1.7624358307 2.3834561288 -0.005575343
C 2.5545628829 0.0907561967 -0.0071738517
O 3.0935630314 1.3195862924 -0.011759739
O -1.6994173493 -2.312386264 0.0063411014
O 3.2201202026 -0.9076636179 -0.0055543534
H 1.0216981854 -2.0371128616 0.0009326184
H 0.84422405 2.2482711632 -0.0097645874
H -1.1260904122 -3.0824226564 0.008120132
H -3.3506602704 -0.9074991923 0.0061071304
H -2.6984840996 2.1577782591 -0.0031412981
H 4.0528869079 1.2093771372 -0.0131007785

M06-2X Gallic Acid (Neutral) -0.004 a.u.

C -0.9507885246 -1.1658966507 0.0020353806
C -1.6859301161 0.0124087664 0.0002505731
C -1.0395888298 1.2413590332 -0.0039670949
C 0.3454639352 1.2930542336 -0.0064452033
C 1.067002236 0.1069809526 -0.0046346127
C 0.4273046477 -1.1283237961 -0.0003940076
O -3.0500650678 0.0035988657 0.0026451722
O -1.7670196344 2.3855830785 -0.005627712
C 2.5564082381 0.0886118307 -0.0071869084
O 3.096900105 1.3141116891 -0.0116573824
O -1.6992338102 -2.3118015721 0.0063207584
O 3.2105378156 -0.9158372339 -0.0055957195
H 1.022894212 -2.0327270841 0.0008769243
H 0.8450315516 2.2505215627 -0.0097968779
H -1.1209441108 -3.0783406544 0.008228975
H -3.342670913 -0.913803523 0.0062264662
H -2.7011374735 2.1540889718 -0.0030215174
H 4.0573967389 1.20763653 -0.0129632134

M06-2X Gallic Acid (Neutral) -0.006 a.u.

C -0.9511225592 -1.162750244 0.0019761382
C -1.6861230748 0.0148350385 0.0001831939
C -1.0406216611 1.2434282825 -0.0040336897
C 0.3446390998 1.2960492233 -0.0065050567
C 1.0659027742 0.1100899718 -0.004688829
C 0.4265027496 -1.1250215131 -0.0004538099
O -3.0540397102 0.0008042457 0.0026197197
O -1.7718273555 2.387739003 -0.0056873226
C 2.558395443 0.0864588861 -0.0071902546
O 3.1005181724 1.3086024949 -0.0115516235
O -1.6991585252 -2.3111559347 0.0062986689

O 3.2010328472 -0.9240070031 -0.0056466015
H 1.0241629328 -2.0282992797 0.0008272978
H 0.8457690484 2.2528999204 -0.0098296751
H -1.1160653897 -3.0742882231 0.0083426153
H -3.33463288 -0.9202012026 0.00634625
H -2.7039788085 2.1503196102 -0.0028819594
H 4.0622078969 1.2057217241 -0.0128310616

M06-2X Gallic Acid (Neutral) -0.008 a.u.

C -0.9514245648 -1.1596046426 0.001917911
C -1.6863967218 0.0172723831 0.0001140639
C -1.0417058024 1.2455741482 -0.0041077601
C 0.3437681926 1.2991314065 -0.0065746185
C 1.0649436263 0.1132789002 -0.004749977
C 0.4257193315 -1.1216858753 -0.0005150011
O -3.0580842775 -0.0021320861 0.0025990692
O -1.7768490228 2.3899082246 -0.0057561779
C 2.5604879114 0.084305828 -0.0072042992
O 3.1043989173 1.3030832199 -0.0114242203
O -1.6991634955 -2.3104697735 0.0062852486
O 3.1915935842 -0.9321413448 -0.0057198692
H 1.0255183124 -2.023818694 0.000778845
H 0.8464388902 2.2553940622 -0.0098766049
H -1.1114000719 -3.0702669564 0.0084582109
H -3.326587718 -0.9266320866 0.0064698602
H -2.7069913909 2.1464534802 -0.0027266711
H 4.0672952998 1.2035748064 -0.0126740096

M06-2X Caffeic Acid (Radical) -0.010 a.u.

C 1.2575165929 0.0590618059 -0.7637227252
C 0.0047402538 -0.0844206433 -0.0161062812
C -0.0316841158 -0.14287602 1.3469805547
C 1.171313847 -0.064002947 2.0764234868
C 2.4065909611 0.0776210782 1.3700538573
C 2.4618637826 0.1383302643 0.0141665107
O -1.0939402115 -0.1544205401 -0.7759417324
C 1.2364700487 -0.12024824 3.5132891064
C 0.2077698568 -0.2406951528 4.3675065379
C 0.5085001173 -0.2810611515 5.8336993005
O -0.6057115925 -0.3713181707 6.5514381396
O 1.1960696864 0.1014601747 -2.009084192
O 1.619808995 -0.2361833263 6.2709128941
H 2.2224779369 -0.0571383165 3.9637289607
H -0.8294946921 -0.3087741091 4.0668802013
H -0.3816981808 -0.3913362825 7.495077022
H -0.7597398549 -0.0847514599 -1.6862890736

H 3.3993016017 0.2474608529 -0.514131256
H 3.3143310511 0.1363933535 1.9571471246
H -0.9828340835 -0.2505821699 1.8497445638

M06-2X Caffeic Acid (Radical) -0.002 a.u.

C 1.2537793085 0.0568200808 -0.7636269273
C 0.0020756762 -0.0814980767 -0.0045299046
C -0.0142180355 -0.138146478 1.3645321546
C 1.1937821342 -0.0623883739 2.0707203048
C 2.4256446872 0.0719786876 1.3588550193
C 2.4714358255 0.1303090674 0.004090342
O -1.1030689619 -0.146568233 -0.7334055032
C 1.259507087 -0.1134011654 3.5152438761
C 0.2287526372 -0.2410624026 4.3600265554
C 0.4922282279 -0.271874315 5.8178618312
O -0.6441572807 -0.4003436775 6.5187854893
O 1.1812977586 0.1016595035 -1.9967793751
O 1.5753941272 -0.1925559339 6.3256052761
H 2.2465541704 -0.0387185613 3.9612483298
H -0.801734149 -0.3242125447 4.0442907044
H -0.4110137986 -0.4137274022 7.456600301
H -0.8126744791 -0.0826970728 -1.6607055507
H 3.4009785712 0.2324404637 -0.5385572752
H 3.3391456141 0.1266279895 1.9374586912
H -0.9620571203 -0.2401225556 1.874058661

M06-2X Caffeic Acid (Radical) -0.004 a.u.

C 1.2543299444 0.0569602447 -0.7634892444
C 0.0028302914 -0.0820513742 -0.0066511887
C -0.0176210251 -0.1391988513 1.3611416304
C 1.1892326276 -0.0630551084 2.0718025924
C 2.4215959703 0.0727122678 1.3611126955
C 2.4691254108 0.131655762 0.0060337901
O -1.1012867418 -0.1478670568 -0.7420864406
C 1.2548251994 -0.1150129277 3.5155629683
C 0.2244681646 -0.2411777524 4.3609658536
C 0.4957140243 -0.2733722704 5.8214931221
O -0.6358502795 -0.3951850625 6.5251242138
O 1.1837858326 0.1020434205 -1.9995198006
O 1.5854090118 -0.1993936881 6.3130118527
H 2.2414745351 -0.0424029875 3.9627593211
H -0.8073974476 -0.3214379088 4.0481037518
H -0.4062114653 -0.4095286217 7.4646112508
H -0.8009606329 -0.0826484578 -1.6656182026
H 3.4003505852 0.2354005149 -0.5335408133
H 3.3338873673 0.1282103447 1.9414737273

H -0.9660493723 -0.2421314872 1.8694819204

M06-2X Caffeic Acid (Radical) -0.006 a.u.

C 1.2550564106 0.0590709708 -0.7633607831
C 0.0035884697 -0.0836756791 -0.0093439862
C -0.0216116451 -0.1423972956 1.3569600158
C 1.1839095252 -0.064487959 2.0730546203
C 2.4168860809 0.0748362093 1.3638006836
C 2.466591292 0.1356201176 0.0085203979
O -1.0989648098 -0.1516111019 -0.7522188614
C 1.2494398683 -0.1186329555 3.5152470718
C 0.2194247592 -0.2409244358 4.3625014915
C 0.4996423616 -0.2764828415 5.8251687422
O -0.627004102 -0.382526003 6.5330527488
O 1.1871471791 0.1034784952 -2.0023959993
O 1.5967878038 -0.2166976415 6.2991938844
H 2.2359931803 -0.0510944371 3.9634632026
H -0.8143448063 -0.3145584466 4.053384422
H -0.3996492525 -0.399470909 7.4739491803
H -0.7880112733 -0.0835151371 -1.6715920887
H 3.3996286238 0.242416932 -0.5274757706
H 3.3277519744 0.1317729994 1.9461960832
H -0.9706096398 -0.2486018815 1.863667945

M06-2X Caffeic Acid (Radical) -0.008 a.u.

C 1.2560927898 0.0595752992 -0.7634363236
C 0.0041956563 -0.0844412397 -0.0124312213
C -0.0262680474 -0.143550853 1.3523038414
C 1.1780040844 -0.0648116111 2.0746146623
C 2.4119619768 0.0763987333 1.3667439314
C 2.4641961167 0.1377454338 0.0112045987
O -1.0965480614 -0.1537380512 -0.7634122878
C 1.2434341959 -0.1203606456 3.5145066089
C 0.2139431589 -0.2405094624 4.3646561629
C 0.5038914623 -0.2788757131 5.8292603347
O -0.6170219166 -0.3751627345 6.5416700878
O 1.1911204485 0.1033652238 -2.0055439041
O 1.6081087317 -0.2282767189 6.2853349552
H 2.229807957 -0.0561259196 3.9637405956
H -0.8216063722 -0.3098783293 4.059512175
H -0.391691674 -0.3939938512 7.483977784
H -0.7743840203 -0.0843387479 -1.6784331999
H 3.3992664645 0.2463568629 -0.5210961735
H 3.3213063706 0.1344281614 1.951397827
H -0.9761573215 -0.2512868368 1.8572025454

M06-2X Gallic Acid (Radical) -0.010 a.u.

C -0.9449575942 -1.2080082736 0.0030754053
C -1.7474163086 0.000511975 0.0014330251
C -1.0179965685 1.2669132534 -0.003431902
C 0.3538107926 1.3275023344 -0.0064025258
C 1.0584757551 0.1243841813 -0.0046864317
C 0.4183995689 -1.1271605043 0.0000162187
O -2.9916155576 0.0249585155 0.0040073264
O -1.7908419126 2.3534571286 -0.004758766
C 2.560630881 0.0852510985 -0.0078351907
O 3.1055244264 1.2981030666 -0.012207983
O -1.6340256597 -2.3638905678 0.0077325894
O 3.1682806833 -0.9435322577 -0.0064022543
H 1.0436819416 -2.0126025176 0.0010996238
H 0.8738937244 2.2741271738 -0.0099969599
H -1.0109132048 -3.0976606513 0.0090673157
H -2.7007195811 2.0121308997 -0.0016408781
H 4.070880614 1.2086381455 -0.0137736129

M06-2X Gallic Acid (Radical) -0.002 a.u.

C -0.9434144574 -1.2177001867 0.0031175269
C -1.7460538287 -0.0036348445 0.001587989
C -1.0167208112 1.2643380039 -0.003396517
C 0.3574315282 1.3174893114 -0.0063665637
C 1.0598381839 0.1139014586 -0.0045658177
C 0.4223318426 -1.1388988006 0.000113652
O -2.9809016293 0.0176474831 0.0042207901
O -1.7721160352 2.3536769641 -0.0047890944
C 2.5507637811 0.0929469261 -0.0076092527
O 3.0924378914 1.3173892862 -0.0125836447
O -1.6409711148 -2.359535546 0.0075948919
O 3.2022415242 -0.913522327 -0.0058826332
H 1.039914785 -2.0285711221 0.0011863523
H 0.8733886333 2.2655549515 -0.0100432968
H -1.0411647798 -3.1116728568 0.0086596408
H -2.6944405642 2.0432895874 -0.001799401
H 4.0525270509 1.2104247114 -0.0141496217

M06-2X Gallic Acid (Radical) -0.004 a.u.

C -0.9438591538 -1.2152167258 0.0031005988
C -1.7462774438 -0.0025680626 0.0015434289
C -1.0169655353 1.264866056 -0.0034066842
C 0.3566275232 1.3198115715 -0.0063739893
C 1.0592499387 0.116387809 -0.0045910659
C 0.4213160019 -1.1359516185 0.0000883872
O -2.9834329925 0.0196035486 0.0041627346

O -1.7764881677 2.3536313393 -0.0047824536
C 2.5530727302 0.0909796298 -0.0076436886
O 3.0952943518 1.3125435127 -0.0125061478
O -1.6391374647 -2.3606500746 0.007617544
O 3.1936678828 -0.9210569214 -0.0059881481
H 1.0406952796 -2.0246136269 0.0011680661
H 0.8736395048 2.2674723752 -0.0100246319
H -1.0331982736 -3.1080324544 0.0087591225
H -2.6957967081 2.0356422212 -0.0017476349
H 4.0566845264 1.2102744207 -0.0140804379

M06-2X Gallic Acid (Radical) -0.006 a.u.

C -0.9442663927 -1.2127838795 0.0030913638
C -1.7465603615 -0.0015176891 0.0015105978
C -1.017231759 1.265474926 -0.0034197127
C 0.3557784294 1.3222525518 -0.0064004619
C 1.058849921 0.118940867 -0.0046404502
C 0.4203209549 -1.1330352881 0.0000543871
O -2.9860610774 0.0214446538 0.0041226787
O -1.7809846922 2.3536215042 -0.0047740874
C 2.5553917219 0.0890684084 -0.0077313295
O 3.0983341719 1.3078238275 -0.012403868
O -1.6373742166 -2.361756548 0.0076603063
O 3.1851555871 -0.9285247508 -0.0060961173
H 1.0415724085 -2.0206649631 0.0011351972
H 0.8738482244 2.2695305794 -0.0100382066
H -1.0255093605 -3.1044942474 0.0088625365
H -2.6971862438 2.0278727538 -0.0016930364
H 4.0610146846 1.2098702941 -0.0139447974

M06-2X Gallic Acid (Radical) -0.008 a.u.

C -0.9446244684 -1.2103854369 0.003082114
C -1.7469504998 -0.0004918561 0.0014718932
C -1.0175843804 1.2661657259 -0.0034271476
C 0.3548317812 1.3248241494 -0.0064050823
C 1.0585828851 0.1216205461 -0.0046665183
C 0.4193514216 -1.130096661 0.0000330424
O -2.9887818373 0.0232388196 0.0040662075
O -1.785804942 2.3535488011 -0.0047665927
C 2.5579352467 0.0871466149 -0.007785175
O 3.1017824215 1.3029698342 -0.01230737
O -1.6356667738 -2.3628325211 0.0076951677
O 3.1766815985 -0.9360408526 -0.0062391755
H 1.0425887817 -2.0166409062 0.0011160899
H 0.8739194458 2.2717593859 -0.0100216315
H -1.0180864181 -3.1010377497 0.0089648309

H -2.698871952 2.0200396341 -0.0016599666
H 4.0657896895 1.2093354725 -0.0138556859

M06-2X Caffeic Acid (Neutral) Zero field

C 1.2637419987 0.0484522436 -0.7102414337
C 0.0461384129 -0.0690011709 -0.0276648946
C 0.0379937369 -0.1164961627 1.3488024771
C 1.2340880772 -0.0480359223 2.0721572619
C 2.4346852291 0.0712187544 1.3776085758
C 2.451339216 0.1181405495 -0.0099050246
O -1.1162276822 -0.1342859427 -0.7155785985
C 1.2718233721 -0.0974655029 3.5312471743
C 0.239852298 -0.2477918447 4.3621854379
C 0.4801616176 -0.2721316353 5.8166536017
O -0.666972443 -0.4328027174 6.5060480556
O 1.1644639126 0.0881712668 -2.068784973
O 1.5451837721 -0.1655829395 6.3625162014
H 2.253335241 -0.001709355 3.9868413718
H -0.7837974363 -0.3571960805 4.0333580871
H -0.432905991 -0.4395708958 7.4425620273
H 2.0331274091 0.1625664373 -2.469979127
H -0.9250338604 -0.0836137429 -1.6581179027
H 3.3876720386 0.2104610795 -0.5473451678
H 3.3650666369 0.1265350663 1.9269727353
H -0.9186245558 -0.2061894848 1.8452481147

M06-2X Caffeic Acid (Neutral) 0.010 a.u.

C 1.2721230102 0.0512247053 -0.7108576941
C 0.0479588369 -0.0703746104 -0.0153476223
C 0.0496757424 -0.1182189479 1.3576608174
C 1.2542263876 -0.0453090165 2.0783726216
C 2.4539447743 0.0780166599 1.3735878309
C 2.4663777627 0.1249557258 -0.0120207634
O -1.109275044 -0.1387994324 -0.6875841978
C 1.2955067338 -0.0975675748 3.5203903703
C 0.2548054393 -0.2346204257 4.3662872358
C 0.4641394128 -0.2732346985 5.799970368
O -0.7104172136 -0.4243290135 6.4845255014
O 1.1446916236 0.0857460355 -2.0422784727
O 1.5019144092 -0.1916737635 6.4205207023
H 2.2814496117 -0.0182691064 3.9713047857
H -0.7655140213 -0.3264958511 4.0248995517
H -0.4507595799 -0.4465282425 7.4109661169
H 1.9823607088 0.1598419265 -2.5115568787
H -0.9480209857 -0.1000457112 -1.6396337499
H 3.3976801223 0.2184836157 -0.5560126958

H 3.3883480533 0.1352896605 1.9171703994
H -0.9061047843 -0.2144199346 1.8542197734

M06-2X Caffeic Acid (Neutral) 0.002 a.u.

C 1.2651423493 0.0491646211 -0.7098956417
C 0.0469755493 -0.0684719922 -0.0240663025
C 0.0417493452 -0.1158746781 1.351737479
C 1.2398892023 -0.0468330221 2.0731720279
C 2.4395176428 0.0727416993 1.3766138065
C 2.4541885861 0.1193576308 -0.0110151159
O -1.1151034801 -0.1340216296 -0.7076711868
C 1.2779912971 -0.0969485693 3.5299562725
C 0.243973459 -0.2455388018 4.36179871
C 0.4761586618 -0.2724539377 5.8130845977
O -0.6769888977 -0.4334637424 6.4991518705
O 1.1585694997 0.0877551289 -2.0632255776
O 1.5348566519 -0.1687678693 6.3749877488
H 2.2600798933 -0.0036610632 3.9850738366
H -0.7785728883 -0.3524666871 4.0294747387
H -0.4401020226 -0.4422769179 7.4342605704
H 2.0212059148 0.158864304 -2.4789258012
H -0.9303452607 -0.086923363 -1.6523030123
H 3.389188076 0.2115491871 -0.5502961526
H 3.3711905383 0.1283092212 1.9239628961
H -0.9144531177 -0.2063675186 1.8487082356

M06-2X Caffeic Acid (Neutral) 0.004 a.u.

C 1.2666670962 0.0498190001 -0.7097862992
C 0.0476458845 -0.068613195 -0.0210843716
C 0.0448297726 -0.1161517528 1.3540775248
C 1.2447744644 -0.0462153468 2.0742681087
C 2.4438219244 0.0741818707 1.3757417355
C 2.4570824517 0.120785895 -0.011758856
O -1.1137948961 -0.134763406 -0.7009212697
C 1.2834139609 -0.097051165 3.5282355291
C 0.2474869698 -0.2429615042 4.3620007294
C 0.4726176641 -0.2727511583 5.809641861
O -0.6863306899 -0.432100791 6.4935886451
O 1.1536804706 0.0873969247 -2.0578157875
O 1.5255163807 -0.1737724326 6.3868502453
H 2.2662863976 -0.0071071579 3.9826438583
H -0.7742345362 -0.3463218251 4.0266824413
H -0.4454973875 -0.4435706199 7.4270137188
H 2.0101286572 0.157839085 -2.4874798763
H -0.9352644689 -0.0903890371 -1.6475185698
H 3.3908946553 0.2132175469 -0.5526025283

H 3.3764948778 0.1301603078 1.921578747
H -0.9111086492 -0.2079592386 1.8512284141

M06-2X Caffeic Acid (Neutral) 0.006 a.u.

C 1.2683520604 0.0504180704 -0.7098955093
C 0.0480665616 -0.0691207689 -0.0186638619
C 0.0471785718 -0.1168652643 1.3558212982
C 1.2487705115 -0.0458942841 2.0754736573
C 2.4476167465 0.0755538832 1.3749982858
C 2.4600405361 0.1223039938 -0.0121562483
O -1.1123355142 -0.1360556163 -0.6953831578
C 1.2880667399 -0.0973928079 3.526068355
C 0.2503912779 -0.2402079226 4.3627801726
C 0.469484872 -0.2730030427 5.8062967377
O -0.6949391183 -0.4296514416 6.4893439479
O 1.149740945 0.0870314072 -2.0525343094
O 1.5170327502 -0.1797216703 6.3982349003
H 2.2718610252 -0.0111723993 3.9795649107
H -0.7707408698 -0.3395389813 4.0250382402
H -0.4489938521 -0.444281663 7.420785294
H 1.999948113 0.158118329 -2.4957192481
H -0.939747213 -0.0937870658 -1.6438506449
H 3.3928470109 0.2151569704 -0.5542717895
H 3.3810693475 0.1320076832 1.9197125266
H -0.9085995023 -0.2102254091 1.852940443

M06-2X Caffeic Acid (Neutral) 0.008 a.u.

C 1.2701776103 0.0508927078 -0.7102420753
C 0.04818415 -0.0697347374 -0.01677464
C 0.0487796776 -0.1175914931 1.357000417
C 1.2518949224 -0.0456085234 2.0768296816
C 2.4509604542 0.0768460572 1.3743158832
C 2.4631207518 0.1237183462 -0.0122282324
O -1.1108001501 -0.1374595974 -0.6909837539
C 1.2920375631 -0.0976045523 3.5234572541
C 0.2527845083 -0.2374093127 4.3641910712
C 0.4666959169 -0.2731781211 5.8030609894
O -0.7028996169 -0.4269518126 6.4863451489
O 1.1467518103 0.0864616857 -2.0473539897
O 1.5092407183 -0.1858206348 6.4093452204
H 2.2768529305 -0.0150007021 3.9758129509
H -0.7679005531 -0.3328346634 4.0244728097
H -0.4506625678 -0.4451696604 7.4154642696
H 1.9907000094 0.1588971568 -2.503694695
H -0.9439357629 -0.0970239688 -1.6412585918
H 3.3950986027 0.2169499933 -0.5553735034

H 3.3849815207 0.133741223 1.9182934878
H -0.9069514958 -0.2124473905 1.8539042977

M06-2X Gallic Acid (Neutral) Zero field

C -0.9500148272 -1.1722007197 0.0021468286
C -1.685770671 0.0076103003 0.0003697177
C -1.0376858094 1.2374967185 -0.0038498132
C 0.3469677907 1.2873565572 -0.0063346031
C 1.069645658 0.1010244616 -0.0045252164
C 0.4289660388 -1.134838198 -0.000271866
O -3.0423190125 0.00868457 0.002684758
O -1.7580647769 2.3813613807 -0.0055282476
C 2.5528158024 0.0929006088 -0.0071643303
O 3.0904879622 1.3250523468 -0.0118549811
O -1.6996982299 -2.3129202947 0.0063645802
O 3.2297642741 -0.8994748358 -0.005517357
H 1.0205866165 -2.0414498809 0.0009898635
H 0.8433525407 2.2461427956 -0.0097406417
H -1.1314938855 -3.0865389084 0.0080136626
H -3.3586162508 -0.9012828681 0.0059851538
H -2.6960095221 2.1613968612 -0.003243817
H 4.048647302 1.2109041052 -0.0132296909

M06-2X Gallic Acid (Neutral) 0.010 a.u.

C -0.9470573824 -1.1886667641 0.0024025001
C -1.6867299839 -0.0042795349 0.0006302047
C -1.033706445 1.2296735628 -0.0035975841
C 0.3496833039 1.2750348131 -0.006097297
C 1.0792500385 0.0878424654 -0.0042552758
C 0.4334995872 -1.1505144417 0.0000429029
O -3.0236981548 0.0188355789 0.0027947289
O -1.7394357304 2.3713822192 -0.0053153291
C 2.5452547159 0.1033465129 -0.0070620144
O 3.079048265 1.3522113602 -0.0123425002
O -1.701695874 -2.3154757246 0.0064665711
O 3.2786346373 -0.8590824994 -0.0053169858
H 1.0170015086 -2.0619199342 0.0013096708
H 0.8377168543 2.2376557429 -0.0096571022
H -1.1616189623 -3.1081890537 0.0075300385
H -3.3994127586 -0.8706497115 0.0052695847
H -2.6865026519 2.1789340766 -0.003566547
H 4.0313300327 1.2150863321 -0.013941566

M06-2X Gallic Acid (Neutral) 0.002 a.u.

C -0.949552351 -1.1753773124 0.002201138
C -1.6857947366 0.0052287845 0.0004262451

C -1.0368072607 1.2357038445 -0.0037967665
C 0.3476359274 1.284669851 -0.0062863086
C 1.0711976947 0.0981938457 -0.0044746233
C 0.4298288 -1.1380414495 -0.0002114883
O -3.0385293083 0.0110048908 0.0027074087
O -1.7539223527 2.3792960856 -0.0054847523
C 2.5511577385 0.0950332581 -0.007155619
O 3.0876896123 1.3304780639 -0.0119461586
O -1.7000381976 -2.3134358053 0.0063893203
O 3.2394287713 -0.891315587 -0.0054823147
H 1.0196173831 -2.0456923829 0.0010481291
H 0.8424012123 2.2441561072 -0.0097223987
H -1.1370941829 -3.090700693 0.0079126078
H -3.366613762 -0.8951098429 0.0058553979
H -2.693732603 2.1649423301 -0.0033299151
H 4.0446886151 1.2121910116 -0.0133559017

M06-2X Gallic Acid (Neutral) 0.004 a.u.

C -0.9490335194 -1.1786006462 0.0022540499
C -1.6858960389 0.0028455907 0.0004809877
C -1.0359825142 1.2340109487 -0.0037448937
C 0.3482389441 1.2821041165 -0.0062391933
C 1.0729063062 0.0954749015 -0.0044237307
C 0.4307182633 -1.1411984895 -0.000150429
O -3.0347893358 0.0132047985 0.002730523
O -1.7500091809 2.3772517071 -0.0054420009
C 2.5495920444 0.0971371342 -0.0071446525
O 3.0851691763 1.3358520255 -0.0120404962
O -1.7003965628 -2.3139595332 0.0064124725
O 3.2491035404 -0.88322128 -0.00544268
H 1.0188172401 -2.0498228208 0.0011080375
H 0.841355122 2.2423240547 -0.0097061809
H -1.1428536935 -3.0949321251 0.0078170129
H -3.3747294581 -0.8889272613 0.0057141671
H -2.6916597287 2.1684306958 -0.0034013099
H 4.0410103956 1.213251183 -0.0134876835

M06-2X Gallic Acid (Neutral) 0.006 a.u.

C -0.9484523131 -1.1818879886 0.0023060175
C -1.6860866408 0.0004583451 0.0005346022
C -1.0352023292 1.2324310686 -0.0036940156
C 0.3487791506 1.2796506676 -0.006193732
C 1.0747980961 0.0928551998 -0.0043731638
C 0.4316325181 -1.1443162065 -0.0000889217
O -3.0310816726 0.0152681394 0.0027557908
O -1.746305387 2.3752342529 -0.0053990413

C 2.5481016211 0.0992138271 -0.0071322666
O 3.0829093962 1.3412234243 -0.0121367686
O -1.7007683355 -2.3144901113 0.0064346614
O 3.2588287412 -0.8751738145 -0.0053993029
H 1.0181500604 -2.0538725382 0.0011696847
H 0.8402140783 2.2406414084 -0.0096930098
H -1.1488061455 -3.099255488 0.0077242817
H -3.3829584233 -0.8827441046 0.0055641638
H -2.6897781695 2.1719026824 -0.0034617382
H 4.0375867545 1.2140862359 -0.0136232418

M06-2X Gallic Acid (Neutral) 0.008 a.u.

C -0.9477969024 -1.1852399287 0.002356164
C -1.6863645682 -0.0019197215 0.0005855803
C -1.0344470204 1.2309805711 -0.0036450638
C 0.3492615016 1.2772978072 -0.0061488329
C 1.0769041471 0.0903165475 -0.0043204248
C 0.4325627781 -1.1474136114 -0.0000260018
O -3.0273911216 0.0171527362 0.0027809702
O -1.742785518 2.3732727609 -0.0053565501
C 2.5466591311 0.1012782333 -0.0071115472
O 3.0808741721 1.3466593016 -0.0122353874
O -1.7011889351 -2.3150039882 0.0064544629
O 3.2686541092 -0.8671370828 -0.0053546581
H 1.0175580534 -2.0578909648 0.0012348543
H 0.8389981914 2.23909053 -0.0096805102
H -1.1550332763 -3.1036750365 0.0076296396
H -3.3912064244 -0.8766376315 0.0054138063
H -2.6880655748 2.1754020903 -0.0035151822
H 4.0343682572 1.2146923873 -0.0137673189

M06-2X Caffeic Acid (Radical) Zero field

C 1.2537415845 0.0547834346 -0.7640775519
C 0.0010789182 -0.0795260134 -0.0027501268
C -0.0118544058 -0.1335519231 1.3675189323
C 1.197312997 -0.0594224674 2.069986357
C 2.4292587961 0.0709949517 1.3568205031
C 2.4740493484 0.1263901661 0.0023964931
O -1.1048000827 -0.1428305071 -0.7257194294
C 1.2632157058 -0.1085656045 3.5145604542
C 0.2326216524 -0.2427914234 4.3595515418
C 0.4890629382 -0.2706655628 5.8143605155
O -0.6511358916 -0.4105508812 6.5133415861
O 1.1798961062 0.0976258341 -1.9943908128
O 1.5654969942 -0.1812057601 6.3377715493
H 2.2502925883 -0.0274325504 3.9594285335

H -0.7960874899 -0.3346286385 4.0413264116
H -0.4137325733 -0.4214350366 7.4493532597
H -0.8233436476 -0.0821905901 -1.6565914154
H 3.4023326972 0.2246622529 -0.5430642226
H 3.3438202704 0.1243782708 1.9339556474
H -0.959574506 -0.2315189513 1.8779947743

M06-2X Caffeic Acid (Radical) 0.010 a.u.

C 1.2574620963 0.0570223942 -0.769005036
C -0.0055791363 -0.0809455524 -0.0003600734
C -0.0083222025 -0.1345341942 1.3736696308
C 1.2053174961 -0.0588492931 2.069646518
C 2.4429520292 0.0720506359 1.3492868183
C 2.4888976186 0.1280107879 0.000082785
O -1.1074882558 -0.1454489962 -0.7039700508
C 1.2744764481 -0.106732739 3.5025968988
C 0.2418182286 -0.2371501019 4.3660076063
C 0.4778688723 -0.2679897603 5.7983954682
O -0.6812011262 -0.412708847 6.5053325079
O 1.1817490994 0.1024553518 -1.9833734637
O 1.5309741855 -0.1830971499 6.3893408262
H 2.2662581981 -0.0291116027 3.9386666035
H -0.784610466 -0.3263347645 4.0424622492
H -0.4064459084 -0.4279970042 7.4277820496
H -0.8678656988 -0.089629762 -1.6503451142
H 3.4120101405 0.2245804224 -0.5549131938
H 3.3588409891 0.1237176194 1.9253794083
H -0.9554606078 -0.234788444 1.8850905616

M06-2X Caffeic Acid (Radical) 0.002 a.u.

C 1.2538402423 0.0542860775 -0.7645584883
C 0.0000368351 -0.0790211707 -0.0014419314
C -0.0098758077 -0.1321466604 1.36979201
C 1.2003662024 -0.0583767795 2.0694522194
C 2.4325704406 0.0707310996 1.355115553
C 2.4766043271 0.125222228 0.0012341738
O -1.1060229723 -0.1418670009 -0.7193076024
C 1.266541108 -0.1067869586 3.5132104947
C 0.2356784601 -0.2423372293 4.3596662257
C 0.4863373709 -0.2697038877 5.8110156876
O -0.6578934293 -0.4149814278 6.509206501
O 1.1789200396 0.096911075 -1.9919242534
O 1.5569286131 -0.1767795847 6.3490680729
H 2.2542054508 -0.0241447309 3.9566599564
H -0.7919859697 -0.3364248905 4.0394643645
H -0.4152850639 -0.4254119888 7.4431645902

H -0.8334478257 -0.0830590577 -1.6535344822
H 3.4035721534 0.2219951536 -0.5467122896
H 3.3478934218 0.1234942457 1.9312419603
H -0.9573315966 -0.2290795119 1.8809602378

M06-2X Caffeic Acid (Radical) 0.004 a.u.

C 1.2542230046 0.0545184391 -0.7651993469
C -0.0011199884 -0.0791159724 -0.0005537643
C -0.008490696 -0.1320060911 1.3714894464
C 1.2027481927 -0.0580538328 2.0691402602
C 2.4355599994 0.0708520872 1.3536206072
C 2.4792837762 0.1252315005 0.0004846273
O -1.1068926914 -0.1420527238 -0.7139550388
C 1.2693014749 -0.1061858219 3.5112970457
C 0.2380454141 -0.2413876491 4.3602958168
C 0.4839112723 -0.2690947062 5.807712467
O -0.6642476036 -0.4163321484 6.5063405177
O 1.1786575007 0.0974874668 -1.9895324467
O 1.5493740412 -0.1760538019 6.3596090838
H 2.257775678 -0.0237741278 3.9531962493
H -0.7889537198 -0.3355249787 4.038623875
H -0.4153267687 -0.4271712201 7.4379485891
H -0.8429355753 -0.084415852 -1.6513603511
H 3.4050548903 0.221429079 -0.5496124141
H 3.3513983194 0.1232490273 1.9291293088
H -0.9557145206 -0.2290796737 1.8830984675

M06-2X Caffeic Acid (Radical) 0.006 a.u.

C 1.2549496741 0.0551922457 -0.766089327
C -0.002426345 -0.0795795561 -0.0000882405
C -0.0077771702 -0.1326164847 1.3726432031
C 1.2043587588 -0.0581791126 2.0690695814
C 2.438239152 0.0711778744 1.3522433842
C 2.4821810687 0.1259256058 0.00012038
O -1.1074053695 -0.1429200418 -0.7096927318
C 1.2714800249 -0.1062415722 3.5088530157
C 0.2397791403 -0.2401205949 4.361519195
C 0.4817530831 -0.2686581989 5.8044723272
O -0.670155211 -0.4158492037 6.5047634721
O 1.1790827988 0.0988548096 -1.987250891
O 1.5426684715 -0.1774895851 6.3696397372
H 2.26093468 -0.0250919858 3.949030831
H -0.7868512632 -0.3330180341 4.0388836537
H -0.4137555966 -0.4277223392 7.4336876767
H -0.8517831593 -0.0860409272 -1.6501533132
H 3.406910073 0.2220846689 -0.5518280282

H 3.354336483 0.123331477 1.9275484757
H -0.9548672937 -0.230520045 1.8844005987

M06-2X Caffeic Acid (Radical) 0.008 a.u.

C 1.255978464 0.0564580863 -0.7672906276
C -0.0038801472 -0.0805183237 -0.0000314701
C -0.0076362592 -0.1342310872 1.3733435261
C 1.205272122 -0.0589347788 2.0692142437
C 2.4407125786 0.0716515097 1.3508456644
C 2.4853127082 0.1274481241 0.0000388213
O -1.1075770181 -0.1446569256 -0.7063979378
C 1.2732388467 -0.1071023383 3.5059301583
C 0.2409847039 -0.2383167367 4.3634147876
C 0.4797780705 -0.2683173166 5.8013683321
O -0.6759007096 -0.4132950984 6.5044383105
O 1.1800452654 0.1013985858 -1.9851433645
O 1.5367028234 -0.1811865857 6.3794623066
H 2.2639062156 -0.028526099 3.9441110455
H -0.7856049417 -0.3282581098 4.0402456684
H -0.4109095687 -0.4270855456 7.4303323984
H -0.8600336605 -0.0879855323 -1.6498197392
H 3.4090833714 0.224236083 -0.5535886425
H 3.3568400861 0.1236513285 1.9263166227
H -0.9546609507 -0.2339102398 1.8849828962

M06-2X Gallic Acid (Radical) Zero field

C -0.9429119638 -1.2202473081 0.0031376008
C -1.7459276454 -0.0047236154 0.001633823
C -1.0165227094 1.263912325 -0.0033853769
C 0.358166233 1.315298191 -0.0063569748
C 1.0605916131 0.111515479 -0.0045392738
C 0.4233687888 -1.1418571328 0.0001424424
O -2.9784532019 0.0155929382 0.0042768757
O -1.7679627537 2.3537200595 -0.0047957179
C 2.5485628198 0.0949292274 -0.0075799994
O 3.0898657045 1.322235936 -0.0126520955
O -1.6428608374 -2.3584079829 0.0075766909
O 3.2108502288 -0.9059992352 -0.0057966601
H 1.0392569954 -2.032497493 0.0012080666
H 0.8730610775 2.2637944187 -0.0100613775
H -1.0494075307 -3.1154104754 0.0085607326
H -2.6932455917 2.050865204 -0.0018588088
H 4.0486607731 1.2104024639 -0.0142149471

M06-2X Gallic Acid (Radical) 0.010 a.u.

C -0.9391701868 -1.234504414 0.0032307864

C -1.7470046211 -0.0106342731 0.0017041649
C -1.0158946548 1.2635870472 -0.0033236897
C 0.3608064549 1.3064055114 -0.006265612
C 1.0672735046 0.1010688465 -0.0044071748
C 0.4286826255 -1.1571615454 0.0003151333
O -2.967177564 0.0033783344 0.00464571
O -1.7499333987 2.3542870284 -0.0048071277
C 2.5383489489 0.1052736202 -0.0074606714
O 3.0808345188 1.3474605984 -0.0128644684
O -1.6531087004 -2.3528367857 0.0075487183
O 3.2547115561 -0.868353752 -0.0056262008
H 1.0376560673 -2.0519389867 0.0013848003
H 0.8705778291 2.2572750025 -0.0100836011
H -1.0951234068 -3.1358672375 0.008120873
H -2.6892780217 2.0883559983 -0.0022782283
H 4.0328910492 1.2073280072 -0.014538412

M06-2X Gallic Acid (Radical) 0.002 a.u.

C -0.9423376644 -1.2228815582 0.0031606546
C -1.7459110734 -0.0058372972 0.0016821293
C -1.0163626098 1.2636003901 -0.0033735
C 0.3588346548 1.313233637 -0.006346156
C 1.0615250713 0.1092238529 -0.0045113286
C 0.4244256237 -1.1448420849 0.0001752869
O -2.9760768789 0.0134246979 0.0043292072
O -1.7640169718 2.3537697626 -0.0048020061
C 2.5464493601 0.096936986 -0.0075545793
O 3.0875745538 1.3271183281 -0.0127153263
O -1.6448089767 -2.3572706585 0.0075614987
O 3.2195195972 -0.89846452 -0.0057230365
H 1.0387050781 -2.0364169229 0.0012342512
H 0.8726628448 2.2621843669 -0.0100803393
H -1.057955926 -3.1192636567 0.0084593623
H -2.6922093224 2.0584028398 -0.0019217283
H 4.0450746397 1.2102048371 -0.0142793897

M06-2X Gallic Acid (Radical) 0.004 a.u.

C -0.9416805462 -1.2256205549 0.0031874627
C -1.746008369 -0.0069809563 0.0017359571
C -1.0162306001 1.2634108768 -0.0033614656
C 0.3594341829 1.3113007199 -0.0063347387
C 1.0626542997 0.1070291768 -0.0044803642
C 0.4254956832 -1.1478613823 0.0002136119
O -2.9737646664 0.0111308309 0.0043728962
O -1.7602740663 2.3538412711 -0.0048090766
C 2.5443958954 0.0989829012 -0.0075296562

O 3.0855715609 1.3320670076 -0.0127729551
O -1.6468164981 -2.3561382815 0.0075485737
O 3.2282647926 -0.8909010402 -0.0056627755
H 1.0382480563 -2.0403383393 0.0012663104
H 0.872195986 2.2607265332 -0.0101018591
H -1.0668237107 -3.1232509933 0.0083534549
H -2.6913347205 2.0659237731 -0.0019840716
H 4.0417647204 1.2098014571 -0.0143463043

M06-2X Gallic Acid (Radical) 0.006 a.u.

C -0.9410086726 -1.2284243728 0.0032108436
C -1.746201147 -0.0081236409 0.0017710501
C -1.0161146214 1.2633527702 -0.0033561103
C 0.3600059002 1.3095141691 -0.0063459788
C 1.0639973806 0.1048827765 -0.004487374
C 0.4265780216 -1.1509399522 0.0002312671
O -2.9716491325 0.0087758102 0.0044634132
O -1.7566643992 2.353992394 -0.0048128928
C 2.5424304253 0.1010156261 -0.0075671434
O 3.0836732215 1.3371225362 -0.0127887888
O -1.6488756947 -2.3550563491 0.0075599076
O 3.2370452734 -0.8834861373 -0.0056059616
H 1.0378785363 -2.0443027704 0.0012774944
H 0.8717553446 2.2594225537 -0.0101502694
H -1.0758390814 -3.1272931039 0.0082784978
H -2.6904855428 2.0733181354 -0.0020488751
H 4.038566188 1.2093525552 -0.0143340795

M06-2X Gallic Acid (Radical) 0.008 a.u.

