Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Electronic Supplementary Information

## Kinetics of Chain Reaction Driven by Proton-Coupled Electron Transfer: α-Hydroxyethyl Radical and Bromoacetate in Buffered Aqueous Solutions

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Cartesian coordinates (Å), harmonic vibrational frequencies ($cm^{-1}$), and final electronic energies (a.u.) of all the stationary points discussed in the paper. The PCM-M06-2X-D3/6-311+G(2d,p) level of theory is used.

**(1) •EtOH**

| | | | |
|---|---|---|---|
| H | -1.305175 | -0.992398 | -0.693189 |
| H | 1.979329 | 0.170388 | 0.038554 |
| C | -1.225643 | -0.163111 | 0.014179 |
| O | 1.163426 | -0.340321 | 0.015967 |
| H | -1.387230 | -0.574934 | 1.019511 |
| C | 0.091413 | 0.505538 | -0.105181 |
| H | -2.028501 | 0.544080 | -0.191267 |
| H | 0.239550 | 1.520873 | 0.244670 |

| | | |
|---|---|---|
| 192.3080 | 344.4690 | 415.5523 |
| 588.8889 | 938.3350 | 1022.7212 |
| 1067.9020 | 1217.7023 | 1280.9191 |
| 1390.2752 | 1455.1216 | 1462.2450 |
| 1484.0047 | 3002.7873 | 3081.8942 |
| 3144.0629 | 3178.3141 | 3883.4188 |

E = -154.362934925 a.u.

**(2) •EtOH/$HCO_3^-$**

| | | | |
|---|---|---|---|
| H | -3.450931 | 1.005164 | -0.781387 |
| H | -3.984000 | -0.473047 | 0.017623 |
| C | -3.355099 | 0.413084 | 0.140282 |
| H | -3.757212 | 1.007896 | 0.960608 |
| C | -1.945410 | 0.028732 | 0.412570 |
| O | -1.385055 | -0.814101 | -0.489852 |
| H | -1.267840 | 0.730111 | 0.892009 |
| H | -0.402041 | -0.886285 | -0.298317 |
| O | 1.178492 | 1.094267 | -0.392958 |
| O | 1.126948 | -1.061968 | 0.086908 |
| C | 1.848759 | -0.038398 | 0.033293 |
| H | 1.825005 | 1.809980 | -0.391915 |
| O | 3.048055 | 0.080012 | 0.306466 |

| | | |
|---|---|---|
| 30.6532 | 50.1479 | 60.5322 |
| 104.8405 | 123.6838 | 200.7508 |
| 204.4911 | 442.5625 | 516.1273 |
| 583.1604 | 600.3738 | 681.6361 |
| 839.4967 | 938.5112 | 984.6939 |
| 1000.7644 | 1023.7308 | 1111.6461 |
| 1227.5645 | 1246.5062 | 1363.9788 |
| 1381.1835 | 1412.2329 | 1458.1172 |
| 1484.7445 | 1535.7212 | 1701.7178 |
| 2954.3472 | 2986.9261 | 3069.7346 |
| 3130.4513 | 3149.6648 | 3866.7260 |

E = -418.938458575 a.u.

**(3) •EtOH/$HPO_4^{2-}$**

| | | | |
|---|---|---|---|
| H | 4.227889 | -0.009155 | -0.718274 |
| H | 3.975136 | -0.119410 | 1.022576 |
| C | 3.612964 | -0.486438 | 0.058296 |
| H | 3.792089 | -1.560919 | 0.010226 |
| C | 2.165859 | -0.183007 | -0.115828 |
| O | 1.800831 | 1.104061 | 0.031805 |
| H | 1.568722 | -0.773805 | -0.810679 |
| O | -1.278272 | -1.188985 | -1.070341 |
| O | -0.602894 | 1.201078 | -0.517027 |
| H | 0.773925 | 1.180726 | -0.213023 |
| P | -1.403591 | -0.050051 | -0.078689 |
| H | 0.287262 | -0.731982 | 1.122959 |
| O | -0.644425 | -0.548506 | 1.316895 |
| O | -2.805753 | 0.280101 | 0.377634 |

| | | |
|---|---|---|
| 59.3882 | 71.3191 | 91.5605 |
| 124.9742 | 153.0368 | 216.8145 |
| 246.6276 | 345.8615 | 369.5551 |
| 442.4747 | 464.1065 | 501.8782 |
| 513.1373 | 553.3224 | 648.3546 |
| 743.4552 | 938.2538 | 943.8073 |
| 1023.3270 | 1054.6621 | 1102.7288 |
| 1116.6625 | 1165.9267 | 1193.2832 |
| 1261.7166 | 1381.4102 | 1427.0363 |
| 1459.9316 | 1484.6610 | 1614.3569 |
| 2096.0768 | 2986.2609 | 3068.1013 |
| 3105.8151 | 3133.6840 | 3750.4871 |

E = -797.644940773 a.u.

**(4) •EtOH/$HCO_3^-$ + 1 × $H_2O$**

| | | | |
|---|---|---|---|
| H | 2.853913 | -1.267071 | -1.269713 |
| H | 0.662799 | 0.611928 | -0.576481 |
| C | 2.268820 | -1.351761 | -0.343877 |
| O | 1.510788 | 0.975060 | -0.192743 |
| H | 2.738833 | -2.110074 | 0.282176 |
| C | 2.203965 | -0.048349 | 0.378183 |

| | | | |
|---|---|---|---|
| H | 1.271657 | -1.702626 | -0.622882 |
| H | 3.054151 | 0.290325 | 0.957826 |
| O | -0.802237 | -0.991654 | 1.118244 |
| H | 0.049379 | -0.530322 | 1.147646 |
| C | -1.445455 | -0.703321 | -0.066193 |
| O | -2.529025 | -1.254536 | -0.230544 |
| O | -0.853202 | 0.097676 | -0.851633 |
| H | -1.050172 | 1.920641 | -0.234798 |
| O | -0.809793 | 2.768906 | 0.172223 |
| H | 0.123205 | 2.644167 | 0.383170 |

| | | |
|---|---|---|
| 23.5075 | 45.2340 | 53.4258 |
| 84.6833 | 109.1358 | 133.2258 |
| 135.4737 | 175.2974 | 206.9362 |
| 224.0512 | 283.3340 | 335.6747 |
| 446.6703 | 540.8139 | 561.4429 |
| 614.9451 | 635.6779 | 685.5137 |
| 843.9482 | 887.0211 | 929.1738 |
| 1000.1713 | 1033.6328 | 1112.9878 |
| 1233.3426 | 1261.7278 | 1340.5171 |
| 1375.7354 | 1412.6137 | 1459.4567 |
| 1483.2083 | 1536.3733 | 1671.1999 |
| 1725.9072 | 3001.5331 | 3061.6617 |
| 3083.2386 | 3139.7198 | 3193.4709 |
| 3726.7759 | 3771.9511 | 3874.5286 |

E = -495.377452128 a.u.

**(5) •EtOH/$HCO_3^-$ + 2 × $H_2O$**

| | | | |
|---|---|---|---|
| H | 2.597610 | -1.074753 | -2.140893 |
| H | 0.779220 | 0.716536 | -0.584473 |
| C | 2.348449 | -1.224143 | -1.081831 |
| O | 1.697761 | 1.073905 | -0.526509 |
| H | 2.986973 | -2.018249 | -0.695091 |
| C | 2.544556 | 0.029154 | -0.298719 |
| H | 1.309761 | -1.562019 | -1.037258 |
| H | 3.544226 | 0.352749 | -0.036476 |
| O | 0.155423 | -1.183059 | 1.477837 |
| H | 0.917236 | -0.642216 | 1.216927 |
| C | -0.925979 | -0.861121 | 0.698678 |
| O | -1.946677 | -1.509821 | 0.887130 |
| O | -0.754577 | 0.085935 | -0.137931 |
| H | -0.565882 | 1.754222 | 0.856803 |
| O | -0.142696 | 2.523440 | 1.270131 |
| H | 0.766270 | 2.457163 | 0.953596 |
| H | -2.636033 | 1.074972 | -2.427332 |
| O | -2.925192 | 0.386870 | -1.821702 |
| H | -2.173865 | 0.260093 | -1.206226 |

| | | |
|---|---|---|
| 19.3697 | 25.9637 | 38.2339 |
| 53.6502 | 61.8188 | 87.7226 |
| 90.9552 | 114.6234 | 120.8794 |
| 141.9886 | 161.8108 | 186.3300 |
| 212.4415 | 219.7083 | 287.3210 |

| | | |
|---|---|---|
| 322.5066 | 401.4831 | 442.5088 |
| 535.2562 | 579.6366 | 620.8034 |
| 641.6353 | 682.5756 | 689.6085 |
| 795.2880 | 844.3925 | 927.8614 |
| 1014.9247 | 1034.7992 | 1108.0134 |
| 1225.9023 | 1260.4510 | 1345.2508 |
| 1373.1449 | 1409.1091 | 1460.1286 |
| 1483.1157 | 1505.8564 | 1648.5201 |
| 1667.6371 | 1733.5516 | 3005.4510 |
| 3085.3854 | 3139.8597 | 3193.3475 |
| 3342.8828 | 3521.8307 | 3737.9275 |
| 3752.5127 | 3873.2750 | 3920.2384 |

E = -571.817849941 a.u.

