Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

An Efficient Buffer-Mediated Control between Free Radical Substitution and Proton-Coupled Electron Transfer: Dehalogenation of Iodoethane by α-Hydroxyethyl Radical in Aqueous Solution

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Figure S1 (the stationary structures with HPO_4^{2-}); Figure S2 (the natural atomic charges); the additional experimental details; Figure S3 (the CASSCF active spaces); Figure S4 (the stationary structures without a base); Cartesian coordinates (Å), harmonic vibrational frequencies (cm^{-1}), total free energies in solution (a.u.) and gas-phase CASSCF/CASPT2 energies (a.u) of all stationary structures.

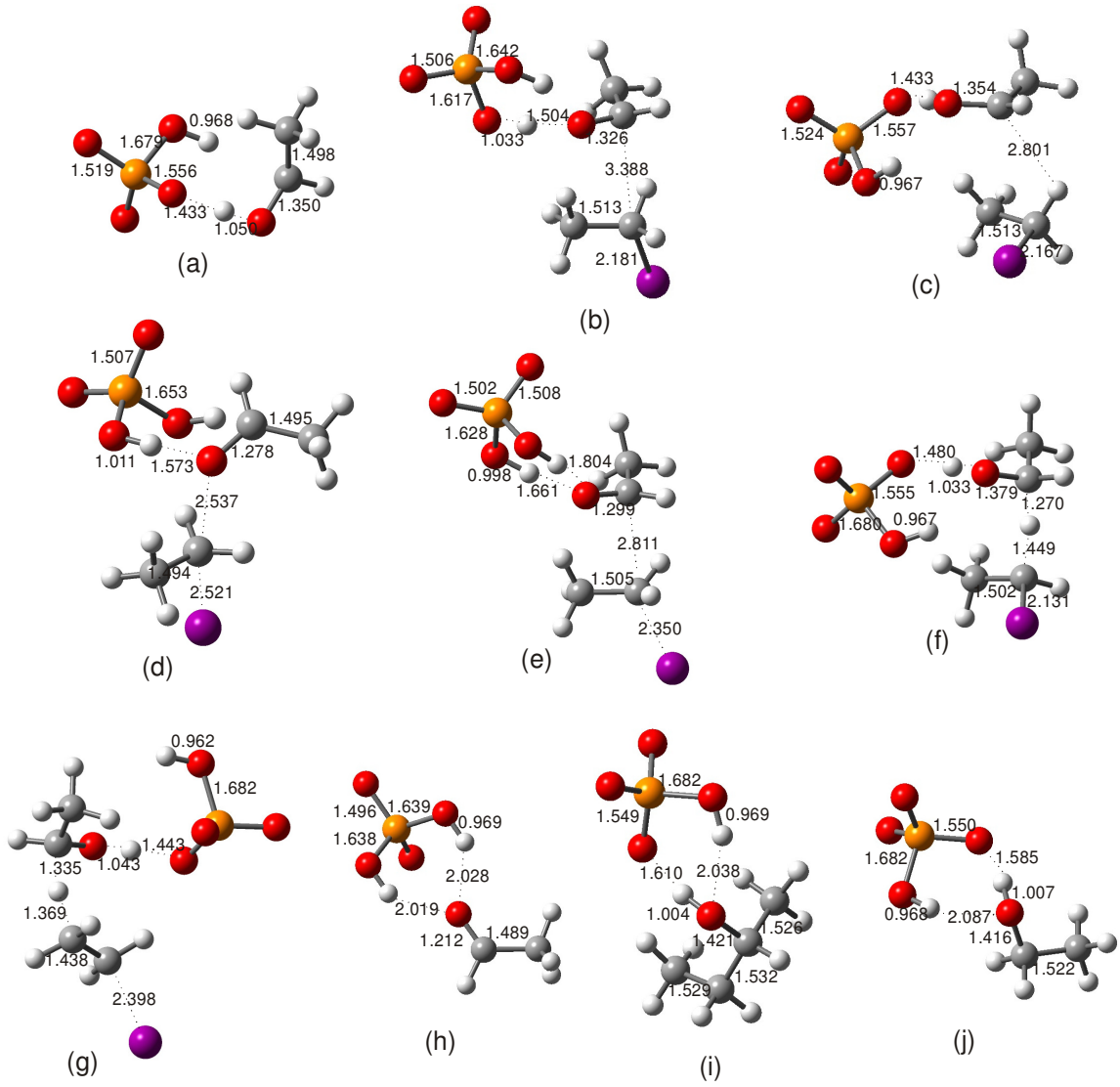

Figure S1. Structures (bond lengths in Å) in the aqueous reaction of iodoethane with α-hydroxyethyl radical/HPO_4^{2-}: (a) the α-hydroxyethyl radical/HPO_4^{2-} complex, (b) the **FRS** vdW complex, (c) the **αHab** vdW complex, (d) the **PCET** transition state, (e) the **FRS** transition state, (f) the **αHab** transition state, (g)the **βHab** transition state, (h) acetaldehyde/$H_2PO_4^-$ complex, (i) 2-butanol/HPO_4^{2-} complex, and (j) ethanol/HPO_4^{2-} complex. The level of theory is PCM-M06-2X/6-311+G(d,p)/LANL2DZdp(I).

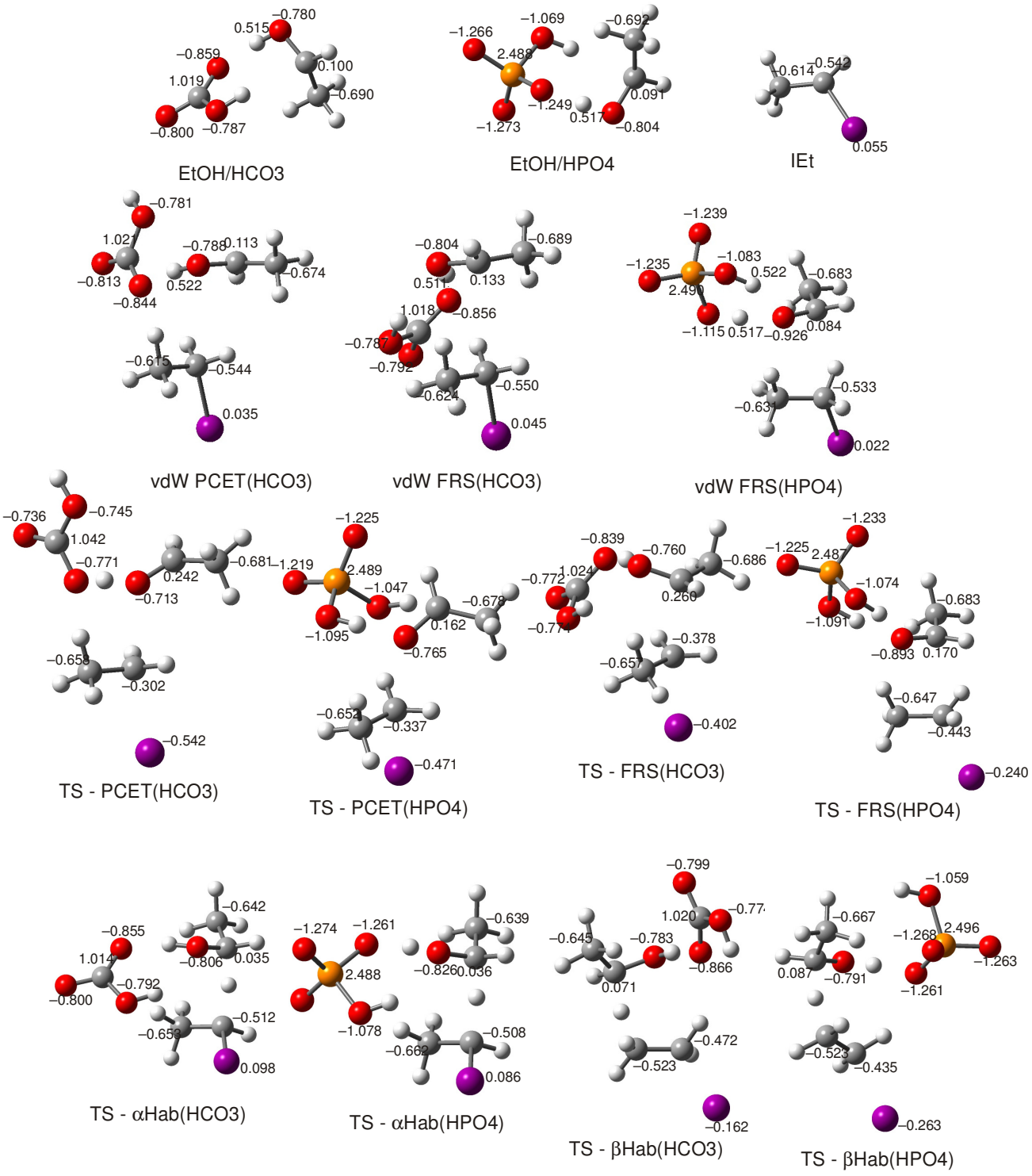

Figure S2. The natural atomic charges at the PCM-M06-2X/6-311+G(d,p)/LANL2DZdp(I)level of theory.