C -0.9402081994 -1.2313716571 0.0032413778
C -1.7465476649 -0.0093213976 0.0018319851
C -1.016039869 1.263429399 -0.003353471
C 0.36046064 1.3078927365 -0.0063699001
C 1.0655338919 0.1028910007 -0.0045004033
C 0.4276523505 -1.1540303529 0.0002496705
O -2.9695653946 0.0062424704 0.0045429234
O -1.7533022839 2.3541645976 -0.0048193993
C 2.5404904632 0.1030968805 -0.0076256772
O 3.0821848166 1.3422102273 -0.0127888911
O -1.65096416 -2.3539954437 0.0075743747
O 3.2458835505 -0.876035881 -0.0055513754
H 1.0376558508 -2.0481909484 0.0012829751
H 0.8711979546 2.2582993064 -0.0102235175
H -1.0852013433 -3.1315166094 0.008195315
H -2.6898837369 2.0807854862 -0.0020896066
H 4.035745134 1.2085731853 -0.01430138

M11 Caffeic Acid (Neutral) -0.010 a.u.

C 1.2543318116 0.0741322851 -0.7057322172
C 0.0468395268 -0.143542231 -0.0517127935
C 0.0224176309 -0.2481782386 1.3237248126
C 1.2000127495 -0.1337355371 2.0630966991
C 2.3994176271 0.0746048955 1.388274875
C 2.4281822672 0.1817334032 0.0078517714
O -1.1006218229 -0.254847577 -0.7831906996
C 1.2372763101 -0.2240817484 3.5292262919
C 0.2109838864 -0.1772347906 4.3653203853
C 0.505108318 -0.270604092 5.8305593052
O -0.607308858 -0.197559392 6.5614173393
O 1.1940772115 0.1665147652 -2.0900299745
O 1.6090831746 -0.3934533885 6.2768578544
H 2.2223578694 -0.3173744495 3.9857170206
H -0.8260379121 -0.0612511173 4.0666076163
H -0.3820525854 -0.2540205683 7.5031596576
H 2.0674020765 0.3893495632 -2.4164915444
H -0.8745854406 -0.1377383034 -1.7102905337
H 3.3683115577 0.3492340539 -0.5136551822
H 3.3182069666 0.1594748998 1.9590620095
H -0.9282913651 -0.427750432 1.8148113071

M11 Caffeic Acid (Neutral) -0.002 a.u.

C 1.2620981448 0.037954529 -0.7049096025
C 0.0447133356 -0.0527778308 -0.0261393649
C 0.0327066772 -0.084683141 1.350109919
C 1.2272312902 -0.027235414 2.0703816101
C 2.4286111224 0.0694237767 1.3797149818
C 2.448704542 0.0999416619 -0.0069104703
O -1.1135374259 -0.1064282933 -0.7272774249
C 1.2621513631 -0.0685930105 3.5352144622
C 0.2363334989 -0.2653945406 4.3550202131
C 0.483800007 -0.273614908 5.8147031819
O -0.6467799471 -0.4869087206 6.512388679
O 1.168644195 0.0644526789 -2.0708724032
O 1.5502552419 -0.1135446974 6.3439238986
H 2.2370509274 0.0695739042 4.0018926417
H -0.7839297379 -0.4266945748 4.0259072011
H -0.4204110271 -0.479642291 7.4522070202
H 2.038796426 0.1207733036 -2.4717108546
H -0.9138588486 -0.0671091028 -1.6690028857
H 3.3896159813 0.1743546295 -0.5455740142
H 3.3598485095 0.119340866 1.9344931211
H -0.9269342757 -0.1495168253 1.8510240905

M11 Caffeic Acid (Neutral) -0.004 a.u.

C 1.2603733305 0.0525461813 -0.7059929609
C 0.0455151178 -0.0801401844 -0.0329722612
C 0.0305086975 -0.1361067918 1.3430496174
C 1.2208578137 -0.0606089393 2.067941743
C 2.4215179575 0.0718224955 1.3810611753
C 2.4437342168 0.128332188 -0.0043041535
O -1.1104938228 -0.1523177748 -0.7410604631
C 1.2573285084 -0.1156413772 3.5336475843
C 0.2260834034 -0.2402737715 4.3589941756
C 0.4904615718 -0.2741699087 5.8197837467
O -0.6437979339 -0.3911744875 6.528257332
O 1.1750360668 0.1006048626 -2.0764994645
O 1.5763897875 -0.2064108247 6.3257327176
H 2.2411865875 -0.0456221733 3.9965675876
H -0.8073366242 -0.3198315741 4.0401468032
H -0.4142499286 -0.4062937579 7.4679595621
H 2.0496851723 0.1926494924 -2.4599138393
H -0.9043945432 -0.0901490062 -1.6795588563
H 3.3844870684 0.2332098781 -0.5387612521
H 3.3497540726 0.1324727493 1.9396725746
H -0.9275355196 -0.2392252759 1.8408326314

M11 Caffeic Acid (Neutral) -0.006 a.u.

C 1.2563415355 0.071740742 -0.7043443695
C 0.0483709414 -0.1255416751 -0.0384535024
C 0.033816657 -0.2182016663 1.3363855398
C 1.2189154855 -0.1136649485 2.0653809409
C 2.4154395372 0.0747718747 1.3832160808
C 2.4360041019 0.1704238434 0.0006009609
O -1.1039005044 -0.2273425953 -0.7537580803
C 1.2561925828 -0.1933095123 3.5310365629
C 0.2216622298 -0.1913968914 4.3601026168
C 0.492962537 -0.2706936983 5.8220733644
O -0.6383987062 -0.2513906358 6.5384794042
O 1.1762194701 0.1512958906 -2.0786711151
O 1.5867987997 -0.3415960652 6.3076113787
H 2.242931615 -0.2443900552 3.9902454281
H -0.8152190907 -0.1251256852 4.0481182544
H -0.4117177523 -0.3005254017 7.4784966174
H 2.0464154482 0.3260984605 -2.4419503404
H -0.8938946382 -0.1313612712 -1.6879904265
H 3.3733758092 0.3217355293 -0.5292420302
H 3.340196415 0.1525074762 1.9453633504
H -0.9174014735 -0.3803607153 1.8318843648

M11 Caffeic Acid (Neutral) -0.008 a.u.

C 1.2548694551 0.0740146176 -0.7048042521
C 0.0478427737 -0.136910051 -0.0446913276
C 0.028999431 -0.2363867292 1.3304166782
C 1.2102617658 -0.1244045822 2.0642254756
C 2.4075986044 0.077061374 1.3856423767
C 2.4315632873 0.179613726 0.0041604643
O -1.1020055793 -0.2461944855 -0.7677072788
C 1.2475957399 -0.2100505897 3.5302438327
C 0.2167893428 -0.1825187126 4.3623508513
C 0.4986406742 -0.2702585924 5.8260920222
O -0.6237515724 -0.22068968 6.5492929488
O 1.184090897 0.1602863418 -2.0840805191
O 1.5974752552 -0.3708576699 6.2924444024
H 2.2334459836 -0.2854371311 3.9881495558
H -0.8199923176 -0.0874369271 4.0565781433
H -0.3983525464 -0.2746469319 7.4902250391
H 2.05658202 0.3570963311 -2.4294808649
H -0.8843911272 -0.1400727484 -1.6985989036
H 3.3697894579 0.3416808842 -0.5216938147
H 3.3293749123 0.16010316 1.9518605491
H -0.9213154573 -0.4103196036 1.8239586213

M11 Gallic Acid (Neutral) -0.010 a.u.

C -0.9503482771 -1.1530200248 0.001870543
C -1.6820326153 0.0225432943 0.0000167307
C -1.0395032928 1.2497623345 -0.0041999463
C 0.3447831549 1.3032085266 -0.0066780163
C 1.0597842659 0.1166196534 -0.0048244912
C 0.4251100274 -1.1174666279 -0.0005856249
O -3.0581948808 -0.0065852701 0.0026112385
O -1.7887122909 2.3881372087 -0.0057754146
C 2.5611222036 0.0810989278 -0.0072891934
O 3.1097641851 1.2959074001 -0.0111915867
O -1.7023831321 -2.3056236098 0.0062569466
O 3.1791139499 -0.943227897 -0.0059798492
H 1.0346634315 -2.0173833362 0.0007758103
H 0.8572897394 2.2580250351 -0.009912935
H -1.1209061579 -3.0712502025 0.0087227065
H -3.316315679 -0.9350756557 0.0065188067
H -2.7171739009 2.1368944299 -0.0025836918
H 4.0755002691 1.2086608137 -0.0124580328

M11 Gallic Acid (Neutral) -0.002 a.u.

C -0.9490498741 -1.1660847954 0.0020873298

C -1.6808985363 0.0124140889 0.0002819103
C -1.0349502793 1.2407956112 -0.0038761129
C 0.3485176017 1.2905755445 -0.0063573969
C 1.064342185 0.1035817738 -0.0045303407
C 0.4285450862 -1.1311277384 -0.0003125772
O -3.0416112076 0.0051356667 0.0026472236
O -1.7682188905 2.3791089768 -0.005479247
C 2.5530653392 0.0902125515 -0.0071668371
O 3.0940791379 1.3189171751 -0.0119411381
O -1.7022504182 -2.3084740643 0.0062501092
O 3.2184174724 -0.9093996481 -0.0053863067
H 1.028520585 -2.0362325396 0.0010116935
H 0.8538184899 2.2482778357 -0.0096639565
H -1.1406665585 -3.0877968643 0.0082210457
H -3.3501898435 -0.908268959 0.0058952409
H -2.7050093919 2.152675197 -0.0030718713
H 4.0551001026 1.2169151879 -0.0133147688

M11 Gallic Acid (Neutral) -0.004 a.u.

C -0.9494153781 -1.1627775298 0.0020325701
C -1.6810655585 0.0149504267 0.000219038
C -1.0360226748 1.2429470845 -0.0039540758
C 0.3476400147 1.2936310705 -0.0064377164
C 1.062988243 0.1067526096 -0.0046079744
C 0.4276542659 -1.1277332047 -0.0003849847
O -3.045630517 0.0023506501 0.0026399183
O -1.7730524289 2.3813564394 -0.005548117
C 2.5549028726 0.0879347196 -0.0072005799
O 3.0976572697 1.3131762877 -0.011759755
O -1.7021917394 -2.3077586046 0.006248105
O 3.2084115583 -0.9179536062 -0.0055156722
H 1.0298910549 -2.0315850829 0.0009474869
H 0.8547787426 2.2505658771 -0.0097252841
H -1.1354432338 -3.0835691583 0.0083376996
H -3.3415527116 -0.9150588814 0.0060672473
H -2.7078227861 2.1488643024 -0.0029669451
H 4.0598340065 1.2151316003 -0.0130969608

M11 Gallic Acid (Neutral) -0.006 a.u.

C -0.9497521233 -1.1594962592 0.0019756094
C -1.6813112142 0.0174883282 0.0001500928
C -1.0371444986 1.245167577 -0.004035036
C 0.3467185749 1.2967630262 -0.0065153175
C 1.0617762497 0.1099905161 -0.0046791526
C 0.4267828949 -1.1243205485 -0.0004537305
O -3.049735344 -0.0005487446 0.0026249627

O -1.7780892854 2.3836165871 -0.0056219483
C 2.5568602363 0.0856557669 -0.0072221189
O 3.1014845714 1.3074149763 -0.0115765016
O -1.702197405 -2.3070397479 0.006244071
O 3.1985143064 -0.9264535331 -0.0056592032
H 1.0313759009 -2.026885245 0.000889139
H 0.8556747947 2.2529584458 -0.0097820134
H -1.1304242054 -3.0794036263 0.0084625207
H -3.3330016711 -0.9218180836 0.0062336069
H -2.7108016397 2.1449781699 -0.0028495391
H 4.0648308576 1.2131573948 -0.0128914415

M11 Gallic Acid (Neutral) -0.008 a.u.

C -0.9500606939 -1.1562440864 0.0019216096
C -1.6816333391 0.0200203366 0.0000827935
C -1.0383016762 1.2474396498 -0.0041182783
C 0.3457678613 1.299953127 -0.0065979118
C 1.0607127236 0.113276659 -0.0047540404
C 0.4259346113 -1.1209011266 -0.0005220651
O -3.053919071 -0.0035335683 0.0026169866
O -1.7832998153 2.3858812978 -0.0056989104
C 2.5589232723 0.0833787884 -0.0072565799
O 3.1055082122 1.3016679301 -0.0113814203
O -1.7022642318 -2.3063248357 0.0062487456
O 3.1887480065 -0.9348748021 -0.0058175989
H 1.0329618484 -2.0221570356 0.0008301412
H 0.8565131891 2.2554426346 -0.0098479674
H -1.1255867424 -3.0752970844 0.0085907916
H -3.3245703517 -0.9285006757 0.0063892983
H -2.7139114911 2.1409985465 -0.0027219413
H 4.0700386878 1.2109992452 -0.0126696524

M11 Caffeic Acid (Radical) -0.010 a.u.

C 1.2564168591 0.0559671504 -0.7594935767
C 0.0010588293 -0.0835466392 -0.0117891299
C -0.0356625718 -0.1402115555 1.3491489119
C 1.1678431435 -0.061911833 2.0745680616
C 2.4034263277 0.0777367435 1.3693174523
C 2.4617866367 0.135760547 0.0171729072
O -1.0885434824 -0.1505754249 -0.7839397484
C 1.2328857128 -0.1175842743 3.512261738
C 0.2039938436 -0.2397863943 4.3605032629
C 0.5111566248 -0.2803019017 5.8280386076
O -0.5970566945 -0.3775192056 6.55541432
O 1.1902025463 0.0951002545 -2.0029704685
O 1.6257345524 -0.229902136 6.259172724

H 2.2189959105 -0.0546555876 3.9708785482
H -0.8370176057 -0.3115550291 4.0623323909
H -0.3759541502 -0.3974343888 7.5003751027
H -0.743599944 -0.08378715 -1.6929783976
H 3.4014761076 0.2432597485 -0.5130881622
H 3.3124748449 0.1385781801 1.960589089
H -0.9879654906 -0.2451121039 1.8562593669

M11 Caffeic Acid (Radical) -0.002 a.u.

C 1.2509978383 0.0585607165 -0.7595918917
C -0.0013826324 -0.084297938 0.0015713086
C -0.0156102186 -0.1424782901 1.3678585513
C 1.1937980411 -0.0636957369 2.0692378438
C 2.4241078962 0.0756058312 1.3578292862
C 2.4705452975 0.1360485873 0.0064963909
O -1.098807298 -0.1515464865 -0.7388440533
C 1.2596459509 -0.1179317474 3.5149233314
C 0.2264173581 -0.2375227402 4.3526755757
C 0.4928560427 -0.2751895057 5.8117329207
O -0.6413448838 -0.3844644121 6.5210609296
O 1.1728357217 0.1016336999 -1.9901267362
O 1.5804836744 -0.2162064951 6.3150915015
H 2.2476516632 -0.0537999107 3.968611092
H -0.808060286 -0.3098379193 4.0367126386
H -0.4106301793 -0.4036697731 7.4600377639
H -0.7998772625 -0.0865282621 -1.6653531402
H 3.4012561357 0.2427540281 -0.538975291
H 3.3401121652 0.1342889421 1.9384269245
H -0.9633430246 -0.2492035877 1.8823980537

M11 Caffeic Acid (Radical) -0.004 a.u.

C 1.2521178993 0.0573165113 -0.7594052474
C -0.0006683069 -0.0837684243 -0.0012088047
C -0.0199817078 -0.1411242262 1.3640073751
C 1.1879395132 -0.0628542295 2.0701756797
C 2.4193028366 0.0758860757 1.3602972993
C 2.4684137163 0.1352692727 0.0087880453
O -1.0964932768 -0.150652415 -0.7487386144
C 1.253485836 -0.1171834384 3.5150385813
C 0.2214270715 -0.2386932882 4.3537795057
C 0.4969198942 -0.2763940486 5.8153578202
O -0.631020094 -0.3840797659 6.5284292829
O 1.1763412072 0.0994460064 -1.9929746834
O 1.5910860159 -0.2178325933 6.3015742687
H 2.2408122275 -0.0519765673 3.9700386859
H -0.8144126049 -0.3124675721 4.0417717999

H -0.4033375331 -0.4029590401 7.4689964001
H -0.7865758703 -0.0856279845 -1.6712942388
H 3.4012165471 0.2417447937 -0.5332097334
H 3.3337506513 0.1350305149 1.9432348346
H -0.9686720224 -0.2465605811 1.8771147437

M11 Caffeic Acid (Radical) -0.006 a.u.

C 1.2531318547 0.0581067707 -0.7593388732
C 0.0000036202 -0.084597002 -0.0042868846
C -0.0243747382 -0.1428967521 1.3596537767
C 1.1820569578 -0.063712766 2.0713524376
C 2.4144414374 0.0769986988 1.3628994324
C 2.4661168804 0.1372373178 0.0112323091
O -1.0940036058 -0.1523278798 -0.7593223301
C 1.247552616 -0.1193156253 3.5145962482
C 0.2162029251 -0.2381459459 4.3554917185
C 0.5012803562 -0.277955165 5.8193965164
O -0.6210344765 -0.3779001766 6.5365345557
O 1.1799743757 0.0998583139 -1.9960328798
O 1.6023365686 -0.2263552229 6.2880053419
H 2.234649885 -0.0575596662 3.9706930483
H -0.8214649814 -0.3077248315 4.0475242611
H -0.3962287341 -0.3981302984 7.4786308299
H -0.7731754933 -0.085541105 -1.6776549084
H 3.4008705207 0.2454509765 -0.5271506582
H 3.3271787155 0.1370793584 1.948439241
H -0.973862684 -0.2500499994 1.8711098173

M11 Caffeic Acid (Radical) -0.008 a.u.

C 1.2546540173 0.0569587134 -0.7593677265
C 0.0005240689 -0.0840293542 -0.007780982
C -0.029768092 -0.1414305021 1.3547428092
C 1.1752313489 -0.0627200213 2.072835841
C 2.4091215669 0.0773858759 1.3659179994
C 2.463996616 0.1364387787 0.0140378811
O -1.0914071596 -0.1513787106 -0.7710427039
C 1.2405156419 -0.1183525744 3.5136999704
C 0.2103950657 -0.2391320972 4.357658678
C 0.5060177403 -0.279203784 5.8235403886
O -0.6094766006 -0.3777118081 6.5454635625
O 1.184745321 0.0973294169 -1.9993602342
O 1.6137780642 -0.2281810987 6.2738407607
H 2.2270689001 -0.0557480536 3.9710694444
H -0.828857257 -0.3100940853 4.0543364133
H -0.3867915766 -0.3977119623 7.489022826
H -0.7587563064 -0.0846624214 -1.6848863238

H 3.4011358156 0.2442412495 -0.5204334863
H 3.320070292 0.1378575626 1.9542279156
H -0.9805454667 -0.2473361238 1.8642499665

M11 Gallic Acid (Radical) -0.010 a.u.

C -0.9441688992 -1.2066983609 0.0031086156
C -1.7449514041 0.0035269704 0.0014080515
C -1.0144237789 1.2712029932 -0.0034547466
C 0.3551717842 1.3299310717 -0.0064451804
C 1.0538257014 0.1253767828 -0.0047458428
C 0.4170567514 -1.1255397259 -0.0000654132
O -2.9865871028 0.031861328 0.003976016
O -1.7984594027 2.349586401 -0.0047129623
C 2.5589424352 0.0834041388 -0.0079581019
O 3.1075614557 1.2951310246 -0.0119172312
O -1.6338418855 -2.362811399 0.0078473734
O 3.1639020427 -0.9477694931 -0.0068224229
H 1.0497039142 -2.0099405834 0.0010333158
H 0.8824683357 2.2760599452 -0.0100183281
H -1.0185408776 -3.1038095896 0.0093209918
H -2.7070088041 1.9993093592 -0.0017297057
H 4.0744417342 1.2143021371 -0.013529429

M11 Gallic Acid (Radical) -0.002 a.u.

C -0.942459488 -1.216703116 0.0031358448
C -1.7436935977 -0.0006723017 0.0015652857
C -1.0128326471 1.26845876 -0.0034003362
C 0.3588184913 1.3196284633 -0.006374626
C 1.0556324312 0.1143738142 -0.004578148
C 0.4214980432 -1.1377398641 0.0000634184
O -2.9756462641 0.0241597405 0.0040739839
O -1.7793343605 2.3500943683 -0.0047169307
C 2.5491380566 0.0916179827 -0.007651625
O 3.0940301785 1.3151973871 -0.0125268547
O -1.6408010151 -2.3584387992 0.0076410306
O 3.1989575935 -0.9167794703 -0.0059756293
H 1.0454636871 -2.0268734606 0.0011762549
H 0.8813921016 2.2674221147 -0.0100136366
H -1.0501402316 -3.1183872314 0.0087945762
H -2.7006951129 2.0318011838 -0.0017836879
H 4.0557641342 1.2159634286 -0.0141339199

M11 Gallic Acid (Radical) -0.004 a.u.

C -0.9429409086 -1.2141078136 0.0031231693
C -1.7438847284 0.000442885 0.0015184462
C -1.0131545739 1.2690767772 -0.0034149197

C 0.3580011608 1.3220890847 -0.0063906578
C 1.0549341628 0.1170465955 -0.0046172493
C 0.4203517025 -1.134625083 0.0000288004
O -2.9781902747 0.0262806527 0.0040438363
O -1.7839343752 2.3499403099 -0.0047150057
C 2.5514323399 0.0895159349 -0.0077085973
O 3.0971004618 1.3100993584 -0.0123796976
O -1.638953147 -2.3595249435 0.0076842855
O 3.1899895189 -0.9246453006 -0.006179911
H 1.0463693355 -2.0226143175 0.0011431998
H 0.8817922963 2.2694137256 -0.0100078869
H -1.0418072527 -3.1145752777 0.008930749
H -2.702121211 2.0235438774 -0.0017629534
H 4.0601074929 1.2157665346 -0.0140006079

M11 Gallic Acid (Radical) -0.006 a.u.

C -0.9433921339 -1.2115997492 0.003117587
C -1.7441500435 0.0015199857 0.0014849964
C -1.0135041757 1.2697223205 -0.0034321196
C 0.3571595439 1.3245923972 -0.0064228606
C 1.0544549748 0.1197203137 -0.0046749805
C 0.4192399512 -1.1316086422 -0.000011047
O -2.9808815267 0.0282672538 0.0040260326
O -1.7885539545 2.3498538723 -0.0047120938
C 2.5537857989 0.0874548929 -0.007809821
O 3.1002386354 1.3051925674 -0.0122244756
O -1.6371999673 -2.3606336914 0.0077415268
O 3.1812344229 -0.9324007075 -0.0063658956
H 1.047342665 -2.0184614565 0.0010988178
H 0.8821378832 2.271490013 -0.0100300156
H -1.0337855973 -3.1108940812 0.0090623115
H -2.7035474567 2.0154409602 -0.0017351855
H 4.0645129803 1.2154667512 -0.0138177773

M11 Gallic Acid (Radical) -0.008 a.u.

C -0.9437962564 -1.2091302836 0.0031125236
C -1.744512167 0.0025457881 0.0014468742
C -1.0139302637 1.2704432801 -0.0034443552
C 0.3562059055 1.327217381 -0.0064368331
C 1.0540686377 0.1225110333 -0.0047133228
C 0.4181367465 -1.1285678343 -0.0000404491
O -2.983667405 0.0301274756 0.0039998146
O -1.7934235767 2.3497214081 -0.0047120528
C 2.5562956273 0.0854175912 -0.007886201
O 3.1037677012 1.3001655431 -0.0120682937
O -1.6354935379 -2.361722513 0.0077943851

O 3.1725252306 -0.9401094138 -0.0065916172
H 1.048462942 -2.0142138931 0.0010643764
H 0.8823581612 2.2737115578 -0.0100275683
H -1.0260377552 -3.1073037952 0.0091944614
H -2.705203675 2.0073394922 -0.0017280427
H 4.0693356848 1.2149701825 -0.0136686995

M11 Caffeic Acid (Neutral) Zero field

C 1.2632740544 0.0410143927 -0.7044339864
C 0.0463178566 -0.056161931 -0.0218923586
C 0.0382086423 -0.0916849331 1.3535949183
C 1.2348261896 -0.0310220437 2.0712491972
C 2.4343181656 0.0713814899 1.3784128692
C 2.4513577821 0.105516333 -0.0084786525
O -1.1121061312 -0.1130383546 -0.7176840714
C 1.2703242647 -0.0755660728 3.5341954061
C 0.2403993677 -0.2594811755 4.354296272
C 0.479093666 -0.2738263549 5.8109781158
O -0.660223794 -0.4746406842 6.5046411629
O 1.1613551444 0.0696457938 -2.0649827654
O 1.540898634 -0.1289454414 6.3567060289
H 2.2474287872 0.0496301506 4.0000762829
H -0.780598486 -0.4057842613 4.0213645961
H -0.4311721943 -0.4716611023 7.4431104431
H 2.0247193926 0.1270226715 -2.4810687554
H -0.9200596784 -0.0732917744 -1.661569162
H 3.3903044397 0.1844055558 -0.549370905
H 3.3671317814 0.1230662591 1.9305364556
H -0.9206868842 -0.1629065171 1.8549029085

M11 Caffeic Acid (Neutral) 0.010 a.u.

C 1.2716846292 0.0508083105 -0.704709796
C 0.0502748928 -0.0695218147 -0.0087354534
C 0.0532919862 -0.1170438993 1.362699442
C 1.2581815904 -0.0449199304 2.0775766537
C 2.4545989094 0.0770664496 1.3748589804
C 2.4657684369 0.1238903997 -0.0106382655
O -1.1034125917 -0.1370733709 -0.6875912606
C 1.2974085384 -0.0972670225 3.5231065001
C 0.2543697576 -0.2366591765 4.3586127682
C 0.4619492547 -0.2728035008 5.7939213522
O -0.7109743815 -0.4285773683 6.4829839648
O 1.1392280616 0.0851342561 -2.0372836492
O 1.5001001263 -0.1850578484 6.4143327813
H 2.283380046 -0.0165106538 3.9817758597
H -0.7673143832 -0.3323733019 4.0129058134

H -0.4538510642 -0.4460702872 7.4109331507
H 1.9676284041 0.1578671632 -2.5237678444
H -0.9435200646 -0.0975042082 -1.640817939
H 3.398569255 0.2172609554 -0.5578774496
H 3.3920635185 0.1343856441 1.9198724854
H -0.9043139218 -0.2113587956 1.8624259058

M11 Caffeic Acid (Neutral) 0.002 a.u.

C 1.2645955174 0.0440760006 -0.7041400332
C 0.0477593474 -0.0600589189 -0.0182144264
C 0.0430340191 -0.0994412018 1.3564783553
C 1.241548496 -0.0354273379 2.072186482
C 2.4394701595 0.0729805656 1.3773235055
C 2.4540022798 0.1110883196 -0.0096832847
O -1.1104482251 -0.1201878451 -0.7093077003
C 1.2776700659 -0.0828217433 3.5327885227
C 0.2440434986 -0.253579621 4.3541277464
C 0.4748526108 -0.273809912 5.8074287481
O -0.672799268 -0.4609389294 6.4980777415
O 1.1548707812 0.0750829115 -2.0592155963
O 1.5321445817 -0.1448820906 6.3690022085
H 2.2569854375 0.0293189155 3.997575569
H -0.7776583612 -0.3848295716 4.0179068926
H -0.4401901054 -0.4625605506 7.4349942022
H 2.0112751876 0.1354291011 -2.4901484255
H -0.9256199557 -0.079447392 -1.6552056812
H 3.391175354 0.1946580469 -0.552443864
H 3.3736343471 0.1264455402 1.9271958216
H -0.9152347683 -0.1774222868 1.8578572162

M11 Caffeic Acid (Neutral) 0.004 a.u.

C 1.2660514727 0.0468206379 -0.703988993
C 0.0489454164 -0.0635037933 -0.0150613727
C 0.0470534293 -0.1062840588 1.3588650383
C 1.2472896249 -0.0393556228 2.0732619115
C 2.4440836056 0.0743110051 1.3764504513
C 2.456715115 0.1159993537 -0.0104712132
O -1.1087048585 -0.1264684358 -0.702048631
C 1.28407443 -0.0889792945 3.531025034
C 0.2472884326 -0.2481706783 4.3544269133
C 0.4709997181 -0.2736643118 5.8039518987
O -0.6841482867 -0.4487628093 6.4925624343
O 1.1493342063 0.0799999191 -2.0535407392
O 1.5236567796 -0.1589987992 6.3807900682
H 2.265358709 0.0117623486 3.9945542058
H -0.7747907814 -0.3662926999 4.0152058778

H -0.4470489796 -0.4548828615 7.4276868939
H 1.9987657013 0.1427324041 -2.4989537539
H -0.9307308967 -0.0851972746 -1.6498777858
H 3.3923325998 0.203674799 -0.5548188145
H 3.3793595777 0.1292705895 1.9245311944
H -0.9107740155 -0.1903384171 1.8600333815

M11 Caffeic Acid (Neutral) 0.006 a.u.

C 1.2677479222 0.0488432631 -0.7039929573
C 0.0497824454 -0.0663754251 -0.0123803204
C 0.0501174701 -0.1116848391 1.3607042361
C 1.2520289261 -0.0423649142 2.0745013161
C 2.4481180691 0.0753643994 1.3758077322
C 2.4595398926 0.1197623544 -0.0109205098
O -1.1068875223 -0.1315392951 -0.6960404779
C 1.2894600324 -0.0935035694 3.5288476772
C 0.2500920505 -0.243452305 4.3552172715
C 0.4675861924 -0.2734050993 5.8005213114
O -0.6942494821 -0.4389951025 6.4881311163
O 1.1447727543 0.0832615276 -2.0479880469
O 1.5154562912 -0.1706056335 6.3921903931
H 2.2724693994 -0.0019060676 3.9909697318
H -0.7720927503 -0.3511194237 4.0134769414
H -0.4516484835 -0.4493507058 7.4211985606
H 1.9871293559 0.1496248351 -2.5075064079
H -0.9352283889 -0.0902256801 -1.6457106854
H 3.3939435449 0.2104612945 -0.5564622766
H 3.3843546644 0.1314804881 1.922406126
H -0.9073813841 -0.2005981018 1.8616132683

M11 Caffeic Acid (Neutral) 0.008 a.u.

C 1.2696365122 0.0499899341 -0.7042354348
C 0.0502360742 -0.0682225726 -0.0102760557
C 0.0521782414 -0.1148961422 1.3620024418
C 1.2556294251 -0.0439760459 2.0759393185
C 2.4516091609 0.0762520615 1.3753006334
C 2.4625590461 0.1221197608 -0.0109725468
O -1.1051299523 -0.1348106255 -0.6912099431
C 1.2938437622 -0.0959252522 3.5262425595
C 0.2524726502 -0.2397753588 4.3565802445
C 0.464579456 -0.2731151768 5.7971799949
O -0.7030587327 -0.432909674 6.4849008791
O 1.1414335087 0.0845570343 -2.0425900347
O 1.5075160458 -0.1786698881 6.4033485437
H 2.2783444307 -0.0105174904 3.9867750683
H -0.769490232 -0.3405385809 4.0126436762

H -0.4538489369 -0.4469004556 7.4156061932
H 1.9767444599 0.1545901912 -2.5157821568
H -0.9394755252 -0.0941997686 -1.6426795993
H 3.3960417252 0.2144561858 -0.5574875005
H 3.3885727464 0.1330866027 1.9208871109
H -0.9052828658 -0.2069227388 1.8624106076

M11 Gallic Acid (Neutral) Zero field

C -0.9486421438 -1.1694168966 0.0021405185
C -1.6808074711 0.0098825663 0.0003408381
C -1.0339193982 1.238715384 -0.0038039757
C 0.3493518979 1.2875983319 -0.0062825229
C 1.0658559072 0.1004807511 -0.0044557147
C 0.4294564252 -1.1345040171 -0.0002412758
O -3.0376642359 0.0077879243 0.0026539578
O -1.763571101 2.3768897959 -0.0054168822
C 2.5513152529 0.0924936927 -0.0071371394
O 3.090730742 1.3246612483 -0.0121087162
O -1.7023738324 -2.3091816821 0.006255403
O 3.2285092083 -0.9007956457 -0.0052719211
H 1.0272556161 -2.0408338857 0.0010755358
H 0.8527888314 2.2461002267 -0.0096093561
H -1.1461037978 -3.0920861886 0.0081085331
H -3.3588741127 -0.901482647 0.0057314131
H -2.7023476245 2.1564348104 -0.0031654043
H 4.0506008363 1.218481231 -0.013519291

M11 Gallic Acid (Neutral) 0.010 a.u.

C -0.9456682203 -1.1866719216 0.0023659696
C -1.6814108677 -0.0025978696 0.0005670175
C -1.0293753719 1.2299090871 -0.0035369328
C 0.352694287 1.2742339649 -0.0059977108
C 1.0761021992 0.0862775379 -0.0041398005
C 0.4343554131 -1.1510483671 0.0000768057
O -3.0185591747 0.018393581 0.002670675
O -1.7433191036 2.366448529 -0.0051967385
C 2.543747493 0.103831128 -0.0070090227
O 3.0776606634 1.3535166422 -0.0127109237
O -1.703974453 -2.3123223416 0.0063094976
O 3.2797661908 -0.8577290166 -0.0049366885
H 1.0225652037 -2.063052017 0.0013755591
H 0.8466030181 2.2371287824 -0.0094333728
H -1.1774869113 -3.1146706121 0.0076317152
H -3.4022398771 -0.8685348654 0.0050969902
H -2.69158794 2.1749772426 -0.0034905227
H 4.0316884511 1.2231355159 -0.0143485168

M11 Gallic Acid (Neutral) 0.002 a.u.

C -0.9481831165 -1.1727725195 0.0021910238
C -1.6807863369 0.0073615884 0.0003948915
C -1.0329312889 1.2367169435 -0.0037390432
C 0.3501359853 1.284712608 -0.0062147221
C 1.0675323775 0.0974626431 -0.0043859142
C 0.4303879612 -1.1378566649 -0.0001728156
O -3.0337859239 0.0102895005 0.0026598589
O -1.7591190006 2.3747100419 -0.0053621549
C 2.5496503298 0.0947750325 -0.0071117669
O 3.0876244097 1.3303946463 -0.0122578868
O -1.702562534 -2.3098774084 0.0062637382
O 3.2386569255 -0.8921692882 -0.0051751827
H 1.0261047285 -2.0453769935 0.0011374348
H 0.851687866 2.2440436485 -0.0095627946
H -1.1517660184 -3.0964367529 0.0080021186
H -3.367581041 -0.894732901 0.0055813855
H -2.6998491638 2.160154511 -0.0032476409
H 4.0463448406 1.2198263647 -0.0137065296

M11 Gallic Acid (Neutral) 0.004 a.u.

C -0.9476682718 -1.1761631842 0.0022381788
C -1.6808311029 0.0048519794 0.0004438869
C -1.0319859068 1.2348193586 -0.0036804503
C 0.3508667739 1.2819294916 -0.0061529849
C 1.069373239 0.094533092 -0.0043200687
C 0.4313429992 -1.1411851884 -0.0001072857
O -3.0299589576 0.0126259881 0.0026639742
O -1.7548706038 2.3725690751 -0.0053132609
C 2.5480803384 0.0970476656 -0.0070872644
O 3.0847630273 1.3361109622 -0.0123933927
O -1.7028141161 -2.3105536068 0.0062726711
O 3.248847494 -0.8835474804 -0.0050906503
H 1.0250736848 -2.0498590768 0.0011975282
H 0.8505238029 2.2421129581 -0.0095224682
H -1.1576870727 -3.1008604202 0.0079025455
H -3.3763031404 -0.8880330061 0.0054434177
H -2.6975246368 2.1638454099 -0.003318387
H 4.0423334491 1.2209809823 -0.0138819893

M11 Gallic Acid (Neutral) 0.006 a.u.

C -0.9470882909 -1.179608342 0.0022826887
C -1.6809436595 0.0023511282 0.0004888979
C -1.0310745745 1.233043597 -0.0036269005
C 0.3515461372 1.279251984 -0.0060965888

C 1.0713988771 0.0916880726 -0.0042576164
C 0.4323259926 -1.1444929514 -0.0000442542
O -3.0261510943 0.0147775784 0.0026674035
O -1.750815652 2.3704670991 -0.0052680224
C 2.5465887983 0.0993083562 -0.0070626947
O 3.0821291198 1.3418517907 -0.0125189813
O -1.703126123 -2.3111985494 0.006282111
O 3.2590895626 -0.8749326015 -0.005014944
H 1.0241481041 -2.0542963461 0.0012568299
H 0.8493035238 2.2403097683 -0.009487935
H -1.1639211132 -3.1053782285 0.0078080107
H -3.3850226256 -0.8813967115 0.0053139919
H -2.6953672554 2.1675295098 -0.0033794093
H 4.0385412731 1.2219498461 -0.014048587

M11 Gallic Acid (Neutral) 0.008 a.u.

C -0.9464265072 -1.1831135315 0.0023254723
C -1.6811328934 -0.0001344079 0.0005300549
C -1.0301961202 1.2314034051 -0.003578172
C 0.3521657711 1.2766808207 -0.0060437742
C 1.0736380117 0.0889276778 -0.0041962142
C 0.4333330314 -1.1477844805 0.0000180815
O -3.0223448678 0.0167138151 0.0026693555
O -1.7469501534 2.3684202777 -0.0052278166
C 2.5451445774 0.1015638192 -0.007034513
O 3.0797258257 1.3476616829 -0.0126303971
O -1.7035106944 -2.3117904837 0.0062935734
O 3.2693921713 -0.8663243976 -0.0049584024
H 1.0233109408 -2.0587013133 0.0013177333
H 0.8480128936 2.238640134 -0.0094570405
H -1.1705145688 -3.1099840047 0.0077161787
H -3.3936745804 -0.8748750255 0.0051944006
H -2.6933717641 2.1712282797 -0.0034357913
H 4.0349599267 1.2226927325 -0.0142087288

M11 Caffeic Acid (Radical) Zero field

C 1.2504963914 0.0569081257 -0.7599374273
C -0.0023176933 -0.0827298424 0.0039166702
C -0.0124440723 -0.139032974 1.3712036443
C 1.1985123444 -0.0618013379 2.0686169469
C 2.4285011847 0.0743044457 1.3557188085
C 2.4730599455 0.1327869575 0.0045653138
O -1.1011024953 -0.1485524431 -0.7300489951
C 1.2645428508 -0.1142869804 3.514412599
C 0.2308961601 -0.2384702226 4.3520062612
C 0.4891737881 -0.2734584882 5.8081925625

O -0.6498213167 -0.3941579607 6.5145084437
O 1.1706708231 0.0993032019 -1.9875929087
O 1.5697654852 -0.2043164028 6.3283211459
H 2.252810534 -0.0450558993 3.9668525671
H -0.8017575677 -0.3172389499 4.032615399
H -0.4153266332 -0.4111177662 7.4518511878
H -0.8122371657 -0.0862449235 -1.6603440599
H 3.4021623549 0.2365989541 -0.5442070306
H 3.3459280429 0.131748574 1.9342460296
H -0.959860961 -0.2426670677 1.886875842

M11 Caffeic Acid (Radical) 0.010 a.u.

C 1.2531012413 0.0576331094 -0.7641767447
C -0.0089464351 -0.0821053067 0.0092017931
C -0.0070204919 -0.1366771215 1.37952789
C 1.2098631635 -0.0602909699 2.069040251
C 2.4443924684 0.0730014614 1.3485159836
C 2.4876258798 0.1304834016 0.0013649465
O -1.1059760137 -0.1467861463 -0.7034320307
C 1.2791466221 -0.1096620964 3.5033364027
C 0.2429799527 -0.236920781 4.356917569
C 0.4759439264 -0.2692593858 5.7913311848
O -0.6834770279 -0.4061420264 6.5011828294
O 1.1702156328 0.1019709233 -1.9765558175
O 1.5298149015 -0.1907561033 6.3829222626
H 2.2719078115 -0.0363946352 3.9463516845
H -0.7853525773 -0.3221647782 4.0286442079
H -0.4129130104 -0.4215873201 7.4256028017
H -0.8616970143 -0.0905239534 -1.6498676326
H 3.4112155683 0.2302632583 -0.5582257574
H 3.364761488 0.1273479014 1.9234577752
H -0.9539340858 -0.2389104313 1.8966334007

M11 Caffeic Acid (Radical) 0.002 a.u.

C 1.2501882757 0.0569226942 -0.7603222516
C -0.0033174562 -0.0824155989 0.0058677388
C -0.0097379034 -0.1383288437 1.3739483575
C 1.2026286733 -0.0614008844 2.0681882571
C 2.432458193 0.0738296947 1.3539411164
C 2.4754882584 0.1320341538 0.0031218505
O -1.1028742639 -0.1479130546 -0.7224000555
C 1.268959872 -0.1132035662 3.5133184473
C 0.2346514076 -0.238275265 4.3518138032
C 0.4858722036 -0.2723823148 5.8046950589
O -0.6579626796 -0.3976053305 6.5091895496
O 1.1690030818 0.0995781044 -1.985061357

O 1.5602639991 -0.199966225 6.3404146745
H 2.2578658256 -0.0426645942 3.9643093157
H -0.7967406568 -0.3188126076 4.0296072834
H -0.4186615185 -0.4139074044 7.4446082396
H -0.8237772171 -0.0869203338 -1.6562207354
H 3.4030357242 0.2348410904 -0.5485151884
H 3.3510442544 0.1305769222 1.9308000214
H -0.9567360732 -0.2414676367 1.890468874

M11 Caffeic Acid (Radical) 0.004 a.u.

C 1.2502801917 0.0566791599 -0.7608074014
C -0.0044137641 -0.0821651849 0.0073535717
C -0.0078108239 -0.1376776115 1.3761037859
C 1.2058896204 -0.0610964528 2.0680231676
C 2.4360120705 0.0734314807 1.3524461538
C 2.4780626176 0.1313947509 0.0020903167
O -1.1043220992 -0.1473773969 -0.7159333614
C 1.2726221524 -0.1122644024 3.5116856319
C 0.2377346424 -0.2380527115 4.3521665853
C 0.482922947 -0.2715119749 5.8012716907
O -0.6653103174 -0.4004780187 6.5051261784
O 1.1681315032 0.1003708791 -1.9826823717
O 1.5515431326 -0.1964768115 6.3518095653
H 2.262283633 -0.0407188234 3.9610609482
H -0.7925871991 -0.3200638124 4.027644414
H -0.4201153918 -0.4162026424 7.4383617763
H -0.8344872005 -0.0879663714 -1.6531116138
H 3.4042717332 0.2334556979 -0.5520337013
H 3.3555140091 0.1296019354 1.928031893
H -0.9545694573 -0.2403626892 1.8931657709

M11 Caffeic Acid (Radical) 0.006 a.u.