**(6) •EtOH/$HPO_4^{2-}$ + 2 × $H_2O$**

| | | | |
|---|---|---|---|
| H | 3.752726 | -1.224700 | -1.022039 |
| H | 4.327305 | 0.283947 | -0.312860 |
| C | 3.609483 | -0.530127 | -0.181965 |
| H | 3.857075 | -1.063620 | 0.735987 |
| C | 2.217374 | -0.009007 | -0.127765 |
| O | 1.842053 | 0.774488 | -1.165916 |
| H | 1.427972 | -0.610455 | 0.319510 |
| O | -1.051252 | -1.187780 | -1.007340 |
| O | -0.601782 | 1.302889 | -0.703755 |
| H | 0.844477 | 0.956809 | -1.070082 |
| P | -1.500379 | 0.096958 | -0.327546 |
| H | -0.619158 | 0.560083 | 1.630543 |
| O | -1.180570 | -0.149934 | 1.283478 |
| O | -2.971794 | 0.399712 | -0.439039 |
| H | 0.152983 | 2.027306 | 0.669319 |
| O | 0.596731 | 2.146243 | 1.543306 |
| H | 1.432797 | 1.672781 | 1.427896 |
| H | -0.370210 | -2.264258 | 0.089313 |
| O | -0.019780 | -2.824929 | 0.829486 |
| H | -0.170257 | -2.242953 | 1.582231 |

| | | |
|---|---|---|
| 16.8516 | 52.5331 | 58.7566 |
| 81.2894 | 89.0806 | 109.7017 |
| 121.0869 | 129.3479 | 155.3582 |
| 183.4043 | 208.5827 | 214.6010 |
| 239.9056 | 296.7559 | 332.1479 |
| 370.0027 | 393.8141 | 420.7531 |
| 436.7269 | 452.0025 | 506.4852 |
| 529.1137 | 543.3312 | 553.7467 |
| 674.3012 | 750.5138 | 830.4614 |
| 837.9311 | 939.7129 | 945.3138 |
| 1027.4548 | 1045.2523 | 1097.0645 |
| 1113.9786 | 1152.4184 | 1217.0514 |
| 1251.9235 | 1381.5027 | 1419.9545 |
| 1459.9236 | 1484.4131 | 1557.2849 |
| 1676.2910 | 1700.1274 | 2700.6593 |
| 2989.3411 | 3073.7856 | 3130.1608 |
| 3145.0887 | 3230.2942 | 3347.3088 |

3742.1427 3801.2679 3892.3284

E = -950.537377055 a.u.

**(7) •EtOH/$HPO_4^{2-}$ + 2 × $H_2O$ (for TS with 3 × $H_2O$)**

| | | | |
|---|---|---|---|
| H | -4.344380 | 1.317776 | -0.039801 |
| H | -3.330045 | 2.759064 | 0.005215 |
| C | -3.443489 | 1.779805 | -0.467020 |
| H | -3.617831 | 1.928259 | -1.532596 |
| C | -2.234793 | 0.943514 | -0.243626 |
| O | -1.847848 | 0.788698 | 1.041683 |
| H | -2.011598 | 0.114051 | -0.914507 |
| O | 0.723170 | -1.280923 | -1.539068 |
| O | 0.032513 | -0.875126 | 0.872926 |
| H | -1.057966 | 0.133854 | 1.049183 |
| P | 1.059989 | -0.578383 | -0.248662 |
| H | 0.003279 | 1.281947 | -0.725989 |
| O | 0.919961 | 1.054431 | -0.508411 |
| O | 2.493797 | -0.717182 | 0.230248 |
| H | 3.239835 | 0.779676 | 0.446406 |
| O | 3.583996 | 1.705395 | 0.528298 |
| H | 2.834807 | 2.214433 | 0.201518 |
| H | -2.793613 | -1.824819 | 0.516188 |
| O | -2.091861 | -2.477351 | 0.431060 |
| H | -1.262446 | -1.951937 | 0.534288 |

| | | |
|---|---|---|
| 26.3100 | 44.4041 | 52.9271 |
| 63.6617 | 88.7640 | 98.5675 |
| 109.1845 | 129.2299 | 152.2478 |
| 157.3315 | 190.8362 | 212.6852 |
| 214.0541 | 237.6308 | 274.9271 |
| 345.0766 | 387.6400 | 427.4523 |
| 437.3627 | 447.9928 | 458.7245 |
| 506.3314 | 523.2608 | 546.8808 |
| 636.3498 | 756.1444 | 786.8055 |
| 787.8332 | 941.6081 | 950.8386 |
| 1023.1183 | 1051.4460 | 1104.6197 |
| 1110.5344 | 1137.9235 | 1169.8591 |
| 1252.5157 | 1381.8912 | 1421.7140 |
| 1458.8715 | 1484.5010 | 1560.3672 |
| 1675.2798 | 1693.6123 | 2579.0969 |
| 2995.2176 | 3076.4342 | 3117.4394 |
| 3140.1145 | 3254.8471 | 3342.1330 |
| 3749.9278 | 3896.7473 | 3905.5635 |

E = -950.535226842 a.u.

**(8) $BrAc^-$**

| | | | |
|---|---|---|---|
| O | 1.478945 | 1.330754 | 0.000001 |
| H | 0.436873 | -1.471283 | 0.886034 |
| C | 1.638875 | 0.100667 | 0.000000 |
| C | 0.420058 | -0.844458 | 0.000003 |
| Br | -1.335588 | 0.032027 | -0.000001 |

| | | | |
|---|---|---|---|
| O | 2.710833 | -0.545210 | -0.000002 |
| H | 0.436873 | -1.471289 | -0.886024 |

| | | |
|---|---|---|
| 56.4952 | 196.4473 | 366.0822 |
| 565.9325 | 660.9911 | 690.1656 |
| 918.5137 | 924.3608 | 1167.9788 |
| 1236.0269 | 1406.1678 | 1432.8868 |
| 1663.4347 | 3137.0427 | 3204.5066 |

E = -2802.18521788 a.u.

**(9) $BrAc^-$ + 1 × $H_2O$**

| | | | |
|---|---|---|---|
| O | -1.121895 | -0.905330 | 0.000002 |
| H | 0.475072 | 1.620905 | 0.885920 |
| C | -1.013974 | 0.328676 | 0.000001 |
| C | 0.367286 | 1.002931 | 0.000000 |
| Br | 1.897162 | -0.216879 | 0.000000 |
| O | -1.937789 | 1.183858 | 0.000000 |
| H | 0.475071 | 1.620905 | -0.885920 |
| H | -3.368812 | -1.301536 | -0.000002 |
| O | -4.024954 | -0.593664 | -0.000001 |
| H | -3.424784 | 0.181940 | -0.000002 |

| | | |
|---|---|---|
| 23.9663 | 47.9524 | 52.7174 |
| 176.0199 | 188.3056 | 304.3710 |
| 313.9879 | 386.7984 | 567.9933 |
| 667.8875 | 700.7636 | 727.9418 |
| 924.6265 | 931.1647 | 1175.1676 |
| 1239.7152 | 1410.1018 | 1436.1119 |
| 1651.2718 | 1686.2081 | 3139.3603 |
| 3205.6591 | 3502.2153 | 3864.1766 |

E = -2878.62825376 a.u.

**(10) TS PCET (•EtOH + $BrAc^-$)**

| | | | |
|---|---|---|---|
| H | 2.476340 | -2.388424 | -0.241427 |
| H | 1.950985 | 0.918617 | -1.107899 |
| C | 2.903078 | -1.708127 | 0.497692 |
| O | 2.628244 | 0.122015 | -1.027513 |
| H | 3.994260 | -1.800066 | 0.443635 |
| C | 2.497635 | -0.311699 | 0.210166 |
| H | 2.587740 | -2.005876 | 1.496502 |
| H | 2.512767 | 0.428174 | 1.009162 |
| O | -0.080368 | 1.841343 | 1.250526 |
| H | 0.112905 | -0.797895 | 1.182781 |
| C | 0.275371 | 1.225525 | 0.242024 |
| C | 0.132892 | -0.281254 | 0.234812 |
| Br | -2.159172 | -0.476973 | -0.129861 |
| O | 0.791433 | 1.741035 | -0.809423 |
| H | 0.367690 | -0.842278 | -0.654480 |

```
-371.0901                71.9754                93.7186
  97.5269               130.1356               142.3990
 164.9963               218.8661               280.9736
 358.8308               439.3821               471.5472
 663.9625               761.2495               808.7038
 912.9579               931.7898               951.8574
 997.4183              1003.9582              1040.2688
1065.9991              1125.0221              1214.4024
1339.0028              1390.0373              1430.3734
1446.5880              1460.1179              1488.2109
1507.0556              1682.2492              2320.8090
3032.8973              3105.5795              3129.0415
3160.0490              3201.0098              3322.4208

E = -2956.54687507 a.u.
```

**(11) TS PCET (•EtOH/$HCO_3^-$ + $BrAc^-$)**

```
H        2.442845    1.504313    2.509182
H        2.364706    1.038671   -0.346384
C        1.537273    1.062966    2.075036
O        1.821577    1.925675   -0.186458
H        0.765533    1.043814    2.844072
C        1.085684    1.869428    0.901832
H        1.776050    0.036232    1.789123
H        0.484193    2.756879    1.075088
O        1.447302   -1.536729   -0.392095
H        0.947444   -0.806614   -0.884199
C        2.767230   -1.278840   -0.255262
O        3.477686   -2.193743    0.172324
O        3.173694   -0.109469   -0.567661
O       -1.325179    1.940211   -1.413605
H       -1.391170    1.274159    1.110603
Br      -2.796270   -0.763778    0.300398
C       -0.957795    0.540585    0.448866
C       -0.749265    0.920741   -1.000257
H       -0.330056   -0.223641    0.878867
O       -0.006189    0.151445   -1.676454

-396.7541                34.1643                61.1475
 78.1837                 92.0476               103.9329
 131.9025               141.6012               144.7893
 154.8349               167.4152               200.6393
 211.8465               230.3427               299.7782
 338.3516               465.1817               492.8396
 647.4233               675.7523               700.1683
 748.3604               790.1819               852.3958
 924.8850               939.9922               955.5202
1026.9375              1035.4851              1051.3817
1063.9886              1097.2613              1118.2450
1153.2645              1275.6842              1311.9037
1370.4838              1383.3072              1394.6497
1435.7433              1462.9129              1471.1695
1491.2591              1580.0006              1640.9821
1656.4216              2192.6081              2833.0706
```

| | | |
|---|---|---|
| 3022.4755 | 3100.2486 | 3146.2885 |
| 3167.9580 | 3201.4280 | 3318.9336 |

E = -3221.12828918 a.u.