Additional Experimental Details

Possible fates of the I atom formed in the current aqueous solutions include the recombination reaction (S1) followed by the equilibrium (S2), as well as the reaction sequences (S3–S4):

$I\bullet + I\bullet \rightarrow I_2$ ($k_{S1} = 8 \times 10^9$ dm^3 mol^{-1} s^{-1})[S1] (S1)

$I_2 + I^- \rightleftharpoons I_3^-$ ($K_{S2} = 7.14 \times 10^2$ dm^3 mol^{-1})[S2] (S2)

$I\bullet + I^- \rightleftharpoons I_2\bullet^-$ (S3)

($K_{S3} = 1.1 \times 10^5$ dm^3 mol^{-1}; $k_f = 1.1 \times 10^{10}$ dm^3 mol^{-1} s^{-1})[S1]

$I_2\bullet^- + I_2\bullet^- \rightarrow I_3^- + I^-$ ($k_{S4} = 3.2 \times 10^9$ dm^3 mol^{-1} s^{-1})[S1] (S4)

$I\bullet + CH_3CH_2OH \not\rightarrow \bullet CH(CH_3)OH + I^- + H^+$ (S5)

$I\bullet + R\bullet \rightarrow RI$ (R$\bullet$ = $\bullet CH(CH_3)OH$ or $\bullet CH_2CH_3$) (S6)

Considering the high rate constants for (S3) and (S4), in addition to the high equilibrium constant K_{S3}, and because iodide ion is the only stable reactant in reactions (S1–S4) accumulating in the solution during irradiation, it can be concluded that these two consecutive reactions represent the most important pathway of iodine atom conversion into stable molecular products, viz. I_2 or its anionic form I_3^-. Two remaining, in principle possible, reactions of I$\bullet$, (S5) and (S6), are expected not to interfere – the former is shown to be unfeasible by the present computations, while that the latter is not concurrent with the other iodine atom reactions was proven experimentally by scavenging the I atoms with the I^- anion added in the concentration of 1 mmol dm^{-3} prior to the irradiation (the last two entries in Table 3).

References:

S1. P. Neta, R. E. Huie, A. B. Ross, *J. Phys. Chem. Ref. Data*, 1988, **17**, 1027–1284.

S2. (a) G. Picardi, R. Guidelli, *J. Phys. Chem.*, 1968, **72**, 2782–2788. (b) G. V. Buxton, R. M. Sellers, *J. Chem. Soc. Faraday Trans. 1*, 1985, **81**, 449–471. (c) I. Štefanić, K.-D. Asmus, M. Bonifačić, *Phys. Chem. Chem. Phys.*, 2003, **5**, 2783–2789.