C 1.250796541 0.0566628642 -0.7615918932
C -0.0057166742 -0.0820101533 0.0083777383
C -0.0067229223 -0.1371432983 1.377704015
C 1.2081821008 -0.0607887011 2.06808595
C 2.439143869 0.0731789596 1.351137627
C 2.4808945991 0.1309258138 0.0014932457
O -1.1053553676 -0.1470102775 -0.7106619922
C 1.2754710247 -0.1113651145 3.5095024023
C 0.2401210183 -0.2377474523 4.3531057922
C 0.4803634906 -0.2707212442 5.7979513084
O -0.6718791856 -0.4028381748 6.502393675
O 1.1681141667 0.1010098507 -1.9804965063
O 1.5436694788 -0.1938744238 6.3625599146
H 2.2660350659 -0.0390428717 3.9570071555

H -0.7893573705 -0.3210080217 4.0268825828
H -0.4196524368 -0.4182387171 7.4331365235
H -0.8443003483 -0.0889818802 -1.6510091688
H 3.4059990649 0.232246003 -0.5547816289
H 3.3592544719 0.1287765818 1.9259658681
H -0.9534085863 -0.2395107426 1.895010391

M11 Caffeic Acid (Radical) 0.008 a.u.

C 1.2517560861 0.0566394178 -0.7626914743
C -0.0072126174 -0.0819672299 0.0089377427
C -0.0064641752 -0.1367537381 1.37879179
C 1.2095121612 -0.0605740935 2.0684021792
C 2.4419127603 0.0730099645 1.3499117728
C 2.4840369887 0.130604507 0.0012760079
O -1.1059553003 -0.146800316 -0.706542089
C 1.2775857556 -0.1105597519 3.5067542415
C 0.2418369169 -0.2373369653 4.3546983173
C 0.4780875314 -0.2699873824 5.7946976066
O -0.6778490968 -0.4046676958 6.5010637748
O 1.1688734838 0.1019190059 -1.9784946552
O 1.5365544894 -0.1920598612 6.3728160733
H 2.2691972408 -0.0377441249 3.952129413
H -0.7870057789 -0.3215758137 4.0272870544
H -0.4172501815 -0.4199950295 7.4289112909
H -0.8533116753 -0.0901246935 -1.649941657
H 3.4082564783 0.2313316733 -0.5568097518
H 3.3623189805 0.1280774155 1.924503935
H -0.9532280478 -0.2389162883 1.8960714279

M11 Gallic Acid (Radical) Zero field

C -0.9419255895 -1.2193766542 0.0031520242
C -1.7435944466 -0.0018274237 0.0016139803
C -1.0125510433 1.267920108 -0.0033840157
C 0.3595739714 1.3172664965 -0.0063539581
C 1.0564911185 0.1117696441 -0.0045352738
C 0.4226623401 -1.1408935907 0.0001022186
O -2.9732079125 0.0219155213 0.0041023775
O -1.7748847223 2.350258852 -0.0047201244
C 2.5469404592 0.0937457309 -0.0075987254
O 3.0911844414 1.3203284067 -0.0126653809
O -1.6427151481 -2.3573549454 0.0076023245
O 3.2080257419 -0.9088587509 -0.0057940509
H 1.0446751726 -2.0311308775 0.0012111149
H 0.88092535 2.2655528728 -0.0100156128
H -1.0587714324 -3.1223074304 0.0086601577
H -2.6993856819 2.0400985748 -0.0018163216

H 4.0516493815 1.2160164657 -0.014265734

M11 Gallic Acid (Radical) 0.010 a.u.

C -0.9378546067 -1.2343302388 0.0032041541
C -1.7444511265 -0.0081400482 0.0016257097
C -1.0114337 1.2669298994 -0.0032843247
C 0.3624889591 1.3074430253 -0.0061678876
C 1.0636492117 0.1001913875 -0.0043259813
C 0.4287587439 -1.1572723897 0.0002941961
O -2.9620300693 0.0088933663 0.0044690394
O -1.7553028331 2.3511876191 -0.0047090698
C 2.5365928538 0.10488435 -0.0073862736
O 3.0805071094 1.3470750525 -0.0131698179
O -1.6531022027 -2.351872252 0.007496914
O 3.2541464671 -0.8687883925 -0.0052729497
H 1.0427805783 -2.0522118596 0.0014014107
H 0.8778277123 2.2584625225 -0.0098827682
H -1.1069852489 -3.1436663106 0.0081301654
H -2.6947783154 2.0812653603 -0.0022623467
H 4.0342784668 1.2130719084 -0.0148651697

M11 Gallic Acid (Radical) 0.002 a.u.

C -0.9412680714 -1.2222985116 0.0031648163
C -1.7435705373 -0.0029616341 0.0016521595
C -1.0122183976 1.2675814436 -0.0034207783
C 0.3605290647 1.3148135423 -0.0065446255
C 1.0575887031 0.1089612752 -0.0047931877
C 0.4240044957 -1.1443677372 -0.00003415
O -2.97067608 0.0196648393 0.0044794069
O -1.7704890418 2.3502933737 -0.0047028831
C 2.5450491651 0.0957359185 -0.0080607185
O 3.0878561419 1.3257162552 -0.0125528343
O -1.6446792241 -2.3561315934 0.0077257578
O 3.2172157918 -0.9010980485 -0.0055023847
H 1.0442116339 -2.0356536709 0.001027388
H 0.880838662 2.2635315008 -0.0102971004
H -1.068114638 -3.1264258305 0.0086696902
H -2.6982235322 2.0489646723 -0.0017858701
H 4.0470378643 1.2167972052 -0.0137296861

M11 Gallic Acid (Radical) 0.004 a.u.

C -0.9406682028 -1.2249948145 0.0031867025
C -1.7436525044 -0.0042276635 0.0016940184
C -1.0120903978 1.2671183682 -0.0033530034
C 0.3609500003 1.3128650976 -0.0063186358
C 1.0587885114 0.1067557554 -0.004472127

C 0.4250760663 -1.1473676956 0.0001703015
O -2.9686833214 0.0171708203 0.0042040162
O -1.7664986655 2.3506363562 -0.0047247483
C 2.5428020393 0.0980519138 -0.0075505204
O 3.0860924078 1.3307925894 -0.0128891801
O -1.6467152081 -2.3552291093 0.0075549793
O 3.2264131082 -0.8929903864 -0.0054856933
H 1.0434676439 -2.0397001066 0.0012662414
H 0.8798417183 2.2622141119 -0.010028487
H -1.0768631753 -3.1304545706 0.008422503
H -2.6971771214 2.0568001359 -0.0019203059
H 4.0440091013 1.2156821978 -0.0144610612

M11 Gallic Acid (Radical) 0.006 a.u.

C -0.9398984822 -1.2279628721 0.003210573
C -1.7438405459 -0.0054809357 0.001747433
C -1.0119051606 1.2669144558 -0.0033386307
C 0.3615281063 1.31089496 -0.0063096254
C 1.0602082521 0.1044282411 -0.0044510008
C 0.4263028893 -1.150635149 0.0002024443
O -2.9665458322 0.0145911068 0.0042547618
O -1.762611517 2.3508435306 -0.0047274422
C 2.5407972432 0.1002666018 -0.0075571756
O 3.0840047704 1.3360923071 -0.0129717057
O -1.6487887522 -2.3541659783 0.0075434615
O 3.2356556683 -0.8850128186 -0.0053585398
H 1.0430665633 -2.0439265851 0.0012852117
H 0.8791913204 2.2608051033 -0.0100520732
H -1.0864134853 -3.1347187897 0.0083116571
H -2.6962807394 2.0650521 -0.0019695525
H 4.0406217016 1.2151377219 -0.0145247966

M11 Gallic Acid (Radical) 0.008 a.u.

C -0.9390179892 -1.2310450841 0.0032372618
C -1.7441151821 -0.006766817 0.001808292
C -1.0117296254 1.2668478974 -0.0033285532
C 0.3620489735 1.3091045443 -0.0063142554
C 1.0618306017 0.1022299948 -0.0044438963
C 0.427544398 -1.1539347044 0.0002285506
O -2.9644771945 0.0118822322 0.0043198704
O -1.7589161241 2.3510600327 -0.0047323038
C 2.5388183983 0.1025221258 -0.007596413
O 3.0821906441 1.3414748633 -0.0130227133
O -1.6509019074 -2.353100472 0.0075430972
O 3.2449087754 -0.8770429607 -0.0052502335
H 1.0427940125 -2.0481274056 0.0012936494

H 0.8784822873 2.2595957425 -0.0100969647
H -1.0963366146 -3.1391200728 0.008211156
H -2.6955028782 2.0731967862 -0.0020146756
H 4.0374714247 1.2143462974 -0.0145468686

ωB97 Caffeic Acid (Neutral) -0.010 a.u.

C 1.2564615631 0.0694163564 -0.7170775022
C 0.0468198623 -0.15180399 -0.0602067395
C 0.0228508904 -0.2564820956 1.3191520576
C 1.2029395506 -0.1404676114 2.0623111654
C 2.4045511714 0.0700869436 1.384395648
C 2.4327304936 0.1778064663 -0.0001488442
O -1.1118308848 -0.2679359294 -0.7832590064
C 1.2413263015 -0.226977622 3.533418505
C 0.2143052309 -0.1821370768 4.3757237677
C 0.5018227576 -0.2671766666 5.8435391502
O -0.6200395652 -0.1847823455 6.5665734054
O 1.1997577649 0.1637407903 -2.105532844
O 1.6047445493 -0.3906293782 6.3034782794
H 2.228787634 -0.3160632188 3.9843868112
H -0.8226809478 -0.0712282076 4.0734863602
H -0.38580361 -0.2360621856 7.5059980508
H 2.0669809923 0.4300806296 -2.4138338916
H -0.889156426 -0.1324394931 -1.7082145799
H 3.3743981077 0.3453376604 -0.519901472
H 3.3255235576 0.156439175 1.9517925386
H -0.9293779935 -0.4350502012 1.8085031402

ωB97 Caffeic Acid (Neutral) -0.002 a.u.

C 1.2623571662 0.0502299896 -0.7159820537
C 0.0446028693 -0.0736237078 -0.0345394518
C 0.0352761781 -0.124793081 1.3444971487
C 1.232282013 -0.0542308786 2.0685380127
C 2.4334073237 0.0697062717 1.3750961166
C 2.4508949824 0.1214478177 -0.0154393629
O -1.1242363641 -0.1422326904 -0.7279116007
C 1.2700339052 -0.1050478202 3.5380458157
C 0.2366975846 -0.2454902731 4.3670879221
C 0.4809502846 -0.2723153853 5.8292264745
O -0.6675703419 -0.4181669617 6.5215672877
O 1.1695270601 0.093593416 -2.0859518698
O 1.5555613867 -0.1782995912 6.3672669878
H 2.2544654037 -0.0180894182 3.9958711111
H -0.7919471115 -0.3440783627 4.0373972532
H -0.4319090928 -0.4260148829 7.4588229099
H 2.043843063 0.1839094319 -2.4699705739

H -0.9243991377 -0.0885332297 -1.668245584
H 3.3916538012 0.218322868 -0.5517401098
H 3.3666672906 0.1263760065 1.9264159928
H -0.9230472643 -0.2189975189 1.8445315738

ωB97 Caffeic Acid (Neutral) -0.004 a.u.

C 1.2612546044 0.0505266577 -0.7166900764
C 0.0436032863 -0.0771775558 -0.0394942438
C 0.0303110923 -0.130880735 1.3401609057
C 1.2246412518 -0.058981411 2.0675492854
C 2.4273369618 0.0683560117 1.3765028746
C 2.4479433229 0.1227462729 -0.0133855248
O -1.1245389396 -0.1471453094 -0.7386687842
C 1.2623815275 -0.110565038 3.5382920893
C 0.2308621419 -0.2448453394 4.3687306752
C 0.4861779315 -0.2718303563 5.8329464206
O -0.6563621309 -0.4073295824 6.5314069099
O 1.1773501625 0.0968840241 -2.0917259235
O 1.568849038 -0.1848784409 6.3530089183
H 2.2472259015 -0.0287566409 3.9960841507
H -0.8003760113 -0.3370685911 4.04455446
H -0.4211227297 -0.4156244414 7.469483995
H 2.0567538363 0.1979783028 -2.4602941744
H -0.9176477794 -0.0882408066 -1.6766335112
H 3.3903108396 0.2226010486 -0.5469421595
H 3.3586367488 0.1260034399 1.9308385689
H -0.9284800562 -0.2280995096 1.8388591443

ωB97 Caffeic Acid (Neutral) -0.006 a.u.

C 1.2603586103 0.0518423208 -0.7175866083
C 0.0427653912 -0.0846670386 -0.04541834
C 0.0249609371 -0.14351524 1.3347260094
C 1.216115441 -0.067959001 2.0663714711
C 2.4204079604 0.0670897546 1.3782630086
C 2.4447069112 0.1269676882 -0.0107770381
O -1.1239134282 -0.1585001851 -0.7513684676
C 1.2539813143 -0.1219828661 3.5379293494
C 0.2240372816 -0.2414181262 4.3711470031
C 0.4920778694 -0.2713332834 5.8369433965
O -0.6446287085 -0.3844048152 6.5431397076
O 1.1860547602 0.1038039158 -2.0976284792
O 1.5840098827 -0.2029032581 6.3375926703
H 2.2401373852 -0.0535932211 3.9951058139
H -0.8109220588 -0.3175083431 4.0538974586
H -0.4085236451 -0.3953369739 7.4817384857
H 2.0695199982 0.2236237771 -2.4497645433

H -0.9098316173 -0.0890985641 -1.6864909144
H 3.3886708956 0.2333543824 -0.5409170549
H 3.3492986857 0.1271873127 1.9362125306
H -0.9341728666 -0.2479762355 1.831468541

ωB97 Caffeic Acid (Neutral) -0.008 a.u.

C 1.2566511438 0.0743762117 -0.7161885215
C 0.0458259979 -0.1308413204 -0.053014757
C 0.0268121302 -0.2289801593 1.3259503099
C 1.2115209525 -0.1234809656 2.0635260811
C 2.4121644079 0.072302923 1.381799125
C 2.4362565774 0.1743730061 -0.0040256831
O -1.115888226 -0.2381411876 -0.7677117603
C 1.2501673016 -0.208203719 3.5343613212
C 0.2191368197 -0.1895484707 4.3734315605
C 0.4960966154 -0.2741860194 5.8393950481
O -0.6349757647 -0.2221216935 6.5561871039
O 1.189742389 0.1605540961 -2.0996752946
O 1.5947059295 -0.3743913255 6.3172232499
H 2.2386470949 -0.2776834267 3.9864129661
H -0.8181498145 -0.1029803018 4.0653966984
H -0.400009167 -0.2738522778 7.4945265709
H 2.0674596437 0.3577095918 -2.4300445894
H -0.8987488103 -0.1276398533 -1.6976757001
H 3.3770643061 0.3309419035 -0.5280366131
H 3.3366739909 0.150975146 1.9446200127
H -0.9260425179 -0.3955101575 1.8181268714

ωB97 Gallic Acid (Neutral) -0.010 a.u.

C -0.9538037561 -1.1573719584 0.0021042954
C -1.6913481898 0.0196751832 0.0003051724
C -1.0461651954 1.2494390677 -0.0040882237
C 0.3418774382 1.3055131046 -0.0066818485
C 1.0649480123 0.1184758269 -0.004832807
C 0.4251246951 -1.118609594 -0.0004485301
O -3.0727684038 -0.0060492094 0.0028843372
O -1.7880018079 2.3991069303 -0.0057781855
C 2.5684491739 0.0825638359 -0.0073420611
O 3.1195331627 1.3006107596 -0.0111794435
O -1.7006807887 -2.3178359 0.0065024798
O 3.1915169765 -0.9440375307 -0.0061000254
H 1.0309850769 -2.0207934225 0.0008619161
H 0.8466264377 2.2645378464 -0.0100498575
H -1.1047109624 -3.0714007484 0.008186623
H -3.3275000191 -0.9344978115 0.0063384121
H -2.7155271223 2.1463029725 -0.0029571015

H 4.0830062723 1.1955956479 -0.0124311522

ωB97 Gallic Acid (Neutral) -0.002 a.u.

C -0.9530509516 -1.1699887775 0.002278237
C -1.6907131082 0.0098545656 0.0005073352
C -1.0419290753 1.2406334583 -0.0038924855
C 0.3453819662 1.2925309786 -0.0065052908
C 1.0691362956 0.1051138938 -0.004662832
C 0.4280161604 -1.1323281245 -0.0002663156
O -3.0571010539 0.0058506279 0.002956486
O -1.7675126429 2.3905981945 -0.0056208519
C 2.5609509084 0.0917570227 -0.0072819559
O 3.1040948322 1.3233344267 -0.0115578701
O -1.7014027548 -2.3206833034 0.0065734343
O 3.2310297383 -0.9099845708 -0.0058543766
H 1.023533141 -2.0403985966 0.0010474717
H 0.8438171608 2.2541660983 -0.0099586189
H -1.1235216634 -3.0871566564 0.0078129812
H -3.3589942473 -0.9088547991 0.0059285489
H -2.7030913437 2.1620197531 -0.0032947252
H 4.0629176383 1.2047608086 -0.0129151719

ωB97 Gallic Acid (Neutral) -0.004 a.u.

C -0.9532824379 -1.1667237424 0.0022396176
C -1.6907517984 0.0123763855 0.0004633664
C -1.0429303324 1.2427998892 -0.0039369671
C 0.34456476 1.295668233 -0.006548077
C 1.0678704036 0.1083447673 -0.0047058827
C 0.4272517821 -1.1289351679 -0.000310671
O -3.0608780877 0.0027719 0.0029440702
O -1.7723148009 2.392797366 -0.0056576601
C 2.5626346922 0.0894607404 -0.0073041835
O 3.1075765466 1.3176944746 -0.0114592549
O -1.7013087534 -2.3197934253 0.0065586098
O 3.221043308 -0.9185401416 -0.0059226388
H 1.0252028563 -2.0355928469 0.0010015442
H 0.8446485443 2.25659179 -0.0099821391
H -1.1188779405 -3.0830565074 0.0079068841
H -3.3504846397 -0.9157347581 0.006019648
H -2.7059444711 2.1583446628 -0.0032230472
H 4.067541369 1.2027513806 -0.0127892187

ωB97 Gallic Acid (Neutral) -0.006 a.u.

C -0.9534659773 -1.1635362856 0.0021979966
C -1.6908686903 0.0148490741 0.0004158094
C -1.0439911393 1.2450062809 -0.0039841166

C 0.3436818745 1.2989317012 -0.0065923145
C 1.0667292371 0.1117059012 -0.0047493702
C 0.4265303005 -1.1254747936 -0.0003563425
O -3.0647391526 -0.0002392184 0.0029293166
O -1.7773824888 2.3949446394 -0.0056955705
C 2.5644001289 0.0871384817 -0.0073227826
O 3.1113627428 1.3119599724 -0.0113637972
O -1.7011114396 -2.3190410018 0.0065421545
O 3.2109928526 -0.927159661 -0.0059838483
H 1.0271719905 -2.0305874632 0.0009539222
H 0.8453547741 2.2591899224 -0.010006145
H -1.114129558 -3.0790677192 0.0079996292
H -3.3424316793 -0.9222807164 0.0061178305
H -2.7090160202 2.1544719921 -0.0031433457
H 4.0724732445 1.2004138937 -0.0126650258

ωB97 Gallic Acid (Neutral) -0.008 a.u.

C -0.9536324248 -1.1604428355 0.0021525278
C -1.6910665779 0.0172625817 0.0003626274
C -1.0450790328 1.2472110795 -0.0040339515
C 0.34277288 1.3022406563 -0.0066350071
C 1.0657420357 0.1151139416 -0.0047893532
C 0.4258306947 -1.1220126729 -0.0004014435
O -3.0687092781 -0.0031081105 0.0029075529
O -1.7826457343 2.3970247612 -0.0057353811
C 2.5663264145 0.0848229524 -0.0073300431
O 3.1153793809 1.3062178125 -0.0112741297
O -1.700834021 -2.3184490379 0.0065219067
O 3.2010784612 -0.9357169627 -0.0060408217
H 1.0292032287 -2.0255764605 0.0009078685
H 0.8459860142 2.2618730982 -0.0100257491
H -1.1092842193 -3.075201816 0.008092414
H -3.3349242488 -0.928409803 0.006222409
H -2.7122399876 2.1504057054 -0.0030547174
H 4.0776574145 1.1979701101 -0.0125527088

ωB97 Caffeic Acid (Radical) -0.010 a.u.

C 1.2557231539 0.0556435611 -0.7689128399
C 0.0005185244 -0.0815853866 -0.0198262866
C -0.0347720367 -0.1377090674 1.3448200768
C 1.1736465615 -0.0616436249 2.0762982866
C 2.4119145565 0.0753426479 1.365702974
C 2.4666362943 0.1324098354 0.0093125909
O -1.1024873633 -0.1476657502 -0.7858195156
C 1.2393167832 -0.1150924616 3.5173116554
C 0.2076322448 -0.241677404 4.3718763771

C 0.5060290892 -0.2770467655 5.8413795358
O -0.6117783827 -0.391861865 6.5599318144
O 1.1965643621 0.0953571209 -2.016687122
O 1.6184724047 -0.2090863025 6.2878219481
H 2.2264557204 -0.0460794899 3.9714503153
H -0.831300883 -0.3199058035 4.0676815381
H -0.3817472949 -0.4071921928 7.5022908685
H -0.7609202166 -0.0807393507 -1.6947092167
H 3.405992675 0.2370875906 -0.5231484177
H 3.3236239883 0.1336116514 1.9529295563
H -0.9878681811 -0.2396479428 1.8520688611

ωB97 Caffeic Acid (Radical) -0.002 a.u.

C 1.2499258489 0.0541141527 -0.7689300698
C -0.0028174896 -0.0798134993 -0.0064654712
C -0.0157403968 -0.1337360585 1.363159002
C 1.1991945654 -0.0588435848 2.0710242849
C 2.4326620574 0.07286919 1.3544263164
C 2.4752972745 0.1276570991 -0.0017734768
O -1.1138363828 -0.1438589481 -0.7411500349
C 1.2658076176 -0.108868758 3.5198875388
C 0.2309960761 -0.2412133435 4.3639049026
C 0.4881740391 -0.2723499475 5.8261079306
O -0.6539150235 -0.4097557375 6.5248203325
O 1.1798291479 0.0955498319 -2.0044703569
O 1.5719248231 -0.1870039187 6.3445017832
H 2.2543424128 -0.0313761449 3.969079756
H -0.8008173962 -0.3295497664 4.0421472968
H -0.4174160622 -0.4217431993 7.4621782207
H -0.8145576578 -0.0832335364 -1.6664270044
H 3.4056775581 0.2272873556 -0.5498465085
H 3.3514166952 0.1285783014 1.9309712737
H -0.964495707 -0.2321904879 1.8786272843

ωB97 Caffeic Acid (Radical) -0.004 a.u.

C 1.2508542889 0.054285959 -0.7687541302
C -0.0019935912 -0.0800770221 -0.0090160988
C -0.0195426837 -0.1344192808 1.3596140386
C 1.1939412681 -0.0593731178 2.0720118622
C 2.4281835011 0.0733270859 1.3566470007
C 2.4731599844 0.1285168645 0.0003959268
O -1.1115511896 -0.1444485209 -0.7504627497
C 1.2602865873 -0.1100872191 3.52004125
C 0.2260965427 -0.2416549383 4.3649525137
C 0.4919564859 -0.2733774857 5.82949166
O -0.6447708561 -0.4060352713 6.5319060728

O 1.1828153667 0.0952759842 -2.0071563333
O 1.582487609 -0.191297481 6.3312574516
H 2.2482275177 -0.0339892113 3.970777421
H -0.8071489491 -0.32832207 4.0465891397
H -0.4109498904 -0.4186067757 7.4706956747
H -0.802309181 -0.0825288127 -1.6720015612
H 3.4054766323 0.2291615497 -0.5443339289
H 3.3454557719 0.1295759899 1.935411433
H -0.9690232148 -0.2334072265 1.8737063575

ωB97 Caffeic Acid (Radical) -0.006 a.u.

C 1.2520381594 0.0554863463 -0.7686151095
C -0.0010971559 -0.0810658866 -0.0120391569
C -0.0238022544 -0.1367708307 1.3554259391
C 1.188067295 -0.0609127571 2.0732212937
C 2.4232997215 0.0741113369 1.3592630136
C 2.4709464414 0.1307548958 0.0030267057
O -1.1087835219 -0.1463981396 -0.7609702668
C 1.254251471 -0.1129347635 3.5196496916
C 0.2205230556 -0.2409802694 4.3665863364
C 0.4961775695 -0.2744603055 5.8331025272
O -0.6349931574 -0.3997631794 6.5400706206
O 1.1862920604 0.0964331248 -2.0099561049
O 1.5939305973 -0.1984395105 6.3173814597
H 2.241965698 -0.0408108394 3.9716193279
H -0.8146061813 -0.3227260813 4.0522783125
H -0.403141464 -0.4136819536 7.4801634406
H -0.7894559072 -0.0821230959 -1.6786161607
H 3.4052916925 0.2334931138 -0.5380188062
H 3.3388863064 0.1311454037 1.940559048
H -0.974138426 -0.2378376088 1.8676408883

ωB97 Caffeic Acid (Radical) -0.008 a.u.

C 1.2536851342 0.0555569894 -0.7686810976
C -0.0003061459 -0.0813122289 -0.0155956849
C -0.0289302373 -0.1372473221 1.3505469682
C 1.1812893364 -0.0612871122 2.0746674445
C 2.4179038401 0.0746940838 1.3622504785
C 2.4688274106 0.1315539746 0.0059688779
O -1.1058421104 -0.146989317 -0.7726528919
C 1.2472364667 -0.1140141202 3.518770603
C 0.2144236672 -0.241342543 4.3688337212
C 0.5008324674 -0.2756806184 5.8370035778
O -0.6239569153 -0.3960014051 6.5493333514
O 1.1909629164 0.0958615048 -2.013142874
O 1.6057949872 -0.2033752186 6.3029178503

H 2.2345741928 -0.043385043 3.9719779992
H -0.8224953202 -0.3213796554 4.0591751495
H -0.3933428491 -0.4105659494 7.4906052562
H -0.775700309 -0.0813966228 -1.6860863445
H 3.4055481833 0.2352388071 -0.5310165685
H 3.331647019 0.1323271562 1.9463582434
H -0.9804997342 -0.2387363601 1.8605389403

ω B97 Gallic Acid (Radical) -0.010 a.u.

C -0.9475960018 -1.2094833111 0.0031613615
C -1.7528158908 0.0020594738 0.0014466567
C -1.0214832897 1.2703697585 -0.0033766731
C 0.3520130937 1.3321112539 -0.0064133977
C 1.0610601747 0.1261878807 -0.0047018528
C 0.4177036404 -1.128522869 0.0000871043
O -2.9994530016 0.0268309311 0.0039485556
O -1.8011290253 2.3603905116 -0.0046674318
C 2.5673727002 0.084892252 -0.0078961463
O 3.1172772721 1.3007228233 -0.012148845
O -1.6381282901 -2.371851888 0.0078319075
O 3.1787984152 -0.9478635178 -0.0066310324
H 1.0456310028 -2.015784236 0.0012062798
H 0.8723524295 2.2821962346 -0.0100231588
H -1.0098909226 -3.1013187404 0.0089958832
H -2.7086149706 2.0096226653 -0.0017679033
H 4.0819946639 1.2025637777 -0.0137563074

ω B97 Gallic Acid (Radical) -0.002 a.u.

C -0.9463049824 -1.2191641377 0.0032064647
C -1.7516851172 -0.0018428886 0.0015954979
C -1.020073297 1.2682205551 -0.0033414223
C 0.3554950726 1.3224596531 -0.006389582
C 1.0623660883 0.1157480648 -0.0046078367
C 0.4216938555 -1.1402701012 0.0001592469
O -2.9889495126 0.0202069082 0.0041396659
O -1.7830448969 2.3608395406 -0.0046825329
C 2.5576238731 0.0928763481 -0.0077051714
O 3.1046444708 1.3196566257 -0.0124762285
O -1.6454550417 -2.3676376466 0.0077443893
O 3.2124366083 -0.9177458898 -0.00613275
H 1.0421098533 -2.0317842854 0.0012778672
H 0.8718078641 2.2740688079 -0.0100802789
H -1.0393617506 -3.1147197632 0.0086020017
H -2.7023229944 2.0388606286 -0.0019192728
H 4.0641119068 1.2033505806 -0.014095058

ω B97 Gallic Acid (Radical) -0.004 a.u.

C	-0.9466472767	-1.2166463432	0.0031902143
C	-1.7518287404	-0.0008046118	0.0015516504
C	-1.0204019168	1.2687230806	-0.0033483138
C	0.3546727606	1.3248614802	-0.0063925054
C	1.0617462092	0.1183814279	-0.0046293476
C	0.4207027895	-1.1371960028	0.0001365073
O	-2.9913763345	0.0220294617	0.0040894193
O	-1.7874978401	2.3606961324	-0.0046730991
C	2.5598315529	0.0907762588	-0.0077357793
O	3.1075802303	1.3147154687	-0.0124121291
O	-1.6434651927	-2.3686971081	0.0077601544
O	3.2036065154	-0.9255511263	-0.0062269962
H	1.0431915685	-2.0274887238	0.0012526168
H	0.8719941813	2.2760611919	-0.010057373
H	-1.0315124174	-3.1111901262	0.0087000801
H	-2.7038398499	2.0313692321	-0.0018796512
H	4.0683357606	1.2030833078	-0.0140304479

ω B97 Gallic Acid (Radical) -0.006 a.u.

C	-0.9469720697	-1.2142019451	0.0031759741
C	-1.7520756135	0.0001847299	0.0015091631
C	-1.0207408618	1.2692399088	-0.0033563681
C	0.3538210033	1.3272491858	-0.0063952437
C	1.0613299935	0.1209804884	-0.0046501013
C	0.4197039372	-1.1342334384	0.0001170051
O	-2.9939340678	0.0237293308	0.0040418252
O	-1.7919730899	2.3605807959	-0.0046678336
C	2.5622142718	0.0887450124	-0.0077717181
O	3.1106411549	1.3099217867	-0.012337322
O	-1.6415850825	-2.3697578981	0.0077787804
O	3.1950900923	-0.9331616795	-0.0063425356
H	1.0440919962	-2.0234358144	0.0012324086
H	0.87215275	2.2780565412	-0.010035964
H	-1.02398857	-3.1077810641	0.0087998623
H	-2.7053892135	2.0240702764	-0.0018438755
H	4.0727053695	1.2029367833	-0.013959057

ω B97 Gallic Acid (Radical) -0.008 a.u.

C	-0.9473120055	-1.2118455045	0.003169859
C	-1.7524065104	0.0011347122	0.001486236
C	-1.0210817755	1.2697847652	-0.0033666483
C	0.3529639797	1.3296217366	-0.0064094934
C	1.0611354141	0.1235233607	-0.0046802067
C	0.4186979707	-1.131392398	0.0000991079
O	-2.9966427111	0.0252891766	0.0039919005

O -1.7964054884 2.3605198405 -0.004666645
C 2.5646923772 0.0868253337 -0.0078387171
O 3.1137903731 1.3053921246 -0.0122507761
O -1.6398435867 -2.3708162233 0.0078047493
O 3.1869587088 -0.9404834614 -0.0064624707
H 1.0448077671 -2.0196438437 0.0012131633
H 0.8723156113 2.2800503869 -0.0100383391
H -1.0168760607 -3.1045499254 0.0088931286
H -2.7068718467 2.0168806037 -0.0017964175
H 4.0771697829 1.2028323157 -0.0138534306

ωB97 Caffeic Acid (Neutral) Zero field

C 1.2635660887 0.0506096733 -0.715489162
C 0.0456054425 -0.0716203959 -0.0302437277
C 0.0397679982 -0.1216457625 1.3481482823
C 1.239125893 -0.0514470911 2.0695272342
C 2.4388879687 0.0710585292 1.3739132783
C 2.4537274551 0.1215411831 -0.0170730275
O -1.1235575506 -0.1397022462 -0.7184371708
C 1.2770383962 -0.1022455453 3.5373812034
C 0.2417653561 -0.2446338039 4.366040512
C 0.4762764541 -0.2726106539 5.8256835822
O -0.6781801287 -0.4239776517 6.5130575141
O 1.1624955177 0.0922598291 -2.0803040828
O 1.5435153619 -0.1763072898 6.3807375271
H 2.2615908589 -0.0141261037 3.9949065506
H -0.784949705 -0.3449387878 4.0316330642
H -0.44109317 -0.4324478818 7.4492745367
H 2.0313812722 0.1745490247 -2.4791547365
H -0.9304651341 -0.0901665029 -1.6609656143
H 3.3929544053 0.2170623507 -0.5557148956
H 3.3738222017 0.127337086 1.9226515624
H -0.9181639818 -0.2148759598 1.8490115697

ωB97 Caffeic Acid (Neutral) 0.010 a.u.

C 1.2724058588 0.0525341605 -0.716023763
C 0.0477125264 -0.0703952742 -0.0179730547
C 0.051242598 -0.1196216776 1.3566702632
C 1.2593296378 -0.0474229103 2.0757524091
C 2.4576937401 0.0756338804 1.3709608234
C 2.468582009 0.1248340574 -0.0193072844
O -1.1169208748 -0.1390761287 -0.690569999
C 1.2990704525 -0.0991935529 3.5270573048
C 0.2561891423 -0.2363211824 4.3693085267
C 0.4603134353 -0.2721099713 5.8090888515
O -0.7181946547 -0.4288849132 6.4910907431

O 1.1420292943 0.0898605643 -2.0539857609
O 1.4984588647 -0.183539713 6.4375761771
H 2.2869593096 -0.0187525686 3.9808767486
H -0.7658528583 -0.3304266019 4.0218842589
H -0.4563611474 -0.4438572719 7.4178145151
H 1.9813710901 0.1632510372 -2.5197507425
H -0.9524437273 -0.0988522546 -1.6421469258
H 3.4029584561 0.2191940464 -0.5643595321
H 3.3971572608 0.1322056547 1.9133906373
H -0.9065894133 -0.2153873803 1.8572298035

ωB97 Caffeic Acid (Neutral) 0.002 a.u.

C 1.2649672792 0.0509916652 -0.7151853755
C 0.0465038656 -0.0706961338 -0.0265829634
C 0.0436245479 -0.1201789999 1.3511388004
C 1.2450899816 -0.0498502896 2.070551397
C 2.4437854758 0.0721647281 1.3729641013
C 2.4565557979 0.1219865952 -0.0183155418
O -1.1225619541 -0.1387005553 -0.7102847281
C 1.2831816936 -0.1008276347 3.5362880986
C 0.246038304 -0.2432408414 4.3655146679
C 0.4721109738 -0.2726743889 5.8222228738
O -0.6879305669 -0.4269446131 6.5059206172
O 1.156396561 0.0914460977 -2.0748119577
O 1.5325779332 -0.1763299216 6.3933305117
H 2.2680949553 -0.0132651666 3.9934181688
H -0.7791843645 -0.343320616 4.0271557725
H -0.4482909559 -0.4363812807 7.4408476798
H 2.0195088639 0.1695513252 -2.4878895789
H -0.9358771346 -0.0919113872 -1.6548313462
H 3.3944151764 0.2168407627 -0.5589208474
H 3.3801261847 0.1283516381 1.9195596437
H -0.9140216178 -0.2133389836 1.8524940063

ωB97 Caffeic Acid (Neutral) 0.004 a.u.

C 1.2665895162 0.0514531811 -0.7150708679
C 0.047203142 -0.0703272303 -0.0235434894
C 0.0466866422 -0.1196489522 1.3534361723
C 1.250073726 -0.0489333436 2.0716444567
C 2.4480274972 0.0731453195 1.3722666544
C 2.4593948529 0.1226987828 -0.019170164
O -1.121308498 -0.1384651106 -0.7035392098
C 1.2883683037 -0.1001927986 3.5347328522
C 0.2495255752 -0.2415068692 4.3655638436
C 0.4685063007 -0.2725837071 5.8188495262
O -0.6967022557 -0.4283404541 6.5001880762

O 1.1512590855 0.0910544237 -2.0694703443
O 1.5227377751 -0.1774793104 6.4051481345
H 2.2738301535 -0.0141944737 3.9913347184
H -0.7745845496 -0.3402492954 4.0240780019
H -0.4533098304 -0.4389981756 7.4335396983
H 2.0084824821 0.1666001407 -2.4963024493
H -0.9405474412 -0.0937682194 -1.6499591918
H 3.3961220489 0.2173150743 -0.5612881589
H 3.3855314847 0.129393258 1.9171341929
H -0.910775011 -0.2133002399 1.8550115477

ωB97 Caffeic Acid (Neutral) 0.006 a.u.

C 1.2683741274 0.0518062136 -0.7151867504
C 0.0476807731 -0.0701574825 -0.0211349652
C 0.048998593 -0.1193412932 1.355125886
C 1.2540944091 -0.0481966279 2.0728367591
C 2.4517507016 0.0740307805 1.3717259319
C 2.4623310886 0.1233401144 -0.0196185924
O -1.1199274969 -0.1384353289 -0.6980097117
C 1.2926838562 -0.0996708314 3.53272207
C 0.2523589559 -0.2398768372 4.3661701454
C 0.4653701999 -0.2724693145 5.8155620321
O -0.7045740849 -0.4291496184 6.4958227378
O 1.147171694 0.0905599761 -2.0642537617
O 1.5137953095 -0.1789899515 6.4163676767
H 2.2787997122 -0.0152439516 3.9886358849
H -0.7708444624 -0.3373419464 4.0221732779
H -0.4563098513 -0.4410560118 7.4273223131
H 1.9984397891 0.1647285426 -2.5044039875
H -0.9448527814 -0.095450468 -1.646216673
H 3.398096736 0.2177458125 -0.5629960368
H 3.3901468687 0.1303584608 1.9153537515
H -0.9084731373 -0.213518237 1.8565860123

ωB97 Caffeic Acid (Neutral) 0.008 a.u.

C 1.2703270273 0.0521519089 -0.7154987703
C 0.0478663756 -0.0701628318 -0.0192905287
C 0.0505077795 -0.1192964167 1.3561996036
C 1.2571642281 -0.0476649214 2.0741904482
C 2.4549468748 0.074864281 1.3713246595
C 2.4653792432 0.1240319867 -0.0196630037
O -1.11844079 -0.1386060119 -0.6937166528
C 1.2961959774 -0.099315237 3.5301864946
C 0.2545508142 -0.2381918634 4.3673922153
C 0.4626717445 -0.2723189533 5.8123066106
O -0.7116653532 -0.4293785493 6.4927922624

O 1.1440869421 0.0901405764 -2.0591053367
O 1.5057451608 -0.1809677749 6.4270900865
H 2.2831009342 -0.0166806353 3.9852143563
H -0.7679687096 -0.3341852637 4.021458415
H -0.4572690623 -0.4426809213 7.4220975366
H 1.9893909233 0.1635448102 -2.5122216563
H -0.9487525733 -0.0971080978 -1.6436339554
H 3.400375103 0.2183353074 -0.5639941633
H 3.3939944841 0.1313011118 1.9141439876
H -0.9070961237 -0.2141405047 1.857311391

ωB97 Gallic Acid (Neutral) Zero field

C -0.9527494326 -1.1732228145 0.0023142899
C -1.6907334699 0.0073764691 0.0005483073
C -1.0410099866 1.2386130118 -0.00385101
C 0.3461166784 1.2895698271 -0.0064653539
C 1.0705198569 0.1020499533 -0.004621854
C 0.4288208701 -1.1356318643 -0.0002235872
O -3.0533574875 0.0086160458 0.0029689033
O -1.7629794408 2.3884707306 -0.0055857612
C 2.5593046507 0.0940273465 -0.007260327
O 3.1009355089 1.3288704017 -0.0116554009
O -1.701638612 -2.3214328529 0.0065876564
O 3.2408962332 -0.9015236125 -0.0057831761
H 1.0221736176 -2.044973785 0.0010914141
H 0.8428801211 2.2519456532 -0.0099380193
H -1.1285433027 -3.0912661519 0.0077196442
H -3.3672105396 -0.9022899563 0.0058448142
H -2.7004714153 2.1656690229 -0.0033596126
H 4.0586071502 1.2063575755 -0.0130369272

ωB97 Gallic Acid (Neutral) 0.010 a.u.

C -0.950153395 -1.1897266237 0.0024642095
C -1.6918637421 -0.0046494163 0.0007166662
C -1.0371996677 1.2304733694 -0.0036808245
C 0.3487174705 1.2767922333 -0.0062848447
C 1.0799509346 0.0885494425 -0.0044119486
C 0.4332017926 -1.1514035111 -0.0000122684
O -3.0350123187 0.0190827553 0.0030181412
O -1.7437326281 2.3787785554 -0.005442006
C 2.551743159 0.1051117899 -0.0070848411
O 3.0892584396 1.3560818948 -0.0121509272
O -1.704166787 -2.3242025579 0.0066424778
O 3.2901461588 -0.8600227002 -0.005410409
H 1.0181587946 -2.0659325167 0.0013046575

H 0.8368192097 2.2432931985 -0.0098491778
H -1.1581356949 -3.1126155126 0.0072268876
H -3.4067873204 -0.872007358 0.0055319845
H -2.6903562644 2.1837656129 -0.0036196408
H 4.0409728589 1.2098563445 -0.0136641361

ωB97 Gallic Acid (Neutral) 0.002 a.u.