**(12) TS PCET ($\bullet$EtOH/$HPO_4^{2-}$ + $BrAc^-$)**

| | | | |
|---|---|---|---|
| O | 2.092395 | 1.768853 | 1.277305 |
| H | 1.736953 | 0.956387 | -1.129096 |
| C | 1.273773 | 0.868641 | 1.013147 |
| C | 1.276816 | 0.305033 | -0.398125 |
| Br | 2.588463 | -1.306461 | -0.356624 |
| O | 0.466721 | 0.335605 | 1.828285 |
| H | 0.352956 | -0.159651 | -0.723182 |
| H | -0.308328 | 4.426790 | -1.273385 |
| H | 0.762785 | 3.764401 | -0.031927 |
| C | 0.243509 | 3.524412 | -0.966537 |
| H | 0.999020 | 3.321407 | -1.729040 |
| C | -0.662053 | 2.349301 | -0.778382 |
| O | -1.608277 | 2.417923 | 0.124110 |
| H | -0.788692 | 1.642532 | -1.602438 |
| O | -1.591753 | -0.924604 | -1.384684 |
| O | -2.973915 | 0.388853 | 0.301176 |
| H | -2.334040 | 1.250288 | 0.189527 |
| P | -2.372897 | -1.026386 | -0.098145 |
| H | -0.655857 | -0.702312 | 1.291954 |
| O | -1.355230 | -1.395787 | 1.106659 |
| O | -3.474920 | -2.048625 | -0.035226 |

| | | |
|---|---|---|
| -314.4043 | 31.1969 | 43.7805 |
| 60.4873 | 71.5599 | 82.3308 |
| 103.4254 | 107.9572 | 126.0172 |
| 145.1341 | 161.2969 | 166.4610 |
| 178.3970 | 182.6370 | 240.6494 |
| 266.1793 | 364.1338 | 381.6708 |
| 470.2615 | 482.8540 | 504.7049 |
| 506.1399 | 523.7612 | 587.7429 |
| 665.9221 | 790.8030 | 837.0175 |
| 908.3982 | 920.1662 | 930.8435 |
| 946.1130 | 957.8872 | 1005.1883 |
| 1063.4268 | 1096.5474 | 1114.4666 |
| 1163.8163 | 1178.4357 | 1186.3284 |
| 1242.2694 | 1292.4627 | 1369.2629 |
| 1380.1250 | 1421.2507 | 1452.4914 |
| 1464.7451 | 1486.2601 | 1492.9312 |
| 1626.9165 | 1847.8551 | 2958.3819 |
| 2992.0882 | 3040.1985 | 3069.0275 |
| 3107.9722 | 3143.9120 | 3252.0991 |

E = -3599.83659128 a.u.

**(13) TS PCET ($\bullet$EtOH/$HCO_3^-$ + $BrAc^-$) 1 × $H_2O$**

| | | | |
|---|---|---|---|
| H | -2.501472 | 2.557729 | -1.785067 |
| H | -2.420569 | 1.047080 | 0.646217 |
| C | -1.586761 | 1.990403 | -1.573987 |
| O | -1.840440 | 1.897241 | 0.847607 |
| H | -0.827950 | 2.284634 | -2.298256 |
| C | -1.119334 | 2.273590 | -0.184759 |
| H | -1.815993 | 0.931601 | -1.712617 |
| H | -0.514115 | 3.155863 | -0.000843 |
| O | -1.558541 | -1.326647 | -0.317774 |
| H | -1.058476 | -0.813515 | 0.380171 |
| C | -2.893334 | -1.056449 | -0.304883 |
| O | -3.612840 | -1.780333 | -0.993315 |
| O | -3.274654 | -0.073768 | 0.408762 |
| O | 1.285847 | 1.498472 | 1.951003 |
| H | 1.357656 | 1.860524 | -0.638273 |
| Br | 2.828820 | -0.290341 | -0.658041 |
| C | 0.948431 | 0.918200 | -0.309480 |
| C | 0.747136 | 0.702834 | 1.170574 |
| H | 0.338815 | 0.358886 | -1.002016 |
| O | 0.034846 | -0.299967 | 1.494030 |
| H | -0.315955 | -3.024311 | 0.371569 |
| O | 0.423629 | -3.047280 | 0.990587 |
| H | 0.509767 | -2.109787 | 1.238554 |

| | | |
|---|---|---|
| -390.3492 | 25.4598 | 50.6900 |
| 63.5492 | 69.9072 | 83.0447 |
| 95.2302 | 108.6889 | 132.6648 |
| 137.7561 | 143.7229 | 151.3464 |
| 162.8862 | 180.8073 | 197.3079 |
| 225.3331 | 236.5625 | 291.8737 |
| 295.3472 | 345.7891 | 350.7266 |
| 456.9345 | 493.3174 | 571.4500 |
| 646.9436 | 672.7547 | 699.2679 |
| 758.1978 | 790.5584 | 847.7216 |
| 926.1540 | 937.6802 | 957.9024 |
| 1010.2835 | 1031.2763 | 1040.0168 |
| 1053.7678 | 1068.9707 | 1115.9709 |
| 1159.4743 | 1274.8955 | 1316.7203 |
| 1350.5898 | 1376.7162 | 1394.5197 |
| 1435.7571 | 1459.2089 | 1472.2433 |
| 1491.5743 | 1573.1271 | 1639.5577 |
| 1674.0204 | 1690.4206 | 2240.5503 |
| 3023.7884 | 3071.9999 | 3101.2690 |
| 3147.8068 | 3172.2500 | 3200.3186 |
| 3317.6477 | 3681.1176 | 3870.4574 |

E = -3297.56966255 a.u.

**(14) TS PCET ($\bullet$EtOH/$HCO_3^-$ + $BrAc^-$) 2 × $H_2O$**

| | | | |
|---|---|---|---|
| H | -1.954430 | 3.109359 | -1.667283 |
| H | -2.230204 | 1.145894 | 0.395692 |
| C | -1.104402 | 2.440779 | -1.486092 |

| | | | |
|---|---|---|---|
| O | -1.646573 | 1.884554 | 0.821621 |
| H | -0.250957 | 2.811594 | -2.052168 |
| C | -0.790447 | 2.408274 | -0.028223 |
| H | -1.375016 | 1.451376 | -1.861119 |
| H | -0.177934 | 3.194168 | 0.401199 |
| O | -1.382324 | -1.065574 | -0.989694 |
| H | -0.941332 | -0.748163 | -0.155394 |
| C | -2.696190 | -0.709919 | -1.039358 |
| O | -3.363480 | -1.169540 | -1.961110 |
| O | -3.108874 | 0.078870 | -0.122058 |
| O | 1.238594 | 1.074053 | 2.172238 |
| H | 1.694080 | 1.944716 | -0.255210 |
| Br | 3.065377 | -0.262696 | -0.549277 |
| C | 1.194699 | 0.991535 | -0.184367 |
| C | 0.801148 | 0.488297 | 1.178755 |
| H | 0.671273 | 0.618615 | -1.050656 |
| O | 0.029926 | -0.530839 | 1.187285 |
| H | -0.362213 | -2.991248 | -0.436746 |
| O | 0.273935 | -3.186032 | 0.261635 |
| H | 0.392583 | -2.317843 | 0.683479 |
| H | -2.861969 | -0.689022 | 1.668219 |
| O | -2.397894 | -0.989756 | 2.464537 |
| H | -1.467381 | -0.814752 | 2.234761 |

| | | |
|---|---|---|
| -366.5907 | 24.6783 | 35.9948 |
| 43.0228 | 55.1369 | 65.5706 |
| 76.8303 | 89.4601 | 101.5501 |
| 116.9927 | 125.8715 | 135.1410 |
| 143.4507 | 151.5557 | 173.0599 |
| 183.2828 | 189.5916 | 199.9611 |
| 230.1767 | 239.7877 | 273.6547 |
| 275.7738 | 327.4089 | 350.3715 |
| 400.9822 | 466.2412 | 483.1695 |
| 498.7507 | 546.6362 | 637.5502 |
| 644.6492 | 675.8357 | 694.1926 |
| 762.6940 | 788.8718 | 850.6513 |
| 927.4143 | 942.0486 | 960.4687 |
| 986.7058 | 1030.9148 | 1036.9156 |
| 1043.5599 | 1055.1965 | 1089.9619 |
| 1124.7114 | 1273.8728 | 1318.0263 |
| 1345.2912 | 1372.8168 | 1395.0739 |
| 1437.2567 | 1459.7649 | 1471.0226 |
| 1492.8850 | 1561.6771 | 1645.7735 |
| 1668.4567 | 1686.6632 | 1718.2649 |
| 2464.3410 | 3028.4078 | 3104.6008 |
| 3152.5783 | 3158.2835 | 3180.9514 |
| 3202.4321 | 3321.4050 | 3653.8099 |
| 3705.5697 | 3764.2553 | 3874.2575 |

E = -3374.01544372 a.u.