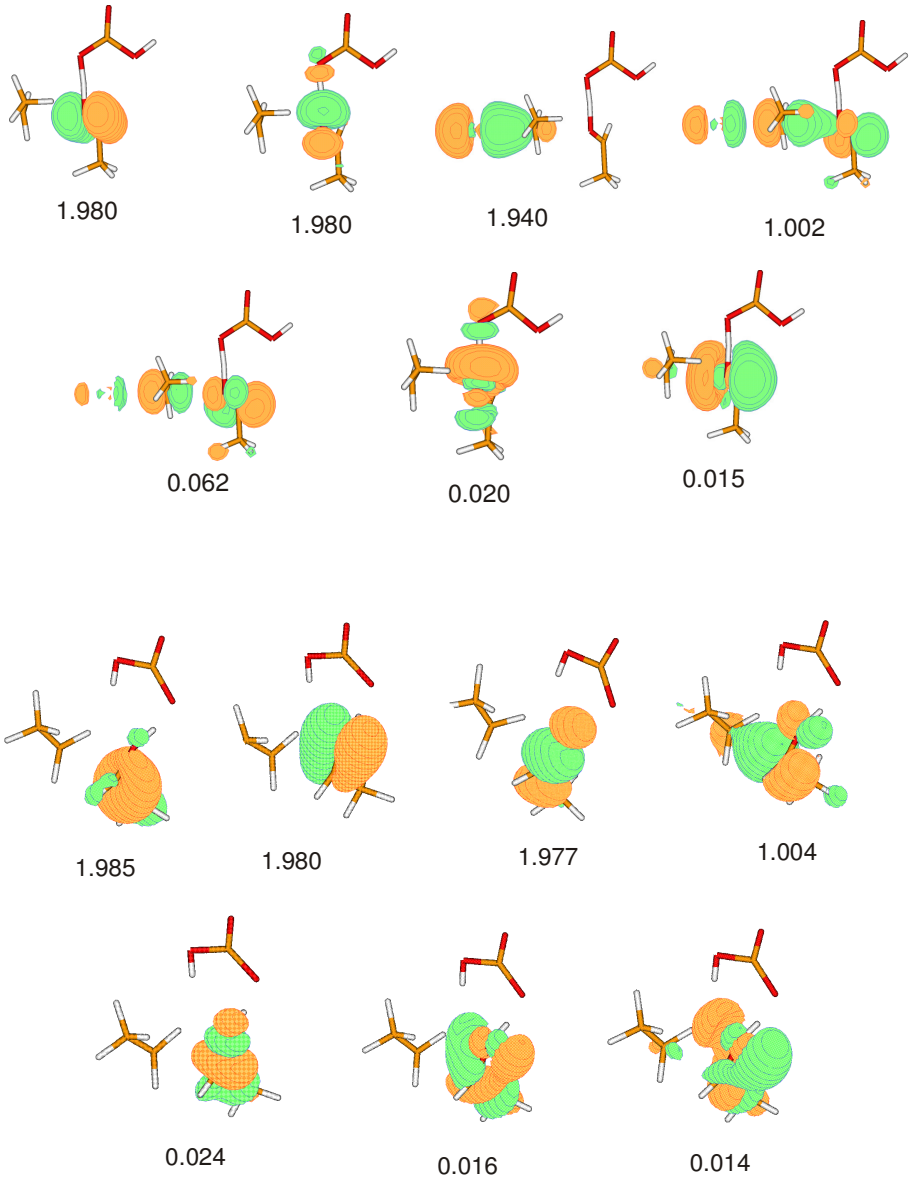

Figure S3. The gas phase (7,7) CASSCF active space and the occupation numbers of the **PCET/**HCO_3^- (upper panel) and **FRS/**HCO_3^- (lower panel) transition state at the CASSCF(7,7)/ANO-RCC level.

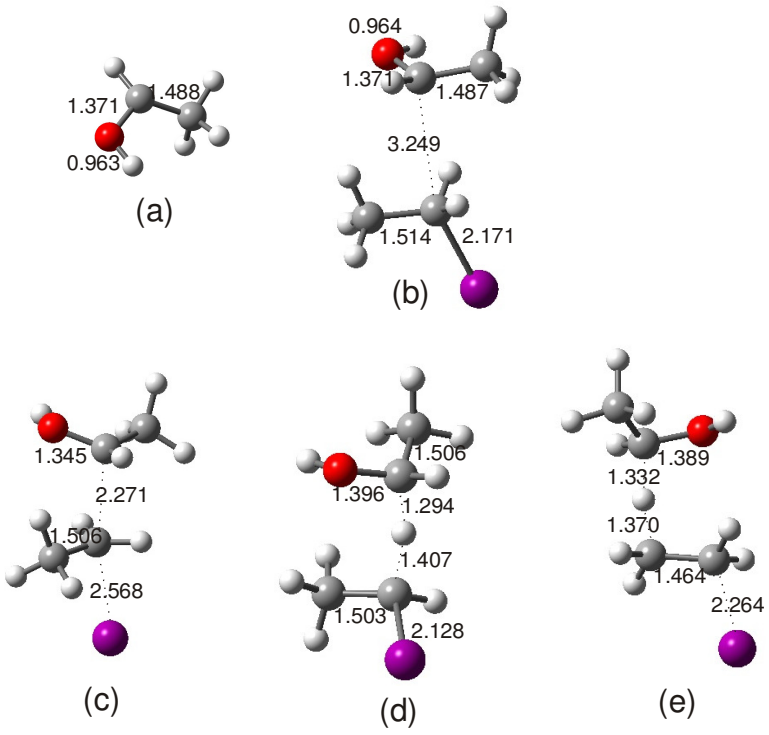

Figure S4. Structures of the reactant and transition states (bond lengths in Å) in the aqueous reaction of iodoethane with α-hydroxyethyl radical without a base: (a) the α-hydroxyethyl radical, (b) the **•EtOH/EtI** vdW complex, (c) the **FRS** transition state, (d) the **αHab** transition state, and (e) the **βHab** transition state. The level of theory is PCM-M06-2X/6-311+G(d,p)/LANL2DZdp(I).