C -0.9523802831 -1.1764434233 0.002347329
C -1.6908176581 0.0049378439 0.0005862752
C -1.0401557661 1.2367226431 -0.0038131849
C 0.3467796586 1.2867495618 -0.0064296472
C 1.0720457297 0.0991182875 -0.0045845909
C 0.4296513842 -1.1388774569 -0.000183678
O -3.049654754 0.0111111446 0.002981718
O -1.7586795092 2.3864186134 -0.0055530041
C 2.5577052107 0.0962854268 -0.0072418357
O 3.0980572178 1.3343482162 -0.0117494755
O -1.7019995206 -2.3220765678 0.0066009445
O 3.2507256421 -0.8931136788 -0.0057091969
H 1.0210268695 -2.0493973961 0.0011314571
H 0.8418626039 2.2498881232 -0.0099219156
H -1.1339042448 -3.0953979138 0.0076291961
H -3.3752148352 -0.8959841862 0.0057712545
H -2.6980544678 2.1693134126 -0.0034174108
H 4.0545677224 1.2076223497 -0.0131502347

ωB97 Gallic Acid (Neutral) 0.004 a.u.

C -0.9519521462 -1.1797104581 0.0023780236
C -1.6909725157 0.0024987931 0.000621846
C -1.039345514 1.2349254226 -0.0037783858
C 0.3473828502 1.2840445397 -0.0063964308
C 1.0737332307 0.0962921285 -0.0045487224
C 0.4305046424 -1.1420821832 -0.0001453292
O -3.0459987173 0.0134933473 0.0029943505
O -1.7545991425 2.3843930408 -0.0055229513
C 2.5561796618 0.098521947 -0.0072216386
O 3.0954317717 1.3397841253 -0.0118416797
O -1.7023818617 -2.3227347242 0.0066134033
O 3.2605705454 -0.8847508527 -0.0056333938
H 1.0200455587 -2.0537134171 0.001168861
H 0.8407591949 2.2479756305 -0.0099081968
H -1.1394154446 -3.0996056604 0.0075383779
H -3.3833299964 -0.8896561756 0.0057072162
H -2.6958271124 2.1728985301 -0.003470524
H 4.0507759951 1.2086509663 -0.0132608261

ω B97 Gallic Acid (Neutral) 0.006 a.u.

C -0.951450277 -1.1830118835 0.0024069613
C -1.691193938 0.0000808952 0.0006556894
C -1.0385799386 1.2332679482 -0.0037455966
C 0.3479191284 1.2814770994 -0.0063638023
C 1.0755973402 0.0935824062 -0.0045112794
C 0.431385647 -1.1452387643 -0.0001064186
O -3.0423450353 0.0156485584 0.0030069768
O -1.7507370836 2.3824265205 -0.0054945934
C 2.5546972783 0.1007316929 -0.0071930898
O 3.0930640886 1.3452021345 -0.0119388309
O -1.7028583235 -2.3233214175 0.0066245192
O 3.2704120419 -0.8764533822 -0.0055515659
H 1.0192421439 -2.0579112591 0.0012066932
H 0.8395588724 2.2462337874 -0.0098945892
H -1.1452555515 -3.1038772145 0.0074409493
H -3.3913341001 -0.8834962718 0.0056499296
H -2.6937894377 2.1764749974 -0.0035203227
H 4.0472281446 1.2094091527 -0.0133776299

ω B97 Gallic Acid (Neutral) 0.008 a.u.

C -0.950854019 -1.1863404918 0.0024349708
C -1.6914880654 -0.0022987497 0.0006873136
C -1.0378706076 1.2317856089 -0.00371361
C 0.3483649104 1.2790681611 -0.006328019
C 1.0776564781 0.0910093187 -0.0044674976
C 0.432289519 -1.1483385443 -0.0000636252
O -3.03868055 0.0174983077 0.0030161598
O -1.7471169776 2.3805535531 -0.0054676297
C 2.553219554 0.1029235892 -0.0071493947
O 3.0910065449 1.3506169919 -0.012042006
O -1.7034646699 -2.3237933562 0.0066336112
O 3.2802413887 -0.8682273807 -0.0054728827
H 1.0186384268 -2.06196469 0.0012495444
H 0.8382436668 2.2446823033 -0.0098764101
H -1.1515132085 -3.1082026758 0.0073378359
H -3.3991089605 -0.8776404125 0.0055938645
H -2.6919660222 2.180087632 -0.0035689495
H 4.0439635918 1.2098058351 -0.013509276

ω B97 Caffeic Acid (Radical) Zero field

C 1.2493617934 0.0536932747 -0.7692576721
C -0.0037477847 -0.0793925679 -0.0043548156
C -0.0126112542 -0.1325782983 1.3661086401
C 1.2037074419 -0.0579638527 2.070274546
C 2.4367735711 0.0725005111 1.352518656

C 2.4775589986 0.1265143731 -0.0035878109
O -1.115870547 -0.1429909405 -0.732864626
C 1.2705588792 -0.1072155754 3.5192458968
C 0.2352399158 -0.2410372725 4.3632938583
C 0.4847954522 -0.2714743036 5.8228517364
O -0.6621096003 -0.4138000211 6.518852575
O 1.1777355356 0.0951636406 -2.0020194426
O 1.5620319203 -0.1827661708 6.3569761518
H 2.2596368743 -0.0278450009 3.9670129446
H -0.7951897628 -0.3317695918 4.0384916233
H -0.4221707053 -0.4251058626 7.4546347347
H -0.8262000774 -0.0838245862 -1.6616650797
H 3.4062382653 0.2248502315 -0.5546640833
H 3.3567714582 0.1276721386 1.9272548325
H -0.9608583741 -0.2301111252 1.8826703348

ω B97 Caffeic Acid (Radical) 0.010 a.u.

C 1.2522450116 0.0559930714 -0.7736429281
C -0.0097170447 -0.0806886599 -0.0001585325
C -0.0067596373 -0.1340148198 1.3728439155
C 1.2146526474 -0.0582159071 2.0699822064
C 2.4522451342 0.0724872007 1.3461047562
C 2.491461941 0.1271304242 -0.0066706061
O -1.1206293924 -0.1446491056 -0.7066063121
C 1.2838880617 -0.105875831 3.5080367452
C 0.2460697896 -0.2375914362 4.3676218677
C 0.4726344076 -0.2684876247 5.8067281838
O -0.6931651964 -0.4173877264 6.5067195832
O 1.1789037514 0.101893164 -1.9920440691
O 1.5246217617 -0.1803390621 6.4087934864
H 2.2771318273 -0.0275534303 3.948169439
H -0.781234796 -0.328653129 4.035655562
H -0.4199576158 -0.4290277934 7.43042293
H -0.8754640081 -0.0892047557 -1.6509861535
H 3.4143503384 0.2240579799 -0.567900812
H 3.3747019502 0.1259663994 1.9179856919
H -0.9543269312 -0.2333199583 1.8907180461

ω B97 Caffeic Acid (Radical) 0.002 a.u.

C 1.249166179 0.0537549488 -0.7696897911
C -0.0046835691 -0.079380621 -0.0026370556
C -0.0100150831 -0.132333965 1.3684918359
C 1.2075794759 -0.0576596407 2.0697795612
C 2.4405718339 0.0723526968 1.3509343683
C 2.4799216452 0.1261537069 -0.0049436253
O -1.1175926078 -0.1428470403 -0.7255262003

C 1.2746500128 -0.1064646193 3.5180622306
C 0.2387316331 -0.2404651936 4.3630889997
C 0.4817446212 -0.2707184238 5.819553051
O -0.6696464776 -0.4159983402 6.5139565185
O 1.1764601136 0.095723529 -1.999677452
O 1.5530006004 -0.1805692145 6.3685373204
H 2.2643774457 -0.0265533046 3.9644855725
H -0.7906442756 -0.3320390766 4.0358310736
H -0.4252503771 -0.4270306661 7.4479227757
H -0.8374961245 -0.084664939 -1.6577330691
H 3.4070324781 0.2238496933 -0.5587191908
H 3.3615995542 0.1271650393 1.9242027583
H -0.9578550782 -0.2297555693 1.8858533186

ω B97 Caffeic Acid (Radical) 0.004 a.u.

C 1.249409264 0.0537305657 -0.770349044
C -0.0057321232 -0.0792975739 -0.0014478939
C -0.0081291779 -0.1318843416 1.3702552704
C 1.2106232829 -0.0572283137 2.0694573846
C 2.4440001115 0.0722611686 1.3496046847
C 2.482497213 0.12570448 -0.0059204861
O -1.1190354079 -0.1425922995 -0.719172953
C 1.277894078 -0.1055734533 3.5163829554
C 0.2415082843 -0.2401146903 4.3633568837
C 0.4790394187 -0.2700823998 5.816318883
O -0.676303832 -0.4180876443 6.5103124222
O 1.1762719961 0.0961464999 -1.9975915056
O 1.5447451381 -0.1786606688 6.3793307703
H 2.2682738576 -0.0249056576 3.9614805516
H -0.7869552023 -0.3329121415 4.0341695409
H -0.4264251621 -0.4287958387 7.4422099922
H -0.848357259 -0.0855494371 -1.6546345244
H 3.4082977018 0.2226697291 -0.5619971653
H 3.3657802654 0.1267025727 1.9218765596
H -0.9557504468 -0.229011556 1.8881306738

ω B97 Caffeic Acid (Radical) 0.006 a.u.

C 1.2500035242 0.0541957764 -0.7711890642
C -0.006873132 -0.0795483992 -0.0006258872
C -0.0068698899 -0.1321660016 1.3715438835
C 1.2129226839 -0.0572686194 2.0693881343
C 2.4471280486 0.0722902607 1.3484334913
C 2.4852582439 0.1258590213 -0.006501317
O -1.120090599 -0.1429526587 -0.7137983737
C 1.2805405279 -0.1053496747 3.5141519022
C 0.2436382933 -0.2394339448 4.3641172051

C 0.4766193444 -0.269511489 5.8130626712
O -0.6824415345 -0.4187314947 6.5077955921
O 1.1767074535 0.0974884024 -1.9956086648
O 1.537275139 -0.1782927186 6.3895255046
H 2.2717184391 -0.0249470674 3.9578348381
H -0.7842049369 -0.3322540838 4.0335203211
H -0.4260129116 -0.4294864626 7.4373334087
H -0.8586245793 -0.0867051309 -1.6524025429
H 3.4099004074 0.2225660253 -0.5645906772
H 3.3694206836 0.1264178028 1.9201066382
H -0.9543632058 -0.2296505436 1.8896759367

ωB97 Caffeic Acid (Radical) 0.008 a.u.

C 1.2509204656 0.0554561132 -0.7722237959
C -0.0081378073 -0.0803698853 -0.0002297734
C -0.0063148117 -0.1337368765 1.3723441294
C 1.2143250496 -0.0581676819 2.0695340483
C 2.4498769424 0.0724049727 1.3473365017
C 2.4881639605 0.1269698244 -0.0066853225
O -1.1205927592 -0.1442805548 -0.7096520679
C 1.2825522591 -0.1062072775 3.5113514364
C 0.2450739092 -0.2381971794 4.365523958
C 0.4745313125 -0.2689611757 5.8098695872
O -0.6881255169 -0.4171261167 6.5066336974
O 1.17753528 0.1004572687 -1.9937132352
O 1.5307605762 -0.1801126801 6.3992128887
H 2.2747783038 -0.0276307961 3.9533652956
H -0.7825326153 -0.3290892889 4.0340999962
H -0.4239342709 -0.4285300412 7.433464187
H -0.8676641595 -0.0881084406 -1.651200922
H 3.4117710267 0.224200114 -0.5665196398
H 3.3724085167 0.1262700905 1.918842895
H -0.9537436612 -0.2327213888 1.8904191357

ωB97 Gallic Acid (Radical) Zero field

C -0.946013737 -1.2219347476 0.0032446845
C -1.7519027756 -0.0029327871 0.0017195606
C -1.019736554 1.2679494733 -0.0033768816
C 0.3563922685 1.3199980709 -0.0065720139
C 1.0631280242 0.1129786804 -0.0048151221
C 0.4226652858 -1.143578584 0.0000610283
O -2.9867399321 0.0177027661 0.0043832519
O -1.7782334932 2.3612384804 -0.0046896282
C 2.5557962611 0.0949702388 -0.008089978
O 3.1014956443 1.3248640481 -0.0123648237
O -1.6476160498 -2.3666681883 0.0078464186

O 3.2214662092 -0.9098861385 -0.0059086891
H 1.040983359 -2.0363674657 0.0011317555
H 0.8719326944 2.2719329468 -0.0103717845
H -1.0479428806 -3.1186546143 0.0085764187
H -2.7003123979 2.0469256645 -0.0018448137
H 4.0597300737 1.2045851562 -0.0136343832

ω B97 Gallic Acid (Radical) 0.010 a.u.

C -0.9425563667 -1.2365521856 0.0033129609
C -1.7533178649 -0.0093602948 0.0019095161
C -1.0190688652 1.266741733 -0.0033442357
C 0.3588211775 1.3098901668 -0.0064462339
C 1.069956516 0.101369802 -0.0045511006
C 0.4280026898 -1.1599931832 0.0002747755
O -2.9769356609 0.0050339086 0.0045356683
O -1.7583959935 2.3626852365 -0.0047794342
C 2.5457908247 0.1062938462 -0.0076516829
O 3.0916343935 1.3508092672 -0.0127535874
O -1.6581978836 -2.3617080313 0.0076879863
O 3.2670249259 -0.8702167648 -0.005620347
H 1.0377620609 -2.0581042474 0.0013673405
H 0.8688577684 2.264476271 -0.0103309213
H -1.0922135263 -3.1388716897 0.008078862
H -2.695335505 2.0883692609 -0.0020940898
H 4.0432633095 1.2022599048 -0.0143004767

ω B97 Gallic Acid (Radical) 0.002 a.u.

C -0.9455190267 -1.224653486 0.0032458038
C -1.7519410457 -0.0041633735 0.0017135947
C -1.019517046 1.2674409259 -0.0033592396
C 0.3570485462 1.3176021725 -0.006508208
C 1.0641054896 0.1103353835 -0.0047280044
C 0.4237158343 -1.1468610115 0.0001188225
O -2.984538065 0.0153893452 0.004397868
O -1.7737390111 2.3614715887 -0.00469939
C 2.5536528668 0.0972353381 -0.0079280954
O 3.0988373398 1.3300880448 -0.0124808619
O -1.6496546202 -2.3656001096 0.0077952334
O 3.2306619447 -0.9017422797 -0.0058580052
H 1.0398405488 -2.0409828473 0.0012116786
H 0.8714816163 2.2700283787 -0.0102998219
H -1.0562169321 -3.1223476099 0.008470325
H -2.6988907789 2.0552891166 -0.0019296702
H 4.0557643392 1.2045934236 -0.0138670294

ω B97 Gallic Acid (Radical) 0.004 a.u.

C -0.9449394948 -1.2274789065 0.0032452619
C -1.7521020502 -0.0054695302 0.0017013444
C -1.019396156 1.2670021313 -0.003339466
C 0.3575723353 1.3153197949 -0.0064352251
C 1.0652429723 0.1078032209 -0.0046272767
C 0.4247888875 -1.1501716704 0.0001833264
O -2.9824665011 0.012856458 0.0044031705
O -1.7694494573 2.361743964 -0.0047087153
C 2.5515993225 0.0995101122 -0.0077448862
O 3.0965392742 1.3352599827 -0.0126111405
O -1.6517191243 -2.3645727637 0.0077380858
O 3.2398972702 -0.8936113697 -0.0058133655
H 1.0389421447 -2.0455005778 0.0012994207
H 0.8708575283 2.2682776598 -0.0102146353
H -1.0647326771 -3.126186502 0.0083615635
H -2.6977039376 2.0639649076 -0.0020171733
H 4.0521616634 1.2043760888 -0.0141252893

ωB97 Gallic Acid (Radical) 0.006 a.u.

C -0.9442729617 -1.2304047372 0.0032503966
C -1.7524197668 -0.0067758782 0.0017080878
C -1.0193588237 1.2667374061 -0.0033288974
C 0.3580063581 1.3132719347 -0.0064059252
C 1.0665647871 0.1054678536 -0.0045803191
C 0.4258689674 -1.1534485943 0.0002191687
O -2.9804914804 0.0102241381 0.0044602458
O -1.7655287931 2.3619676536 -0.0047179378
C 2.549639638 0.1018070106 -0.0076637974
O 3.0947505998 1.3403885631 -0.0126934726
O -1.6538137028 -2.3635376865 0.0077097253
O 3.2491053834 -0.8855446233 -0.0057472346
H 1.0383091353 -2.0498423758 0.0013443265
H 0.8701502831 2.2667746551 -0.0101943168
H -1.073667447 -3.1302452208 0.0082709411
H -2.6967940029 2.0724469809 -0.0020810063
H 4.0490438263 1.2038359203 -0.0142549843

ωB97 Gallic Acid (Radical) 0.008 a.u.

C -0.9434609807 -1.2333978927 0.0032889474
C -1.7528343345 -0.0080246113 0.0018350958
C -1.0191820285 1.2666635866 -0.0033340985
C 0.3584568422 1.3115535497 -0.0064055431
C 1.0682298433 0.1034170073 -0.0045246919
C 0.4269211438 -1.1566663599 0.0002730138
O -2.978764236 0.0078225035 0.0044222904
O -1.7619647128 2.362383494 -0.0047573662

C 2.5477306404 0.1039944055 -0.0075993351
O 3.0930978989 1.3455521263 -0.0127506214
O -1.6559985312 -2.3627163492 0.0076756693
O 3.2579919908 -0.8780070254 -0.0057096535
H 1.0379753568 -2.0539426513 0.0013838497
H 0.8695510286 2.2655903458 -0.010242525
H -1.0826775542 -3.1345576921 0.0081641345
H -2.6960929102 2.0803075165 -0.0020764953
H 4.0461125434 1.2031510467 -0.014347671

ωB97XD Caffeic Acid (Neutral) -0.010 a.u.

C 1.2565618626 0.0611430417 -0.7143536483
C 0.0471514096 -0.1450515764 -0.0578933758
C 0.0225962559 -0.2408490908 1.3194608299
C 1.1991571873 -0.130386074 2.0643748753
C 2.4005627302 0.0661938073 1.3849522173
C 2.4299576463 0.163625236 0.0037856908
O -1.108764221 -0.253629141 -0.7726695277
C 1.239157991 -0.2057524332 3.5272235998
C 0.2169630151 -0.1931678809 4.3751599837
C 0.5056060371 -0.2595646181 5.8377246103
O -0.6166476972 -0.2180049572 6.5545805844
O 1.2029271164 0.1467448181 -2.0957016082
O 1.6088197827 -0.3377276659 6.2983735246
H 2.227879162 -0.256887041 3.9736619684
H -0.8209173502 -0.1233416621 4.0754650787
H -0.3879578499 -0.2558000763 7.4930092931
H 2.0679918485 0.4083163129 -2.4065355977
H -0.8894251719 -0.1355530761 -1.6980214279
H 3.3722386378 0.3196827606 -0.5117984164
H 3.3204801433 0.1500405012 1.9477404295
H -0.9292275355 -0.4063591846 1.8060449163

ωB97XD Caffeic Acid (Neutral) -0.002 a.u.

C 1.2625079987 0.0478349989 -0.7125176663
C 0.0454123919 -0.0692068654 -0.0351117257
C 0.0335574534 -0.117893287 1.3418395689
C 1.2247950263 -0.0514733528 2.0699358222
C 2.4261379809 0.0669260667 1.3777411972
C 2.4466978577 0.1153754877 -0.0079226865
O -1.1182991655 -0.1331585818 -0.7232918183
C 1.2639663353 -0.0989372901 3.5302206539
C 0.2396812429 -0.2515810382 4.3674037164
C 0.4853687329 -0.2708585224 5.8223542596
O -0.6570986025 -0.4306906079 6.5123886085
O 1.1751675286 0.0894431718 -2.0750366177

O 1.5562499207 -0.1601534856 6.3582528328
H 2.2462218657 0.0024340857 3.9819979768
H -0.7855079341 -0.3669193512 4.0432651069
H -0.4251710283 -0.4329623901 7.447810289
H 2.0474665211 0.1750572107 -2.4583519592
H -0.9227493281 -0.0827336571 -1.6619141539
H 3.3877461762 0.2078807616 -0.5378226632
H 3.356807076 0.1215502858 1.9267128464
H -0.9238470498 -0.2062616393 1.8366304125

ωB97XD Caffeic Acid (Neutral) -0.004 a.u.

C 1.2614361855 0.0464301402 -0.7134021962
C 0.0442173432 -0.0702417778 -0.0397228417
C 0.0284909614 -0.1186754965 1.3378967579
C 1.2174190016 -0.0527010805 2.0690726281
C 2.4203580313 0.0653816828 1.3789920791
C 2.443943674 0.1136884173 -0.0063484738
O -1.1190774275 -0.1338582321 -0.7333344238
C 1.2564475754 -0.0992912328 3.5309015802
C 0.2348185636 -0.2538676334 4.368926049
C 0.4905895461 -0.2706078979 5.8265340232
O -0.6457439152 -0.4283123672 6.5213397297
O 1.1828410547 0.0886020325 -2.0810044175
O 1.5681840657 -0.1590474983 6.3453126439
H 2.2384454426 0.0045364834 3.9826737023
H -0.7917669021 -0.3717630812 4.0493108878
H -0.4157092726 -0.4293438048 7.4578803723
H 2.0603269579 0.1826565279 -2.4493757079
H -0.9166262511 -0.0799446518 -1.6697414845
H 3.3868270317 0.2061218315 -0.5336785755
H 3.349318029 0.1199632761 1.9307064399
H -0.9296286951 -0.2060536372 1.8316452275

ωB97XD Caffeic Acid (Neutral) -0.006 a.u.

C 1.2606236798 0.045547123 -0.7143481205
C 0.0429596591 -0.0720079362 -0.0449565696
C 0.022691381 -0.1212562072 1.3332280706
C 1.2090230511 -0.0552983332 2.0682320256
C 2.4138389195 0.0635405591 1.3805680338
C 2.4411148063 0.1127069564 -0.0042971795
O -1.1194828295 -0.1354270661 -0.7448524171
C 1.2480111878 -0.1012722926 3.5311225818
C 0.2291180116 -0.2553631154 4.3709500473
C 0.4962540453 -0.2700248668 5.8307424524
O -0.6332973134 -0.4237708361 6.5316017632
O 1.1912515924 0.089380873 -2.0870851355

O 1.5810681714 -0.1589981003 6.3316398198
H 2.2301001331 0.0030443312 3.9825831399
H -0.7994396228 -0.3736074718 4.0570409515
H -0.4037937292 -0.4237325978 7.4690101226
H 2.0738164764 0.1922207111 -2.4399877994
H -0.9092865009 -0.077399545 -1.6788382689
H 3.3859723364 0.2059941539 -0.528659715
H 3.3408314399 0.1182908877 1.9354179047
H -0.9362638952 -0.208895227 1.8254722924

ωB97XD Caffeic Acid (Neutral) -0.008 a.u.

C 1.2600452182 0.0445175932 -0.7155425645
C 0.0418580451 -0.0770667678 -0.0509570793
C 0.0165747224 -0.1289663505 1.3277224065
C 1.1999501467 -0.0615424051 2.0672944889
C 2.4068019082 0.0607451047 1.3823337847
C 2.4382308224 0.1125049097 -0.0018867001
O -1.1192392198 -0.1414974579 -0.7578643582
C 1.2390219595 -0.1074629602 3.5308700635
C 0.2226268496 -0.2555104028 4.3736563413
C 0.5024528686 -0.2687644496 5.8352636809
O -0.620562243 -0.4108514806 6.5433735192
O 1.2005412374 0.0919099222 -2.0933703399
O 1.5954064252 -0.1647328131 6.3171580123
H 2.2219284748 -0.007212651 3.9815548813
H -0.8087866144 -0.3685665321 4.0663869055
H -0.3906370011 -0.4104066323 7.4814630125
H 2.0866950693 0.2152778793 -2.4297555384
H -0.901174148 -0.0745302305 -1.6890076426
H 3.3851238509 0.2086356366 -0.5228314407
H 3.3315008328 0.1165927989 1.9407731822
H -0.9432482047 -0.219400711 1.8179493851

ωB97XD Gallic Acid (Neutral) -0.010 a.u.

C -0.9524086356 -1.1558917552 0.0021391585
C -1.6894532404 0.0181443987 0.0003857233
C -1.0454887611 1.2462205497 -0.0039567498
C 0.3391234794 1.301655915 -0.0065431361
C 1.0643549827 0.1185456814 -0.0047214753
C 0.4233898062 -1.1146683051 -0.0003653079
O -3.0635914284 -0.0063011166 0.0028762923
O -1.7804574338 2.3919775493 -0.0056282651
C 2.5624330182 0.0824411271 -0.0072152685
O 3.1120246182 1.2951936271 -0.0116030013
O -1.6926366478 -2.3119246298 0.0063676682
O 3.1829029731 -0.9419237396 -0.0056100544

H 1.0250655864 -2.0156559506 0.0009274636
H 0.8399417123 2.2586696983 -0.0099474391
H -1.0986397483 -3.0635943381 0.0079810792
H -3.3211098643 -0.9310565021 0.0060286721
H -2.7068329831 2.1454783642 -0.0030119482
H 4.0729435663 1.1939144263 -0.0128094116

ωB97XD Gallic Acid (Neutral) -0.002 a.u.

C -0.9512981742 -1.1685566628 0.0023017005
C -1.6885807936 0.0085502416 0.0005735352
C -1.0411334856 1.237874738 -0.0037695699
C 0.3427083578 1.2892162551 -0.0063682249
C 1.0686646791 0.1055465734 -0.0045451514
C 0.4264808165 -1.1284219603 -0.0001759601
O -3.0475047048 0.0049813948 0.0029353954
O -1.7604218302 2.3834806468 -0.0054816875
C 2.5539548926 0.0915020597 -0.0071496753
O 3.0961646266 1.3178720837 -0.0120161096
O -1.6935303198 -2.3143828731 0.0064182708
O 3.2210958476 -0.9085321563 -0.0053273052
H 1.0192354638 -2.0343525981 0.0011214528
H 0.8376230914 2.2485802103 -0.0098586876
H -1.1181825676 -3.0793828017 0.0075822589
H -3.3516637879 -0.9060097008 0.0056671152
H -2.6945580195 2.1611044741 -0.0033241859
H 4.052506908 1.2021550756 -0.0132891712

ωB97XD Gallic Acid (Neutral) -0.004 a.u.

C -0.9516035177 -1.1652895789 0.0022663239
C -1.6886645034 0.0109988025 0.000533533
C -1.0421716795 1.2399192753 -0.0038108279
C 0.3418612551 1.292246985 -0.0064090071
C 1.0673440945 0.1087260916 -0.0045882236
C 0.4256844701 -1.1249899901 -0.0002211957
O -3.0513696052 0.0020922797 0.002925812
O -1.7651455796 2.3856524637 -0.0055148406
C 2.5558619555 0.0892156285 -0.0071706553
O 3.0997735595 1.3121721566 -0.0119139505
O -1.6933573166 -2.3136148571 0.0064079653
O 3.2113238771 -0.9169898023 -0.0053984687
H 1.0206510699 -2.0296645684 0.0010736497
H 0.8383000309 2.250973829 -0.0098798036
H -1.1132950511 -3.0752824569 0.0076799029
H -3.3434752714 -0.9126616625 0.005742316
H -2.6973962756 2.157399014 -0.0032578632
H 4.0572394875 1.2003213903 -0.0131706666

ωB97XD Gallic Acid (Neutral) -0.006 a.u.

C	-0.9518833055	-1.1620997145	0.0022272592
C	-1.6888329844	0.0134083689	0.0004891917
C	-1.0432449803	1.2419966485	-0.0038554545
C	0.3409743533	1.2953505028	-0.0064517322
C	1.0661815901	0.111970518	-0.0046321611
C	0.4249095204	-1.1215406602	-0.0002683159
O	-3.0553281807	-0.0007322308	0.0029131987
O	-1.770081355	2.3877841589	-0.0055496379
C	2.5578907263	0.086935215	-0.0071878829
O	3.1036324611	1.3064722868	-0.0118136643
O	-1.6931273367	-2.3129691755	0.006395643
O	3.2016535563	-0.925407082	-0.0054647175
H	1.0221559346	-2.0249403945	0.001024363
H	0.8389034242	2.2534740027	-0.0099015041
H	-1.1083731473	-3.0712954051	0.0077783406
H	-3.3356926414	-0.9190091568	0.0058269704
H	-2.7004076206	2.1535330454	-0.0031834105
H	4.0622309856	1.1982940722	-0.0130524858

ωB97XD Gallic Acid (Neutral) -0.008 a.u.

C	-0.9521515712	-1.1590045724	0.0021846966
C	-1.6890985884	0.0157611191	0.0004403354
C	-1.0443430194	1.2440704332	-0.0039041953
C	0.3400629414	1.2984826902	-0.0064974228
C	1.0651884321	0.1152423519	-0.0046779153
C	0.424147585	-1.1181000473	-0.0003175912
O	-3.0594067005	-0.0034119525	0.0028975964
O	-1.7751918783	2.3898550819	-0.0055870157
C	2.5600731314	0.0846745568	-0.0072040039
O	3.1077127919	1.3008124591	-0.0117105661
O	-1.6928026881	-2.3124954572	0.0063825633
O	3.1921689154	-0.9337257115	-0.005531553
H	1.0236539119	-2.0202572542	0.000973454
H	0.8394429607	2.2560394313	-0.009925198
H	-1.1033307084	-3.0674327526	0.0078786081
H	-3.3284695297	-0.9249391988	0.0059231195
H	-2.703555679	2.1495009976	-0.003100805
H	4.0674606933	1.1961528254	-0.012930107

ωB97XD Caffeic Acid (Radical) -0.010 a.u.

C	1.256734821	0.055319813	-0.763364758
C	0.0031768551	-0.079981503	-0.0187963928
C	-0.0364439529	-0.1375482345	1.3435155153
C	1.1652822324	-0.0634717415	2.0761781279

C 2.400862689 0.0716106893 1.3694624684
C 2.4589854118 0.128554802 0.0147369758
O -1.0912009744 -0.1417403031 -0.7833733958
C 1.2321084521 -0.1144830119 3.5111072326
C 0.210219738 -0.2460324273 4.3731169183
C 0.5113499838 -0.2747581981 5.8369584196
O -0.6009523432 -0.3944429347 6.5532281514
O 1.195658992 0.0952469804 -2.009473786
O 1.621233574 -0.1975370496 6.2797037479
H 2.2184019815 -0.0371674106 3.9583430201
H -0.8263080782 -0.3341081496 4.0746598351
H -0.3759894441 -0.4055922069 7.4939523887
H -0.7430275084 -0.0742160205 -1.6886595011
H 3.4000376223 0.232115864 -0.5084458725
H 3.3103507862 0.12858745 1.9539339998
H -0.9888288379 -0.2378374073 1.8449899055

ωB97XD Caffeic Acid (Radical) -0.002 a.u.

C 1.2520478351 0.0509374367 -0.7633211331
C 0.0001766911 -0.0759420508 -0.0058309643
C -0.0179453356 -0.1279744242 1.3618923336
C 1.1899822283 -0.0569064876 2.0711061577
C 2.4210459035 0.0688476244 1.3581999029
C 2.4680709784 0.1200145083 0.004013171
O -1.1025550607 -0.1349021513 -0.7385365059
C 1.2577552709 -0.1033364898 3.5137699804
C 0.2335720483 -0.2470350225 4.3652434617
C 0.4936752732 -0.2701681377 5.8210146333
O -0.641986441 -0.421054995 6.5178118864
O 1.1808840002 0.0900576319 -1.9974727716
O 1.5742619219 -0.1682323152 6.3357333752
H 2.2446202885 -0.012078823 3.9564185218
H -0.7952654564 -0.3521706107 4.0497534629
H -0.4094588369 -0.4272924615 7.4534128766
H -0.798760442 -0.077358795 -1.6611971057
H 3.4008101819 0.2150224334 -0.534428398
H 3.3372360635 0.122558736 1.9326422822
H -0.9665151122 -0.2204666064 1.8715478327

ωB97XD Caffeic Acid (Radical) -0.004 a.u.

C 1.2528319849 0.0513202032 -0.7632466935
C 0.0009411214 -0.0765403866 -0.0083252733
C -0.0216314333 -0.1295295915 1.3582667023
C 1.1849088759 -0.0581066169 2.072048161
C 2.4167302689 0.0692475877 1.3604025279

C 2.4659129413 0.1213558562 0.0060755906
O -1.100384563 -0.1358151279 -0.7477275636
C 1.2524510198 -0.1052662021 3.5138585097
C 0.228845161 -0.2472674063 4.3663075691
C 0.4974984969 -0.2710788091 5.8246780156
O -0.6330824757 -0.4161015017 6.5248442188
O 1.1836551578 0.0908751254 -2.0001868446
O 1.5847921969 -0.1732991311 6.3229971352
H 2.2389550397 -0.0161302977 3.9577843583
H -0.8015437812 -0.3498193085 4.0542741604
H -0.4037931088 -0.4231944157 7.4619703464
H -0.786524953 -0.0766035534 -1.666565968
H 3.4004640682 0.2180111662 -0.5290883691
H 3.3315055598 0.1236409657 1.9369240206
H -0.9708795774 -0.2231795559 1.8664823963

ωB97XD Caffeic Acid (Radical) -0.006 a.u.

C 1.2538634602 0.0521748988 -0.7632133229
C 0.0016546529 -0.0774225185 -0.0112257512
C -0.0259595606 -0.1316532898 1.354061646
C 1.1791242889 -0.0595960891 2.0732278281
C 2.4119515437 0.0698572656 1.3629643187
C 2.4637052145 0.1232120374 0.0085299552
O -1.0978146119 -0.1372341639 -0.7581531487
C 1.2464928991 -0.1077280433 3.5134357261
C 0.2234902116 -0.2473633969 4.3679235446
C 0.5017006459 -0.2722262621 5.8284727624
O -0.6234360128 -0.4097396835 6.5329457129
O 1.1869840191 0.0920575204 -2.0030410084
O 1.5961087499 -0.1801577213 6.3095029277
H 2.2327674349 -0.0214443683 3.9585444139
H -0.8086899471 -0.3464799031 4.0599003157
H -0.3964690554 -0.4178848659 7.4714155167
H -0.7731619291 -0.0757815838 -1.6728297508
H 3.4002374223 0.2218422076 -0.5230185356
H 3.3251421191 0.1250438512 1.9418375792
H -0.9760395452 -0.2269568914 1.8604922705

ωB97XD Caffeic Acid (Radical) -0.008 a.u.

C 1.2551612364 0.0533002733 -0.7632498301
C 0.0023550349 -0.0785482838 -0.0146160476
C -0.0308923767 -0.1341769819 1.3492175243
C 1.1726488284 -0.0612819953 2.0746172068
C 2.4067053926 0.0707057044 1.3659370489
C 2.4614144659 0.1255546468 0.011381352
O -1.0948299155 -0.1391870706 -0.7698730833

C 1.2397793102 -0.1106455975 3.5125063318
C 0.2173646966 -0.2472557066 4.3701005308
C 0.5062720195 -0.2736487585 5.832480553
O -0.6128647196 -0.401995726 6.5422928442
O 1.1909517419 0.0936736785 -2.0061007967
O 1.6082511761 -0.1890794787 6.2950516733
H 2.2259236152 -0.0279823357 3.9587916051
H -0.8168075865 -0.3420220645 4.0665402188
H -0.3873846262 -0.4115171022 7.4819656002
H -0.7586700968 -0.0751930961 -1.6800210134
H 3.4000987388 0.2265220427 -0.5161971022
H 3.3181453151 0.1268318174 1.9474275413
H -0.9819702504 -0.2315349655 1.853520843

ω B97XD Gallic Acid (Radical) -0.010 a.u.

C -0.9470804191 -1.2051425427 0.0031065045
C -1.74915265 0.0019131634 0.0014482671
C -1.019252223 1.26693503 -0.003313314
C 0.3508564486 1.3294455251 -0.0063649602
C 1.059778956 0.1278919748 -0.0046612613
C 0.4159949246 -1.1210962896 0.0001030675
O -2.9938839228 0.031487863 0.0038514171
O -1.7947608574 2.3507332141 -0.0045299432
C 2.561601896 0.0841679946 -0.0077636021
O 3.1119770501 1.2934312456 -0.0125668672
O -1.6289702684 -2.3643438772 0.0076382071
O 3.1683360978 -0.9476422374 -0.005975512
H 1.0409083309 -2.0066546832 0.0012319652
H 0.8668129117 2.2779484353 -0.0099885619
H -1.002153669 -3.0916097038 0.0087644137
H -2.6999154825 1.9978374902 -0.0016604056
H 4.0739948765 1.1978203978 -0.0140244148

ω B97XD Gallic Acid (Radical) -0.002 a.u.

C -0.9457032051 -1.214670679 0.0031515694
C -1.7475649346 -0.0019281858 0.0016034167
C -1.0175927779 1.2643628359 -0.0032597048
C 0.3546083063 1.3193178904 -0.0063015751
C 1.0613428549 0.1168694705 -0.0045211901
C 0.4200853043 -1.1332814433 0.0002036754
O -2.9831657304 0.0245494869 0.0040598801
O -1.7761530781 2.3511181213 -0.0045510767
C 2.5516805633 0.0921607273 -0.0075262232
O 3.0982074173 1.3131392649 -0.0130018787
O -1.636519136 -2.3598525461 0.0075034455
O 3.2025729783 -0.9171667655 -0.0053900594

H 1.0368964894 -2.0234492748 0.0013216914
H 0.8668122302 2.2691725086 -0.0100026114
H -1.0322970309 -3.1051154658 0.0083124492
H -2.6933189494 2.0281162569 -0.0018502109
H 4.0552006983 1.1997807974 -0.0144565973

ωB97XD Gallic Acid (Radical) -0.004 a.u.

C -0.9460921763 -1.2122692212 0.0031346317
C -1.7478943759 -0.0009814613 0.0015590053
C -1.0179615186 1.2648587727 -0.0032685009
C 0.3537319538 1.3215980315 -0.0063094547
C 1.0607276564 0.1194273604 -0.0045489057
C 0.4190472121 -1.1302788852 0.0001761023
O -2.9857098582 0.0262306761 0.0039978966
O -1.7803933876 2.351119293 -0.0045385197
C 2.5540477462 0.0901131833 -0.0075593599
O 3.1012040974 1.3082238199 -0.0129266411
O -1.6345223582 -2.3610409194 0.0075262996
O 3.1940185362 -0.9247946913 -0.0054877632
H 1.0376663894 -2.0193973433 0.0012951082
H 0.8668688642 2.2710885852 -0.0099840699
H -1.0243585482 -3.1016498848 0.0084190193
H -2.6947462038 2.0211331756 -0.0018012314
H 4.0594579711 1.1997425091 -0.0143886164

ωB97XD Gallic Acid (Radical) -0.006 a.u.

C -0.9464567539 -1.2099015094 0.0031260715
C -1.7482537818 -0.0000320462 0.0015321845
C -1.018324073 1.2654152773 -0.0032864958
C 0.3528478332 1.3239719515 -0.0063490255
C 1.0602994348 0.1220290644 -0.0046123668
C 0.4180113243 -1.1273314382 0.0001346123
O -2.9883428938 0.0278772579 0.0039693551
O -1.7847378169 2.3511140628 -0.004533029
C 2.5564058594 0.088166988 -0.0076674419
O 3.1043562823 1.3035030933 -0.0128016996
O -1.6326483792 -2.3621855245 0.0075737076
O 3.1856170901 -0.9322376235 -0.0056064615
H 1.0384385235 -2.0154188261 0.0012487601
H 0.8669480673 2.2730983167 -0.0100155826
H -1.0167641552 -3.0982650855 0.0085382374
H -2.6961555196 2.0138598129 -0.0017387261
H 4.0638509585 1.1994592286 -0.0142170997

ωB97XD Gallic Acid (Radical) -0.008 a.u.

C -0.946798128 -1.2075440466 0.0031159858

C -1.7486911851 0.0009224275 0.0014909675
C -1.0187419174 1.2660949609 -0.0032996452
C 0.3519033134 1.3265410329 -0.0063587746
C 1.0600001913 0.1248052219 -0.0046392418
C 0.4169841877 -1.1243032867 0.0001164473
O -2.9910697932 0.0296445965 0.0039115603
O -1.7894966307 2.3509839637 -0.0045305139
C 2.5589875694 0.0861857736 -0.0077176348
O 3.1079177655 1.2985926113 -0.0126873495
O -1.6308152315 -2.3632933528 0.0076060971
O 3.1771689136 -0.9398161909 -0.0057796491
H 1.0394087094 -2.0112682758 0.0012371262
H 0.8669444716 2.2753379138 -0.0100042698
H -1.0093967628 -3.0949371304 0.008651153
H -2.6978918942 2.0062015035 -0.0016980394
H 4.068678421 1.1989752774 -0.0141192189

ωB97XD Caffeic Acid (Neutral) Zero field

C 1.2635438692 0.0489406343 -0.7119688929
C 0.0464263879 -0.0688151117 -0.030744459
C 0.0383586238 -0.1176910359 1.345536285
C 1.2319406809 -0.0505385262 2.0709135166
C 2.4318288781 0.0684416281 1.3764295428
C 2.4494592418 0.117009835 -0.009514277
O -1.1174773392 -0.1333671729 -0.7137714793
C 1.2714365495 -0.0988114547 3.5293348268
C 0.2446016013 -0.2489097362 4.3664616184
C 0.4805848998 -0.2710004186 5.8186730775
O -0.6685470762 -0.4316467233 6.5039034886
O 1.1680077853 0.0899560802 -2.0692364547
O 1.5446465562 -0.1629865758 6.3715091803
H 2.2542974837 -0.0006042165 3.9806645394
H -0.7792204383 -0.3608011264 4.0374999563
H -0.4349801305 -0.4357549373 7.4382621294
H 2.0346395973 0.1702690927 -2.4672102003
H -0.9290194528 -0.0858775461 -1.6545137096
H 3.3888079107 0.2097702426 -0.5417788042
H 3.3641432087 0.1233317353 1.9227938751
H -0.9183678371 -0.2072426666 1.8413402407

ωB97XD Caffeic Acid (Neutral) 0.010 a.u.