**(15) TS PCET (•EtOH/$HCO_3^-$ + $BrAc^-$) 3 × $H_2O$**

| | | | |
|---|---|---|---|
| H | 1.872647 | -2.952999 | -1.500371 |
| H | 1.895906 | -0.950276 | 0.535081 |

| | | | |
|---|---|---|---|
| C | 0.969461 | -2.344771 | -1.372187 |
| O | 1.363346 | -1.718673 | 0.947257 |
| H | 0.172614 | -2.783947 | -1.970614 |
| C | 0.586147 | -2.316033 | 0.068590 |
| H | 1.186637 | -1.343899 | -1.751057 |
| H | 0.021287 | -3.142639 | 0.485964 |
| O | 0.948953 | 1.198555 | -0.956059 |
| H | 0.497613 | 0.867533 | -0.126020 |
| C | 2.276927 | 0.935124 | -0.959698 |
| O | 2.950625 | 1.394293 | -1.873752 |
| O | 2.716373 | 0.206660 | 0.004548 |
| O | -1.588343 | -1.059884 | 2.173714 |
| H | -1.905121 | -2.044002 | -0.236301 |
| Br | -3.427317 | 0.053030 | -0.628750 |
| C | -1.466880 | -1.060432 | -0.181206 |
| C | -1.160337 | -0.481688 | 1.173033 |
| H | -0.958503 | -0.668983 | -1.048205 |
| O | -0.462164 | 0.590433 | 1.167569 |
| H | -0.244573 | 3.063602 | -0.481661 |
| O | -0.920996 | 3.206630 | 0.190558 |
| H | -0.976216 | 2.337631 | 0.622899 |
| H | 2.368755 | 0.967075 | 1.798590 |
| O | 1.848580 | 1.225794 | 2.573746 |
| H | 0.945026 | 0.989515 | 2.295823 |
| H | 5.550637 | -1.039806 | 0.382725 |
| O | 5.375820 | -0.463047 | -0.366102 |
| H | 4.439940 | -0.194112 | -0.263638 |

| | | |
|---|---|---|
| -349.8203 | 18.5689 | 27.5273 |
| 38.6150 | 48.2272 | 52.3273 |
| 60.1893 | 62.3503 | 80.1784 |
| 92.2990 | 96.5351 | 103.7341 |
| 113.9989 | 125.2339 | 136.0106 |
| 138.9736 | 150.8415 | 170.6743 |
| 183.1709 | 185.8617 | 198.8597 |
| 206.6557 | 230.7117 | 240.5814 |
| 263.1875 | 273.4973 | 325.0055 |
| 354.8914 | 387.5568 | 401.4770 |
| 466.0623 | 469.7084 | 495.5308 |
| 551.3015 | 625.5635 | 651.9728 |
| 671.3393 | 678.8003 | 696.7003 |
| 777.0109 | 790.5288 | 849.3502 |
| 928.9950 | 943.5496 | 964.5366 |
| 1003.6502 | 1035.4283 | 1043.2489 |
| 1046.7212 | 1049.8307 | 1078.3915 |
| 1123.8741 | 1273.6132 | 1321.4059 |
| 1347.4311 | 1379.2025 | 1396.0218 |
| 1435.6599 | 1460.0202 | 1472.0427 |
| 1492.7798 | 1553.5346 | 1646.1338 |
| 1648.0374 | 1671.7896 | 1690.0078 |
| 1724.6856 | 2649.0963 | 3031.3816 |
| 3045.0271 | 3107.0912 | 3155.0097 |
| 3184.8861 | 3203.6928 | 3323.8866 |
| 3531.7522 | 3649.7113 | 3712.3192 |
| 3784.9952 | 3879.7291 | 3920.6107 |

E = -3450.45599668 a.u.

**(16) TS PCET (•EtOH/$HPO_4^{2-}$ + $BrAc^-$) 1 × $H_2O$**

| | | | |
|---|---|---|---|
| O | 1.846540 | 1.964101 | 1.150319 |
| H | 1.938160 | 0.884840 | -1.199465 |
| C | 1.177467 | 0.951973 | 0.879265 |
| C | 1.385267 | 0.306467 | -0.474483 |
| Br | 2.896075 | -1.226126 | -0.075266 |
| O | 0.347986 | 0.377214 | 1.645694 |
| H | 0.596620 | -0.331719 | -0.852826 |
| H | -0.138394 | 3.993217 | -2.020697 |
| H | 0.998162 | 3.514206 | -0.749939 |
| C | 0.459871 | 3.158054 | -1.633265 |
| H | 1.185782 | 2.879526 | -2.397453 |
| C | -0.406727 | 2.004601 | -1.274434 |
| O | -1.323399 | 2.212807 | -0.349625 |
| H | -0.586490 | 1.187288 | -1.967524 |
| O | -1.429704 | -1.050284 | -1.733946 |
| O | -2.762006 | 0.261039 | -0.017244 |
| H | -1.938475 | 1.333170 | -0.226962 |
| P | -2.243647 | -1.147516 | -0.459056 |
| H | -0.631032 | -0.871368 | 1.017778 |
| O | -1.234119 | -1.606319 | 0.745188 |
| O | -3.351516 | -2.175005 | -0.456770 |
| H | -2.556744 | 0.647856 | 1.739683 |
| O | -2.220070 | 0.948256 | 2.608805 |
| H | -1.260474 | 0.909114 | 2.455679 |

| | | |
|---|---|---|
| -450.2250 | 37.2253 | 56.5296 |
| 72.8072 | 81.2737 | 87.0493 |
| 99.5759 | 110.4288 | 116.0896 |
| 127.1411 | 132.2094 | 144.6110 |
| 159.7251 | 177.5529 | 181.2553 |
| 195.0747 | 228.1316 | 265.2620 |
| 320.0838 | 374.5939 | 399.5577 |
| 452.1139 | 465.2340 | 474.5439 |
| 512.2884 | 523.4511 | 546.6898 |
| 571.8013 | 662.4254 | 720.9385 |
| 732.6892 | 789.9228 | 809.5431 |
| 866.1131 | 895.6812 | 938.9319 |
| 949.8081 | 960.6408 | 1022.1275 |
| 1040.6146 | 1068.4034 | 1113.8188 |
| 1124.1354 | 1148.0624 | 1217.8791 |
| 1251.2792 | 1286.4889 | 1372.8939 |
| 1382.5326 | 1440.8939 | 1465.8051 |
| 1471.3252 | 1486.1579 | 1623.3844 |
| 1635.2559 | 1703.2033 | 1826.2254 |
| 3004.6227 | 3074.9702 | 3132.2163 |
| 3155.5018 | 3165.4495 | 3272.3696 |
| 3287.2429 | 3541.7729 | 3703.8954 |

E = -3676.28533652 a.u.

**(17) TS PCET (•EtOH/$HPO_4^{2-}$ + $BrAc^-$) 2 × $H_2O$**

| | | | |
|---|---|---|---|
| O | 1.637561 | 2.272854 | 1.160575 |
| H | 1.819714 | 1.227877 | -1.200568 |
| C | 1.049021 | 1.217992 | 0.874469 |
| C | 1.325856 | 0.595297 | -0.478151 |
| Br | 2.975679 | -0.767790 | -0.074790 |
| O | 0.251026 | 0.579811 | 1.625873 |
| H | 0.595443 | -0.107463 | -0.862287 |
| H | -0.454863 | 4.191624 | -1.992253 |
| H | 0.724533 | 3.771163 | -0.740336 |
| C | 0.196530 | 3.390237 | -1.619737 |
| H | 0.927434 | 3.161281 | -2.395476 |
| C | -0.594969 | 2.184688 | -1.260850 |
| O | -1.517919 | 2.336035 | -0.327471 |
| H | -0.727902 | 1.357027 | -1.951604 |
| O | -1.412594 | -0.916772 | -1.739021 |
| O | -2.844502 | 0.287018 | -0.019876 |
| H | -2.074824 | 1.432510 | -0.214096 |
| P | -2.234922 | -1.072534 | -0.477703 |
| H | -0.640056 | -0.684554 | 1.019148 |
| O | -1.190881 | -1.465445 | 0.738906 |
| O | -3.253466 | -2.185625 | -0.478451 |
| H | -2.664097 | 0.680199 | 1.744669 |
| O | -2.344513 | 0.999901 | 2.612759 |
| H | -1.385502 | 1.029305 | 2.456590 |
| H | 1.458015 | -2.840239 | -0.096576 |
| O | 0.670963 | -3.388347 | 0.011442 |
| H | -0.026867 | -2.742787 | 0.243722 |

| | | |
|---|---|---|
| -433.7167 | 35.9353 | 39.9747 |
| 66.4167 | 75.7865 | 80.4343 |
| 89.7578 | 99.0363 | 110.6944 |
| 114.2451 | 119.4359 | 126.3431 |
| 132.4816 | 140.5396 | 154.6077 |
| 168.1733 | 169.7186 | 185.7893 |
| 213.4768 | 225.9786 | 262.4868 |
| 276.1388 | 309.9729 | 381.9001 |
| 385.5480 | 430.0006 | 453.3215 |
| 466.3339 | 469.9514 | 515.1557 |
| 523.1381 | 535.9214 | 560.2816 |
| 663.5610 | 674.0220 | 707.3626 |
| 741.1270 | 785.8631 | 792.3187 |
| 917.3483 | 926.3272 | 941.2477 |
| 954.9808 | 962.8853 | 1020.9610 |
| 1050.3947 | 1069.6878 | 1113.3549 |
| 1121.8428 | 1159.8338 | 1190.2963 |
| 1259.6699 | 1293.6987 | 1373.9673 |
| 1381.9779 | 1441.0279 | 1464.6294 |
| 1469.8336 | 1484.1184 | 1622.3761 |
| 1636.0590 | 1663.9306 | 1705.8913 |
| 1970.2869 | 3006.2603 | 3074.0293 |
| 3126.5056 | 3134.0521 | 3153.3511 |
| 3162.5400 | 3280.3417 | 3545.8151 |
| 3556.4611 | 3711.7364 | 3844.8596 |

E = -3752.72916800 a.u.