Iodoethane

C	1.399118	0.698880	0.000000
H	1.463579	1.320165	-0.888754
H	1.463577	1.320160	0.888757
C	2.407316	-0.430535	0.000000
H	2.303144	-1.056916	0.886262
H	2.303018	-1.057036	-0.886162
H	3.413337	-0.001460	-0.000101
I	-0.637458	-0.040283	0.000000

E(RM062X) = -90.5430143113
E(MP2) = -373.92735850454

Frequencies:
263.2361 266.3347 512.0897 751.8433 975.8798 1009.0252
1082.2198 1248.8631 1260.1814 1408.8343 1474.2446 1480.7689
1490.3220 3063.7463 3131.6202 3143.1256 3156.8157 3207.2182

•EtOH/HCO_3^-

H	2.367136	-1.971162	-0.453304
H	2.597442	-0.622841	-1.578390
C	1.998292	-0.982299	-0.729295
H	0.967551	-1.080371	-1.081546
C	2.093926	-0.049355	0.435322
H	2.969799	-0.082433	1.074076
O	1.569289	1.199741	0.322352
H	0.682294	1.135174	-0.133394
H	-0.090185	-0.511371	1.055984
O	-1.030947	-0.724217	0.969491
O	-0.819900	0.842499	-0.634168
C	-1.588955	0.034027	-0.048231
O	-2.782643	-0.178177	-0.261450

E(UM062X) = -418.929826432
E(PMP2) = -418.31740488
E(UMP2) = -418.31545416553

Frequencies:
47.9074 63.9120 109.8688 125.9384 137.6769 201.9027 224.5752
437.6974 550.5013 612.6370 636.1273 686.4602 838.4696 908.1011
930.2914 985.4405 1031.8903 1107.3070 1242.0905 1260.2114
1341.7203 1372.4582 1408.3314 1459.4295 1485.2322 1511.0947
1723.8841 3000.3248 3045.5094 3088.0604 3143.1420 3188.2690
3765.8871

vdW PCET/HCO_3^-

H	−1.537539	3.889233	−1.630571
C	−1.982241	2.105550	−0.547620
C	−1.555171	3.529534	−0.600853
O	−2.147227	1.589948	0.696829
H	−2.239292	4.162388	−0.026931
H	−1.684606	1.404429	−1.324111
H	−0.550362	3.677088	−0.175731
H	−0.033359	−0.140080	−0.015953
H	0.687620	−0.912009	2.260109
I	2.610459	−0.353503	−0.281194
C	0.643237	0.152020	2.024351
C	0.739390	0.389951	0.533316
H	−0.321113	0.540116	2.364060
H	1.437370	0.666263	2.567383
H	0.728742	1.444497	0.271109
O	−2.190284	−0.994715	0.386484
O	−3.337666	−2.753242	−0.414369
C	−3.192920	−1.566284	−0.103976
H	−2.233181	0.597737	0.619945
O	−4.268108	−0.717793	−0.312486
H	−4.976085	−1.252184	−0.689005

E(UM062X) = −509.478089856
E(PMP2) = −792.25210516
E(UMP2) = −792.25006357336
E(CASSCF)= −7606.5563383714
E(CASPT2)= −7608.5216733418

Frequencies:
22.3938 30.5071 36.5119 49.0681 53.5710 63.1034 81.8405
100.9429 105.7138 117.6880 134.5425 196.1867 209.5906 264.9068
275.2570 433.3280 509.9581 516.7475 557.9805 586.4249 681.7561
767.1280 837.3825 937.2460 955.9306 980.3242 994.1664
1013.8237 1025.2271 1084.4823 1109.2786 1223.6519 1244.3153
1247.2478 1264.3735 1368.7931 1375.9291 1400.2427 1410.7979
1458.2814 1472.2784 1481.2640 1484.6344 1488.3229 1515.3969
1716.8287 2981.8632 3048.0622 3062.5175 3072.4698 3132.8065
3137.1291 3143.9270 3150.2105 3153.9032 3213.5782 3871.2407

vdW FRS/HCO_3^-

C	−0.204495	−1.149232	0.302339
H	−0.192862	−2.088124	−0.245692
H	0.540585	−0.475667	−0.109008
C	−0.073884	−1.336879	1.798871
H	−0.152966	−0.384810	2.325161
H	−0.835899	−2.015467	2.184065