C 1.2714538641 0.0521034032 -0.7122390649
C 0.0481713998 -0.069763606 -0.0175210758
C 0.0509124937 -0.1197026173 1.3552172244
C 1.2536457669 -0.0488068106 2.0775634865
C 2.4523270677 0.0737821119 1.3720618016

C 2.4645282757 0.1228885412 -0.0120951166
O -1.1110277488 -0.1367846277 -0.6843397462
C 1.2966281387 -0.0991365231 3.5185277644
C 0.2606242727 -0.2379755315 4.3703691338
C 0.4630630998 -0.2708410261 5.801749219
O -0.7133095741 -0.4293101471 6.4803414474
O 1.1467193863 0.0904460076 -2.0424256134
O 1.4980368068 -0.1789028515 6.4308570741
H 2.2837394717 -0.0146282485 3.9651362921
H -0.758867724 -0.3362789274 4.0263667859
H -0.4542522821 -0.4419219306 7.4052606574
H 1.9831679325 0.163580107 -2.5079313122
H -0.9530118067 -0.0968918502 -1.6340750904
H 3.3981338658 0.2167962538 -0.5519286572
H 3.3892052845 0.1300487917 1.9118402514
H -0.9047769908 -0.2150285187 1.8518485386

ωB97XD Caffeic Acid (Neutral) 0.002 a.u.

C 1.2647661322 0.0498114047 -0.7116158169
C 0.047263687 -0.0688172085 -0.0269562128
C 0.0424368714 -0.117949614 1.3486662286
C 1.2381706586 -0.0499874434 2.0719913927
C 2.4369700303 0.0697275103 1.3752976557
C 2.452271462 0.1184565803 -0.0107532099
O -1.1164497531 -0.1339932691 -0.7054634236
C 1.2781134051 -0.0989237492 3.5280691971
C 0.2490050509 -0.2464243714 4.3660903669
C 0.4762514237 -0.2710435625 5.8151160833
O -0.679181071 -0.4316829435 6.496600445
O 1.1617978834 0.0903151402 -2.0636061032
O 1.5337849485 -0.1661525963 6.3842933601
H 2.2616905026 -0.0038402212 3.9787428893
H -0.7736110089 -0.3550052438 4.0329002941
H -0.4429021745 -0.43753272 7.4296634719
H 2.0225139467 0.1675711092 -2.4758164295
H -0.934766577 -0.0885659998 -1.6481886548
H 3.3900942467 0.211523739 -0.5450964662
H 3.3706767625 0.1249362689 1.9194932703
H -0.913785427 -0.2087508098 1.845155662

ωB97XD Caffeic Acid (Neutral) 0.004 a.u.

C 1.2661743899 0.0503878002 -0.7114536117
C 0.0478909598 -0.0688372279 -0.0237832326
C 0.0456861082 -0.1180393402 1.3512128127
C 1.2433687079 -0.0493974516 2.0731826947
C 2.4415224284 0.0708705992 1.3743355823

C 2.4551773678 0.1195468521 -0.0116127179
O -1.1152683108 -0.1345084318 -0.6983861934
C 1.2838554202 -0.098810938 3.5264022896
C 0.2528031831 -0.2443847837 4.3662855623
C 0.4723845044 -0.2710786414 5.8116427728
O -0.6888195965 -0.4317329562 6.4905561099
O 1.1566682742 0.090253722 -2.0581623878
O 1.5237282031 -0.1689606036 6.3964671685
H 2.2681518135 -0.0061796971 3.9763194401
H -0.7687206279 -0.350527069 4.0295148747
H -0.4486161678 -0.4390956115 7.4220329192
H 2.0113648053 0.1656470379 -2.4841785848
H -0.9400218717 -0.090749984 -1.6429825943
H 3.3916776018 0.2127111431 -0.547733652
H 3.3763378636 0.1263371442 1.9168666688
H -0.9102340565 -0.2097795626 1.848058079

ωB97XD Caffeic Acid (Neutral) 0.006 a.u.

C 1.2677704941 0.0510125978 -0.7114674478
C 0.0482870742 -0.0690807998 -0.021138983
C 0.0482026647 -0.1185393492 1.3531527965
C 1.247693073 -0.049126522 2.0744896832
C 2.4455802378 0.0719100133 1.3735274244
C 2.4581538332 0.1207245314 -0.0121088723
O -1.1139330476 -0.1352557929 -0.6925229936
C 1.2888058804 -0.09897143 3.5242592239
C 0.2559399414 -0.2422178734 4.3669880556
C 0.4689221659 -0.2710273096 5.808214465
O -0.6976337476 -0.4311394999 6.4858149678
O 1.1523756464 0.0903846735 -2.0528025572
O 1.5144587252 -0.1721343034 6.4081503724
H 2.2739349936 -0.0091231283 3.9732903486
H -0.7647421469 -0.3456002728 4.0272909443
H -0.452355344 -0.4401389778 7.4154379378
H 2.0010221286 0.1645444384 -2.4922545264
H -0.9446619995 -0.0928944197 -1.6388889625
H 3.3935105088 0.2141502187 -0.549721542
H 3.3813040034 0.1276684757 1.9147448268
H -0.9075240852 -0.2114732701 1.8501288382

ωB97XD Caffeic Acid (Neutral) 0.008 a.u.

C 1.2695428167 0.0515807461 -0.7117134599
C 0.0483954375 -0.0693793951 -0.0190671542
C 0.0499329361 -0.1190749049 1.3544787688
C 1.2510973251 -0.0489108696 2.0759440408
C 2.4491589699 0.0728842876 1.372810927

C 2.4612605627 0.1218321342 -0.0122510847
O -1.1124941645 -0.1359956732 -0.6878853363
C 1.2929933519 -0.0990679024 3.5216438043
C 0.2584930018 -0.2401046063 4.368319595
C 0.4658526569 -0.2709561903 5.8048908049
O -0.7057118557 -0.430341938 6.4824185127
O 1.1490534173 0.0904358227 -2.0475482289
O 1.5059626678 -0.1754477454 6.4194814438
H 2.2790383281 -0.0119077812 3.9696304014
H -0.76152231 -0.3409082078 4.0262598298
H -0.4541304599 -0.4410698556 7.4098599947
H 1.991621203 0.1638024374 -2.5001392236
H -0.9489327866 -0.0949171868 -1.6359578112
H 3.3956622888 0.2154962064 -0.5510826426
H 3.3855644666 0.1289093064 1.9131232276
H -0.9057268537 -0.2131866843 1.8513675907

ωB97XD Gallic Acid (Neutral) Zero field

C -0.9509436934 -1.1717750651 0.0023342236
C -1.6885464961 0.0061650254 0.0006098978
C -1.0401437563 1.2359726907 -0.003733356
C 0.3435057593 1.2863041921 -0.0063332863
C 1.0701356093 0.1024582115 -0.0045074181
C 0.427293133 -1.1318276445 -0.0001341669
O -3.0436741829 0.0075207559 0.0029451632
O -1.7559081041 2.3814036634 -0.0054526888
C 2.5521231809 0.0938030513 -0.0071354548
O 3.0928065131 1.3235792811 -0.012106563
O -1.6939397768 -2.3149575616 0.0064296213
O 3.2309343323 -0.9000358673 -0.005264286
H 1.0178918991 -2.0389997675 0.0011657023
H 0.8369119477 2.2463128742 -0.0098440495
H -1.1235944821 -3.083475962 0.0074905291
H -3.3594106237 -0.899774066 0.0056055534
H -2.6919012384 2.164827235 -0.0033838225
H 4.0480209791 1.2037239532 -0.0133915987

ωB97XD Gallic Acid (Neutral) 0.010 a.u.

C -0.948337384 -1.1891095218 0.0024697327
C -1.6895823004 -0.0061363611 0.0007609901
C -1.0356909007 1.2275363618 -0.0035987111
C 0.3466754172 1.2731066067 -0.0061979484
C 1.080251866 0.0882059754 -0.0043365613
C 0.4316524057 -1.1486013704 0.000061677
O -3.0253020186 0.019680823 0.00298746
O -1.7364738636 2.370980476 -0.0053494964

C 2.544321558 0.105279054 -0.0070319616
O 3.0796880847 1.3522673096 -0.0124997094
O -1.6956485043 -2.3188982446 0.0064836463
O 3.2815062013 -0.8575775719 -0.0049953437
H 1.0128534696 -2.0614854177 0.0013698806
H 0.8322083099 2.2367811568 -0.0098118375
H -1.1517889452 -3.1055788469 0.0070267064
H -3.4025768962 -0.8658286157 0.0054296267
H -2.6813300096 2.1821079326 -0.0036208766
H 4.0291345101 1.2084952542 -0.0138532737

ωB97XD Gallic Acid (Neutral) 0.002 a.u.

C -0.9505504786 -1.1750387067 0.0023647603
C -1.6885896148 0.0037745958 0.0006428465
C -1.0391866631 1.2341310467 -0.0037011918
C 0.3442610329 1.2834574794 -0.0063017011
C 1.0717782142 0.0994247873 -0.0044719808
C 0.428113586 -1.1352364062 -0.0000936539
O -3.0399221829 0.0099953955 0.0029525037
O -1.7515823171 2.3793411025 -0.0054277174
C 2.5504099442 0.0961163229 -0.0071233899
O 3.0896753536 1.3293045581 -0.0121859321
O -1.694381098 -2.3155597796 0.0064416332
O 3.2409167724 -0.8914852254 -0.0052138046
H 1.0165746374 -2.0436572781 0.0012090685
H 0.8361516309 2.2441299802 -0.0098327491
H -1.1291399285 -3.0876389981 0.0074043946
H -3.3673290017 -0.8934547954 0.0055540387
H -2.689403812 2.1684780149 -0.0034384505
H 4.0437649251 1.2051429062 -0.0134846744

ωB97XD Gallic Acid (Neutral) 0.004 a.u.

C -0.9501290194 -1.178513814 0.0023938473
C -1.6887571999 0.0012555623 0.0006740736
C -1.0382416061 1.232236187 -0.0036718178
C 0.344980483 1.2806234965 -0.0062726302
C 1.0736245493 0.0964153184 -0.0044377393
C 0.4289526063 -1.1386608574 -0.0000538809
O -3.036279858 0.0128524685 0.0029588987
O -1.7474385099 2.3771376941 -0.0054048729
C 2.548846165 0.0984270243 -0.0071091363
O 3.0867567181 1.3350565561 -0.0122634063
O -1.6945111226 -2.316547779 0.006453891
O 3.2510867937 -0.8828928937 -0.0051632546
H 1.0153206909 -2.0483281358 0.0012519822
H 0.8352885043 2.2420120487 -0.0098241051

H -1.134205213 -3.0920337651 0.0073150664
H -3.3764095927 -0.8861899406 0.0055113405
H -2.6870547345 2.1718746935 -0.003488804
H 4.0397313454 1.2065011364 -0.0135754524

ωB97XD Gallic Acid (Neutral) 0.006 a.u.

C -0.9496448563 -1.182088497 0.0024208234
C -1.6889966426 -0.0013038831 0.0007043709
C -1.0373235774 1.2304209949 -0.0036455213
C 0.3456434222 1.2779045953 -0.0062470865
C 1.0756652841 0.0935042418 -0.0044052967
C 0.4298213415 -1.1420469956 -0.0000156681
O -3.0326587827 0.0156723515 0.0029676644
O -1.7435318432 2.3749127597 -0.0053845388
C 2.5473537462 0.1007301653 -0.007091041
O 3.0841062203 1.3408143312 -0.0123413797
O -1.694616684 -2.3176165506 0.0064652493
O 3.2613183358 -0.8743253351 -0.0051067437
H 1.0142344845 -2.0529036693 0.0012923361
H 0.8343329537 2.2400457675 -0.0098195332
H -1.1393565212 -3.096561558 0.0072198891
H -3.3858221574 -0.8786876248 0.0054800637
H -2.6849148763 2.1751478516 -0.0035354488
H 4.0359511528 1.2076060546 -0.0136641392

ωB97XD Gallic Acid (Neutral) 0.008 a.u.

C -0.9490508991 -1.1856052833 0.0024457172
C -1.689259991 -0.0037645637 0.0007336478
C -1.0364703603 1.2288571967 -0.0036216862
C 0.3462134365 1.2754082997 -0.006223784
C 1.0778690416 0.0907742602 -0.0043734928
C 0.4307244104 -1.1453501497 0.0000215768
O -3.0289933984 0.017923553 0.0029786937
O -1.73988819 2.3728595712 -0.0053663719
C 2.5458493829 0.1030121176 -0.0070675486
O 3.0817546286 1.3465375913 -0.0124200051
O -1.6950234955 -2.3183768683 0.0064753784
O 3.2714448968 -0.8658885719 -0.0050468702
H 1.0134174929 -2.0572781918 0.0013298821
H 0.8333097369 2.2383106557 -0.0098174464
H -1.1452580804 -3.1010667262 0.0071226112
H -3.3944855471 -0.8719395267 0.0054557298
H -2.6830180681 2.1785475153 -0.0035787477
H 4.0324260034 1.208264121 -0.0137532841

ωB97XD Caffeic Acid (Radical) Zero field

C 1.2515237661 0.0509487931 -0.7635371549
C -0.0006867099 -0.0759983898 -0.0038349881
C -0.0148869899 -0.1278669757 1.3648399601
C 1.1943382408 -0.0567256001 2.0703218826
C 2.4249146501 0.0686548998 1.3562567452
C 2.4702019172 0.1197999061 0.0023121719
O -1.1042848442 -0.1350533462 -0.7306466106
C 1.2624795393 -0.1028486052 3.5130824929
C 0.237673067 -0.2461955326 4.3647952697
C 0.4903254341 -0.2693785134 5.8176366256
O -0.6502992436 -0.4231828102 6.5120891503
O 1.1786154109 0.0912778807 -1.994885488
O 1.5647417834 -0.1662288218 6.3478984247
H 2.2500386961 -0.0114187108 3.954194982
H -0.7900384151 -0.3515243075 4.0464028115
H -0.4137956611 -0.4291732905 7.4460156173
H -0.809833988 -0.0786032375 -1.6567860427
H 3.4012314417 0.2143649425 -0.5390374068
H 3.3422546842 0.1220323217 1.9290392985
H -0.9628607792 -0.2203616024 1.8756152586

ωB97XD Caffeic Acid (Radical) 0.010 a.u.

C 1.2546832326 0.0552815574 -0.7681043999
C -0.0058477003 -0.0787844277 -0.0004768465
C -0.007829358 -0.1329550576 1.371475194
C 1.2062137931 -0.0589508881 2.0698106413
C 2.4404571303 0.069566346 1.3491676989
C 2.4839579312 0.1234171703 -0.0009455733
O -1.1094258571 -0.1397896357 -0.7036180419
C 1.2772974292 -0.1047851827 3.5021956824
C 0.2492710633 -0.2405723261 4.3700393407
C 0.4772277094 -0.2667294342 5.8016847927
O -0.6841778683 -0.4210596759 6.5000755907
O 1.1809458122 0.1012944087 -1.9849919242
O 1.526909917 -0.1707872466 6.4013710551
H 2.2697035067 -0.0195807033 3.9347435672
H -0.7757801139 -0.3395581788 4.0434145286
H -0.4128133196 -0.428812768 7.421748679
H -0.8635747792 -0.0848796301 -1.6459984003
H 3.4089399523 0.2187563468 -0.5526260497
H 3.3602502612 0.1219907998 1.9191415554
H -0.9547567421 -0.2305424741 1.8836659096

ωB97XD Caffeic Acid (Radical) 0.002 a.u.

C 1.2512697495 0.0512412559 -0.7638779492
C -0.0016751335 -0.0761120416 -0.0022987738

C -0.0124863352 -0.1278900092 1.3672092544
C 1.1979825164 -0.0565269828 2.0697324292
C 2.4284314291 0.0686119932 1.3545526456
C 2.4724386143 0.1197035894 0.0009392666
O -1.1057055813 -0.1352469931 -0.7238421827
C 1.2665152598 -0.1023773794 3.5118865796
C 0.2412080784 -0.2454750411 4.3648652875
C 0.4873052544 -0.268709972 5.8144241673
O -0.6578883896 -0.4248343153 6.5075447751
O 1.1771544435 0.0920950491 -1.9924894251
O 1.5558805205 -0.1648793785 6.3595420064
H 2.254845252 -0.0108229422 3.9513722026
H -0.7855072223 -0.3510633661 4.0439595823
H -0.4165719462 -0.4306268025 7.4396082259
H -0.8202045496 -0.0794860206 -1.6532319067
H 3.4019433997 0.2137583528 -0.5430285055
H 3.3467061439 0.1216670968 1.9260392197
H -0.9599895038 -0.2205070927 1.8788661005

ωB97XD Caffeic Acid (Radical) 0.004 a.u.

C 1.2513778327 0.0517423722 -0.7643728994
C -0.0027235224 -0.0764934151 -0.0011082659
C -0.0106642617 -0.1285231827 1.3690965255
C 1.2009632501 -0.056725335 2.0694093878
C 2.4316497207 0.068708673 1.3530780878
C 2.4748272192 0.1200557809 -0.0000421499
O -1.1068487185 -0.1357760323 -0.7179368241
C 1.2699824505 -0.1024467563 3.510193415
C 0.2441020089 -0.2445289063 4.3653771945
C 0.4845421491 -0.2680943831 5.8111987706
O -0.664945975 -0.4253889419 6.5040060121
O 1.1764094639 0.093425959 -1.9902025581
O 1.5477446395 -0.1646563244 6.3705498642
H 2.2592026416 -0.011561445 3.9479970153
H -0.7818743255 -0.3495037735 4.0424383904
H -0.4177446696 -0.4312111457 7.433941296
H -0.8301412233 -0.0803604604 -1.6504675068
H 3.4029590567 0.2140173854 -0.5463381899
H 3.3506537488 0.1215899987 1.9236055818
H -0.9578194857 -0.2217510675 1.8813498531

ωB97XD Caffeic Acid (Radical) 0.006 a.u.

C 1.2519659831 0.0523182063 -0.7651797779
C -0.003786715 -0.0769440983 -0.0003698647
C -0.0093088841 -0.1293049033 1.3704572167
C 1.2033433463 -0.0569929851 2.0693298662

C 2.4347133835 0.0689504366 1.3517615949
C 2.4775233836 0.1205991626 -0.0006634082
O -1.1078816491 -0.1364503061 -0.7126007622
C 1.2728770613 -0.1026442848 3.5080134989
C 0.2463815582 -0.2434869245 4.3663345229
C 0.4819617528 -0.2675743552 5.8079608327
O -0.6715453993 -0.4253954066 6.5015117984
O 1.176834714 0.0948503582 -1.9881719436
O 1.5402020458 -0.1652094548 6.3810411815
H 2.2630280511 -0.0127844151 3.9441743232
H -0.7790305665 -0.3475321701 4.0417510409
H -0.4174342131 -0.4314601751 7.4290396574
H -0.8406055082 -0.0814148679 -1.648331449
H 3.404452118 0.2145995773 -0.5490201168
H 3.3542230836 0.1217232896 1.9217034623
H -0.9562615459 -0.2233276838 1.8830313265

ωB97XD Caffeic Acid (Radical) 0.008 a.u.

C 1.2531342889 0.0531541089 -0.7664624328
C -0.0047806011 -0.0775112276 -0.0001488881
C -0.008267399 -0.1303001134 1.3712574662
C 1.2052106246 -0.057388416 2.069499459
C 2.4377524372 0.0693043872 1.3505000596
C 2.4806378463 0.1214261261 -0.0009582618
O -1.1089182392 -0.1374620558 -0.7075459821
C 1.2753380608 -0.1030381089 3.505362918
C 0.2481299891 -0.2422966535 4.3678048314
C 0.4794729113 -0.2671518812 5.8047348778
O -0.6779462531 -0.424651233 6.500040197
O 1.1786496508 0.0967554003 -1.9865094971
O 1.5331276107 -0.1667564928 6.3912781293
H 2.2664707272 -0.0146637822 3.9398887025
H -0.7768922737 -0.3449290162 4.041922614
H -0.4158942733 -0.431256728 7.4248535095
H -0.8524682739 -0.0829291778 -1.6466759028
H 3.4065267642 0.215635404 -0.5511272471
H 3.3575434393 0.1219622366 1.9202311162
H -0.955175037 -0.2253837768 1.8838273312

ωB97XD Gallic Acid (Radical) Zero field

C -0.9452843247 -1.2171406279 0.003170119
C -1.747332079 -0.0029157395 0.0016500119
C -1.0172562429 1.2639157535 -0.0032532542
C 0.3554390109 1.317096852 -0.0062955701
C 1.0621418546 0.1143483388 -0.0044946114
C 0.4211272517 -1.1363390455 0.0002324321

O -2.9807365673 0.0227755788 0.0041293564
O -1.7720257488 2.3511195679 -0.004568907
C 2.5494442767 0.0942603426 -0.0074979721
O 3.0954144481 1.3181357511 -0.0130645841
O -1.6385934199 -2.3586621655 0.007483788
O 3.2113013893 -0.9094436609 -0.0053120299
H 1.036107212 -2.0275907469 0.0013493154
H 0.866708316 2.2673361272 -0.0100249582
H -1.0405301803 -3.1086903185 0.0082081213
H -2.6919851704 2.0351519962 -0.0019022477
H 4.0511519742 1.1997649967 -0.0145140093

ωB97XD Gallic Acid (Radical) 0.010 a.u.

C -0.9419113921 -1.2316956832 0.0032650699
C -1.7485333087 -0.0095178549 0.0018907423
C -1.0168586484 1.2622242239 -0.0032591924
C 0.3579886659 1.3063830285 -0.0063777219
C 1.0689503709 0.1020982202 -0.0044870879
C 0.4267843817 -1.1531635751 0.0003344967
O -2.9708410986 0.0084061338 0.004505179
O -1.7512988003 2.3529704603 -0.0046507384
C 2.5393952573 0.1055972113 -0.0075664805
O 3.0841920576 1.3449111524 -0.0132501125
O -1.6492479139 -2.3537184413 0.0074632119
O 3.2571294272 -0.8697195081 -0.0049338149
H 1.0333593417 -2.049657918 0.0014358518
H 0.8642997022 2.2590216439 -0.0102952593
H -1.0854544357 -3.1292507833 0.0077896381
H -2.6863934628 2.079697913 -0.0020278708
H 4.0335318559 1.1985367766 -0.0145409111

ωB97XD Gallic Acid (Radical) 0.002 a.u.

C -0.944801786 -1.2197397522 0.0031883118
C -1.7472448547 -0.0040084401 0.0016980805
C -1.0169945697 1.2634876538 -0.003248872
C 0.3561772645 1.3148840617 -0.0062928835
C 1.0631217454 0.1118359468 -0.0044708694
C 0.4221939773 -1.1394933144 0.0002601651
O -2.9784488669 0.0206933993 0.004206206
O -1.7678893968 2.3512133595 -0.004589801
C 2.5473091418 0.0964176817 -0.0074721237
O 3.0927916996 1.3232400929 -0.0131252277
O -1.6406979445 -2.3575234666 0.0074655147
O 3.2202031227 -0.9016125839 -0.0052333092
H 1.0353509152 -2.0318429664 0.0013751539
H 0.866491295 2.2655393929 -0.0100522102

H -1.0490198029 -3.1124290332 0.0081040814
H -2.6907240717 2.0427454243 -0.0019518167
H 4.0472741316 1.1997155441 -0.0145654

ωB97XD Gallic Acid (Radical) 0.004 a.u.

C -0.9442093748 -1.2225535869 0.0032052745
C -1.7473623655 -0.0053064915 0.0017431338
C -1.016871597 1.2630359179 -0.0032463555
C 0.3567532888 1.3126136756 -0.006293318
C 1.0642705268 0.1092982297 -0.0044488243
C 0.4233117922 -1.1428012578 0.0002891722
O -2.9763433113 0.017977341 0.0042753587
O -1.7635716409 2.351539737 -0.0046098096
C 2.5452217682 0.098639224 -0.0074463517
O 3.0902874991 1.3284862459 -0.0131880532
O -1.6427647731 -2.3565267417 0.0074484128
O 3.2292666261 -0.8936573208 -0.0051514707
H 1.0347245258 -2.036217708 0.0014042142
H 0.8660711031 2.2637277274 -0.0100831545
H -1.0576920781 -3.1164122942 0.0080036594
H -2.6895084138 2.0516470686 -0.0019898763
H 4.0435084245 1.1996332336 -0.0146170117

ωB97XD Gallic Acid (Radical) 0.006 a.u.

C -0.943476153 -1.2255888865 0.0032219571
C -1.7476849615 -0.0067906206 0.0017837516
C -1.0168835689 1.2625822072 -0.0032437195
C 0.3571644695 1.3103080272 -0.00629366
C 1.0656114237 0.1067555937 -0.0044235127
C 0.4244902304 -1.1462621851 0.0003250547
O -2.9743938472 0.0146377403 0.0043121021
O -1.7591331868 2.3520875265 -0.0046229487
C 2.5431696324 0.1009294156 -0.0074169518
O 3.0879354254 1.3338890207 -0.0132598811
O -1.6447961858 -2.3556647943 0.0074309296
O 3.2384869783 -0.8855899625 -0.0050674207
H 1.0342528962 -2.0407053608 0.0014448028
H 0.8654418146 2.2619248156 -0.0101142315
H -1.0665984062 -3.1206675322 0.0079075592
H -2.6883697836 2.0618172269 -0.002007592
H 4.0398752224 1.1994607682 -0.0146812389

ωB97XD Gallic Acid (Radical) 0.008 a.u.

C -0.942774248 -1.228583873 0.003239445
C -1.7480705472 -0.0081707119 0.0018230951
C -1.0168975583 1.2623265951 -0.0032520295

C 0.3575897981 1.3082758767 -0.0063388165
C 1.0671607308 0.1043679086 -0.0044623903
C 0.4256311182 -1.149697569 0.0003249371
O -2.9726642489 0.0114636059 0.0044129582
O -1.7550513341 2.3525937719 -0.0046332228
C 2.5412664435 0.1032296594 -0.0075008163
O 3.0859207145 1.3393439325 -0.0132546518
O -1.6469881141 -2.3547431498 0.0074509937
O 3.2477347285 -0.8777018455 -0.0049931682
H 1.0337799796 -2.0451729261 0.0014388765
H 0.8648842688 2.260398388 -0.0102054878
H -1.0757705352 -3.124891538 0.0078606404
H -2.6872561228 2.0709369584 -0.0020150898
H 4.0365969268 1.1991479167 -0.014600273

CAM-B3LYP Caffeic Acid (Neutral) -0.010 a.u.

C 1.2582208532 0.0570247472 -0.7103773349
C 0.0467138611 -0.1195497254 -0.0553809451
C 0.0169035976 -0.2012206228 1.3197091431
C 1.1925595603 -0.1070589182 2.0656565766
C 2.3962236162 0.0633865856 1.3866240457
C 2.4299563961 0.1463122913 0.0064595122
O -1.1091643798 -0.212141483 -0.7767508578
C 1.2320794371 -0.1746705609 3.5266168659
C 0.214606697 -0.2139217674 4.3755532765
C 0.5094749925 -0.2681306203 5.8336601109
O -0.6103870368 -0.2817978968 6.5569460441
O 1.2073511688 0.1308988472 -2.0950480721
O 1.61526371 -0.2942057116 6.2916629996
H 2.220973494 -0.1805671267 3.9721934159
H -0.8255963414 -0.2001598262 4.0813978976
H -0.378579096 -0.3113166292 7.4981446379
H 2.0846939515 0.3474420082 -2.413696966
H -0.8855899402 -0.1028818294 -1.7047756435
H 3.3737885282 0.2809696647 -0.5104914051
H 3.314408167 0.1357507964 1.9518630336
H -0.9387902362 -0.340490223 1.8046176647

CAM-B3LYP Caffeic Acid (Neutral) -0.002 a.u.

C 1.2618365283 0.0531798873 -0.7071510717
C 0.0486448736 -0.0792995834 -0.0317759093
C 0.0360886083 -0.1351535886 1.3420371177
C 1.224851316 -0.060789509 2.0704474364
C 2.4235773321 0.0709823167 1.3792003672
C 2.4435635092 0.1278949877 -0.004283795
O -1.1136035954 -0.1526407108 -0.7252952096

C	1.26383148	-0.1148891589	3.5282214247
C	0.2392266783	-0.2369749148	4.3662620126
C	0.4870016545	-0.2720002945	5.8172389463
O	-0.6583120872	-0.3965727165	6.512347693
O	1.1734295079	0.1001460561	-2.0716580972
O	1.5606576977	-0.2014858401	6.3518923768
H	2.2485365787	-0.0465968705	3.9776547019
H	-0.7894138518	-0.3136514481	4.0460984637
H	-0.4256572238	-0.4122599562	7.4504032253
H	2.0449019723	0.1957276232	-2.4610379292
H	-0.9181881913	-0.0957275544	-1.6662510845
H	3.3819546096	0.2310972726	-0.5353121855
H	3.3516524451	0.1302451787	1.9300961364
H	-0.919468842	-0.2375591764	1.8354493799

CAM-B3LYP Caffeic Acid (Neutral) -0.004 a.u.

C	1.2607831451	0.0531134028	-0.7078687231
C	0.0476784946	-0.0835171544	-0.0367446185
C	0.0311328068	-0.1418528866	1.3375866249
C	1.2172424805	-0.0658469822	2.0693852149
C	2.417360906	0.0695693102	1.3806640039
C	2.4405056355	0.129071284	-0.0023507735
O	-1.1138783694	-0.1586931177	-0.7361120541
C	1.2562470546	-0.1208689446	3.528578969
C	0.2336449502	-0.2361616727	4.3679732176
C	0.4922024214	-0.2717593873	5.8211015418
O	-0.6470514079	-0.3844005298	6.5220886402
O	1.1812694687	0.1029210079	-2.0776088474
O	1.5737760555	-0.2095286003	6.3377335895
H	2.2413915352	-0.0583342004	3.9777923477
H	-0.7974499604	-0.3056223836	4.0533520885
H	-0.4150650034	-0.4004636843	7.4610216259
H	2.0576074563	0.213029668	-2.4510040672
H	-0.9113680649	-0.094931908	-1.6745609114
H	3.3805118593	0.2353080942	-0.5305430491
H	3.3434766979	0.1300451035	1.9345480527
H	-0.9249071616	-0.2474044185	1.8295511277

CAM-B3LYP Caffeic Acid (Neutral) -0.006 a.u.

C	1.2597366348	0.0544078391	-0.7086969895
C	0.046851777	-0.0905587522	-0.0423000294
C	0.0261060897	-0.1539168172	1.3324301783
C	1.2092286655	-0.0743439496	2.0682447108
C	2.4106746597	0.0683762319	1.3823371242
C	2.4371549775	0.1330290442	-0.0000014517
O	-1.1134691219	-0.1692925333	-0.7482185098

C	1.2484000645	-0.131914551	3.5284422463
C	0.2274796402	-0.2320481668	4.3701824177
C	0.4978313439	-0.271217354	5.8252624934
O	-0.6354270944	-0.363145104	6.5329897561
O	1.1894332044	0.1093185496	-2.0835222202
O	1.5878239679	-0.2267701386	6.3230208364
H	2.2347039978	-0.0830905474	3.9768208036
H	-0.8067858804	-0.2847830985	4.0619195874
H	-0.403796217	-0.3819522834	7.4727538052
H	2.0697858782	0.2383619595	-2.4402990689
H	-0.9036550536	-0.096829306	-1.6839192659
H	3.3786584347	0.245362333	-0.5249503713
H	3.334555703	0.1312126253	1.9395439728
H	-0.9301806716	-0.2665339806	1.8225439745

CAM-B3LYP Caffeic Acid (Neutral) -0.008 a.u.

C	1.2587816932	0.0562272802	-0.7095592998
C	0.0464138652	-0.1021921526	-0.0485020898
C	0.0212629388	-0.173365739	1.3264930908
C	1.2009261243	-0.087708539	2.0670127576
C	2.4035605205	0.0668311128	1.3842860992
C	2.4335495317	0.1394280151	0.0028985615
O	-1.1120428185	-0.1869781082	-0.761707495
C	1.2403656439	-0.1496438612	3.5277835238
C	0.2209865073	-0.2245687736	4.3728127039
C	0.5036760355	-0.2703507669	5.829492107
O	-0.6234005281	-0.3290061765	6.5448168798
O	1.1980329929	0.1190396878	-2.0893497477
O	1.6021354405	-0.2558408696	6.3075657678
H	2.2281669322	-0.1238054081	3.9748724161
H	-0.8166553774	-0.249406677	4.0715078286
H	-0.3916544938	-0.3526609938	7.4852911296
H	2.0799369128	0.2799989972	-2.4282369862
H	-0.89514488	-0.0999535332	-1.6940752298
H	3.3763296148	0.2614289041	-0.518331428
H	3.3248157713	0.1336435332	1.9452614275
H	-0.9349314271	-0.297443932	1.8142519831

CAM-B3LYP Caffeic Acid (Neutral) -0.010 a.u.

C	-0.949994191	-1.1525942847	0.002075535
C	-1.6843984823	0.01969223	0.0002058212
C	-1.0415816246	1.2448530466	-0.0040897301
C	0.3406155806	1.2994399486	-0.0065405099
C	1.0638669078	0.117442342	-0.0046750274
C	0.4231247263	-1.1142413076	-0.0003861814
O	-3.0605047925	-0.0068154567	0.0026577657

O -1.7800306769 2.3907111596 -0.0058325984
C 2.5582637663 0.0831099363 -0.0070721743
O 3.1094766033 1.2962799597 -0.0110293663
O -1.6953131285 -2.3085603192 0.0064646555
O 3.1804222568 -0.9392477607 -0.0065966395
H 1.0250420029 -2.0137185122 0.0009792675
H 0.8431444244 2.2545271719 -0.0097826664
H -1.1064031222 -3.0677171368 0.0083910791
H -3.3186864214 -0.9343475047 0.0061957485
H -2.7093415589 2.1451182435 -0.0029801337
H 4.0738587298 1.1972932444 -0.0126908452

Recover connectivity data from disk.

NAtoms= 18 NQM= 18 NQMF= 0 NMMI= 0 NMMIF=
NMic= 0 NMicF= 0.

CAM-B3LYP Caffeic Acid (Neutral) -0.002 a.u.

C -0.9489490829 -1.1654676607 0.0022506124
C -1.6835211495 0.0099395847 0.0004456894
C -1.0369700283 1.23629258 -0.0038962789
C 0.3443204033 1.2867269318 -0.0064491928
C 1.0685047769 0.1041862112 -0.0046275514
C 0.4261498145 -1.1280873147 -0.0002752765
O -3.0441372297 0.0051486191 0.0028384448
O -1.759716731 2.3818642697 -0.0056310748
C 2.5502559932 0.092039598 -0.00722289
O 3.0931270488 1.3194354497 -0.011429692
O -1.6957653048 -2.311320584 0.0065721555
O 3.21941972 -0.9055157262 -0.0061030087
H 1.0185624708 -2.0328404772 0.0010615818
H 0.8407831713 2.2442068675 -0.0098145052
H -1.1257472873 -3.0837044975 0.0079638184
H -3.350685647 -0.9080208052 0.0058590856
H -2.6968091851 2.1602226574 -0.0033123802
H 4.0527392467 1.2061192963 -0.0129355373

CAM-B3LYP Caffeic Acid (Neutral) -0.004 a.u.

C -0.9492765438 -1.1622132491 0.0022119514
C -1.6836218345 0.0123842551 0.00039715
C -1.0380231019 1.2383155767 -0.0039417392
C 0.3434797554 1.2897344565 -0.006483663
C 1.0671356326 0.1073358908 -0.0046583234
C 0.4253452025 -1.1246925623 -0.0003126968
O -3.0481125179 0.0023387606 0.0028122357
O -1.7644275988 2.3840714639 -0.0056755602
C 2.552095562 0.0897926121 -0.00722527
O 3.0967298314 1.3137044552 -0.011321312

O	-1.6955808653	-2.3106538139	0.0065545757
O	3.2095977418	-0.9139708485	-0.00620908
H	1.0199626401	-2.0281991388	0.0010261648
H	0.8415201632	2.2465575875	-0.0098262363
H	-1.1206239821	-3.0796091441	0.0080686627
H	-3.3425389464	-0.9146146154	0.0059445128
H	-2.6996226821	2.1565952104	-0.0032391932
H	4.0575225436	1.2043481034	-0.0128281791

CAM-B3LYP Caffeic Acid (Neutral) -0.006 a.u.

C	-0.9495562482	-1.1589881158	0.0021700674
C	-1.683801326	0.0148184004	0.0003399054
C	-1.0391524293	1.2404168347	-0.0039875017
C	0.3425734576	1.2928677518	-0.0065045954
C	1.0659041259	0.1106094507	-0.0046692033
C	0.4245767514	-1.1212461356	-0.0003395795
O	-3.0521689686	-0.0005920653	0.0027680308
O	-1.7693988741	2.3862791167	-0.0057239663
C	2.5540529692	0.0875567418	-0.0071890321
O	3.1006921626	1.3079130972	-0.0112237258
O	-1.6954493805	-2.3099651671	0.0065280324
O	3.1998286033	-0.9224289135	-0.0063319301
H	1.0215141674	-2.0234580708	0.0010053448
H	0.8421361345	2.249081054	-0.0098167301
H	-1.1156950853	-3.0755738308	0.0081748932
H	-3.334500288	-0.9212031181	0.0060234015
H	-2.7026703895	2.1528571563	-0.0031615265
H	4.0626756176	1.2022808136	-0.0127678845

CAM-B3LYP Caffeic Acid (Neutral) -0.008 a.u.

C	-0.94979313	-1.1557848022	0.0021247536
C	-1.6840596863	0.0172539296	0.0002772538
C	-1.0403333454	1.2425962551	-0.0040375736
C	0.3416218333	1.2960982485	-0.0065270386
C	1.0648208712	0.1139716569	-0.0046793459
C	0.4238360451	-1.1177682437	-0.0003666132
O	-3.0562909403	-0.0036457929	0.0027200767
O	-1.7745913203	2.3884938126	-0.0057762143
C	2.5560960662	0.0853338677	-0.0071462519
O	3.1049294035	1.3021235582	-0.0111230916
O	-1.6953611975	-2.3092690039	0.006499907
O	3.1901103595	-0.9308426584	-0.0064587373
H	1.0232021211	-2.0186394162	0.0009863132
H	0.842685702	2.2517297157	-0.0098073359
H	-1.1109641744	-3.0716157775	0.008282734
H	-3.3265496802	-0.9277798876	0.0061105165

H -2.7059032798 2.1490417623 -0.0030747186
H 4.0681053522 1.1999277758 -0.0127106339

CAM-B3LYP Caffeic Acid (Radical) -0.010 a.u.

C 1.255379458 0.0545689847 -0.7568686119
C 0.0051568821 -0.0821906597 -0.0153297901
C -0.0342584522 -0.1374085053 1.3437880846
C 1.1657615125 -0.0610221723 2.0774948169
C 2.3991160995 0.076098131 1.3710853824
C 2.4559029486 0.1328114208 0.0186564488
O -1.0884555251 -0.149525593 -0.7841797832
C 1.2312208335 -0.1151133322 3.5088519342
C 0.2101325661 -0.2382199711 4.3710840654
C 0.5118750849 -0.2778409785 5.8301954032
O -0.5994007179 -0.3873803637 6.5511575709
O 1.1944998017 0.0932650489 -2.0036182309
O 1.6226055914 -0.2181156293 6.2712698036
H 2.2170767787 -0.0505379208 3.9558609563
H -0.8269178123 -0.310710592 4.0753263745
H -0.3744640506 -0.4068659502 7.4949823811
H -0.7389191906 -0.0826985499 -1.6918540851
H 3.3942269239 0.2376510227 -0.507500208
H 3.3066434752 0.1354182744 1.9564246136
H -0.9855302073 -0.2396636646 1.8449458738

CAM-B3LYP Caffeic Acid (Radical) -0.002 a.u.

C 1.2498842983 0.0551309562 -0.7564738842
C 0.0024701002 -0.0818209017 -0.0018335628
C -0.0140501701 -0.1370478609 1.3623511102
C 1.1923825256 -0.0609011508 2.0724431813
C 2.4205310756 0.0738997599 1.3594309987
C 2.4647270345 0.1308826253 0.007709594
O -1.1001186219 -0.1481893925 -0.7375208926
C 1.2593474729 -0.1127010275 3.5113038606
C 0.2343019217 -0.2367305521 4.362655153
C 0.4938414566 -0.2727464346 5.8145208671
O -0.6441300439 -0.3993343894 6.514661335
O 1.1783310695 0.0972543047 -1.9908628062
O 1.5756623275 -0.2005352633 6.3294059309
H 2.2470273114 -0.0439625728 3.9529262432
H -0.7960538177 -0.3140666771 4.0487785712
H -0.4123457625 -0.4165427563 7.4532845444
H -0.7982525327 -0.0856198136 -1.6631980564
H 3.3936364073 0.2332998407 -0.5344939546
H 3.3349281677 0.1310769582 1.9344461734
H -0.9604682198 -0.2388266525 1.8722385938

CAM-B3LYP Caffeic Acid (Radical) -0.004 a.u.

C	1.2507492489	0.0547357444	-0.7564107983
C	0.0031561063	-0.0819014369	-0.0043788813
C	-0.0181227507	-0.1371875599	1.3587410542
C	1.1868892275	-0.0610910928	2.0734330522
C	2.4159161794	0.0742714825	1.3617331931
C	2.4625503691	0.1312742725	0.0098536293
O	-1.0977746058	-0.1484378278	-0.7472619678
C	1.2536280757	-0.1134221237	3.511423391
C	0.2294013085	-0.2370536343	4.3638749112
C	0.497770871	-0.2737000385	5.8181857658
O	-0.6345305733	-0.396818408	6.5218829432
O	1.1810354287	0.0966807177	-1.9936444788
O	1.5863145313	-0.2038967394	6.3162012087
H	2.2408221641	-0.0456452359	3.9543281318
H	-0.8023801249	-0.3131600001	4.053643009
H	-0.4058449835	-0.4145228115	7.462039449
H	-0.7848194201	-0.085031289	-1.6689126531
H	3.3934591658	0.234442086	-0.5289076495
H	3.3288576835	0.1320072861	1.9389053413
H	-0.9654259014	-0.2390243912	1.8670443489

CAM-B3LYP Caffeic Acid (Radical) -0.006 a.u.