**(18) TS PCET (•EtOH/$HPO_4^{2-}$ + $BrAc^-$) 3 × $H_2O$**

| | | | |
|---|---|---|---|
| O | -1.577957 | -2.404997 | 1.253734 |
| H | -1.681577 | -1.577679 | -1.199028 |
| C | -1.152628 | -1.284359 | 0.933658 |
| C | -1.366157 | -0.825911 | -0.491360 |
| Br | -3.298030 | 0.253044 | -0.360206 |
| O | -0.566513 | -0.459943 | 1.700322 |
| H | -0.753409 | -0.012824 | -0.862592 |
| H | 1.175130 | -4.073232 | -1.503122 |
| H | -0.223752 | -3.818196 | -0.447474 |
| C | 0.339863 | -3.396084 | -1.284456 |
| H | -0.304556 | -3.356717 | -2.162178 |
| C | 0.840150 | -2.043721 | -0.930989 |
| O | 1.633361 | -1.967994 | 0.125158 |
| H | 0.927466 | -1.247051 | -1.663999 |
| O | 1.116909 | 1.100516 | -1.565998 |
| O | 2.574425 | 0.330772 | 0.362344 |
| H | 1.981450 | -0.988060 | 0.235732 |
| P | 1.757397 | 1.515597 | -0.260409 |
| H | 0.117691 | 0.905012 | 1.105841 |
| O | 0.552122 | 1.761298 | 0.829652 |
| O | 2.544263 | 2.800409 | -0.274214 |
| H | 2.289607 | 0.010733 | 2.155611 |
| O | 1.922460 | -0.326926 | 2.994957 |
| H | 1.011937 | -0.541839 | 2.730106 |
| H | -2.193354 | 2.559720 | -0.384544 |
| O | -1.539765 | 3.255693 | -0.241440 |
| H | -0.767293 | 2.772148 | 0.112165 |
| H | 3.891094 | -1.790088 | -1.313230 |
| O | 4.326166 | -0.931886 | -1.300902 |
| H | 3.748535 | -0.387525 | -0.719971 |

| | | |
|---|---|---|
| -401.7258 | 32.6654 | 35.8443 |
| 41.5602 | 48.1410 | 74.1380 |
| 78.1094 | 90.4018 | 100.3261 |
| 109.7883 | 113.2084 | 115.5901 |
| 121.2155 | 133.4704 | 137.2763 |
| 144.6093 | 155.6882 | 156.3391 |
| 168.9316 | 178.6316 | 187.8759 |
| 193.3577 | 227.5273 | 241.6564 |
| 250.0264 | 277.3205 | 326.5079 |
| 377.5348 | 393.5420 | 418.7514 |
| 422.2909 | 461.2318 | 469.3944 |
| 474.5530 | 519.2162 | 526.6515 |
| 536.6379 | 558.3685 | 664.3707 |
| 667.9938 | 699.5871 | 728.0854 |
| 745.3358 | 788.6608 | 806.1152 |
| 907.6689 | 934.6534 | 946.1068 |
| 962.2563 | 973.0958 | 1027.2027 |
| 1057.5335 | 1066.5455 | 1110.4733 |
| 1122.0278 | 1166.1691 | 1185.2931 |
| 1266.4581 | 1310.5137 | 1374.0843 |

| | | |
|---|---|---|
| 1383.7692 | 1443.1196 | 1465.7677 |
| 1472.5018 | 1486.7419 | 1600.4692 |
| 1635.3525 | 1661.3610 | 1676.6713 |
| 1707.6546 | 2251.4553 | 3013.5663 |
| 3060.5405 | 3080.0868 | 3141.6512 |
| 3156.1760 | 3176.1329 | 3285.4778 |
| 3424.7464 | 3574.7588 | 3613.8105 |
| 3708.6272 | 3838.3813 | 3905.8556 |

E = -3829.17229381 a.u.

**(19) TS PCET no H bond (•EtOH/$HCO_3^-$ + $BrAc^-$)**

| | | | |
|---|---|---|---|
| O | 2.823384 | 1.291843 | -0.206259 |
| H | 0.800193 | 0.217092 | -1.429348 |
| C | 1.825149 | 0.902808 | 0.441401 |
| C | 0.749589 | 0.182405 | -0.351997 |
| Br | 1.514222 | -1.988398 | -0.226928 |
| O | 1.614783 | 1.040008 | 1.668266 |
| H | -0.195702 | -0.044985 | 0.118620 |
| H | -0.040230 | 4.357388 | -0.719819 |
| H | 0.938128 | 3.444274 | 0.442416 |
| C | 0.479253 | 3.406458 | -0.547784 |
| H | 1.262941 | 3.294137 | -1.293798 |
| C | -0.487490 | 2.283496 | -0.624801 |
| O | -1.404522 | 2.217581 | 0.321864 |
| H | -0.762101 | 1.872544 | -1.593649 |
| H | -2.087596 | 1.476167 | 0.071476 |
| O | -3.694639 | -1.661619 | -0.238560 |
| O | -2.200467 | -0.889874 | 1.201378 |
| C | -2.897892 | -0.642572 | 0.222029 |
| H | -4.174540 | -1.321993 | -1.003539 |
| O | -2.982354 | 0.440027 | -0.432057 |

| | | |
|---|---|---|
| -369.4349 | 23.4296 | 35.2765 |
| 48.9625 | 70.5597 | 81.9072 |
| 105.2375 | 108.5367 | 125.2070 |
| 139.6484 | 145.7446 | 162.5207 |
| 195.3289 | 208.6218 | 259.4864 |
| 334.6326 | 448.8125 | 477.9807 |
| 517.2950 | 610.5572 | 656.3776 |
| 678.3777 | 776.1108 | 796.3141 |
| 839.4595 | 929.7906 | 947.3609 |
| 956.7293 | 1004.7982 | 1016.1093 |
| 1038.5726 | 1080.4112 | 1122.3097 |
| 1206.1795 | 1238.1520 | 1266.7573 |
| 1356.8549 | 1365.8219 | 1387.5883 |
| 1429.3502 | 1451.8576 | 1457.9637 |
| 1482.7566 | 1580.4779 | 1632.9919 |
| 1706.4647 | 2395.7963 | 3020.6713 |
| 3101.0580 | 3140.8545 | 3165.8614 |
| 3187.3050 | 3311.6991 | 3863.1169 |

E = -3221.11857729 a.u.

**(20) TS PCET no H bond (•EtOH/$HPO_4^{2-}$ + $BrAc^-$)**

| | | | |
|---|---|---|---|
| O | 2.224571 | 0.757043 | -1.875473 |
| H | 0.264112 | -0.063617 | -0.385188 |
| C | 2.362820 | 0.668270 | -0.631943 |
| C | 1.205404 | 0.044870 | 0.136990 |
| Br | 1.742882 | -2.016495 | 0.328940 |
| O | 3.360626 | 1.014712 | 0.041432 |
| H | 1.127556 | 0.321693 | 1.178903 |
| H | 0.840547 | 4.487313 | 0.462669 |
| H | 1.679407 | 3.231353 | 1.376975 |
| C | 1.212589 | 3.452872 | 0.412285 |
| H | 1.983299 | 3.401786 | -0.357165 |
| C | 0.108979 | 2.488023 | 0.129632 |
| O | -0.819030 | 2.307602 | 1.037199 |
| H | -0.149751 | 2.291217 | -0.914552 |
| O | -1.848884 | -0.756553 | -1.346109 |
| O | -2.714220 | 1.188166 | 0.048026 |
| H | -1.817784 | 1.678183 | 0.522852 |
| P | -2.631610 | -0.376052 | -0.117086 |
| H | -4.410664 | -0.602158 | -1.335666 |
| O | -2.294368 | -1.053907 | 1.180164 |
| O | -4.206470 | -0.763550 | -0.408640 |

| | | |
|---|---|---|
| -573.0526 | 46.6630 | 60.7242 |
| 68.5249 | 76.3441 | 78.8557 |
| 87.7188 | 93.2952 | 116.2897 |
| 116.4300 | 147.2115 | 152.2950 |
| 156.8652 | 168.4766 | 183.7261 |
| 237.9476 | 287.0283 | 323.2914 |
| 380.3860 | 446.6621 | 460.2924 |
| 482.7919 | 517.4373 | 531.7386 |
| 637.0347 | 658.9405 | 769.7237 |
| 793.0099 | 887.9369 | 926.8707 |
| 944.3028 | 957.5734 | 983.7719 |
| 1013.4017 | 1044.8305 | 1068.9631 |
| 1117.2153 | 1124.6270 | 1167.2303 |
| 1205.5284 | 1306.0165 | 1372.9026 |
| 1388.9866 | 1414.7583 | 1432.9775 |
| 1450.8507 | 1462.2068 | 1470.5822 |
| 1531.0899 | 1621.5536 | 2973.3130 |
| 3061.8638 | 3066.8236 | 3133.3523 |
| 3169.4405 | 3277.0727 | 3885.8432 |

E = -3599.82499104 a.u.

**(21) •$CH_2CO_2H$**

| | | | |
|---|---|---|---|
| O | -0.853825 | -0.949662 | -0.000153 |
| H | 1.663260 | -1.312696 | 0.000229 |
| C | -0.015873 | 0.105232 | 0.000012 |
| C | 1.375196 | -0.273263 | 0.000137 |
| O | -0.418108 | 1.252281 | 0.000009 |

| | | | |
|---|---|---|---|
| H | 2.116709 | 0.509110 | -0.000635 |
| H | -1.760445 | -0.609177 | 0.000670 |

| | | |
|---|---|---|
| 338.3436 | 438.0225 | 528.1537 |
| 591.8826 | 640.1443 | 769.7149 |
| 944.8668 | 1003.2593 | 1211.5923 |
| 1378.6162 | 1474.9697 | 1729.4571 |
| 3203.9084 | 3327.9363 | 3814.8720 |

E = -228.413655202 a.u.