C	1.2519002303	0.0551723112	-0.7563831094
C	0.0038320419	-0.081958438	-0.0074398341
C	-0.0228716057	-0.1373575214	1.354470223
C	1.1805843319	-0.0610489067	2.0746087087
C	2.4107937269	0.0748492959	1.3644314199
C	2.4603625984	0.1318046416	0.0124280071
O	-1.0950134148	-0.1487259275	-0.7582714611
C	1.2470676499	-0.1139969579	3.5110313224
C	0.2237951098	-0.2375396114	4.3656366479
C	0.5020545969	-0.2750397596	5.8218920843
O	-0.6239441779	-0.3941826045	6.5303917896
O	1.1846903531	0.0948938958	-1.9966564352
O	1.5975768564	-0.2075352796	6.3022513592
H	2.2337916459	-0.0471233462	3.9552164672
H	-0.8095553142	-0.3125847688	4.0596470149
H	-0.3972574248	-0.4121785091	7.4718983911
H	-0.7705308834	-0.0836991589	-1.6756085506
H	3.3935265876	0.2352553891	-0.5225497725
H	3.3221184416	0.1329437747	1.9440244261
H	-0.9712693498	-0.2394295187	1.8607543014

CAM-B3LYP Caffeic Acid (Radical) -0.008 a.u.

C	1.2534287885	0.0549598183	-0.7565488866
C	0.0044880771	-0.0820031729	-0.0110585901
C	-0.0282132829	-0.1373231317	1.3495405466
C	1.1735882987	-0.06101131	2.0759807228
C	2.4052697626	0.0753717629	1.3675134878
C	2.4581833501	0.1321760264	0.0153371974
O	-1.0919290149	-0.1489687311	-0.7705166963
C	1.2396983475	-0.114480073	3.5101999765
C	0.2174683173	-0.23785266	4.3680234117
C	0.5067602307	-0.2762451014	5.8259558294
O	-0.6123261063	-0.391536802	6.5400468421
O	1.1890594741	0.0937603097	-1.9999595081
O	1.6096020663	-0.2116079795	6.2874789528
H	2.2260137266	-0.048592474	3.9556714352
H	-0.81762037	-0.3117613954	4.0667751078
H	-0.3870460342	-0.4101076484	7.4828065403
H	-0.7554088425	-0.082952272	-1.6832726537
H	3.3937980247	0.2361418463	-0.5154929795
H	3.3147909838	0.1339707607	1.9498432819
H	-0.9779537972	-0.2394187727	1.8534489821

CAM-B3LYP Caffeic Acid (Radical) -0.010 a.u.

C	-0.9448570347	-1.2021114765	0.0031669541
C	-1.7436363667	0.003458874	0.0014093252
C	-1.0160737775	1.2655202031	-0.0034168414
C	0.3515765774	1.3266723367	-0.0064254812
C	1.0593528666	0.1266115984	-0.0047449497
C	0.415362031	-1.1207210901	0.0000227822
O	-2.9886260432	0.0341481949	0.0038920544
O	-1.7945370927	2.3490587687	-0.0047300033
C	2.5568370922	0.0846429146	-0.0079853649
O	3.1088101007	1.2943672884	-0.0117449519
O	-1.6290836402	-2.3622750358	0.0079345765
O	3.1648725577	-0.9454134503	-0.0071732459
H	1.039537074	-2.0054554232	0.0011426362
H	0.869349812	2.2732220949	-0.0099921627
H	-1.0054873287	-3.095795516	0.00920011
H	-2.7026036447	1.9961009404	-0.0018070633
H	4.0742988168	1.2010917777	-0.0134533741

CAM-B3LYP Caffeic Acid (Radical) -0.002 a.u.

C	-0.9435526984	-1.2120037212	0.0032022407
C	-1.7423184172	-0.0008039981	0.0015485112
C	-1.0145231221	1.2624786493	-0.0033769245
C	0.3551586458	1.3159311873	-0.0064000176
C	1.0611623132	0.1151432098	-0.0046510873

C	0.419387141	-1.1332909269	0.0000978352
O	-2.9781203099	0.0261874555	0.0040443125
O	-1.7747627619	2.3497945308	-0.0047293237
C	2.5473945251	0.0927671698	-0.007777446
O	3.0946418364	1.3148147458	-0.0121418229
O	-1.636653959	-2.3579513528	0.0078291737
O	3.2004229208	-0.9141358497	-0.0065626636
H	1.0348761924	-2.0229287825	0.0012349796
H	0.8689140522	2.2639010174	-0.0100405397
H	-1.0362948371	-3.1097515581	0.0087849643
H	-2.6955712164	2.0291400076	-0.0019161553
H	4.054931695	1.2038312161	-0.0138510366

CAM-B3LYP Caffeic Acid (Radical) -0.004 a.u.

C	-0.9439461237	-1.2094700277	0.0031913973
C	-1.7425320481	0.0003236403	0.0015091833
C	-1.0148090106	1.2631547259	-0.0033854599
C	0.3543770494	1.3184341908	-0.0064026975
C	1.0604837126	0.117846829	-0.0046706249
C	0.4183441842	-1.1301535016	0.0000792196
O	-2.9805627872	0.0283700521	0.0039991644
O	-1.7794314205	2.3496199185	-0.0047275569
C	2.5496278817	0.0906774835	-0.0078175472
O	3.0977537108	1.3097018857	-0.0120484781
O	-1.634704393	-2.3590359119	0.0078515113
O	3.1915115019	-0.921984453	-0.0067100373
H	1.0358417932	-2.0186368492	0.0012146685
H	0.8691874426	2.2659912341	-0.0100211433
H	-1.02826423	-3.1061340871	0.0088887519
H	-2.6971234738	2.0208844112	-0.0018894298
H	4.0593382107	1.2035334594	-0.0137659217

CAM-B3LYP Caffeic Acid (Radical) -0.006 a.u.

C	-0.9442912789	-1.2069786896	0.0031812868
C	-1.7428233806	0.0014112232	0.0014707824
C	-1.0151595922	1.2638949973	-0.0033945481
C	0.3535195104	1.3210644383	-0.0064049764
C	1.0599548122	0.1206642715	-0.0046894758
C	0.4173227321	-1.1270096286	0.0000619839
O	-2.983120618	0.030434605	0.0039569801
O	-1.7842960277	2.349435062	-0.0047274782
C	2.5519549131	0.0886185174	-0.0078589275
O	3.1011551354	1.3045741626	-0.0119517537
O	-1.6327910386	-2.3601186199	0.0078751428
O	3.1826078911	-0.9298333627	-0.0068659184
H	1.0369436331	-2.0142868614	0.001194697

H	0.8693566767	2.2682444614	-0.0100019035
H	-1.0204528516	-3.1026006546	0.0089930277
H	-2.6988256823	2.0126134169	-0.0018651735
H	4.0640371658	1.2029956613	-0.0136787457

CAM-B3LYP Caffeic Acid (Radical) -0.008 a.u.

C	-0.9445889564	-1.2045384307	0.0031757593
C	-1.7431855357	0.0024590641	0.001446757
C	-1.0155665711	1.2646783056	-0.0034077867
C	0.352601092	1.3237973967	-0.0064266063
C	1.0595895122	0.1235627939	-0.0047301367
C	0.4163341194	-1.1238917945	0.000035684
O	-2.9858028805	0.0323294231	0.0039305112
O	-1.7892685474	2.3492717242	-0.0047277094
C	2.5542974319	0.0866313241	-0.007943853
O	3.1047798239	1.2995484742	-0.0118435233
O	-1.6309300993	-2.361192042	0.0079100369
O	3.1737564028	-0.9375882748	-0.0070022279
H	1.0381626224	-2.0099311116	0.001159816
H	0.8694324781	2.2706377156	-0.0100143803
H	-1.0128938403	-3.099165313	0.0090972508
H	-2.7005751473	2.0043601764	-0.0018258574
H	4.0689500952	1.2021535687	-0.013538734

CAM-B3LYP Caffeic Acid (Neutral) Zero field

C	1.2630694805	0.053112576	-0.7066151142
C	0.0496070647	-0.0774879086	-0.0273812177
C	0.0406195754	-0.1320492388	1.345845448
C	1.2317721914	-0.0582235182	2.0715633489
C	2.4292915249	0.0718448903	1.3779274771
C	2.4466018869	0.1273187319	-0.0058353353
O	-1.1128873167	-0.1500955098	-0.715670164
C	1.2709143578	-0.1118836628	3.5274218136
C	0.2442351597	-0.236625568	4.3652055523
C	0.4821696711	-0.2721531767	5.813358705
O	-0.6693057004	-0.402637814	6.5037223615
O	1.1665029452	0.0980944968	-2.0658193644
O	1.5484575153	-0.1978357099	6.365245978
H	2.2555620579	-0.041595276	3.976821045
H	-0.7824492619	-0.3160613527	4.0401610971
H	-0.4345967904	-0.4183811072	7.4405578698
H	2.0319829619	0.189021868	-2.4703736781
H	-0.9244488444	-0.0968429124	-1.6588203821
H	3.383461397	0.2287998729	-0.5393113899
H	3.3590269657	0.1305422737	1.9262791123
H	-0.9144758416	-0.2331899543	1.8403008371

CAM-B3LYP Caffeic Acid (Neutral) 0.010 a.u.

C	1.2714650225	0.0524698789	-0.7071632661
C	0.0508829107	-0.0719588809	-0.0138017199
C	0.0521370473	-0.1218496581	1.3559962894
C	1.2527701834	-0.0491085419	2.0788064239
C	2.4498629081	0.0758031719	1.3735564021
C	2.4624100584	0.1257549454	-0.0084438832
O	-1.1071141898	-0.1416805554	-0.6856476021
C	1.2953746471	-0.1009537593	3.5169683813
C	0.2612439634	-0.2330964841	4.3690525536
C	0.464265392	-0.2715249171	5.7963978874
O	-0.7126405606	-0.422565053	6.4791693118
O	1.1457762768	0.0898008386	-2.0387732826
O	1.4989587186	-0.1899694226	6.4263858556
H	2.2825319941	-0.0259100306	3.9616274699
H	-0.758818632	-0.3208855759	4.0280594475
H	-0.4519807648	-0.441270193	7.4061752711
H	1.9805795669	0.1667038449	-2.5127035462
H	-0.9486326342	-0.1011208258	-1.6382169072
H	3.3943386301	0.2212478292	-0.5495498231
H	3.3844062832	0.1329703336	1.9151458718
H	-0.9027058211	-0.2191849449	1.851542865

CAM-B3LYP Caffeic Acid (Neutral) 0.002 a.u.

C	1.2645540231	0.0524766527	-0.7062330137
C	0.0502993972	-0.0748901873	-0.0234950032
C	0.0441320963	-0.1273771902	1.3490972874
C	1.2375554295	-0.0546221349	2.0728349262
C	2.4343188885	0.072679343	1.3768985174
C	2.4497227704	0.1258413356	-0.0070557667
O	-1.1121216781	-0.1460850508	-0.7073351356
C	1.2769264545	-0.1074243716	3.5262826442
C	0.2486385326	-0.2370918689	4.364679402
C	0.4777797219	-0.2720917871	5.8095263434
O	-0.6789922765	-0.4114358301	6.4962439145
O	1.1606163922	0.0949916197	-2.0602303407
O	1.5368308375	-0.1919467855	6.3780138655
H	2.2613838668	-0.0328811619	3.9755795946
H	-0.7760118587	-0.3220323695	4.0353407843
H	-0.4409375159	-0.4266973458	7.4315763954
H	2.0202405665	0.1797410056	-2.4794936447
H	-0.929974338	-0.09686786	-1.6525450349
H	3.3853839124	0.2247530279	-0.5425641768
H	3.3655047772	0.1305865873	1.9230775545
H	-0.9107389994	-0.2259536283	1.844384887

CAM-B3LYP Caffeic Acid (Neutral) 0.004 a.u.

C	1.2660836408	0.0524823234	-0.7060730047
C	0.050883634	-0.0737802868	-0.0202106455
C	0.0472388885	-0.1254153139	1.3517124215
C	1.2426899019	-0.0528045076	2.0741257286
C	2.4389196192	0.0735392037	1.3759673407
C	2.4527568585	0.1256891148	-0.0079130919
O	-1.1110269338	-0.1445060872	-0.7001658744
C	1.2824977227	-0.1053665135	3.5246418606
C	0.2525000826	-0.2362070045	4.3647390483
C	0.4738612181	-0.2720099725	5.8059577096
O	-0.6883180768	-0.4153817647	6.4900765427
O	1.155427014	0.0935082655	-2.0546834244
O	1.5262226556	-0.1905234627	6.390432873
H	2.2673145946	-0.0301934364	3.9733068866
H	-0.7706732569	-0.3223779133	4.0317265884
H	-0.446268317	-0.4312641104	7.4237659346
H	2.0089356994	0.1750296025	-2.4881434071
H	-0.9350624057	-0.0980086776	-1.6473220129
H	3.3872405334	0.2234934122	-0.5452099053
H	3.3713026275	0.1311625752	1.9203720582
H	-0.9074147005	-0.223393446	1.8474803734

CAM-B3LYP Caffeic Acid (Neutral) 0.006 a.u.

C	1.2677506653	0.0524185924	-0.7061388367
C	0.0512044673	-0.0728488754	-0.0174952259
C	0.049596881	-0.1236884138	1.3537490654
C	1.2469186939	-0.051172359	2.0755385192
C	2.4430172004	0.0743512719	1.3751374146
C	2.4558687958	0.1255350744	-0.0084309499
O	-1.1098179383	-0.1431151467	-0.6941625246
C	1.2873557397	-0.103479998	3.5225595187
C	0.2558521763	-0.2353681639	4.3654263713
C	0.4703462757	-0.2719052931	5.8025471351
O	-0.6969185091	-0.4187894106	6.4851435302
O	1.1512215593	0.0920482859	-2.049268279
O	1.5163785165	-0.1895124131	6.4024983942
H	2.2726996941	-0.0277849969	3.9703000621
H	-0.7660342487	-0.3227011375	4.0292601917
H	-0.4497992182	-0.4353341844	7.4169197929
H	1.9985680423	0.1710565845	-2.4965173933
H	-0.9398099301	-0.098977557	-1.6431816584
H	3.389350571	0.222319239	-0.5472357248
H	3.3763479716	0.1317429125	1.9182050075
H	-0.904986406	-0.2211220111	1.8497295899

CAM-B3LYP Caffeic Acid (Neutral) 0.008 a.u.

C	1.2695464489	0.0524623999	-0.7064995715
C	0.0512475017	-0.0723736319	-0.0153953756
C	0.051239362	-0.1227326742	1.3551349566
C	1.2502536765	-0.0500932245	2.077060272
C	2.4466307465	0.0751017343	1.3743334341
C	2.4590596358	0.125664188	-0.0086154255
O	-1.1084806224	-0.1424174389	-0.689357624
C	1.2915940298	-0.1022109245	3.5199839128
C	0.2586904044	-0.2341723411	4.3668380875
C	0.4671553437	-0.2717245315	5.799358773
O	-0.7049438346	-0.4207689457	6.4816565745
O	1.1480253879	0.0909229697	-2.0439984097
O	1.5073208418	-0.189733285	6.4144064139
H	2.2777365256	-0.0269098605	3.9663938935
H	-0.7621922914	-0.3216270861	4.028056692
H	-0.4516255723	-0.4383752853	7.4112234052
H	1.9891406824	0.1687833857	-2.504648057
H	-0.9442330088	-0.1001566498	-1.640163276
H	3.3916803665	0.2217937285	-0.5486822783
H	3.3806643756	0.1323763978	1.9164818169
H	-0.9033989995	-0.2201369249	1.8510157856

CAM-B3LYP Caffeic Acid (Neutral) Zero field

C	-0.94856132	-1.1687461728	0.0022859543
C	-1.6834876629	0.0074966388	0.000491057
C	-1.0359653292	1.2343542829	-0.0038570403
C	0.3451063174	1.2838326904	-0.0064241657
C	1.070031208	0.1011379735	-0.0046065721
C	0.4269830227	-1.1314500767	-0.0002440672
O	-3.0402162765	0.0078203935	0.0028678174
O	-1.7552392469	2.3796777232	-0.0055909745
C	2.5484713323	0.0943099928	-0.0072334284
O	3.0898203928	1.325173773	-0.011525006
O	-1.6960119204	-2.3119708403	0.0065919318
O	3.2292985058	-0.8970235165	-0.0059981527
H	1.0173001516	-2.0374013609	0.0010900009
H	0.8399712892	2.2419946636	-0.0098142172
H	-1.1310901851	-3.0878697807	0.007864624
H	-3.358892783	-0.9014456802	0.0057901594
H	-2.6942006886	2.1637696755	-0.0033752407
H	4.0482441926	1.2075646209	-0.0130186801

CAM-B3LYP Caffeic Acid (Neutral) 0.010 a.u.

C	-0.9455691348	-1.1858502332	0.0024618572
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C	-1.684304843	-0.0045803419	0.000640375
C	-1.0314004523	1.2263328042	-0.003634398
C	0.3482154468	1.2710199866	-0.0060880368
C	1.0804539027	0.0872905627	-0.0041912749
C	0.4314926802	-1.1479304252	0.0000990904
O	-3.0211087092	0.0186831866	0.0027954127
O	-1.7359397673	2.3694531488	-0.0054188325
C	2.5405640971	0.1056388107	-0.0067333906
O	3.076900805	1.3542117149	-0.0122059282
O	-1.6982113641	-2.3148888353	0.006612677
O	3.2797239824	-0.8547640793	-0.0057598844
H	1.0125710866	-2.0594852552	0.001484306
H	0.8349578411	2.2329755348	-0.0095173143
H	-1.1616999388	-3.1099265386	0.0072738079
H	-3.4003614898	-0.8694245958	0.0052862124
H	-2.6839068626	2.18113282	-0.0037148638
H	4.0291837201	1.211336735	-0.0140958151

CAM-B3LYP Caffeic Acid (Neutral) 0.002 a.u.

C	-0.9481084058	-1.1720441545	0.0023181835
C	-1.6835094722	0.0050644239	0.0005314763
C	-1.0350093803	1.2325083252	-0.0038215724
C	0.3458310105	1.2810635203	-0.0063998763
C	1.0717092488	0.0982028908	-0.0045844213
C	0.4278416271	-1.1347777905	-0.0002129547
O	-3.0363592417	0.0103418189	0.0028921551
O	-1.7510067483	2.3775281945	-0.0055550222
C	2.5467574283	0.0965927698	-0.007238196
O	3.0868129141	1.3308819911	-0.0116140976
O	-1.6963278654	-2.3126030974	0.0066095545
O	3.2392148612	-0.8885346124	-0.0059034643
H	1.0161852211	-2.041868668	0.0011188123
H	0.8390850215	2.2399280272	-0.00981299
H	-1.1366523182	-3.0920957239	0.0077718548
H	-3.3671341091	-0.8949204438	0.0057289283
H	-2.6918105225	2.167244415	-0.0034314603
H	4.0440417308	1.2087131139	-0.0131029097

CAM-B3LYP Caffeic Acid (Neutral) 0.004 a.u.

C	-0.9475974338	-1.1753855283	0.0023493133
C	-1.6836023248	0.0026368807	0.0005680027
C	-1.0340999994	1.2307654102	-0.0037878475
C	0.3464957093	1.2784050942	-0.0063723356
C	1.0735573217	0.0953674942	-0.0045558699
C	0.4287243818	-1.1380732084	-0.0001778034
O	-3.032551091	0.0127063992	0.0029099813

O	-1.7469923911	2.375411721	-0.0055222364
C	2.5451518023	0.098864682	-0.0072296191
O	3.0840776186	1.3365578903	-0.0117029014
O	-1.6966969731	-2.3132137656	0.0066257233
O	3.2491916962	-0.8800788946	-0.0058200872
H	1.0151785652	-2.0462766526	0.0011535366
H	0.8381136965	2.2380043043	-0.009806411
H	-1.1424483119	-3.0963945014	0.0076784643
H	-3.3754346939	-0.8884341423	0.0056690547
H	-2.68961803	2.1706876417	-0.0034844642
H	4.0401114574	1.2096741754	-0.0132005005

CAM-B3LYP Caffeic Acid (Neutral) 0.006 a.u.

C	-0.9470160763	-1.1787931107	0.002381271
C	-1.6837721484	0.000210953	0.0006026504
C	-1.0332144827	1.2291406363	-0.0037555841
C	0.3471105225	1.275845169	-0.006342852
C	1.0756133943	0.0926120934	-0.0045222014
C	0.4296321931	-1.1413505956	-0.0001381164
O	-3.0287577647	0.0148954118	0.0029245219
O	-1.7431626562	2.3733390037	-0.005492337
C	2.5436186021	0.1011301831	-0.0072105388
O	3.0815654674	1.3422842299	-0.0117906785
O	-1.6971172525	-2.3138047547	0.0066443112
O	3.2592654228	-0.8716302662	-0.0057478845
H	1.0142484073	-2.0506652137	0.0011955916
H	0.8370756904	2.2362112049	-0.0097975236
H	-1.1485253572	-3.1007988314	0.0075774944
H	-3.3837966366	-0.8819929716	0.0056103155
H	-2.6875954319	2.174147168	-0.0035366052
H	4.0363891066	1.2104446906	-0.0133078344

CAM-B3LYP Caffeic Acid (Neutral) 0.008 a.u.

C	-0.9463444116	-1.1822775862	0.0024163911
C	-1.6840054385	-0.0022007215	0.0006315388
C	-1.0323203695	1.2276539871	-0.0037154318
C	0.3476867032	1.2733836233	-0.0062821723
C	1.0779038228	0.0899234315	-0.0044449694
C	0.4305606894	-1.1446307172	-0.0000713099
O	-3.024951408	0.0168926592	0.0029130117
O	-1.7394833378	2.3713428693	-0.0054618549
C	2.5421037955	0.1033903676	-0.0071169206
O	3.079188632	1.3481447328	-0.0119152187
O	-1.6976100285	-2.3143719889	0.0066539036
O	3.2694358086	-0.863190659	-0.0057049063
H	1.0133870396	-2.0550593219	0.0012738361

H	0.836016006	2.2345368945	-0.0097469255
H	-1.1549270928	-3.1053172011	0.0074549862
H	-3.392144044	-0.8756372109	0.0055204541
H	-2.6857020942	2.177635862	-0.0036000492
H	4.0327667276	1.2110059793	-0.0135103631

CAM-B3LYP Caffeic Acid (Radical) Zero field

C	1.2493459151	0.055562219	-0.7566653783
C	0.0017085253	-0.0817348139	0.0002484367
C	-0.0106418553	-0.1368626485	1.3653761068
C	1.1971203324	-0.0606779982	2.0716687855
C	2.4247369612	0.0735754729	1.3574347918
C	2.4669601491	0.1305001165	0.0059244314
O	-1.1021484797	-0.1479333884	-0.7288978641
C	1.2643404518	-0.1119697451	3.5107050066
C	0.2385917699	-0.2365022605	4.3619763067
C	0.4902932681	-0.2720553899	5.8110037325
O	-0.652891487	-0.4016886619	6.5085600385
O	1.1764236181	0.0978126054	-1.9882947013
O	1.5656664391	-0.1974160717	6.3419582935
H	2.2525674437	-0.0423071402	3.9509799163
H	-0.7904866538	-0.3150789228	4.044930176
H	-0.4171484229	-0.4182734061	7.4454780183
H	-0.8108752295	-0.08619591	-1.6583491242
H	3.3940769648	0.2321464963	-0.5393938228
H	3.3403896446	0.1301896245	1.9306254299
H	-0.956377355	-0.2385711774	1.87650442

CAM-B3LYP Caffeic Acid (Radical) 0.010 a.u.

C	1.252194144	0.0557117098	-0.7610691044
C	-0.0040227474	-0.0816134185	0.0041656712
C	-0.0043456924	-0.1353265287	1.3728387733
C	1.2084990069	-0.0595254072	2.0711189627
C	2.4401237577	0.0725649799	1.3498760882
C	2.4806135022	0.128568751	0.0018814623
O	-1.1070391065	-0.146884787	-0.7019604089
C	1.2793029142	-0.1078654658	3.5005103979
C	0.2515060587	-0.2345295336	4.3672961266
C	0.4771032846	-0.2684274986	5.7955137952
O	-0.6867430235	-0.4109261787	6.4954970085
O	1.177408254	0.1024256695	-1.9783608016
O	1.5257579038	-0.1882612445	6.3978865067
H	2.2717816083	-0.0348817292	3.9314451453
H	-0.7736259968	-0.3186973859	4.0412944376
H	-0.4161405227	-0.4266990597	7.4199640631
H	-0.8617051887	-0.0911502063	-1.647667078

H	3.4018649637	0.227210238	-0.5542232007
H	3.3584394107	0.1268982543	1.9199363663
H	-0.9493205308	-0.2360721586	1.8858287886

CAM-B3LYP Caffeic Acid (Radical) 0.002 a.u.

C	1.2491420829	0.0559541502	-0.7569942156
C	0.0008502176	-0.0816729666	0.0018942782
C	-0.0079185864	-0.1366111331	1.3678595501
C	1.2010878277	-0.0603784774	2.0711187544
C	2.4285525886	0.0733078763	1.3556996958
C	2.4692922133	0.1300853978	0.0044833672
O	-1.1038665841	-0.1477207918	-0.7213405817
C	1.2686213137	-0.1111128979	3.5096348533
C	0.2422660517	-0.2361099823	4.3618319803
C	0.4870605462	-0.2712177264	5.8076201086
O	-0.6608739143	-0.4039994468	6.5035457672
O	1.1753022193	0.098272343	-1.9859248975
O	1.5563560986	-0.1947630163	6.3538808952
H	2.2574678178	-0.0405994078	3.948468601
H	-0.7856894416	-0.3158873317	4.0420751792
H	-0.4202254209	-0.4202460544	7.4385356613
H	-0.822693637	-0.0868593778	-1.6543412506
H	3.3948283308	0.2309216516	-0.5436203402
H	3.345247745	0.1293718416	1.9274216736
H	-0.9531554689	-0.2382156502	1.8799239201

CAM-B3LYP Caffeic Acid (Radical) 0.004 a.u.

C	1.2492841105	0.0563450611	-0.7575659834
C	-0.0001575459	-0.0816275057	0.0031193808
C	-0.0058727688	-0.136326555	1.3698426981
C	1.2042825308	-0.0600550279	2.0707870829
C	2.4320280134	0.0730874519	1.3541616272
C	2.47179098	0.1296725181	0.0033929362
O	-1.1052478236	-0.1475131588	-0.714823866
C	1.2722427581	-0.1102231271	3.5080876942
C	0.2453983317	-0.2357316482	4.362234171
C	0.4841589955	-0.2704730229	5.8043783415
O	-0.6681894488	-0.406163378	6.4996175246
O	1.1748889077	0.0987381896	-1.9837380902
O	1.5476939058	-0.1924186447	6.3653533731
H	2.2618281222	-0.0388950505	3.9452812781
H	-0.7816017548	-0.3167247232	4.040237859
H	-0.4217552199	-0.422110503	7.4324656441
H	-0.8338086718	-0.0875531206	-1.651198619
H	3.3959342604	0.2296921062	-0.5472264559
H	3.3495415276	0.1286060581	1.9247992097

H -0.9507872102 -0.2378069195 1.8825671942

CAM-B3LYP Caffeic Acid (Radical) 0.006 a.u.

C 1.2499464716 0.0557524109 -0.7583434191
C -0.0012535561 -0.0815218661 0.003908772
C -0.0047894336 -0.135778665 1.3712171995
C 1.2063806078 -0.059810999 2.0707302453
C 2.4349364941 0.0728220043 1.3527810486
C 2.4744572049 0.1291196687 0.0026998938
O -1.1062134027 -0.1471364884 -0.7096884753
C 1.2750521609 -0.1093487995 3.5060104586
C 0.2478077485 -0.2354023812 4.3632765796
C 0.4816708122 -0.2697730816 5.8012339649
O -0.6746198858 -0.4081728034 6.4970864847
O 1.1751353397 0.1000234059 -1.9816728557
O 1.539909902 -0.1904896511 6.3762201455
H 2.2654283357 -0.0372624654 3.9414317854
H -0.7783962566 -0.317645648 4.0396256754
H -0.4210862947 -0.42386302 7.427447936
H -0.8434894783 -0.0888998593 -1.6492254778
H 3.3974592423 0.228701642 -0.5499990845
H 3.3529407168 0.1280041166 1.9228282332
H -0.9496247288 -0.2367985204 1.88420389

CAM-B3LYP Caffeic Acid (Radical) 0.008 a.u.

C 1.2508442938 0.0556366487 -0.7594749001
C -0.0025580159 -0.0815452426 0.0043016097
C -0.0041328385 -0.1355091533 1.372299323
C 1.2079859034 -0.0596412765 2.0708232692
C 2.437765699 0.0726685764 1.3513700964
C 2.477393116 0.1288021152 0.0021562682
O -1.1068742811 -0.1470049968 -0.7051827112
C 1.2775152846 -0.1085826212 3.5034970642
C 0.2499307818 -0.2349098515 4.3648727934
C 0.4792354761 -0.2690474289 5.7982551137
O -0.6809373516 -0.4096881309 6.4955268268
O 1.175947637 0.1012529511 -1.9798642615
O 1.5324688996 -0.1892346057 6.3870996804
H 2.2688764962 -0.0360278602 3.9368345174
H -0.7756494052 -0.3180986415 4.0397899217
H -0.4195406545 -0.4254238001 7.4231502329
H -0.853151312 -0.0901212634 -1.6478731921
H 3.3993860476 0.2279190429 -0.5524301861
H 3.3560903079 0.127446584 1.9211582356
H -0.948944084 -0.2363720458 1.8854632985

CAM-B3LYP Caffeic Acid (Radical) Zero field

C	-0.94310069	-1.2145975887	0.0032146987
C	-1.7421942992	-0.0019721197	0.0015893517
C	-1.0142960317	1.2618810159	-0.0033691905
C	0.3558668917	1.3135540722	-0.0063964912
C	1.0619970561	0.1125512083	-0.0046300677
C	0.4204509612	-1.136428876	0.0001187635
O	-2.9757806872	0.0238807117	0.0040908476
O	-1.7702870533	2.3499593565	-0.004733705
C	2.5452547816	0.0948858884	-0.0077387507
O	3.0918160077	1.3199209775	-0.0122296631
O	-1.6386404938	-2.3568621066	0.007808614
O	3.2093530949	-0.9062893384	-0.006427639
H	1.0340453455	-2.0271704248	0.0012561428
H	0.8685451836	2.2619694113	-0.0100598479
H	-1.0445787032	-3.1134699678	0.0086820243
H	-2.6941697178	2.0373939604	-0.0019459715
H	4.0508103539	1.2039168198	-0.0139341158

CAM-B3LYP Caffeic Acid (Radical) 0.010 a.u.

C	-0.9396065785	-1.2289930917	0.0032974462
C	-1.7429957597	-0.0083643955	0.001838864
C	-1.0136869229	1.2604481781	-0.0033640092
C	0.358530937	1.3036393707	-0.0064513999
C	1.0688786182	0.1011252856	-0.0046054572
C	0.4260865232	-1.1525723932	0.0001981008
O	-2.965337766	0.0104824041	0.0044558077
O	-1.7505400062	2.3508187811	-0.004789171
C	2.5353416124	0.106078857	-0.0077111611
O	3.0814535872	1.3464157312	-0.0125090278
O	-1.649288902	-2.3513107688	0.0077746125
O	3.2546852689	-0.8670460097	-0.0058682503
H	1.0319328256	-2.0480562417	0.0013057887
H	0.865814484	2.2546161178	-0.0102727094
H	-1.0907167424	-3.1338928771	0.0082079893
H	-2.6891187444	2.0784925608	-0.0020925292
H	4.0336595657	1.2012414911	-0.0141198941

CAM-B3LYP Caffeic Acid (Radical) 0.002 a.u.

C	-0.9425740938	-1.2172750562	0.0032292207
C	-1.7421699336	-0.0031818108	0.00163411
C	-1.0141187564	1.2613747793	-0.0033628424
C	0.3565060745	1.3113018878	-0.0063940684
C	1.0630000239	0.1100675624	-0.0046086742
C	0.4215377954	-1.1395803794	0.0001416826
O	-2.9735294093	0.0214310929	0.0041385912

O	-1.7659905872	2.3501210199	-0.0047410575
C	2.5431857052	0.0970450362	-0.0077018096
O	3.089270937	1.3250571769	-0.0123114502
O	-1.6406681859	-2.3557650314	0.0077904098
O	3.2183208312	-0.8984238529	-0.0063032244
H	1.0333482685	-2.0313762547	0.0012778738
H	0.8680895193	2.2601924201	-0.0100820073
H	-1.0531667495	-3.1173163473	0.0085783878
H	-2.6929085143	2.0456651115	-0.0019766667
H	4.046959075	1.2037856455	-0.014013475

CAM-B3LYP Caffeic Acid (Radical) 0.004 a.u.

C	-0.941971481	-1.2202240577	0.0032512009
C	-1.7423558759	-0.0044238442	0.0017127485
C	-1.0139790293	1.2610985351	-0.0034106297
C	0.3572489833	1.3089543397	-0.006628105
C	1.0643233657	0.1074261038	-0.0049122611
C	0.4227509918	-1.1429942888	-0.0000174193
O	-2.9713225957	0.0186979438	0.004511704
O	-1.761535803	2.3502207623	-0.0047326236
C	2.5413361486	0.0991988042	-0.0082198847
O	3.0864404458	1.3305535452	-0.012121733
O	-1.6427098372	-2.3545028355	0.0079382231
O	3.2273970826	-0.8906176909	-0.0060415576
H	1.0328083006	-2.0358767779	0.0010653752
H	0.8678274951	2.2583289739	-0.0104280951
H	-1.0624724981	-3.1213388792	0.0086176602
H	-2.6914783514	2.0544117905	-0.0019037152
H	4.0427846583	1.2042105758	-0.0133858877

CAM-B3LYP Caffeic Acid (Radical) 0.006 a.u.

C	-0.9412489318	-1.223072423	0.0032569286
C	-1.742464293	-0.0057117574	0.001728995
C	-1.0139284514	1.2607426527	-0.0034006141
C	0.3577271037	1.3069319482	-0.0066065036
C	1.0656895424	0.1051289485	-0.0048780953
C	0.423919449	-1.1462165414	0.0000106209
O	-2.9691720549	0.0161212536	0.0045774907
O	-1.7577579475	2.3502421128	-0.0047395017
C	2.5393135884	0.1014856581	-0.0081504372
O	3.0846000019	1.3357957052	-0.0122009492
O	-1.6448115751	-2.3533013878	0.0079130272
O	3.2365692146	-0.8826220849	-0.0059470992
H	1.0323693574	-2.0400743882	0.0010977709
H	0.8671115843	2.2568654918	-0.01041779
H	-1.0716873165	-3.125342132	0.0085234508

H -2.6907253661 2.062727876 -0.0019653658
H 4.0395880946 1.2034220679 -0.013506928

CAM-B3LYP Caffeic Acid (Radical) 0.008 a.u.

C -0.9405033267 -1.2258822918 0.0032781558
C -1.7426326507 -0.0070141739 0.0017806996
C -1.0137680293 1.2604891418 -0.0033597174
C 0.3581111327 1.3053385131 -0.006427197
C 1.0671179263 0.1031966227 -0.0045949551
C 0.4249307723 -1.1492633258 0.0001885019
O -2.9672955997 0.0133913517 0.0043606095
O -1.7541208177 2.3506474995 -0.004774131
C 2.5372547753 0.1037535018 -0.0076872383
O 3.0830156142 1.340934454 -0.0124828676
O -1.6470549887 -2.352442286 0.0077708889
O 3.2454950659 -0.8748771778 -0.0059612847
H 1.0320807664 -2.0439165388 0.001307607
H 0.8664460071 2.2557752857 -0.0102096698
H -1.0807845202 -3.1295475086 0.0082954775
H -2.6898483442 2.070344117 -0.0020672066
H 4.0366482169 1.2021958156 -0.0141226726

ω B97X Caffeic Acid (Neutral) -0.010 a.u.

C 1.2562928518 0.0681854599 -0.7131242302
C 0.0483189992 -0.1484864109 -0.0578041034
C 0.0237126945 -0.2508723828 1.3192129092
C 1.2006944911 -0.1372471965 2.0628911637
C 2.4009529135 0.069067256 1.3855597847
C 2.4297932471 0.1743187314 0.0038902412
O -1.1075745761 -0.2623580101 -0.7776393129
C 1.239337728 -0.2219500292 3.5294677167
C 0.2160338951 -0.1844640751 4.3736443439
C 0.503356031 -0.2671820522 5.8374890183
O -0.6163774792 -0.1952725324 6.5582173623
O 1.2011579098 0.1601973842 -2.0973915796
O 1.6046515594 -0.3809209822 6.2966188013
H 2.2261682703 -0.3041324158 3.9779301227
H -0.8200538405 -0.0812505516 4.0735556801
H -0.3847647404 -0.2445518807 7.4965360238
H 2.0668033233 0.4246593028 -2.4068052349
H -0.8870766356 -0.13093856 -1.7019376049
H 3.3709532764 0.3383385363 -0.5135828799
H 3.3204122196 0.1541430591 1.9512940541
H -0.9276811383 -0.4256106502 1.8065617236

ω B97X Caffeic Acid (Neutral) -0.002 a.u.

C	1.2619906166	0.0499597759	-0.7120220462
C	0.0462317589	-0.0732307947	-0.0332513088
C	0.0357181897	-0.1245186166	1.343548095
C	1.2287393053	-0.0547194796	2.0688792099
C	2.4286365923	0.0687300372	1.3768017472
C	2.4473199235	0.1204504757	-0.010324381
O	-1.119215835	-0.1411156205	-0.7241466588
C	1.2666702961	-0.1049932602	3.5335726877
C	0.2379632759	-0.2459537271	4.365447039
C	0.4831868705	-0.2715412564	5.8229790588
O	-0.6614008281	-0.4182471415	6.5147229414
O	1.1718329334	0.0935102028	-2.0777297317
O	1.5559701613	-0.1759222105	6.3583967523
H	2.2498437404	-0.0165410924	3.9886947918
H	-0.7892292124	-0.3461930046	4.038911771
H	-0.4272648467	-0.4254112673	7.4505672604
H	2.0444155742	0.1835200257	-2.4616450466
H	-0.9220318208	-0.0878621227	-1.6632629174
H	3.3874399907	0.217007255	-0.5435439175
H	3.3598335628	0.1250368086	1.9272137673
H	-0.9215392488	-0.2182929868	1.8407748863

ωB97X Caffeic Acid (Neutral) -0.004 a.u.

C	1.2609316525	0.0498820373	-0.7127516891
C	0.0451619335	-0.0759249405	-0.0381075621
C	0.0306700852	-0.1290146047	1.3392813816
C	1.2211352646	-0.0584302485	2.0678979298
C	2.4225938301	0.0673361513	1.3781812603
C	2.4444126692	0.1209543156	-0.00841285
O	-1.119649447	-0.1446001641	-0.734760168
C	1.259072637	-0.1090393791	3.5339187236
C	0.2324692837	-0.2462149684	4.3670676288
C	0.4884236581	-0.2711639945	5.8268520125
O	-0.6501202696	-0.4100521751	6.5242791644
O	1.179541786	0.0957822248	-2.0835308379
O	1.5687902097	-0.1800830168	6.3447325483
H	2.2425339947	-0.0234512676	3.9888705857
H	-0.7970259328	-0.3427606765	4.0459436727
H	-0.4168228145	-0.4170574702	7.461037427
H	2.0573337899	0.1950284161	-2.4521871009
H	-0.9153159262	-0.0867839574	-1.6715596099
H	3.3862047697	0.2196216585	-0.538939993
H	3.3519010545	0.1243008603	1.9315275066
H	-0.9271312281	-0.2246568004	1.8352439696

ωB97X Caffeic Acid (Neutral) -0.006 a.u.

C	1.2599879305	0.0511409376	-0.7136295338
C	0.0442753046	-0.0825939416	-0.0437891648
C	0.0254047599	-0.1403659908	1.3340731222
C	1.2128542511	-0.0665572856	2.0667720938
C	2.4158536017	0.0661665675	1.3798354624
C	2.4412178521	0.1247898828	-0.0059934714
O	-1.1192399305	-0.154733646	-0.7470106794
C	1.2510126927	-0.1193650753	3.5336745801
C	0.2260291302	-0.2433687965	4.3693889649
C	0.4941995209	-0.2708045992	5.8309400671
O	-0.6386967089	-0.3892542403	6.5355385934
O	1.1879433768	0.1021730738	-2.0894092712
O	1.5834655364	-0.1963720964	6.3299833794
H	2.235764662	-0.0456445648	3.9878925676
H	-0.8069949365	-0.3255631632	4.0548431719
H	-0.4049957027	-0.3985443666	7.4729259781
H	2.0700513707	0.2177763577	-2.4419424608
H	-0.9076996273	-0.087416572	-1.6810795972
H	3.3845877875	0.2293969789	-0.5332676544
H	3.34285897	0.1253204737	1.9366471324
H	-0.9327688411	-0.2425079337	1.8281907196

ωB97X Caffeic Acid (Neutral) -0.008 a.u.

C	1.2560905161	0.0730858659	-0.7122781683
C	0.0475075628	-0.1302977788	-0.0506793702
C	0.0279742522	-0.2253179742	1.3260761413
C	1.2091617241	-0.1187374732	2.0642134571
C	2.4080030399	0.0756712703	1.3830271226
C	2.4325903	0.1745620556	0.0001231477
O	-1.1110692662	-0.2389490376	-0.7621864078
C	1.2483272509	-0.2009640628	3.53052894
C	0.2211097529	-0.1925099759	4.371462436
C	0.4979392267	-0.2733632302	5.8334338141
O	-0.6309512229	-0.2349847873	6.5476886954
O	1.1906399096	0.1560629225	-2.0916339053
O	1.5949287698	-0.3601689038	6.3107335779
H	2.236258563	-0.2601923071	3.9800059144
H	-0.8152979507	-0.1172399547	4.0652855027
H	-0.3984546127	-0.2836433069	7.4849653407
H	2.0672903386	0.3476220911	-2.4234979463
H	-0.8964933367	-0.1326531905	-1.6914738201
H	3.3724757344	0.3300505867	-0.5215488648
H	3.3307405676	0.1558379149	1.9441942424
H	-0.9236601192	-0.3901987241	1.8161441505

ωB97X Gallic Acid (Neutral) -0.010 a.u.

C	-0.9523936536	-1.1554604943	0.0021125216
C	-1.6886174495	0.0191244326	0.0003233448
C	-1.0447317474	1.2467618414	-0.0040444391
C	0.3404412296	1.3024354943	-0.0066246444
C	1.0637174807	0.1182465719	-0.0047866238
C	0.4238277908	-1.1158808113	-0.0004206313
O	-3.0658854015	-0.0061021268	0.0028626024
O	-1.7833147759	2.3936421077	-0.0057311212
C	2.5634930848	0.0827639431	-0.0072818224
O	3.113577466	1.297116116	-0.011301029
O	-1.6961064259	-2.3129747938	0.00645309
O	3.1848622516	-0.9416291868	-0.0059637084
H	1.0278383811	-2.0167358471	0.0008846179
H	0.8435971553	2.2597721984	-0.0099922199
H	-1.1021020056	-3.0659331994	0.0081150246
H	-3.3221665647	-0.9323330915	0.0062243774
H	-2.7099541695	2.144192629	-0.0029759367
H	4.0754783538	1.1942192168	-0.0125594023

ω B97X Gallic Acid (Neutral) -0.002 a.u.

C	-0.9514586139	-1.1680276895	0.0022813591
C	-1.6878537093	0.009452817	0.0005227098
C	-1.0404617856	1.2382164478	-0.0038471078
C	0.3439651034	1.2898212291	-0.0064468052
C	1.0679395662	0.1051837992	-0.0046157218
C	0.4268341877	-1.1294774279	-0.0002386438
O	-3.0500197277	0.005491077	0.0029339795
O	-1.7632026326	2.3851012178	-0.0055676497
C	2.5555807771	0.0917996206	-0.0072216489
O	3.0980319332	1.319627942	-0.0117155729
O	-1.6968640512	-2.3155925206	0.0065129569
O	3.2234213775	-0.908184359	-0.0056638009
H	1.0213981024	-2.0356476589	0.001065143
H	0.8409561802	2.2496660958	-0.0098987554
H	-1.1212024722	-3.0816089538	0.0077273383
H	-3.3531274012	-0.9069897183	0.0058241075
H	-2.6976947978	2.1595822915	-0.003305747
H	4.0553189639	1.2028107902	-0.0130521407

ω B97X Gallic Acid (Neutral) -0.004 a.u.

C	-0.9517278738	-1.1648005635	0.0022439331
C	-1.6879206094	0.0119122832	0.0004798103
C	-1.0414728443	1.2402990746	-0.0038916725
C	0.3431356876	1.2928819028	-0.0064902534
C	1.0666545159	0.1083628833	-0.0046598382
C	0.4260517053	-1.1260962592	-0.0002837009

O -3.0538454235 0.0025795668 0.0029222594
O -1.7679396672 2.3872723575 -0.0056050533
C 2.5573563758 0.0895272995 -0.0072448576
O 3.1015572417 1.31399994 -0.0116104967
O -1.6966889639 -2.3148289639 0.0065008947
O 3.2136029129 -0.9166300796 -0.0057393193
H 1.0229151335 -2.0309430094 0.0010187165
H 0.841718846 2.2520491409 -0.0099233241
H -1.1163525433 -3.0775511998 0.0078234057
H -3.3449361204 -0.9136299354 0.0059127128
H -2.7005220977 2.1559211751 -0.0032351632
H 4.0599747248 1.2008993871 -0.0129240533

ωB97X Gallic Acid (Neutral) -0.006 a.u.

C -0.951965661 -1.16164343 0.0022032692
C -1.6880685834 0.014335591 0.0004322765
C -1.0425304246 1.2424225003 -0.0039387474
C 0.3422593225 1.2960324792 -0.0065329279
C 1.0655139821 0.11162798 -0.0047013287
C 0.4252979408 -1.1226836922 -0.000328347
O -3.0577623332 -0.0002979894 0.0029054961
O -1.7729007471 2.3894109252 -0.0056442054
C 2.5592531496 0.0872489958 -0.0072587775
O 3.1053506116 1.3083321718 -0.0115097887
O -1.6964685132 -2.3141664608 0.0064859459
O 3.2038395613 -0.9250738487 -0.0058120117
H 1.0245803534 -2.0261572537 0.0009736253
H 0.8423919042 2.2545606595 -0.0099449881
H -1.1114939995 -3.0735979382 0.0079190934
H -3.3371106748 -0.9200133843 0.0060070384
H -2.7035360155 2.1521080881 -0.0031570198
H 4.0649111267 1.1987796064 -0.0128046027

ωB97X Gallic Acid (Neutral) -0.008 a.u.

C -0.9521848454 -1.1585560014 0.0021593411
C -1.6883024662 0.0167188637 0.0003806448
C -1.0436131586 1.2445596926 -0.0039897496
C 0.341359161 1.2992183363 -0.0065788942
C 1.0645356294 0.1149263652 -0.0047452159
C 0.424559917 -1.1192750359 -0.0003752586
O -3.0617765618 -0.0031130331 0.0028868272
O -1.7780326199 2.3915092037 -0.0056857366
C 2.5612853358 0.0849915397 -0.0072732764
O 3.1093580443 1.3027001486 -0.0114070997
O -1.6962116653 -2.3136116002 0.0064703816
O 3.1942382407 -0.9334179313 -0.0058827981

H	1.0262561663	-2.0213994543	0.0009267113
H	0.8430090208	2.2571397422	-0.0099694907
H	-1.1066302083	-3.0697484892	0.0080160291
H	-3.329681466	-0.9261105158	0.0061118803
H	-2.7066842997	2.1481610011	-0.0030700896
H	4.0700767759	1.1965321681	-0.0126802061

ωB97X Caffiec Acid (Radical) -0.010 a.u.

C	1.2557918512	0.0557514715	-0.7635758203
C	0.0029113473	-0.0812671837	-0.0177651902
C	-0.0340385309	-0.1381190365	1.3445909878
C	1.1699179639	-0.0626927696	2.0760985619
C	2.4058159169	0.0738910178	1.3681051145
C	2.4616952878	0.1313317599	0.0138215294
O	-1.0957260385	-0.1460915672	-0.7819787476
C	1.2355737931	-0.115474809	3.5138545945
C	0.2093656851	-0.2425645912	4.3704889824
C	0.508449593	-0.2760550431	5.8361145202
O	-0.6055596768	-0.391544147	6.5534871686
O	1.1963844964	0.0957009403	-2.0095553807
O	1.6186391107	-0.2060156096	6.2803909065
H	2.2217692682	-0.0445473266	3.964718309
H	-0.828093851	-0.322907442	4.0694177768
H	-0.3779894265	-0.4058167728	7.4946149434
H	-0.7534999638	-0.0787754059	-1.6893298848
H	3.4008760632	0.2358900259	-0.5147490056
H	3.3156376676	0.1316499074	1.9541525475
H	-0.9862685569	-0.2398244187	1.8488710867

ωB97X Caffeic Acid (Radical) -0.002 a.u.

C	1.2504355839	0.0535940923	-0.7634593481
C	-0.0001221487	-0.078974121	-0.0047407476
C	-0.0150185045	-0.1328969519	1.3628288851
C	1.1952178554	-0.0590916893	2.0708702786
C	2.4262968424	0.0713600074	1.3569644333
C	2.4703763283	0.1258141772	0.0029433065
O	-1.1069458363	-0.1417355134	-0.7373803906
C	1.261599427	-0.1082643201	3.5164738718
C	0.2322940833	-0.2425573522	4.3625412855
C	0.4906499018	-0.2714733103	5.8205726494
O	-0.6472291996	-0.4109750592	6.5186465075
O	1.1805133338	0.0949869183	-1.9974600128
O	1.5724456715	-0.1827770915	6.3360739586
H	2.2488445452	-0.0276734856	3.9628714209
H	-0.7979346958	-0.3345495154	4.043943075
H	-0.4125602861	-0.4215145401	7.4546921771

H -0.8079989427 -0.0816199912 -1.6614230273
H 3.4007782527 0.2246206919 -0.5410743945
H 3.343058377 0.1264223757 1.9325598872
H -0.9630485883 -0.2301763217 1.8753291844

ωB97X Caffeic Acid (Radical) -0.004 a.u.

C 1.2513058688 0.0539618543 -0.763350192
C 0.0006793716 -0.0794246434 -0.0072260218
C -0.0187653732 -0.134039485 1.3592760354
C 1.1900548543 -0.0599310431 2.0718487649
C 2.4219021181 0.0718460754 1.3591561407
C 2.468249507 0.1269797787 0.0050729593
O -1.1047474552 -0.1425685631 -0.7465554765
C 1.2562543516 -0.1098807095 3.5165929797
C 0.2275727944 -0.2428120978 4.3636153192
C 0.494428214 -0.2724854976 5.8240511746
O -0.6382925891 -0.4066118056 6.525580225
O 1.183412056 0.0951687349 -2.0001457677
O 1.5828899062 -0.1876118436 6.3232203014
H 2.2430582985 -0.0311760951 3.9643003433
H -0.8041693448 -0.3324932494 4.0485191735
H -0.4065256864 -0.4178894286 7.4630871499
H -0.7959006089 -0.0809228896 -1.6668772431
H 3.400532919 0.2271065558 -0.5356302503
H 3.3372144351 0.1275245689 1.9368933708
H -0.967501637 -0.2322212166 1.8703440137

ωB97X Caffeic Acid (Radical) -0.006 a.u.

C 1.2523807784 0.055569777 -0.7632632049
C 0.0015104599 -0.0806865321 -0.0102207879
C -0.0230317751 -0.137051786 1.3550275346
C 1.1842101092 -0.0618654858 2.0730324092
C 2.4170438087 0.0727244013 1.3617575094
C 2.4660079847 0.1297043653 0.0076841286
O -1.101976243 -0.1449107635 -0.7571403776
C 1.2503336341 -0.1132999237 3.5161491508
C 0.2221105387 -0.2418758292 4.3653019761
C 0.4986940007 -0.2735885084 5.8278012295
O -0.6286477819 -0.3993629765 6.5337483626
O 1.1867128075 0.0967875092 -2.0029230745
O 1.5943455458 -0.195694765 6.3096634276
H 2.2370943274 -0.0393156224 3.9648501113
H -0.8116381554 -0.3256726067 4.0543800886
H -0.3990221501 -0.4122094664 7.4725843002
H -0.782845831 -0.0804409206 -1.6734860229
H 3.4002756863 0.2322955027 -0.5293347157

H 3.330681771 0.1292692865 1.9419957475
H -0.9725875157 -0.2378566558 1.8641652075

ωB97X Caffeic Acid (Radical) -0.008 a.u.

C 1.2539132441 0.0556474811 -0.7633652423
C 0.0021999539 -0.0809775294 -0.0136873591
C -0.0281938347 -0.1376312913 1.350192114
C 1.1774676422 -0.0623222492 2.0744654186
C 2.4117038242 0.0732717418 1.3646969306
C 2.4638904076 0.1305137995 0.0105511366
O -1.0990618122 -0.145481259 -0.7688366452
C 1.2434088318 -0.1144279801 3.515270981
C 0.2161247652 -0.2422067225 4.3675467317
C 0.5033381795 -0.2747328829 5.8317808208
O -0.6176825774 -0.3955824443 6.5429503919
O 1.1911297777 0.0962921925 -2.006084919
O 1.6061006918 -0.200538199 6.2954520355
H 2.2298457067 -0.0419568766 3.9651021402
H -0.8193955667 -0.3242595367 4.0612301862
H -0.3894659284 -0.4091099476 7.4829878596
H -0.7687291149 -0.0796050375 -1.6808641203
H 3.4004934953 0.2341089544 -0.5224495074
H 3.3235169474 0.1304206621 1.9477033806
H -0.9789526329 -0.2389038755 1.8571306659

ωB97X Gallic Acid (Radical) -0.010 a.u.

C -0.9462230124 -1.2063106501 0.0031451048
C -1.7489350794 0.0020472166 0.0014483604
C -1.0196090074 1.2674076773 -0.0033639905
C 0.3510981568 1.3291690291 -0.0064088855
C 1.059566159 0.1265456965 -0.0047035228
C 0.4167070471 -1.1243934157 0.0000778396
O -2.9937759512 0.0282842159 0.0039232872
O -1.7963293773 2.354209276 -0.0046323854
C 2.5625232359 0.0848644117 -0.0078725772
O 3.1122318322 1.2965017658 -0.0122157125
O -1.6325301268 -2.3662211273 0.0077802518
O 3.1713611638 -0.9462195064 -0.006480265
H 1.0430993055 -2.0102195686 0.001195574
H 0.8694537054 2.2778464478 -0.0100218082
H -1.0060272704 -3.0949565669 0.0089304199
H -2.7028214093 2.0046627107 -0.0017372676
H 4.0753026286 1.1999053873 -0.013769423

ωB97X Gallic Acid (Radical) -0.002 a.u.

C -0.9449760406 -1.2158668447 0.0031871678

C	-1.7475415694	-0.001819613	0.001595984
C	-1.0180753719	1.2650052309	-0.0033188508
C	0.3547584248	1.3192447785	-0.0063626527
C	1.0610374703	0.1158176315	-0.0045849919
C	0.4207027145	-1.1363121016	0.0001628303
O	-2.983215995	0.0216079626	0.0041112638
O	-1.7780057606	2.3545482366	-0.0046468891
C	2.5528428956	0.0928442422	-0.0076475128
O	3.0990230192	1.3157994577	-0.0126053501
O	-1.6400156611	-2.3618573058	0.0076669603
O	3.2053252988	-0.9159652233	-0.0059238641
H	1.0392160887	-2.0266209831	0.001277469
H	0.86924715	2.2693451025	-0.0100502202
H	-1.0358922916	-3.1083573111	0.0085086109
H	-2.6963207646	2.0342030354	-0.0019011979
H	4.0569823928	1.2015067048	-0.0141737565

ω B97X Gallic Acid (Radical) -0.004 a.u.

C	-0.9453275777	-1.2134162834	0.0031720277
C	-1.7477854541	-0.0008191195	0.0015528769
C	-1.0184114851	1.2655179799	-0.0033269919
C	0.3539116924	1.3215853312	-0.0063679654
C	1.0604220883	0.1183999242	-0.0046086063
C	0.4196917812	-1.1332947686	0.0001398619
O	-2.9856859103	0.0233602719	0.0040555694
O	-1.7823487322	2.3544890369	-0.0046376062
C	2.5551070179	0.0907803647	-0.0076816723
O	3.101981351	1.3108981353	-0.0125297708
O	-1.6380287098	-2.362975248	0.0076871911
O	3.1966715907	-0.9236436094	-0.0060328525
H	1.0401182843	-2.0224840406	0.00125454
H	0.8693768467	2.2712962316	-0.0100306675
H	-1.0280134566	-3.1048735016	0.0086112424
H	-2.697796873	2.0269664648	-0.0018593971
H	4.0612095464	1.2013358305	-0.0141027794

ω B97X Gallic Acid (Radical) -0.006 a.u.

C	-0.9456630435	-1.2110270048	0.0031636173
C	-1.7480877107	0.0001541737	0.0015270572
C	-1.0187494975	1.2660715823	-0.0033410137
C	0.3530490255	1.3239727519	-0.0063959425
C	1.0600032963	0.1209860792	-0.0046568475
C	0.4186823285	-1.1303586304	0.0001080252
O	-2.9882742401	0.0250005613	0.0040197401
O	-1.7867093989	2.3544612624	-0.0046330165
C	2.5573963026	0.0888147526	-0.007769092

O	3.1050494051	1.3062109196	-0.012427646
O	-1.6361485211	-2.3640774197	0.0077228376
O	3.1882308871	-0.9311168371	-0.0061427104
H	1.0409573782	-2.0184920978	0.0012181967
H	0.8695037946	2.2733054839	-0.0100486559
H	-1.0204648728	-3.101501665	0.0087173508
H	-2.6992196218	2.0196813894	-0.0018041074
H	4.0655364886	1.2010376983	-0.013962793

ωB97X Gallic Acid (Radical) -0.008 a.u.

C	-0.9459614973	-1.2086693403	0.0031540505
C	-1.7484842853	0.0011042476	0.0014884652
C	-1.0191447585	1.2666947006	-0.0033526626
C	0.3521153116	1.3264758351	-0.0064049227
C	1.0597256241	0.1236799814	-0.0046832762
C	0.4176845656	-1.1274101349	0.0000902783
O	-2.990967442	0.0266526448	0.0039727368
O	-1.7913670137	2.3543629359	-0.0046317701
C	2.5599108326	0.086839157	-0.0078237598
O	3.1084622678	1.3014099348	-0.0123228072
O	-1.6343255971	-2.3651612236	0.0077520588
O	3.1798538074	-0.9386287425	-0.0063023336
H	1.0418995237	-2.0144529774	0.0012033403
H	0.8695321186	2.2754646513	-0.0100384056
H	-1.0131576834	-3.0982061274	0.0088242937
H	-2.7009221564	2.012316293	-0.0017680477
H	4.0702383824	1.2006511648	-0.0138622381

ωB97X Caffeic Acid (Neutral) zero field

C	1.2631937249	0.0505461825	-0.7114611651
C	0.0472408424	-0.0717550196	-0.0289289616
C	0.0402577749	-0.1223261269	1.3472024186
C	1.2356221363	-0.0525586919	2.0699005925
C	2.4341225618	0.0700840467	1.3756436974
C	2.45013268	0.1209949015	-0.0118929155
O	-1.1184369271	-0.1394571803	-0.7147553866
C	1.27369536	-0.1030304816	3.5328346337
C	0.2428379677	-0.2444893277	4.3643987728
C	0.4784392361	-0.2717371458	5.8192867938
O	-0.6721356275	-0.4226258356	6.5062892713
O	1.1647917528	0.0927481932	-2.0720378851
O	1.5441582834	-0.1751782616	6.3715218693
H	2.2570613123	-0.0148069334	3.987751418
H	-0.7826167939	-0.3448441978	4.0331928244
H	-0.4362655763	-0.4307648836	7.4410309802
H	2.0318428259	0.1757073656	-2.4707582349

H	-0.928026281	-0.0898980231	-1.6560262617
H	3.388699391	0.2166945205	-0.5473952708
H	3.3669924782	0.1261886708	1.9234472834
H	-0.916496122	-0.2158197718	1.845339526

ωB97X Caffeic Acid (Neutral) 0.010 a.u.

C	1.2716027303	0.052390235	-0.7118350951
C	0.0492145171	-0.0704356498	-0.0160508929
C	0.0521835988	-0.1200363127	1.3564702556
C	1.2565263043	-0.0482445789	2.0764437119
C	2.4537139457	0.0748557016	1.3721445963
C	2.4650592004	0.1242638223	-0.0143143238
O	-1.1120255843	-0.1387594814	-0.6859021765
C	1.2970668969	-0.0995835124	3.5224454815
C	0.2582352369	-0.2361989974	4.3677563627
C	0.4617473733	-0.2714482162	5.802562861
O	-0.7139652439	-0.4278199549	6.4831219421
O	1.1438085525	0.0901373195	-2.0455427778
O	1.4979844826	-0.1827609676	6.4295724292
H	2.2839211292	-0.0187514688	3.9730950214
H	-0.7622324045	-0.3305924593	4.0223063697
H	-0.4535800316	-0.4425206955	7.4085510721
H	1.9810598545	0.1637690259	-2.5114963623
H	-0.9507475366	-0.0986076767	-1.6361880002
H	3.3984875048	0.218661704	-0.5567540057
H	3.3912419209	0.1312865674	1.9133647028
H	-0.9041914471	-0.2159324043	1.8548328281

ωB97X Caffeic Acid (Neutral) 0.002 a.u.

C	1.2645309028	0.0509552521	-0.7111259008
C	0.0481152051	-0.0709041311	-0.0251759328
C	0.0441724883	-0.1209816065	1.350296501
C	1.2416765456	-0.0510208072	2.0709834735
C	2.4391162903	0.0712234413	1.37463477
C	2.4529642287	0.1215189971	-0.0131374386
O	-1.1174653691	-0.1385849752	-0.7064907208
C	1.2799981375	-0.1016963053	3.5317114639
C	0.247178449	-0.2429815486	4.3638864176
C	0.4741919494	-0.2718124746	5.8157566115
O	-0.6821374992	-0.4253842067	6.4990177999
O	1.158638523	0.0919982475	-2.0665091826
O	1.5331588094	-0.1754918902	6.3841545976
H	2.2637519758	-0.0142349267	3.9861872929
H	-0.7767705871	-0.342852594	4.0285428035
H	-0.4436775588	-0.4345732914	7.432477604
H	2.0198793406	0.1708834124	-2.4794725788

H -0.9335174129 -0.0917639304 -1.649762289
H 3.3901330435 0.2166130249 -0.5506472186
H 3.3734145023 0.1272738468 1.9202485672
H -0.9122409642 -0.2145115343 1.8490073593

ωB97X Caffeic Acid (Neutral) 0.004 a.u.

C 1.2660437161 0.0513152137 -0.7109880757
C 0.0487959783 -0.0704617351 -0.0220259888
C 0.0473510955 -0.120239221 1.3527732324
C 1.2467989096 -0.0499306691 2.0721442132
C 2.4435481466 0.0722389453 1.3738158397
C 2.4558377836 0.1221129131 -0.014008469
O -1.1162947972 -0.13824341 -0.6994861094
C 1.2854488908 -0.1008203314 3.5301502331
C 0.2508717649 -0.2413783386 4.3639292129
C 0.4704356987 -0.2717958459 5.8123386447
O -0.6912575473 -0.4270209276 6.4930312283
O 1.1534430759 0.0913743791 -2.0611251439
O 1.5230726787 -0.1765574236 6.3961862071
H 2.2697554813 -0.0146076033 3.9839941506
H -0.7718531624 -0.3402668488 4.025145697
H -0.4491286705 -0.437373448 7.4249590004
H 2.0087452228 0.1677914583 -2.4878677353
H -0.9384546344 -0.0935317588 -1.6446335096
H 3.3917941629 0.2168270158 -0.5531993103
H 3.379020216 0.1283296355 1.9176823906
H -0.90886301 -0.2140899995 1.8517682922

ωB97X Caffeic Acid (Neutral) 0.006 a.u.

C 1.2677373166 0.0516686901 -0.7110576502
C 0.0492389241 -0.0702805688 -0.0194797129
C 0.049749558 -0.1199015732 1.3546196551
C 1.2509627719 -0.0491520274 2.0734103886
C 2.4474245411 0.0731730213 1.3731657588
C 2.4587856465 0.1227775245 -0.0144925146
O -1.1149614281 -0.1382245281 -0.6937466456
C 1.2900476552 -0.1002465903 3.5281113004
C 0.2539135668 -0.2397188939 4.3645576461
C 0.467150659 -0.2717225844 5.8090115144
O -0.6995139089 -0.4278517685 6.4883877307
O 1.1492416247 0.0908797758 -2.0558602569
O 1.5138993388 -0.1781906982 6.4076669622
H 2.2750540555 -0.0156032785 3.9811305932
H -0.7678486735 -0.3373078795 4.0230155974
H -0.4525529312 -0.4394905496 7.4184951929
H 1.9985448139 0.1657549841 -2.4959921052

H -0.9428957279 -0.0952437303 -1.6406714473
H 3.3937217387 0.217277945 -0.5550430305
H 3.3838173953 0.1293567402 1.9157317433
H -0.9064059366 -0.2142820103 1.8536232802

ωB97X Caffeic Acid (Neutral) 0.008 a.u.

C 1.2695985679 0.0521203083 -0.711319183
C 0.0494084724 -0.0704286548 -0.0175050808
C 0.0513694696 -0.1201353103 1.3558231435
C 1.2541935874 -0.0487815822 2.074832021
C 2.4507789236 0.0740443155 1.3726570109
C 2.4618251181 0.1236551972 -0.0145680448
O -1.1134951306 -0.1386690325 -0.6892882697
C 1.2938758162 -0.1000752947 3.525545264
C 0.2562953894 -0.2377739158 4.365819099
C 0.4643014266 -0.27158267 5.8057361401
O -0.7070504041 -0.4276391161 6.4851144759
O 1.1459995148 0.0906423196 -2.050661751
O 1.5056550359 -0.1807123187 6.4186662627
H 2.2797652988 -0.0176864695 3.9775178866
H -0.7647810518 -0.3333415414 4.022119546
H -0.4539579866 -0.4408743131 7.4130509303
H 1.989281212 0.1648704696 -2.5038091495
H -0.9468997587 -0.097110484 -1.6379156895
H 3.3959221998 0.2182081928 -0.5561683556
H 3.387852941 0.1303874182 1.9143437417
H -0.9048276417 -0.2154455182 1.8545940019

ωB97X Gallic Acid (Neutral) zero field

C -0.9511323665 -1.1712255722 0.0023158196
C -1.6878417465 0.0070401676 0.0005623067
C -1.0395076232 1.2362664538 -0.0038069722
C 0.3447358173 1.2868924137 -0.0064087783
C 1.0693652762 0.1021185602 -0.0045765563
C 0.4276431056 -1.1328120333 -0.0001969156
O -3.0462273387 0.0081035743 0.0029464931
O -1.7586912324 2.3830043444 -0.0055332118
C 2.5538630439 0.0940737187 -0.0072040603
O 3.0947760129 1.32522756 -0.0118141623
O -1.6972168581 -2.3162097589 0.0065253195
O 3.2332414263 -0.8997427455 -0.0055887311
H 1.0200433967 -2.0402446023 0.0011078389
H 0.8401331971 2.2474325514 -0.0098802395
H -1.1264824606 -3.0856803086 0.007634476
H -3.3610063609 -0.9006647487 0.0057475426
H -2.6950621017 2.1632320285 -0.0033686854

H 4.0509278124 1.2044133968 -0.0131674837

ωB97X Gallic Acid (Neutral) 0.010 a.u.

C -0.9485483823 -1.1880047293 0.0024630975
C -1.6888496689 -0.0050312994 0.000723095
C -1.0353181948 1.2279922532 -0.003648204
C 0.3476984008 1.2738778074 -0.0062417024
C 1.0791258991 0.0882193735 -0.0043790718
C 0.4320077039 -1.1490547307 0.0000113886
O -3.027815396 0.019277355 0.0029872588
O -1.7393013272 2.3729823961 -0.0054029225
C 2.5462655871 0.1053215769 -0.0070632065
O 3.0822073553 1.3531145223 -0.0122615745
O -1.6994964548 -2.3193607901 0.0065834357
O 3.2830494194 -0.8578482039 -0.0052757509
H 1.0153729431 -2.0620424864 0.0013228718
H 0.8348528723 2.2383077238 -0.0098077814
H -1.155706286 -3.107263503 0.0071625369
H -3.4018623848 -0.8689006744 0.0054762921
H -2.6846593636 2.1807879746 -0.0036241965
H 4.0325382772 1.2088504344 -0.0137315656

ωB97X Gallic Acid (Neutral) 0.002 a.u.

C -0.9507479194 -1.1744238507 0.0023478249
C -1.6878907049 0.0046563554 0.0005984852
C -1.0386027845 1.2344233143 -0.0037711988
C 0.3454487068 1.2840754892 -0.0063749889
C 1.070943018 0.099153356 -0.0045410231
C 0.4284704474 -1.1361162668 -0.0001576515
O -3.0424864708 0.0105056433 0.0029580016
O -1.7543949234 2.3809666812 -0.0055030022
C 2.552216122 0.0963507689 -0.007190704
O 3.0917772785 1.3308042328 -0.0119013543
O -1.6976825561 -2.3167533821 0.0065382855
O 3.2431004408 -0.8912993758 -0.0055235973
H 1.0188181303 -2.0447622608 0.0011477309
H 0.8392516908 2.245327425 -0.0098663308
H -1.1320639616 -3.0897850808 0.0075478182
H -3.368768406 -0.8945106641 0.0056824112
H -2.6926161108 2.166856756 -0.0034260564
H 4.0467890028 1.205755859 -0.0132706501

ωB97X Gallic Acid (Neutral) 0.004 a.u.

C -0.9503174299 -1.177730551 0.0023779765
C -1.6880286975 0.0022211763 0.0006321091
C -1.0377307456 1.2326134077 -0.003738192

C	0.3461104493	1.2813340226	-0.0063430256
C	1.0726945913	0.0962623898	-0.0045057537
C	0.4293173281	-1.1394026457	-0.000118667
O	-3.0388211139	0.0129893831	0.0029674884
O	-1.7503040499	2.3788913827	-0.0054751073
C	2.5506743374	0.0986146931	-0.0071742641
O	3.0890187732	1.3363588614	-0.0119872348
O	-1.6980367939	-2.3174580081	0.0065504891
O	3.2530403604	-0.8828677577	-0.0054586734
H	1.0177159444	-2.0492204586	0.0011872484
H	0.8382794442	2.2433346567	-0.0098538259
H	-1.1375392728	-3.094021115	0.0074601006
H	-3.3770584158	-0.8879772059	0.0056250592
H	-2.6903460594	2.1703503669	-0.0034782108
H	4.0428923503	1.2069324017	-0.0133735166

ωB97X Gallic Acid (Neutral) 0.006 a.u.

C	-0.9498250275	-1.1811291309	0.0024068321
C	-1.6882438136	-0.0002427914	0.0006645429
C	-1.0368871708	1.2308869539	-0.0037080053
C	0.3467171269	1.2786959324	-0.0063140146
C	1.0746358823	0.0934600167	-0.0044720051
C	0.4301906383	-1.1426591793	-0.0000805583
O	-3.035181115	0.0154238262	0.0029782542
O	-1.7464216838	2.3768135079	-0.0054497408
C	2.5492014642	0.1008619568	-0.0071556272
O	3.0864979469	1.3419136503	-0.0120714568
O	-1.6983623495	-2.3182332509	0.0065634328
O	3.263035605	-0.8744669025	-0.0053921669
H	1.0167615615	-2.0535997803	0.0012257189
H	0.8372156664	2.2414825821	-0.0098449437
H	-1.1431050859	-3.0983806295	0.0073674933
H	-3.3856330782	-0.8812647065	0.0055768115
H	-2.6882589361	2.1737674311	-0.0035268596
H	4.0392233688	1.2078955139	-0.0134737073

ωB97X Gallic Acid (Neutral) 0.008 a.u.

C	-0.9492402221	-1.1845466754	0.0024346582
C	-1.6885110856	-0.0026610033	0.0006953652
C	-1.0360820921	1.2293407874	-0.0036795604
C	0.347251464	1.2762121061	-0.0062845915
C	1.0767703851	0.0907803318	-0.0044354402
C	0.4310903472	-1.1458727584	-0.0000407517
O	-3.0315149801	0.0175231573	0.0029882324
O	-1.7427553295	2.3748384925	-0.0054265346
C	2.5477394172	0.1030945977	-0.0071275856

O 3.0842215182 1.3474840373 -0.0121571126
O -1.698852793 -2.318866207 0.0065759184
O 3.2730271199 -0.8661309117 -0.0053282709
H 1.0159879545 -2.0578669717 0.0012662405
H 0.8360774587 2.239807756 -0.0098352714
H -1.1491575815 -3.1027911411 0.0072702862
H -3.3938956618 -0.8749010518 0.0055328446
H -2.6863647414 2.1772355937 -0.0035738829
H 4.0357698221 1.2085448605 -0.0135805437

ω B97X Caffeic Acid (Radical) Zero field

C 1.2498795118 0.0531861971 -0.7636557186
C -0.0010113343 -0.0786917578 -0.002626166
C -0.0119374497 -0.1320395521 1.3658319447
C 1.1996635422 -0.0584496041 2.0701429829
C 2.4302819437 0.0710138739 1.3550829689
C 2.4725388612 0.1249278642 0.0011966255
O -1.1088082783 -0.1411507234 -0.7293194055
C 1.2662892851 -0.1069799834 3.515837201
C 0.2364016063 -0.2421843029 4.361948796
C 0.487249322 -0.2706194423 5.8171882106
O -0.6554036828 -0.4144602751 6.5127557438
O 1.1782493003 0.0952102172 -1.9948951481
O 1.5627323389 -0.1791266974 6.3482288904
H 2.2540755117 -0.0250394954 3.9608674146
H -0.7925272556 -0.3358964603 4.0403558054
H -0.4169638272 -0.4244290432 7.4471581541
H -0.8191489582 -0.0824642035 -1.6568294937
H 3.4012226322 0.2227416861 -0.545819462
H 3.3482885317 0.125620336 1.928863972
H -0.959419601 -0.2286496335 1.879459684

ω B97X Caffeic Acid (Radical) 0.010 a.u.

C 1.2526453355 0.0560176079 -0.7678228374
C -0.0067483506 -0.0802469912 0.00146337
C -0.0056183187 -0.1340950247 1.3727202579
C 1.2111001977 -0.0589167786 2.0699111658
C 2.4457579991 0.071300391 1.3484631524
C 2.4861801799 0.1261877205 -0.0020016763
O -1.1136981485 -0.1435138205 -0.7027897363
C 1.280369531 -0.1061586903 3.504824785
C 0.2477482344 -0.2381118484 4.366567591
C 0.4746862387 -0.267767443 5.8011913086
O -0.6875906323 -0.4171021857 6.5002473396
O 1.1794980529 0.1021290645 -1.9847468202
O 1.5249721127 -0.1781940218 6.4007900762

H 2.2725911653 -0.0264622924 3.9416378366
H -0.7780212248 -0.3306022976 4.0370128173
H -0.4156331338 -0.4278440787 7.4226201163
H -0.8695755492 -0.088130845 -1.6459677948
H 3.4089167052 0.222884428 -0.5594037352
H 3.3663458258 0.1243309666 1.9192490067
H -0.9522742203 -0.2331848607 1.8878067767

ωB97X Caffeic Acid (Radical) 0.002 a.u.

C 1.2495878093 0.0535697373 -0.7639572325
C -0.0019727009 -0.0788183086 -0.0009016298
C -0.0093987706 -0.1321187816 1.3682747494
C 1.2034785203 -0.0582877104 2.0696481233
C 2.433950623 0.0709507001 1.3534690876
C 2.4747769075 0.1248422483 -0.0001586704
O -1.11036151 -0.141296429 -0.7222363038
C 1.2704138753 -0.1064950381 3.5146656106
C 0.2398830994 -0.2414174994 4.3618155499
C 0.4841993468 -0.2698987951 5.8138904133
O -0.6630104539 -0.4161650821 6.5079315195
O 1.1767126044 0.0958786862 -1.9924653855
O 1.5538279008 -0.1775257727 6.3597251426
H 2.2589161007 -0.0244674239 3.9582464323
H -0.7880296594 -0.3353737478 4.0376618552
H -0.419961676 -0.4260034118 7.4405016705
H -0.8298088425 -0.0832615027 -1.6530294994
H 3.4018834188 0.2221325679 -0.5498777013
H 3.3529792267 0.1252086927 1.9258084018
H -0.9564138199 -0.2289341292 1.8827608667

ωB97X Caffeic Acid (Radical) 0.004 a.u.

C 1.2497459691 0.0535366184 -0.7645273059
C -0.0030259209 -0.078758432 0.0003173189
C -0.0074842118 -0.1317034614 1.3701341908
C 1.2065863531 -0.0578353553 2.0693504742
C 2.437349361 0.0709139048 1.3520802837
C 2.4772636706 0.1244319605 -0.0011796012
O -1.1117428314 -0.1410804776 -0.7159598283
C 1.2737976944 -0.1056002005 3.5130207379
C 0.2427771428 -0.2409519329 4.3621514858
C 0.4814274209 -0.2692650513 5.8106857152
O -0.6698544119 -0.4182628508 6.5042156864
O 1.176317626 0.0961679361 -1.9903115968
O 1.5455036946 -0.1757438232 6.3706607651
H 2.2630014813 -0.0229362175 3.9551498689
H -0.7841941767 -0.3359686556 4.0358665216

H -0.4213093117 -0.4278571374 7.4347317953
H -0.8404637905 -0.0841091978 -1.6499696019
H 3.4030244261 0.2209904859 -0.5532639849
H 3.3571583781 0.124830647 1.9233922005
H -0.9542265631 -0.2282797593 1.8852278745

ω B97X Caffeic Acid (Radical) 0.006 a.u.

C 1.2503185616 0.0539749468 -0.7653247767
C -0.0041138717 -0.0790179211 0.0011428395
C -0.0061109884 -0.1320045253 1.3714863946
C 1.2090128756 -0.0578505081 2.0693088011
C 2.4405052702 0.0710145025 1.3508571541
C 2.4799792329 0.1246393241 -0.0017957589
O -1.1128618426 -0.1414861826 -0.7104568346
C 1.2766314092 -0.1053861913 3.5108301018
C 0.2450486512 -0.240152501 4.3629611014
C 0.4789063052 -0.2687161848 5.807449443
O -0.6762561308 -0.4188998456 6.5015557479
O 1.1767820257 0.0973903485 -1.9883042662
O 1.5379067304 -0.1755378626 6.3810550923
H 2.266687936 -0.0231403632 3.951409181
H -0.7812760235 -0.3350018007 4.035071501
H -0.4211579093 -0.4286241386 7.4297341825
H -0.8510575968 -0.0853123127 -1.6476538982
H 3.4045428204 0.2209586062 -0.5559591278
H 3.3608614669 0.1246650036 1.9215240502
H -0.9526969223 -0.228993394 1.8868820719

ω B97X Caffeic Acid (Radical) 0.008 a.u.

C 1.2512711305 0.0553565065 -0.7663700176
C -0.0052652945 -0.0798964085 0.0014784706
C -0.0053486204 -0.1337245229 1.3722661269
C 1.2106038376 -0.0588238012 2.0694650614
C 2.4433313825 0.0711953582 1.3497232951
C 2.4828752859 0.125925302 -0.001994811
O -1.1135154603 -0.1430085376 -0.7060367789
C 1.2788595424 -0.1064041502 3.5080804119
C 0.2466221422 -0.2387819435 4.3644129972
C 0.4766918626 -0.2682148579 5.8042797284
O -0.6822688988 -0.4170061899 6.5002503332
O 1.1778643387 0.1005285955 -1.9864106446
O 1.5312427419 -0.1777642251 6.3909814576
H 2.2700279745 -0.0262960542 3.9468699529
H -0.7794630979 -0.3313062725 4.0355296482
H -0.4193761551 -0.4274738673 7.4257382081
H -0.8609597726 -0.0869007094 -1.6462855143

H	3.4063618443	0.2228776669	-0.5579601012
H	3.3639631745	0.1246187008	1.9201742454
H	-0.9518659582	-0.2323815897	1.8875809307

ωB97X Gallic Acid (Radical) Zero field

C	-0.9445798581	-1.2184108144	0.0032033196
C	-1.7474130476	-0.0028890278	0.0016401002
C	-1.0177831875	1.2645214039	-0.0033124336
C	0.3555420953	1.3169288219	-0.0063585863
C	1.0618337042	0.1132483184	-0.0045619588
C	0.4217242583	-1.1394130355	0.0001872154
O	-2.9808737659	0.0196625611	0.0041711912
O	-1.7737046737	2.3546540637	-0.0046597964
C	2.5507053185	0.0949601693	-0.0076168223
O	3.0962338731	1.3207942121	-0.0126738513
O	-1.6420660544	-2.3607603976	0.0076490076
O	3.2141661434	-0.9081725578	-0.005826805
H	1.0382965672	-2.0308795225	0.0013019259
H	0.8690423263	2.2674445423	-0.010072305
H	-1.044050721	-3.1119739212	0.0084074202
H	-2.6949155467	2.0417353391	-0.0019439319
H	4.0529345684	1.2016728449	-0.0142386893

ωB97X Gallic Acid (Radical) 0.010 a.u.

C	-0.9412794286	-1.232892299	0.0032941767
C	-1.7486044068	-0.0092344186	0.0018897369
C	-1.0171213833	1.2632513776	-0.0033163873
C	0.3582218666	1.3067003449	-0.0064347252
C	1.0686096816	0.1014550392	-0.004553037
C	0.4271797768	-1.155867016	0.0002739594
O	-2.9709121708	0.0064740144	0.0045375369
O	-1.7536065137	2.3560911183	-0.0047294299
C	2.5408924916	0.1061776075	-0.0076582175
O	3.0855872059	1.3469642009	-0.0128924403
O	-1.6528058308	-2.3556806484	0.0076278149
O	3.2594950021	-0.8688116694	-0.005361213
H	1.0354487681	-2.052530053	0.001364712
H	0.8665655732	2.2597180078	-0.0103252692
H	-1.0889810122	-3.1322853367	0.007968688
H	-2.6894202183	2.0833380565	-0.0020675351
H	4.0358225985	1.200254674	-0.01432337

ωB97X Gallic Acid (Radical) 0.002 a.u.

C	-0.9441017529	-1.2211002265	0.0032195674
C	-1.747435797	-0.0040778008	0.0016843197
C	-1.0175704507	1.2640539133	-0.0033076537

C	0.3562219708	1.3146150996	-0.0063565172
C	1.0628059011	0.1106876231	-0.0045398903
C	0.4227761908	-1.1426216333	0.0002127274
O	-2.9786712953	0.017348885	0.0042300227
O	-1.7693676296	2.3548755478	-0.0046741985
C	2.5486512551	0.0971315541	-0.007587574
O	3.0936039502	1.3258942825	-0.0127414306
O	-1.6441364859	-2.3597267158	0.007632567
O	3.2231602771	-0.9002693502	-0.0057310099
H	1.0374422692	-2.0352431392	0.0013276144
H	0.8687050134	2.265581417	-0.0100974555
H	-1.0524626201	-3.1157730395	0.0083073997
H	-2.6935768493	2.049944251	-0.0019818146
H	4.0490480532	1.2018023321	-0.014301674

ωB97X Gallic Acid (Radical) 0.004 a.u.