**(22) $\bullet CH_2CO_2^-$**

| | | | |
|---|---|---|---|
| O | 0.698137 | -1.123677 | 0.000002 |
| H | -1.899915 | -0.933323 | -0.000021 |
| C | 0.125816 | -0.000003 | -0.000011 |
| C | -1.354003 | -0.000075 | 0.000012 |
| O | 0.697988 | 1.123757 | 0.000002 |
| H | -1.899956 | 0.933149 | -0.000022 |

| | | |
|---|---|---|
| 215.3887 | 456.4259 | 570.9963 |
| 658.6404 | 772.8776 | 974.6505 |
| 995.0257 | 1367.4629 | 1468.5006 |
| 1577.2997 | 3166.8537 | 3280.6355 |

E = -227.947039772 a.u.

**(23) $\bullet CH_2CO_2^-/H_2CO_3$**

| | | | |
|---|---|---|---|
| O | -1.221336 | 1.107841 | -0.140752 |
| H | -3.812522 | 0.929030 | -0.119075 |
| C | -1.816962 | 0.000000 | -0.000001 |
| C | -3.276109 | -0.000004 | -0.000011 |
| O | -1.221330 | -1.107835 | 0.140759 |
| H | -3.812520 | -0.929040 | 0.119039 |
| O | 1.264924 | -1.119936 | -0.148665 |
| O | 3.164893 | 0.000006 | -0.000021 |
| C | 1.948404 | -0.000000 | -0.000001 |
| H | 0.238247 | -1.039062 | -0.025024 |
| O | 1.264918 | 1.119929 | 0.148690 |
| H | 0.238241 | 1.039057 | 0.025043 |

| | | |
|---|---|---|
| 31.5039 | 62.8485 | 118.1601 |
| 163.2821 | 189.7324 | 275.4269 |
| 281.5317 | 482.3686 | 605.3605 |
| 644.8658 | 654.1261 | 692.5981 |
| 771.7631 | 827.2382 | 1004.8744 |
| 1006.7381 | 1050.0498 | 1076.6085 |
| 1117.2000 | 1332.9957 | 1399.6188 |
| 1408.2160 | 1487.6970 | 1529.9979 |

1595.9772 1785.1313 2364.6107
2503.9774 3184.2863 3304.2955

E = -493.000331170 a.u.

**(24) $\bullet CH_2CO_2^-/H_2PO_4^-$**

O 1.730367 1.123486 -0.123992
H 4.291494 0.935409 0.242376
C 2.303769 -0.000021 -0.041683
C 3.756849 0.000086 0.166440
O 1.730485 -1.123585 -0.123945
H 4.291696 -0.935137 0.242172
H 0.129198 -1.213098 -0.386710
O -0.852872 -1.259976 -0.575282
O -3.020828 0.000098 -0.408251
P -1.610246 -0.000041 0.092214
O -1.365455 -0.000843 1.574924
O -0.853125 1.260756 -0.573922
H 0.129026 1.213575 -0.385846

38.6776 41.8260 99.4640
118.8797 149.9770 192.3800
252.5086 365.3973 371.3145
472.8667 494.7324 497.5520
508.7030 586.9579 665.8968
770.1825 838.8291 861.4995
864.8806 909.2283 997.6414
1004.3205 1083.8852 1205.2038
1306.8668 1373.0665 1402.7780
1477.1953 1561.4267 2988.0373
3051.8649 3175.9725 3293.5129

E = -871.715452531 a.u.

**(25) EtOH**

H -1.288567 -0.854827 -0.885930
H 1.983685 0.085327 -0.000751
C -1.220240 -0.221976 -0.000057
O 1.150631 -0.395866 0.000109
H -1.288602 -0.854951 0.885745
C 0.081116 0.547266 0.000045
H -2.066081 0.466245 -0.000007
H 0.144741 1.186722 -0.885298
H 0.144519 1.186674 0.885450

210.3177 269.2318 423.6622
820.1779 912.1185 1048.9847
1117.8955 1181.7489 1267.6676
1307.6402 1399.2185 1455.8293
1479.1623 1491.5774 1528.5129
3040.6437 3065.1999 3075.5711
3140.5134 3143.6191 3888.6957

E = -155.021823243 a.u.

**(26) TS1 (•$CH_2CO_2H$ + EtOH)**

| | | | |
|---|---|---|---|
| O | -0.974734 | -0.833026 | -1.050645 |
| H | -0.566035 | -1.495791 | 1.475603 |
| C | -1.336799 | -0.221189 | -0.061061 |
| C | -0.796046 | -0.456521 | 1.271699 |
| O | -2.212092 | 0.789067 | -0.227414 |
| H | -1.202980 | 0.109124 | 2.101624 |
| H | 1.389155 | 2.226582 | 0.354461 |
| C | 1.555739 | 1.382370 | -0.314906 |
| H | 0.725439 | 1.326388 | -1.022753 |
| H | 2.472859 | 1.561874 | -0.882285 |
| C | 1.677190 | 0.107054 | 0.472663 |
| H | 2.412342 | 0.119265 | 1.275038 |
| H | 0.517422 | -0.017978 | 1.081238 |
| O | 1.815982 | -1.052658 | -0.263986 |
| H | 1.065806 | -1.111927 | -0.877836 |
| H | -2.447755 | 1.185112 | 0.620899 |

| | | |
|---|---|---|
| -1407.3314 | 58.2953 | 92.8976 |
| 133.6146 | 149.0826 | 209.6555 |
| 258.3062 | 436.0372 | 446.9307 |
| 477.4757 | 490.8099 | 535.6527 |
| 622.2696 | 659.3353 | 714.0555 |
| 858.2458 | 920.2448 | 942.4157 |
| 1025.4883 | 1037.0640 | 1092.6941 |
| 1137.8070 | 1175.5052 | 1240.4226 |
| 1322.1648 | 1339.5284 | 1370.2117 |
| 1396.4156 | 1437.3066 | 1446.9948 |
| 1471.7945 | 1476.1444 | 1485.3601 |
| 1734.8559 | 3050.0756 | 3115.4198 |
| 3138.3388 | 3148.7008 | 3153.1943 |
| 3249.7659 | 3738.6348 | 3855.8264 |

E = -383.417359879 a.u.

**(27) TS2 (•$CH_2CO_2H$ + EtOH)**

| | | | |
|---|---|---|---|
| O | -1.072694 | -0.888792 | -0.923356 |
| H | -0.633573 | -1.412618 | 1.528180 |
| C | -1.453735 | -0.045217 | 0.071774 |
| C | -0.803417 | -0.359552 | 1.333549 |
| O | -2.194637 | 0.888885 | -0.149245 |
| H | -1.120601 | 0.244687 | 2.173226 |
| H | 1.343901 | 2.218374 | 0.227920 |
| C | 1.546259 | 1.347154 | -0.395393 |
| H | 0.730405 | 1.238331 | -1.114565 |
| H | 2.469529 | 1.522757 | -0.953667 |
| C | 1.677889 | 0.116014 | 0.457319 |
| H | 2.397914 | 0.183745 | 1.270352 |

```
H        0.516831    0.001625    1.056123
O        1.868803   -1.074621   -0.220068
H        1.197760   -1.146704   -0.913032
H       -1.515918   -0.604371   -1.736682

-1416.1100              65.7859              85.1627
 120.1858              139.7377             207.8856
 250.5974              417.2969             431.6434
 446.5264              520.4099             567.8791
 600.1018              665.9309             710.7270
 860.5693              919.3417             926.2680
1021.8063             1037.3106            1082.9970
1140.3275             1169.3272            1210.5273
1312.9425             1347.6735            1381.6659
1397.3588             1422.4458            1439.4348
1454.2715             1473.8928            1483.2256
1760.5282             3049.0659            3112.8394
3139.7126             3148.9152            3158.8697
3262.3386             3807.5302            3813.1233

E = -383.419978377 a.u.
```

**(28) TS3 ($\bullet CH_2CO_2H$ + EtOH)**

```
O       -1.022943   -0.693930   -1.067035
H       -0.641718   -1.343259    1.501436
C       -1.510426   -0.037646    0.006126
C       -0.836720   -0.297029    1.283192
O       -2.433702    0.731383   -0.146828
H       -1.204712    0.291288    2.114111
H        1.576701    2.235248    0.274070
C        1.697233    1.354157   -0.355456
H        0.891883    1.335060   -1.092542
H        2.647772    1.432044   -0.889087
C        1.669059    0.114569    0.484815
H        2.374106    0.083692    1.314640
H        0.488784    0.088977    1.046334
O        1.700454   -1.037937   -0.305263
H        1.980583   -1.792931    0.225096
H       -0.178757   -1.130552   -0.853108

-1509.1863              67.3568              92.3721
 144.3888              165.8981             206.6777
 256.2262              413.5921             427.6598
 448.8736              521.8005             615.6560
 645.8794              660.7213             699.4740
 865.4015              926.9476             932.5325
1040.8927             1047.6024            1069.8552
1151.8516             1163.9342            1263.3326
1281.1606             1356.6236            1372.3411
1394.9282             1433.7440            1450.3715
1469.9498             1471.3500            1491.9872
1776.6356             3055.5062            3117.4158
3128.8096             3140.3829            3154.0867
3244.0289             3677.3807            3864.7888
```

E = -383.418524723 a.u.

**(29) TS4 (•$CH_2CO_2H$ + EtOH)**

| | | | |
|---|---|---|---|
| O | -1.020134 | -0.730135 | -1.088419 |
| H | -0.541609 | -1.618268 | 1.374269 |
| C | -1.337000 | -0.211802 | -0.028576 |
| C | -0.770048 | -0.564987 | 1.261636 |
| O | -2.193496 | 0.823348 | 0.010716 |
| H | -1.168570 | -0.057458 | 2.130548 |
| H | 1.405190 | 2.180701 | 0.535641 |
| C | 1.559463 | 1.399538 | -0.208957 |
| H | 0.718826 | 1.409113 | -0.906713 |
| H | 2.468358 | 1.627854 | -0.772067 |
| C | 1.687392 | 0.058135 | 0.458368 |
| H | 2.440241 | -0.006635 | 1.241534 |
| H | 0.538300 | -0.116640 | 1.079716 |
| O | 1.802419 | -1.031133 | -0.383623 |
| H | 1.041746 | -1.029667 | -0.986799 |
| H | -2.451642 | 1.029050 | -0.900346 |

| | | |
|---|---|---|
| -1417.6438 | 64.9021 | 92.2099 |
| 134.4754 | 152.6416 | 210.0712 |
| 257.2357 | 432.7727 | 435.4342 |
| 480.5355 | 527.7965 | 565.3676 |
| 600.2193 | 665.6032 | 724.2973 |
| 860.0718 | 920.0915 | 944.8010 |
| 1021.9660 | 1035.0769 | 1092.7301 |
| 1138.1443 | 1170.9305 | 1221.3737 |
| 1323.5482 | 1369.7467 | 1377.1899 |
| 1396.7266 | 1437.3634 | 1448.0914 |
| 1465.6965 | 1475.0364 | 1485.5784 |
| 1717.2344 | 3049.9310 | 3114.6239 |
| 3138.5043 | 3148.6941 | 3162.2577 |
| 3263.3347 | 3741.4166 | 3807.6382 |

E = -383.420578843 a.u.

**(30) TS (•$CH_2CO_2^-$ + EtOH)**

| | | | |
|---|---|---|---|
| O | 0.947371 | -0.931115 | 0.859880 |
| H | 0.744906 | -1.034279 | -1.790706 |
| C | 1.427608 | -0.069494 | 0.051962 |
| C | 0.845278 | -0.055612 | -1.327944 |
| O | 2.307170 | 0.767779 | 0.344767 |
| H | 1.202796 | 0.727093 | -1.989261 |
| H | -1.748538 | 2.189306 | -0.093440 |
| C | -1.708051 | 1.257709 | 0.473481 |
| H | -0.819039 | 1.273595 | 1.108706 |
| H | -2.588341 | 1.207380 | 1.121400 |
| C | -1.662589 | 0.071986 | -0.456026 |
| H | -2.439449 | 0.064353 | -1.221170 |
| H | -0.512082 | 0.184932 | -1.085779 |

```
O       -1.579524   -1.164992    0.166042
H       -0.653870   -1.213288    0.535901

-1590.6039              64.7829              90.2048
 152.9827              186.1189             218.3839
 274.4286              434.7441             440.3568
 521.2979              621.6185             658.5546
 713.9328              836.3796             858.9590
 920.5532              953.4948            1024.4394
1033.9309             1107.4365            1132.2681
1171.1675             1339.2561            1369.0145
1385.9470             1399.3016            1441.8152
1464.1909             1471.3306            1492.1751
1511.8243             1604.7729            3039.1861
3076.2054             3105.4903            3118.7243
3123.1436             3134.0723            3215.3739

E = -382.956780582 a.u.
```

**(31) TS ($\bullet CH_2CO_2^-/H_2CO_3$ + EtOH)**

```
O       -0.287105    0.302773   -1.056211
H       -2.448034    1.775226   -1.203256
C       -0.602830    1.207692   -0.213397
C       -1.995497    1.685437   -0.221105
O        0.200853    1.641037    0.654604
H       -2.234310    2.469423    0.487528
H       -2.363157   -0.790557    2.339494
C       -2.081266   -1.268945    1.400730
H       -1.024724   -1.066234    1.208577
H       -2.204706   -2.350131    1.509722
C       -2.935010   -0.755343    0.272196
H       -4.009180   -0.819061    0.438754
H       -2.657007    0.533607    0.200599
O       -2.625139   -1.247885   -0.986082
H       -1.721207   -0.944778   -1.193315
O        2.295547    0.311511    1.015346
O        3.914272   -0.882797    0.097448
C        2.819736   -0.361767    0.007178
H        1.428339    0.832650    0.796828
O        2.109559   -0.447349   -1.103800
H        1.139286   -0.100924   -1.028988

-1519.3025              25.8502              29.4428
  70.8453               81.9350             115.2906
 138.6423              163.0902             184.7399
 193.6497              220.1094             256.5891
 294.9344              437.9511             473.3175
 525.9204              584.6220             646.5664
 650.8540              659.0433             695.7901
 724.5497              826.3000             865.1506
 921.8129              981.6237            1028.1431
1036.5218             1046.9609            1077.0646
1100.8629             1109.7646            1130.0204
1170.5889             1328.7180            1334.4632
```

| | | |
|---|---|---|
| 1377.4442 | 1389.2074 | 1401.7399 |
| 1411.0637 | 1448.0701 | 1457.3953 |
| 1472.1846 | 1477.2668 | 1487.7927 |
| 1526.0908 | 1590.5810 | 1789.1023 |
| 2417.6419 | 2553.3068 | 3045.7154 |
| 3110.0207 | 3129.8256 | 3141.9740 |
| 3145.6879 | 3244.0651 | 3635.6548 |

E = -648.008525540 a.u.

**(32) TS ($\bullet CH_2CO_2^-/H_2PO_4^-$ + EtOH)**

| | | | |
|---|---|---|---|
| O | 0.875247 | 0.693097 | 1.083847 |
| H | 3.222373 | 1.814700 | 0.746193 |
| C | 1.199752 | 1.380840 | 0.060555 |
| C | 2.649917 | 1.611089 | -0.153804 |
| O | 0.384131 | 1.815348 | -0.790230 |
| H | 2.916538 | 2.202153 | -1.022733 |
| H | 2.440626 | -1.352506 | -2.181287 |
| C | 2.180779 | -1.595356 | -1.149486 |
| H | 1.173670 | -1.223867 | -0.941530 |
| H | 2.165438 | -2.684787 | -1.045732 |
| C | 3.183183 | -0.994152 | -0.200250 |
| H | 4.221972 | -1.255161 | -0.400169 |
| H | 3.092861 | 0.309954 | -0.384887 |
| O | 2.903243 | -1.165214 | 1.148918 |
| H | 2.097669 | -0.635811 | 1.329503 |
| H | -1.195795 | 1.376640 | -0.759352 |
| O | -2.159337 | 1.117920 | -0.727394 |
| O | -3.791173 | -0.543126 | 0.213325 |
| P | -2.329681 | -0.325906 | -0.023380 |
| O | -1.555197 | -1.353687 | -0.797725 |
| O | -1.630344 | -0.098115 | 1.415839 |
| H | -0.684477 | 0.192966 | 1.295961 |

| | | |
|---|---|---|
| -1552.6857 | 24.7632 | 45.8283 |
| 68.7184 | 79.9606 | 107.9765 |
| 114.5375 | 143.7867 | 163.6756 |
| 179.0400 | 197.6183 | 249.3864 |
| 277.2395 | 367.0966 | 367.9932 |
| 442.6211 | 464.2653 | 494.6757 |
| 498.4445 | 506.6714 | 524.6073 |
| 620.1118 | 657.3289 | 691.1006 |
| 720.3645 | 833.7750 | 839.2026 |
| 858.5851 | 861.5703 | 891.1929 |
| 922.0029 | 975.1652 | 1027.3991 |
| 1037.2828 | 1085.2885 | 1105.2041 |
| 1128.6132 | 1167.3263 | 1207.6521 |
| 1291.0223 | 1336.7942 | 1366.2568 |
| 1382.1612 | 1394.1558 | 1403.0529 |
| 1454.4715 | 1457.7026 | 1469.8497 |
| 1483.4080 | 1492.3857 | 1571.9034 |
| 3034.3460 | 3065.9988 | 3099.0512 |
| 3118.3233 | 3126.9315 | 3133.2486 |
| 3138.0376 | 3233.1376 | 3511.1172 |

E = -1026.72434473 a.u.

**(33) $CH_3CO_2H$**

| | | | |
|---|---|---|---|
| O | -0.789961 | -1.023224 | 0.000005 |
| H | 1.656775 | -0.708647 | -0.880396 |
| C | -0.088298 | 0.120597 | -0.000003 |
| C | 1.388030 | -0.124854 | -0.000003 |
| O | -0.622148 | 1.200717 | 0.000001 |
| H | 1.917818 | 0.822175 | 0.000061 |
| H | -1.732851 | -0.799205 | -0.000024 |
| H | 1.656743 | -0.708728 | 0.880349 |

| | | |
|---|---|---|
| 77.0657 | 435.5386 | 539.8086 |
| 595.5013 | 644.2905 | 889.6324 |
| 1012.2182 | 1073.1015 | 1223.1153 |
| 1351.3358 | 1420.2593 | 1462.9675 |
| 1468.7051 | 1818.8027 | 3088.5154 |
| 3156.9560 | 3203.8626 | 3805.5489 |

E = -229.078175796 a.u.

**(34) $CH_3CO_2^-$**

| | | | |
|---|---|---|---|
| O | 0.750716 | 1.122454 | -0.039036 |
| H | -1.744098 | 0.864903 | -0.520859 |
| C | 0.187588 | 0.001205 | -0.010030 |
| C | -1.344932 | -0.007032 | -0.005049 |
| O | 0.763079 | -1.112853 | 0.043162 |
| H | -1.734379 | -0.919602 | -0.453598 |
| H | -1.686139 | 0.030270 | 1.032526 |

| | | |
|---|---|---|
| 52.5289 | 456.9530 | 612.7254 |
| 653.6408 | 922.6435 | 1019.2795 |
| 1054.4046 | 1352.8507 | 1431.4307 |
| 1458.8273 | 1480.1906 | 1603.9752 |
| 3064.8192 | 3134.4686 | 3161.9266 |

E = -228.610958384 a.u.