C	-0.9435907156	-1.2241104843	0.0032445716
C	-1.7478105134	-0.00539441	0.0017699697
C	-1.0174464162	1.2638348182	-0.0033547194
C	0.3569248424	1.3122676196	-0.0065789832
C	1.0639454251	0.1080232648	-0.004814875
C	0.4239071378	-1.1460587529	0.0000755698
O	-2.9766607663	0.0141864439	0.0045627827
O	-1.764556326	2.3552841737	-0.0046716975
C	2.5467380491	0.0993437174	-0.0080676236
O	3.0907480588	1.331337609	-0.0125717979
O	-1.6462012516	-2.3586685816	0.0077645732
O	3.2321476246	-0.8923860681	-0.0054842375
H	1.0367648871	-2.0398118626	0.0011405012
H	0.868491679	2.2636735663	-0.0104311414
H	-1.0615376861	-3.1198880267	0.00833244
H	-2.6916851689	2.0589907079	-0.0018977686
H	4.0449131401	1.2024992654	-0.0137225642

ωB97X Gallic Acid (Radical) 0.006 a.u.

C	-0.9429107316	-1.2269768219	0.0032430081
C	-1.7479838797	-0.0067298578	0.0017513567
C	-1.0173913508	1.2634598531	-0.0033324784
C	0.3573774395	1.3101436174	-0.0064929946
C	1.0652540782	0.105625696	-0.0046960115
C	0.4250286512	-1.1493572524	0.0001532778
O	-2.9746224671	0.01149832	0.0045423155
O	-1.760548534	2.355500675	-0.0046796058
C	2.5446890569	0.1016298345	-0.0078558728
O	3.0887187187	1.3365196496	-0.0127156195
O	-1.6482974364	-2.3575944013	0.0076976364

O	3.2413076865	-0.8843401072	-0.0054542166
H	1.0361752475	-2.0441691221	0.0012444201
H	0.867808944	2.2620908255	-0.0103280064
H	-1.0703668395	-3.1238059198	0.0082217122
H	-2.6907262438	2.0676737388	-0.001984299
H	4.0415796603	1.2019542726	-0.014019622

ωB97X Gallic Acid (Radical) 0.008 a.u.

C	-0.9421362298	-1.229799967	0.0032701313
C	-1.7481807718	-0.007935581	0.0018190385
C	-1.0172329684	1.2632312804	-0.0033074129
C	0.3577979818	1.3084070622	-0.0063935761
C	1.0668543527	0.103560627	-0.0045260971
C	0.4260816403	-1.1525276298	0.0002701767
O	-2.9727715727	0.0092397988	0.0044290035
O	-1.7571797254	2.3558236577	-0.0047107326
C	2.5427824129	0.1038631399	-0.0075946157
O	3.0871645699	1.3416065276	-0.0128907287
O	-1.6505555734	-2.3567292431	0.0076156041
O	3.250362779	-0.8766298026	-0.0054465689
H	1.0357541591	-2.0482787382	0.0013769078
H	0.8671533934	2.2608965129	-0.0102346227
H	-1.0793375972	-3.1279831755	0.0080494406
H	-2.6902198836	2.0753569003	-0.0020524983
H	4.0387550333	1.2010216303	-0.0143784492

Table S1: Thermal enthalpies of all the species at 298.15 K with LC-BLYP/6-311++G(3df,2p)

Gallic Acid (Neutral)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-645.11334	-645.11218	-645.10704
0.008	-645.10915	-645.10853	-645.10433
0.006	-645.10568	-645.10542	-645.10217
0.004	-645.10291	-645.10286	-645.10063
0.002	-645.10077	-645.10083	-645.09968
0.000	-645.09935	-645.09935	-645.09935
-0.002	-645.09859	-645.09845	-645.09969
-0.004	-645.09848	-645.09806	-645.10065
-0.006	-645.09901	-645.09822	-645.10220
-0.008	-645.10019	-645.09893	-645.10437
-0.010	-645.10200	-645.10020	-645.10704

Gallic Acid (Radical)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-644.47568	-644.48458	-644.48197
0.008	-644.47442	-644.48176	-644.47994
0.006	-644.47386	-644.47953	-644.47836
0.004	-644.47401	-644.47789	-644.47724
0.002	-644.47484	-644.47683	-644.47657
0.000	-644.47635	-644.47635	-644.47635
-0.002	-644.47854	-644.47646	-644.47657
-0.004	-644.48139	-644.47716	-644.47723
-0.006	-644.48490	-644.47845	-644.47834
-0.008	-644.48908	-644.48032	-644.47991
-0.010	-644.49392	-644.48279	-644.48193

Gallic Acid (Radical Cation)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-644.81955	-644.80513	-644.80009
0.008	-644.81314	-644.80153	-644.79801
0.006	-644.80742	-644.79864	-644.79639
0.004	-644.80237	-644.79647	-644.79524
0.002	-644.79801	-644.79505	-644.79455
0.000	-644.79433	-644.79433	-644.79433
-0.002	-644.79133	-644.79428	-644.79455
-0.004	-644.78902	-644.79489	-644.79524
-0.006	-644.78741	-644.79611	-644.79639

-0.008	-644.78650	-644.79795	-644.79801
-0.010	-644.78629	-644.80037	-644.80009

Gallic Acid (Anion)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-644.57195	-644.58662	-644.59682
0.008	-644.57045	-644.58323	-644.59474
0.006	-644.57012	-644.58045	-644.59327
0.004	-644.57090	-644.57826	-644.57692
0.002	-644.57278	-644.57668	-644.57598
0.000	-644.57569	-644.57569	-644.57569
-0.002	-644.57959	-644.57529	-644.57599
-0.004	-644.58444	-644.57548	-644.57693
-0.006	-644.59020	-644.57627	-644.59327
-0.008	-644.59684	-644.57766	-644.59475
-0.010	-644.60432	-644.57964	-644.59683

Caffeic Acid (Neutral)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-647.14973	-647.12553	-647.13272
0.008	-647.14230	-647.12391	-647.12937
0.006	-647.13599	-647.12289	-647.12669
0.004	-647.13075	-647.12245	-647.12473
0.002	-647.12653	-647.12258	-647.12355
0.000	-647.12328	-647.12328	-647.12328
-0.002	-647.12099	-647.12455	-647.12394
-0.004	-647.11963	-647.12639	-647.12549
-0.006	-647.11918	-647.12879	-647.12777
-0.008	-647.11963	-647.13177	-647.13076
-0.010	-647.12101	-647.13531	-647.13438

Caffeic Acid (Radical)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-646.51522	-646.51638	-646.51427
0.008	-646.51158	-646.51356	-646.51208
0.006	-646.50909	-646.51131	-646.51036
0.004	-646.50769	-646.50965	-646.50912
0.002	-646.50735	-646.50856	-646.50834
0.000	-646.50803	-646.50803	-646.50803
-0.002	-646.50974	-646.50808	-646.50834

-0.004	-646.51248	-646.50870	-646.50912
-0.006	-646.51624	-646.50988	-646.51036
-0.008	-646.52105	-646.51163	-646.51208
-0.010	-646.52694	-646.51395	-646.51427

Caffeic Acid (Radical Cation)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-646.83191	-646.81290	-646.83564
0.008	-646.82878	-646.81472	-646.83283
0.006	-646.82669	-646.81709	-646.83057
0.004	-646.82577	-646.82001	-646.82891
0.002	-646.82601	-646.82348	-646.82785
0.000	-646.82749	-646.82749	-646.82749
-0.002	-646.83031	-646.83205	-646.82780
-0.004	-646.83460	-646.83714	-646.82882
-0.006	-646.84044	-646.84278	-646.83047
-0.008	-646.84788	-646.84895	-646.83273
-0.010	-646.85691	-646.85567	-646.83559

Caffeic Acid (Anion)	Along C-O bond	Perpendicular to the C-O bond	Perpendicular to the molecular plane
0.010	-646.65971	-646.63725	-646.61821
0.008	-646.64621	-646.63115	-646.61620
0.006	-646.63482	-646.62569	-646.61469
0.004	-646.62558	-646.62086	-646.61368
0.002	-646.61839	-646.61667	-646.61315
0.000	-646.61312	-646.61312	-646.61312
-0.002	-646.60959	-646.61019	-646.61357
-0.004	-646.60766	-646.60790	-646.61450
-0.006	-646.60716	-646.60624	-646.61592
-0.008	-646.60801	-646.60521	-646.61784
-0.010	-646.61010	-646.60482	-646.62025

Table S2: Dipole moment (in Debye) of gallic acid and caffeic acid

	Along C-O bond		Perpendicular to C-O bond		Perpendicular to molecular plane	
	GA	CA	GA	CA	GA	CA
0.010	5.906	10.221	5.164	3.901	4.191	5.444
0.008	5.046	8.779	4.515	3.583	3.609	4.917
0.006	4.222	7.431	3.875	3.408	3.062	4.444
0.004	3.440	6.155	3.250	3.386	2.579	4.063
0.002	2.716	4.939	2.648	3.515	2.223	3.821
0.000	2.088	3.774	2.088	3.774	2.088	3.774
-0.002	1.652	2.674	1.620	4.145	2.228	3.956
-0.004	1.556	1.692	1.344	4.593	2.586	4.306
-0.006	1.843	1.125	1.387	5.101	3.070	4.756
-0.008	2.373	1.524	1.728	5.651	3.618	5.268
-0.010	3.016	2.453	2.239	6.234	4.200	5.818

Table S3: Component of Dipole moment along C-O bond (in Debye) of gallic acid and caffeic acid

	Along C-O bond		Perpendicular to C-O bond		Perpendicular to molecular plane	
	GA	CA	GA	CA	GA	CA
0.010	-5.653	-10.051	-1.501	-3.090	-1.355	-2.688
0.008	-4.758	-8.607	-1.471	-3.192	-1.355	-2.891
0.006	-3.886	-7.253	-1.443	-3.281	-1.358	-3.100
0.004	-3.032	-5.967	-1.417	-3.366	-1.361	-3.297
0.002	-2.194	-4.732	-1.391	-3.451	-1.366	-3.457
0.000	-1.368	-3.533	-1.368	-3.533	-1.368	-3.533
-0.002	-0.553	-2.366	-1.346	-3.619	-1.366	-3.474
-0.004	0.252	-1.217	-1.326	-3.703	-1.362	-3.346
-0.006	1.050	-0.076	-1.308	-3.786	-1.359	-3.195
-0.008	1.843	1.059	-1.292	-3.865	-1.357	-3.039
-0.010	2.630	2.194	-1.277	-3.940	-1.356	-2.888

Table S4: Thermal enthalpies of gallic acid and caffeic acid and their radical at 298.15 K with 6-311++G(3df,2p)

(a) CBS-QB3

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-645.60060	-644.98759	-647.69290	-647.09359
-0.008	-645.59880	-644.98284	-647.69140	-647.08768
-0.006	-645.59767	-644.97876	-647.69073	-647.08288
-0.004	-645.59719	-644.97535	-647.69097	-647.07913
-0.002	-645.59738	-644.97261	-647.69213	-647.07642
0.000	-645.59819	-644.97055	-647.69422	-647.07474
0.002	-645.59962	-644.96917	-647.69727	-647.07410
0.004	-645.60168	-644.96848	-647.70131	-647.07450
0.006	-645.60446	-644.96849	-647.70638	-647.07598
0.008	-645.60795	-644.96921	-647.71253	-647.07856
0.010	-645.61217	-644.97066	-647.71988	-647.08231

(b) B3LYP/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.60146	-645.99410	-648.74132	-648.14782
-0.008	-646.59976	-645.98928	-648.73985	-648.14138
-0.006	-646.59876	-645.98518	-648.73941	-648.13620
-0.004	-646.59846	-645.98179	-648.74002	-648.13223
-0.002	-646.59886	-645.97913	-648.74168	-648.12946
0.000	-646.59998	-645.97719	-648.74441	-648.12787
0.002	-646.60182	-645.97597	-648.74826	-648.12748
0.004	-646.60441	-645.97549	-648.75325	-648.12830
0.006	-646.60775	-645.97577	-648.75945	-648.13035
0.008	-646.61186	-645.97682	-648.76691	-648.13368
0.010	-646.61676	-645.97864	-648.77572	-648.13834

(c) M06-2X/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.35776	-645.74533	-648.48125	-647.88151
-0.008	-646.35603	-645.74059	-648.47979	-647.87541
-0.006	-646.35494	-645.73652	-648.47935	-647.87047
-0.004	-646.35450	-645.73313	-648.47987	-647.86666
-0.002	-646.35473	-645.73041	-648.48128	-647.86396
0.000	-646.35563	-645.72837	-648.48370	-647.86234
0.002	-646.35723	-645.72704	-648.48714	-647.86185
0.004	-646.35952	-645.72641	-648.49160	-647.86248
0.006	-646.36252	-645.72649	-648.49716	-647.86425
0.008	-646.36625	-645.72732	-648.50386	-647.86723
0.010	-646.37073	-645.72890	-648.51179	-647.87146

(d) LC-BLYP/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-645.10200	-644.49392	-647.12101	-646.52694
-0.008	-645.10019	-644.48908	-647.11963	-646.52105
-0.006	-645.09901	-644.48490	-647.11918	-646.51624
-0.004	-645.09848	-644.48139	-647.11963	-646.51248
-0.002	-645.09859	-644.47854	-647.12099	-646.50974
0.000	-645.09935	-644.47635	-647.12328	-646.50803
0.002	-645.10077	-644.47484	-647.12653	-646.50735
0.004	-645.10291	-644.47401	-647.13075	-646.50769
0.006	-645.10568	-644.47386	-647.13599	-646.50909
0.008	-645.10915	-644.47442	-647.14230	-646.51158
0.010	-645.11334	-644.47568	-647.14973	-646.51522

(e) LC- ω PBE/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.17553	-645.56312	-648.29168	-647.69200
-0.008	-646.17372	-645.55834	-648.29018	-647.68611
-0.006	-646.17256	-645.55422	-648.28963	-647.68130
-0.004	-646.17204	-645.55078	-648.29003	-647.67756
-0.002	-646.17218	-645.54800	-648.29136	-647.67486
0.000	-646.17298	-645.54589	-648.29362	-647.67319
0.002	-646.17445	-645.54447	-648.29685	-647.67255
0.004	-646.17660	-645.54373	-648.30107	-647.67296
0.006	-646.17944	-645.54368	-648.30633	-647.67443
0.008	-646.18298	-645.54433	-648.31266	-647.67701
0.010	-646.18724	-645.54570	-648.32015	-647.68073

(f) ω B97/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.48914	-645.88087	-648.61610	-648.02062
-0.008	-646.48733	-645.87604	-648.61461	-648.01465
-0.006	-646.48620	-645.87192	-648.61407	-648.00980
-0.004	-646.48572	-645.86851	-648.61441	-648.00601
-0.002	-646.48585	-645.86580	-648.61571	-648.00330
0.000	-646.48662	-645.86379	-648.61798	-648.00165
0.002	-646.48812	-645.86244	-648.62122	-648.00105
0.004	-646.49030	-645.86172	-648.62548	-648.00153
0.006	-646.49315	-645.86170	-648.63078	-648.00309
0.008	-646.49672	-645.86244	-648.63720	-648.00577
0.010	-646.50105	-645.86393	-648.64481	-648.00964

(g) ω B97X/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.43287	-645.82373	-648.56253	-647.96594
-0.008	-646.43108	-645.81887	-648.56108	-647.95992
-0.006	-646.42999	-645.81473	-648.56056	-647.95504
-0.004	-646.42957	-645.81129	-648.56096	-647.95123
-0.002	-646.42977	-645.80857	-648.56233	-647.94850
0.000	-646.43061	-645.80657	-648.56468	-647.94686
0.002	-646.43218	-645.80527	-648.56802	-647.94631
0.004	-646.43447	-645.80462	-648.57238	-647.94685
0.006	-646.43741	-645.80461	-648.57780	-647.94848
0.008	-646.44105	-645.80535	-648.58435	-647.95122
0.010	-646.44544	-645.80686	-648.59209	-647.95514

(h) ω B97XD/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.38328	-645.77284	-648.51478	-647.91661
-0.008	-646.38155	-645.76792	-648.51326	-647.91047
-0.006	-646.38054	-645.76375	-648.51280	-647.90550
-0.004	-646.38023	-645.76030	-648.51331	-647.90165
-0.002	-646.38052	-645.75759	-648.51480	-647.89890
0.000	-646.38148	-645.75560	-648.51729	-647.89725
0.002	-646.38322	-645.75437	-648.52080	-647.89674
0.004	-646.38567	-645.75387	-648.52536	-647.89737
0.006	-646.38872	-645.75398	-648.53100	-647.89918
0.008	-646.39248	-645.75475	-648.53780	-647.90214
0.010	-646.39701	-645.75634	-648.54585	-647.90623

(i) M11/6-311++G(3df,2p)

Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.33199	-645.71878	-648.43293	-647.83310
-0.008	-646.33013	-645.71391	-648.43138	-647.82699
-0.006	-646.32892	-645.70973	-648.43085	-647.82201
-0.004	-646.32837	-645.70622	-648.43233	-647.81814
-0.002	-646.32848	-645.70341	-648.43265	-647.81536
0.000	-646.32927	-645.70127	-648.43496	-647.81365
0.002	-646.33075	-645.69983	-648.43828	-647.81302
0.004	-646.33293	-645.69909	-648.44261	-647.81349
0.006	-646.33582	-645.69907	-648.44801	-647.81507
0.008	-646.33944	-645.69978	-648.45452	-647.81782
0.010	-646.34380	-645.70123	-648.46222	-647.82177

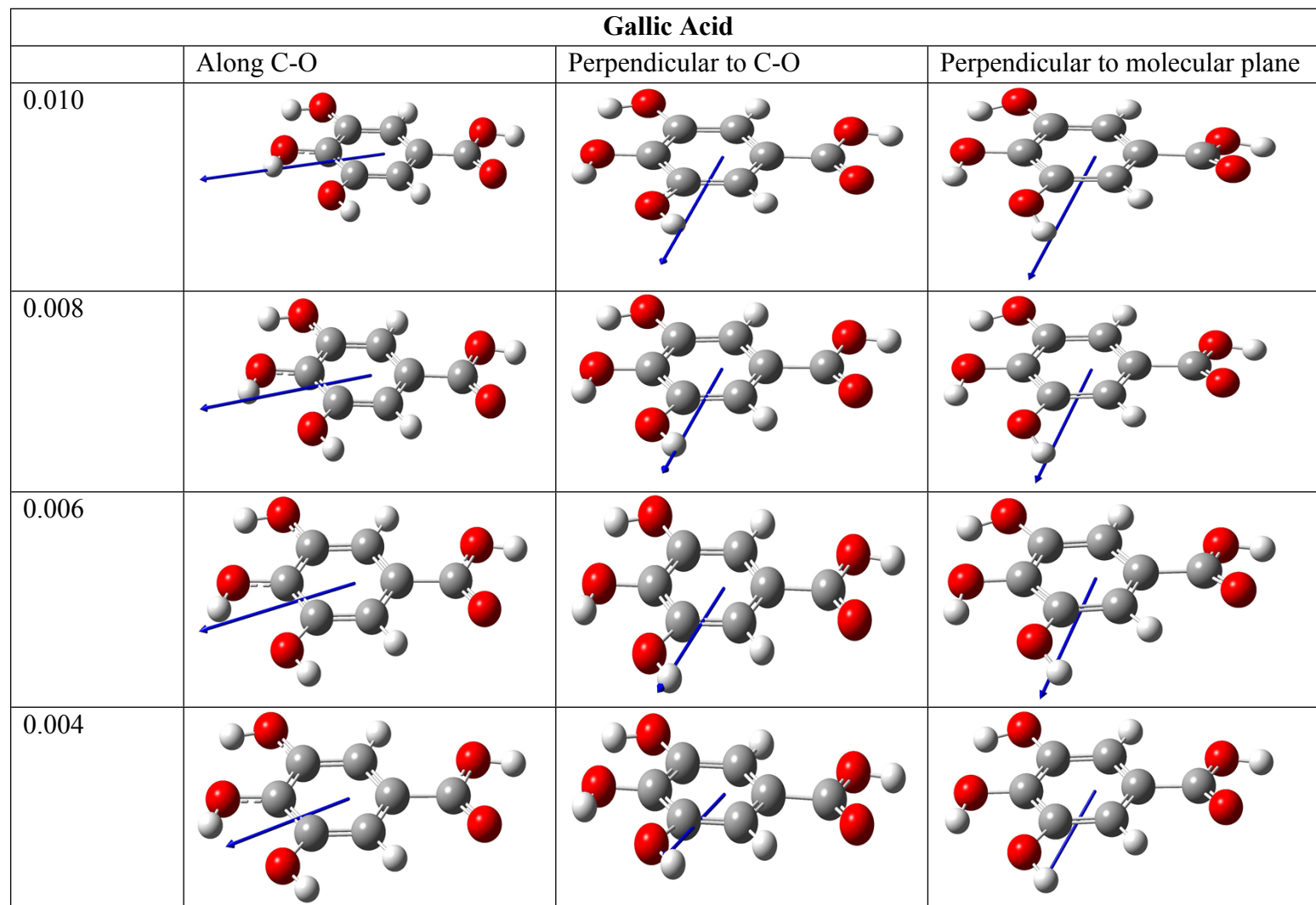
(j) CAMB3LYP/6-311++G(3df,2p)

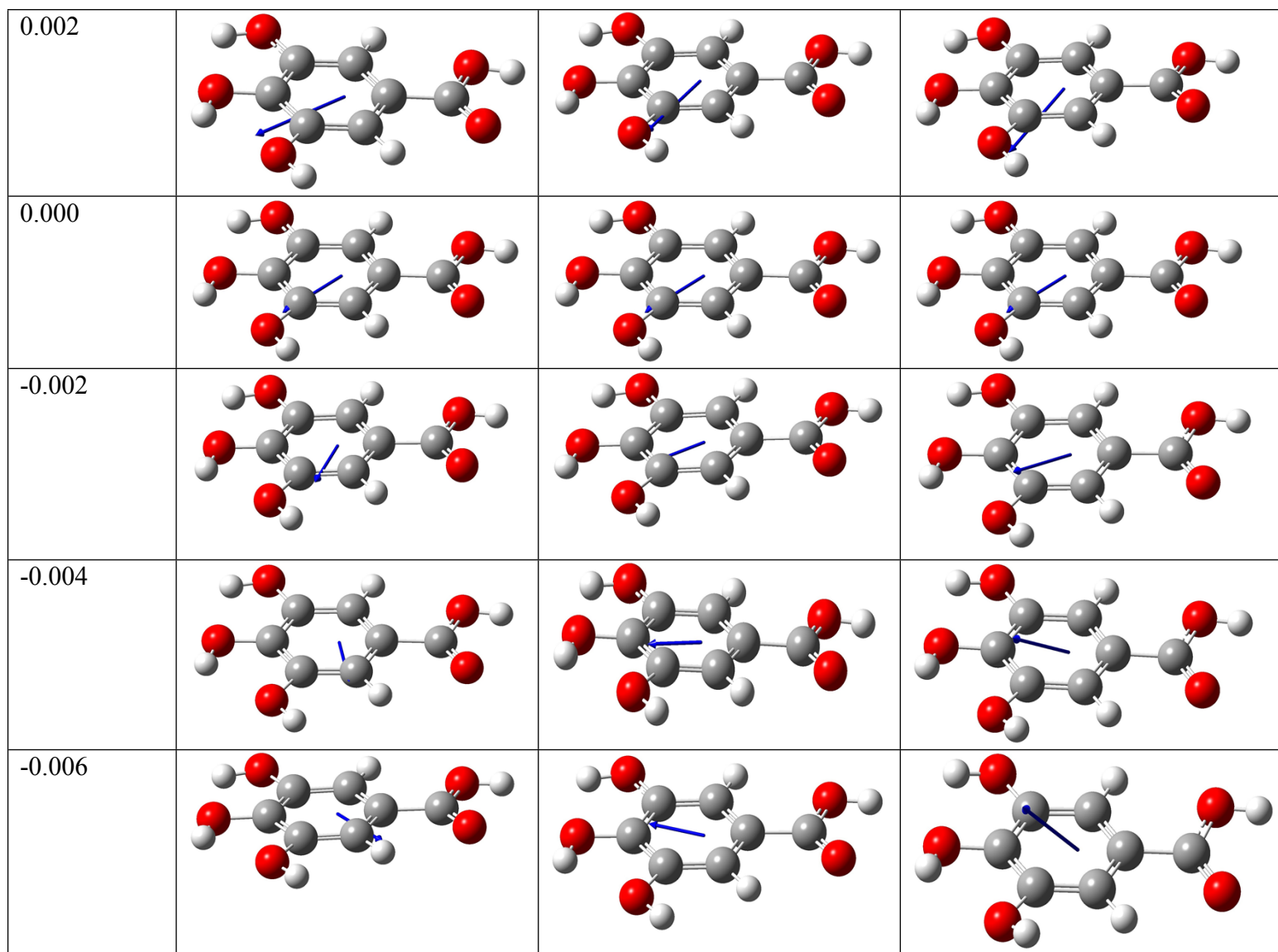
Electric Field (a.u.)	Gallic Acid		Caffeic Acid	
	Neutral	Radical	Neutral	Radical
-0.010	-646.34046	-645.73274	-648.45017	-647.85586
-0.008	-646.33871	-645.72792	-648.44874	-647.84973
-0.006	-646.33762	-645.72379	-648.44827	-647.84475
-0.004	-646.33720	-645.72035	-648.44878	-647.84091
-0.002	-646.33746	-645.71760	-648.45027	-647.83817
0.000	-646.33841	-645.71554	-648.45276	-647.83654
0.002	-646.34005	-645.71419	-648.45628	-647.83600
0.004	-646.34239	-645.71354	-648.46086	-647.83658
0.006	-646.34545	-645.71361	-648.46655	-647.83830
0.008	-646.34925	-645.71441	-648.47340	-647.84120
0.010	-646.35379	-645.71595	-648.48149	-647.84534

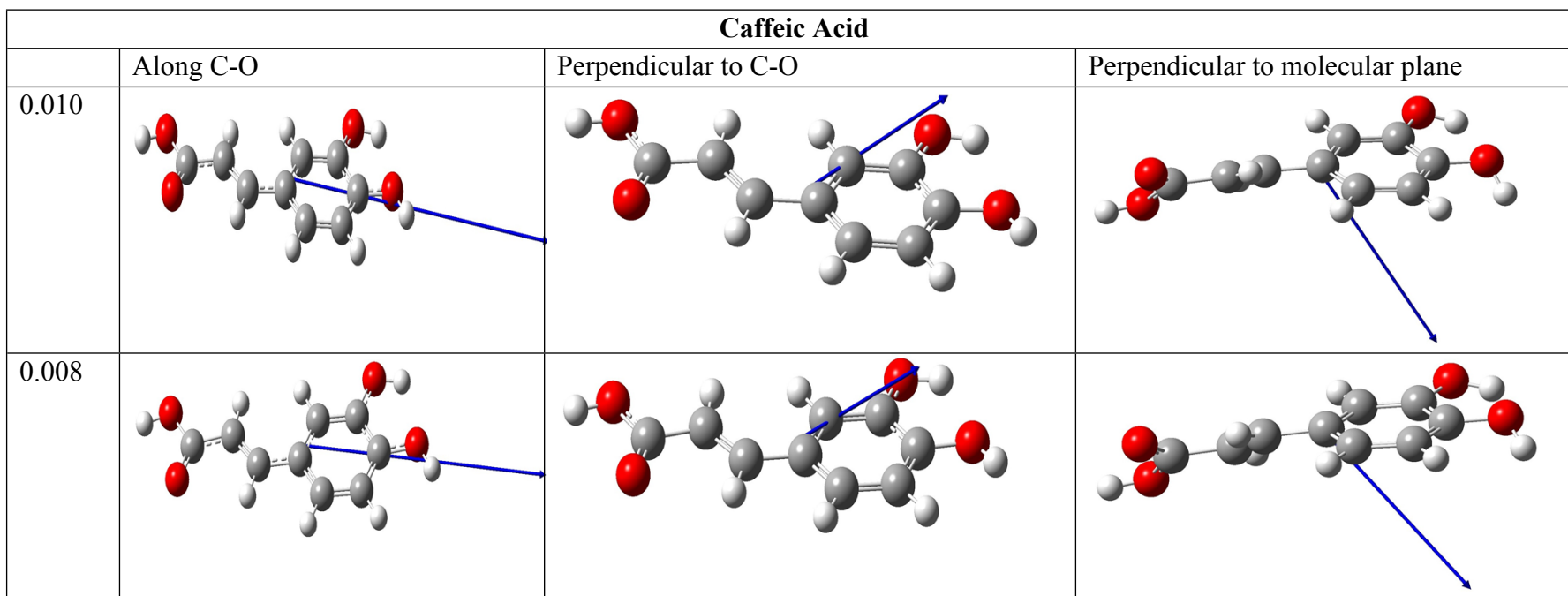
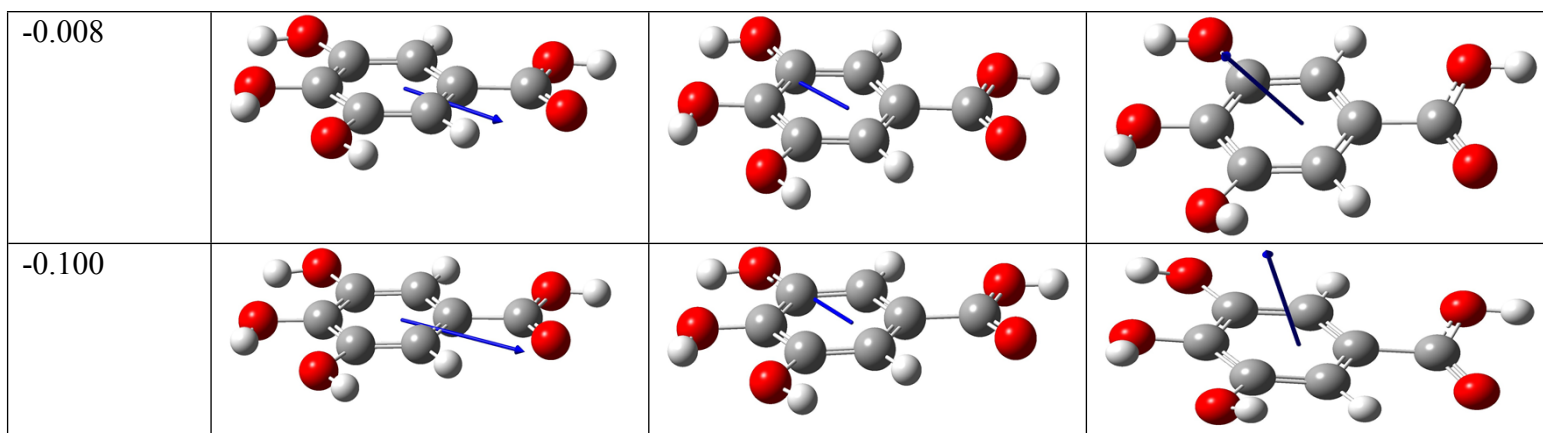
Table S5: O-H bond lengths (Å) of gallic and caffeic acids in presence of varying electric field (in a.u.) along C-O directions in different level of theory.

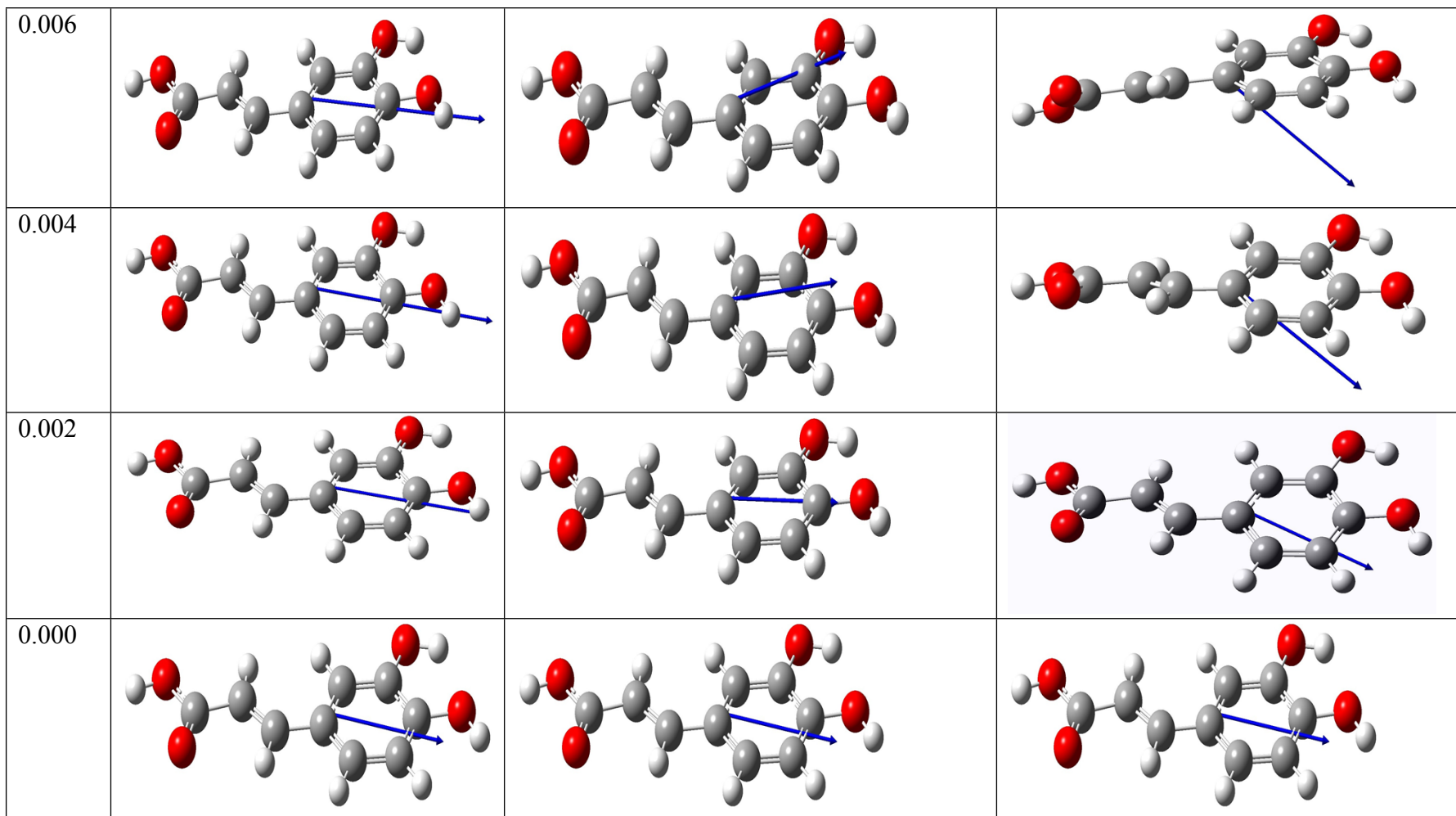
Electric field	B3LYP	M06-2X	LC-BLYP	LC- ω PBE	ω B97	ω B97X	ω B97XD	M11	CAM-B3LYP
	Gallic Acid								
0.010	0.9640	0.9626	0.9638	0.9621	0.9628	0.9610	0.9600	0.9637	0.9628
0.008	0.9641	0.9627	0.9639	0.9621	0.9628	0.9611	0.9600	0.9638	0.9629
0.006	0.9642	0.9628	0.9640	0.9622	0.9630	0.9612	0.9601	0.9638	0.9629
0.004	0.9643	0.9629	0.9641	0.9623	0.9631	0.9613	0.9603	0.9640	0.9631
0.002	0.9645	0.9631	0.9644	0.9625	0.9632	0.9615	0.9604	0.9641	0.9633
0.000	0.9647	0.9634	0.9646	0.9627	0.9635	0.9618	0.9607	0.9643	0.9635
-0.002	0.9650	0.9637	0.9649	0.9630	0.9638	0.9620	0.9610	0.9646	0.9638
-0.004	0.9654	0.9641	0.9653	0.9633	0.9641	0.9624	0.9612	0.9650	0.9642
-0.006	0.9659	0.9645	0.9658	0.9637	0.9645	0.9627	0.9616	0.9654	0.9646
-0.008	0.9664	0.9650	0.9663	0.9642	0.9650	0.9632	0.9620	0.9658	0.9651
-0.010	0.9670	0.9656	0.9669	0.9647	0.9655	0.9637	0.9625	0.9664	0.9657
Caffeic Acid									
0.010	0.9600	0.9582	0.9583	0.9572	0.9582	0.9566	0.9557	0.9586	0.95821
0.008	0.9601	0.9584	0.9585	0.9574	0.9583	0.9567	0.9559	0.9588	0.95839
0.006	0.9604	0.9586	0.9588	0.9576	0.9586	0.9570	0.9561	0.9591	0.95863
0.004	0.9606	0.9590	0.9591	0.9579	0.9589	0.9572	0.9563	0.9594	0.95891
0.002	0.9610	0.9593	0.9595	0.9582	0.9592	0.9576	0.9566	0.9597	0.95928
0.000	0.9614	0.9597	0.9600	0.9586	0.9596	0.9579	0.9570	0.9601	0.95968
-0.002	0.9619	0.9602	0.9605	0.9591	0.9601	0.9584	0.9575	0.9606	0.96017
-0.004	0.9624	0.9608	0.9611	0.9596	0.9606	0.9589	0.9580	0.9612	0.96073
-0.006	0.9631	0.9614	0.9618	0.9602	0.9612	0.9595	0.9586	0.9618	0.96303
-0.008	0.9639	0.9622	0.9626	0.9609	0.9619	0.9602	0.9592	0.9626	0.96215
-0.010	0.9648	0.9630	0.9635	0.9617	0.9627	0.9610	0.9601	0.9634	0.96303

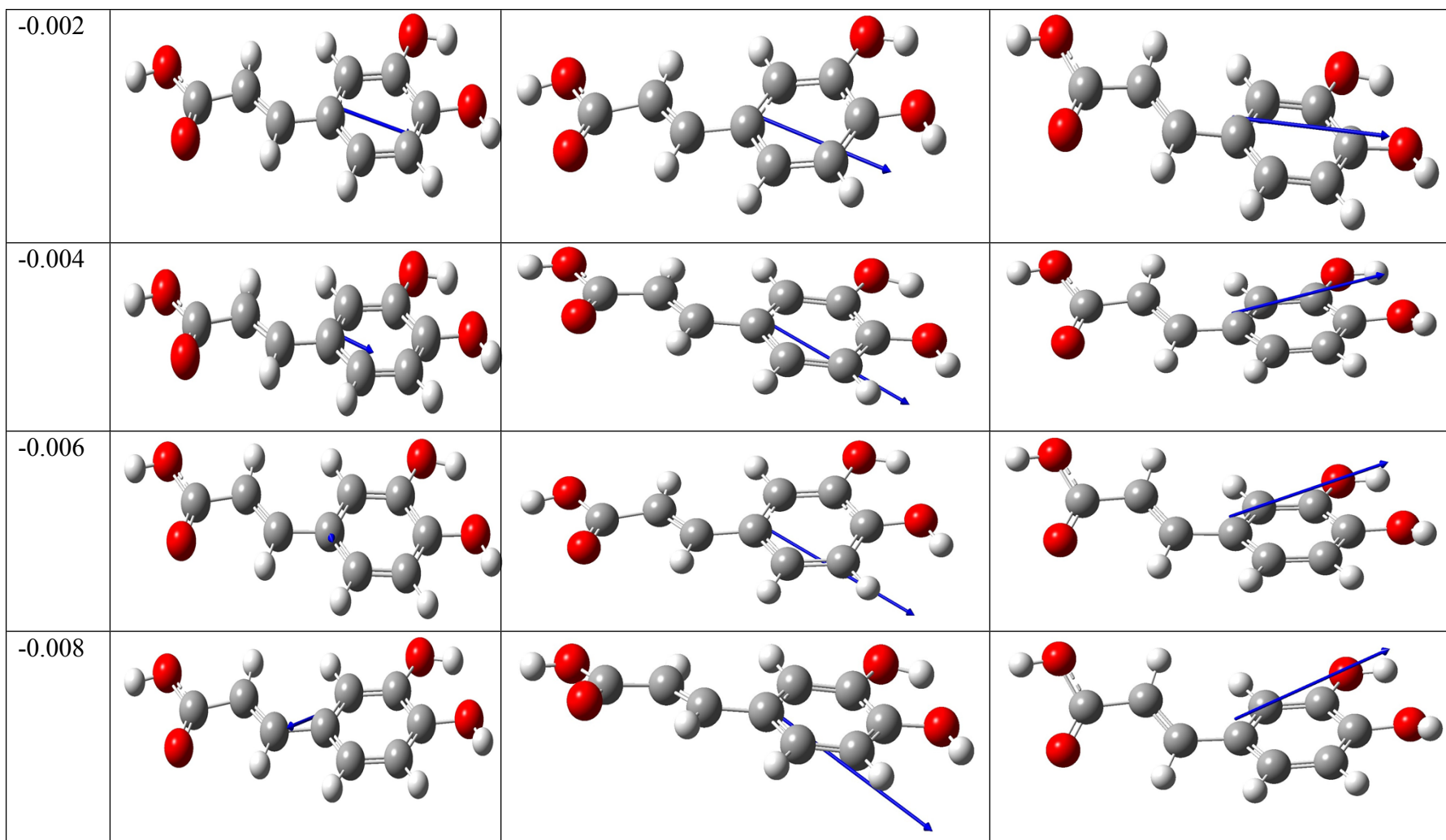
Figure S1: Change of dipole moment vector with the external electric field











-0.100