**(35) $CH_3CO_2^-/H_2CO_3$**

| | | | |
|---|---|---|---|
| O | -1.169102 | -1.108195 | -0.036711 |
| H | -3.664905 | -0.862755 | -0.516369 |
| C | -1.762104 | 0.002288 | -0.016538 |
| C | -3.272357 | -0.002088 | 0.020612 |
| O | -1.170143 | 1.112799 | 0.000529 |
| H | -3.671589 | 0.922223 | -0.389887 |
| H | -3.586115 | -0.080445 | 1.063712 |
| O | 1.333265 | 1.130177 | -0.018613 |
| O | 3.230673 | -0.001406 | 0.013436 |
| C | 2.013916 | -0.000828 | 0.004423 |

| | | | |
|---|---|---|---|
| H | 0.300051 | 1.040230 | -0.010433 |
| O | 1.331351 | -1.130451 | 0.017353 |
| H | 0.297479 | -1.038876 | -0.005970 |

| | | |
|---|---|---|
| 8.3062 | 26.7662 | 57.6981 |
| 121.1097 | 159.2893 | 180.4720 |
| 276.2591 | 494.3784 | 616.2847 |
| 645.7948 | 654.7626 | 688.5234 |
| 826.8809 | 955.7158 | 1033.6067 |
| 1054.4736 | 1067.3251 | 1068.6110 |
| 1121.5958 | 1333.6244 | 1371.5168 |
| 1404.6420 | 1459.8276 | 1465.2339 |
| 1494.5998 | 1528.9192 | 1616.1721 |
| 1785.2790 | 2369.7181 | 2503.1262 |
| 3077.8581 | 3150.9820 | 3184.5239 |

E = -493.664712087 a.u.

**(36) $CH_3CO_2^-/H_2PO_4^-$**

| | | | |
|---|---|---|---|
| O | -1.678039 | -1.117519 | -0.154711 |
| H | -4.210496 | -0.893668 | -0.223513 |
| C | -2.248654 | 0.000047 | -0.069905 |
| C | -3.746410 | 0.000157 | 0.188179 |
| O | -1.677650 | 1.117362 | -0.154628 |
| H | -4.210443 | 0.894426 | -0.222602 |
| H | -3.906498 | -0.000489 | 1.268769 |
| H | -0.076223 | 1.209983 | -0.400320 |
| O | 0.908726 | 1.259756 | -0.576395 |
| O | 3.075502 | -0.000227 | -0.391751 |
| P | 1.660781 | 0.000068 | 0.097208 |
| O | 1.404880 | 0.001075 | 1.578165 |
| O | 0.908880 | -1.260674 | -0.574587 |
| H | -0.076058 | -1.210677 | -0.398849 |

| | | |
|---|---|---|
| 40.3244 | 48.2663 | 53.2168 |
| 100.9835 | 119.6913 | 156.6075 |
| 191.8681 | 364.9336 | 371.5046 |
| 488.0821 | 494.4203 | 498.3437 |
| 508.7954 | 615.6512 | 664.8675 |
| 838.9214 | 861.7435 | 866.8035 |
| 903.4670 | 953.7192 | 1033.5241 |
| 1064.2616 | 1083.5853 | 1204.9055 |
| 1308.9586 | 1365.9677 | 1392.0746 |
| 1456.3927 | 1458.5796 | 1487.2720 |
| 1586.9714 | 2978.2664 | 3039.7698 |
| 3073.0604 | 3144.4577 | 3174.9328 |

E = -872.379704772 a.u.

**Table S1.** TST and CVT rate constants ($s^{-1}$), and Wigner (WTC) and small-curvature tunnelling (SCT) corrections for the unimolecular PCET reactions in the buffered solutions.[a] The pre-reaction H-bonded complex between $\bullet CH(CH_3)OH\cdots HCO_3^-$ (or $HPO_4^{2-}$; structures 37 and 38) and bromoacetate is taken as the reactant. The PCM-M06-2X-D3/6-311+G(2d,p) level of theory is used.

| | $HCO_3^-$ | $HPO_4^{2-}$ |
|---|---|---|
| TST | $2.58 \times 10^8$ | $1.23 \times 10^{12}$ |
| CVT | $2.58 \times 10^8$ | $1.15 \times 10^{12}$ |
| CVT/TST | 1.00 | 0.93 |
| WTC | 1.15 | 1.10 |
| SCT | 1.64 | 1.28 |

[a] The reactions paths were interpolated in the steps of 0.05 bohr starting from the PCET transition states (structures 11 and 12). The number of points along the MEP was 10 (9) and 5 (4) in the forward and reverse direction, respectively, for the $HCO_3^-$ ($HPO_4^{2-}$) case.

**(37) $\bullet CH(CH_3)OH\cdots HCO_3^-$ + $BrAc^-$**

| | | | |
|---|---|---|---|
| H | 2.853684 | 1.214536 | 2.380442 |
| H | 2.478605 | 1.059567 | -0.447211 |
| C | 1.831215 | 1.069628 | 2.003472 |
| O | 2.202292 | 1.999356 | -0.238017 |
| H | 1.144102 | 1.194574 | 2.841472 |
| C | 1.498572 | 2.036361 | 0.916992 |
| H | 1.760732 | 0.034574 | 1.656450 |
| H | 1.164927 | 3.034907 | 1.177042 |
| O | 1.254582 | -1.608844 | -0.358535 |
| H | 0.825227 | -0.851082 | -0.848614 |
| C | 2.607113 | -1.458304 | -0.304048 |
| O | 3.240950 | -2.389201 | 0.212949 |
| O | 3.087717 | -0.387128 | -0.777348 |
| O | -1.409177 | 2.029061 | -1.335882 |
| H | -1.502576 | 1.295985 | 1.106045 |
| Br | -2.788889 | -0.700761 | 0.335320 |
| C | -1.207762 | 0.485153 | 0.450342 |
| C | -0.874020 | 0.971860 | -0.966138 |
| H | -0.428219 | -0.131525 | 0.882169 |
| O | -0.103375 | 0.237621 | -1.639131 |

| | | |
|---|---|---|
| 28.5355 | 48.7349 | 58.9601 |
| 67.0651 | 80.0248 | 89.2618 |
| 99.8251 | 114.5589 | 121.3986 |
| 141.7045 | 166.0459 | 178.2263 |

| | | |
|---|---|---|
| 192.7500 | 220.9518 | 244.2736 |
| 449.0842 | 451.1329 | 520.6049 |
| 605.4281 | 639.4800 | 673.5875 |
| 685.6915 | 817.9207 | 853.3965 |
| 902.0611 | 928.7264 | 930.1955 |
| 942.1994 | 1014.8748 | 1027.2593 |
| 1034.9013 | 1109.0925 | 1132.0569 |
| 1228.3797 | 1253.5120 | 1347.5599 |
| 1359.8302 | 1380.7386 | 1412.7957 |
| 1416.9792 | 1461.6275 | 1473.3368 |
| 1486.5646 | 1525.7313 | 1654.8211 |
| 1667.3785 | 2988.3537 | 3001.6620 |
| 3075.8403 | 3077.2057 | 3129.1544 |
| 3154.9553 | 3176.4862 | 3237.9107 |

E = -3221.13686209 a.u.

**(38) $\bullet CH(CH_3)OH\cdots HPO_4^{2-}$ + $BrAc^-$**

| | | | |
|---|---|---|---|
| O | 1.976647 | 1.947065 | 1.381827 |
| H | 1.653085 | 1.215288 | -1.027361 |
| C | 1.298026 | 0.939465 | 1.110188 |
| C | 1.340906 | 0.438826 | -0.337708 |
| Br | 2.751130 | -0.953912 | -0.463993 |
| O | 0.584882 | 0.275142 | 1.906518 |
| H | 0.426052 | -0.058164 | -0.653412 |
| H | -1.523164 | 4.279899 | -1.585574 |
| H | -0.475230 | 4.297745 | -0.168737 |
| C | -0.740167 | 3.715139 | -1.056889 |
| H | 0.134285 | 3.672870 | -1.708243 |
| C | -1.183028 | 2.344913 | -0.682739 |
| O | -2.192907 | 2.264574 | 0.206985 |
| H | -1.089591 | 1.514247 | -1.377202 |
| O | -1.442116 | -0.965409 | -1.371644 |
| O | -2.884072 | -0.089554 | 0.532982 |
| H | -2.463425 | 1.254057 | 0.321704 |
| P | -2.164591 | -1.315790 | -0.080467 |
| H | -0.449658 | -0.974737 | 1.276606 |
| O | -1.016582 | -1.738226 | 1.019551 |
| O | -3.066782 | -2.532030 | -0.154737 |

| | | |
|---|---|---|
| 30.0144 | 48.5642 | 51.8458 |
| 66.1431 | 80.6158 | 86.8149 |
| 93.3078 | 118.4517 | 126.8646 |
| 133.8321 | 137.4822 | 163.7121 |
| 183.2321 | 230.9320 | 235.4368 |
| 365.3480 | 397.5062 | 447.9535 |
| 459.2856 | 509.9758 | 512.3453 |
| 521.8646 | 553.4786 | 624.1820 |
| 671.2464 | 790.6488 | 807.4610 |
| 821.4663 | 936.3645 | 942.0867 |
| 947.4117 | 953.6607 | 1013.6331 |
| 1046.0118 | 1115.7349 | 1124.9161 |
| 1142.6598 | 1164.7966 | 1233.9049 |
| 1262.0897 | 1267.1823 | 1379.4088 |

| | | |
|---|---|---|
| 1419.6967 | 1425.3208 | 1455.8748 |
| 1482.3498 | 1490.9320 | 1600.7968 |
| 1636.9763 | 2170.4590 | 2970.9935 |
| 3051.6969 | 3105.7949 | 3119.5874 |
| 3151.8795 | 3209.1151 | 3368.5939 |

E = -3599.84064836 a.u.