H	0.911403	-1.766594	2.004841
H	2.085320	-1.244929	-1.833266
H	2.729221	0.292816	-0.118890
C	2.898551	-1.841814	-1.406381
O	3.115788	-0.361680	0.535267
H	3.822097	-1.546814	-1.926284
C	2.996437	-1.635935	0.066568
H	2.708045	-2.891987	-1.632345
H	3.479769	-2.370285	0.700137
I	-2.090627	-0.218975	-0.228095
O	1.142045	1.760639	1.269813
H	1.708312	0.983815	1.385678
C	1.177686	2.154644	-0.059089
O	0.512960	3.151967	-0.331933
O	1.883513	1.445199	-0.830548

E(UM062X) = -509.480504525
E(PMP2) = -792.25406584
E(UMP2) = -792.25203869188
E(CASSCF)= -7606.5479785528
E(CASPT2)= -7608.5199827677

Frequencies:
28.3875 31.6429 54.9949 65.7461 72.6192 92.3239 93.6823
106.4814 120.4969 136.9731 171.8793 220.7056 232.4326 267.1448
276.3907 442.3578 511.4587 582.6271 585.8788 617.9750 686.8414
763.6959 838.8304 929.4812 945.4104 975.9620 984.8830
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1735.6899 2975.7537 2995.9505 3059.1036 3070.7871 3131.1870
3139.2369 3146.1261 3155.1283 3197.5739 3222.0890 3782.3123

TS FRS/HCO_3^-

C	-0.239551	-0.990905	0.324803
H	-0.600594	-1.887211	-0.155390
H	0.331860	-0.300603	-0.278684
C	-0.178678	-0.904748	1.826088
H	-0.249479	0.131427	2.157602
H	-0.993302	-1.469459	2.278860
H	0.766808	-1.309492	2.200959
H	1.855844	-1.279866	-1.937275
H	2.940667	-0.544720	0.019506
C	1.833452	-2.266404	-1.467630
O	2.694520	-1.364030	0.623485
H	2.734387	-2.805501	-1.786578
C	1.811773	-2.148819	0.019453
H	0.964077	-2.818023	-1.825660
H	1.492074	-2.996098	0.619360

I	-2.395944	0.240743	-0.191969
O	1.943037	1.497962	1.112271
H	2.105007	0.586764	1.393732
C	2.520930	1.712717	-0.123892
O	2.432276	2.850396	-0.566277
O	3.073934	0.705966	-0.667604

E(UM062X) = -509.464751586
E(PMP2) = -792.23083712
E(UMP2) = -792.22729754195
E(CASSCF)= -7606.52151472
E(CASPT2)= -7608.4997038455

Frequencies:
-372.6263 17.7327 38.9605 66.2461 90.2371 96.5032 110.4780
129.1373 155.3919 170.1182 189.3510 219.0108 242.3306 279.5014
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807.5342 835.9115 933.9272 939.9831 973.7864 997.6379
1024.5256 1041.0523 1075.6848 1121.3763 1159.0274 1196.7760
1259.8037 1289.3274 1350.9602 1389.7326 1401.3414 1434.0583
1456.5504 1466.6752 1476.2907 1484.1355 1493.7886 1541.6885
1739.5913 2269.2376 3031.1609 3058.4803 3104.9444 3128.3339
3155.7869 3162.1591 3177.1421 3202.3362 3315.5022 3804.0417

TS PCET/HCO_3^-

H	-2.289036	4.096686	-1.010542
C	-2.205400	2.044288	-0.406736
C	-1.830428	3.473561	-0.242996
O	-1.830533	1.185637	0.468955
H	-2.125315	3.846673	0.743518
H	-2.681928	1.693328	-1.324237
H	-0.737964	3.591288	-0.310324
H	0.081400	-0.102695	-0.470587
H	0.393710	-1.501013	1.595593
I	2.963151	-0.265448	-0.211907
C	0.293763	-0.422296	1.723082
C	0.506704	0.301188	0.435541
H	-0.720402	-0.217809	2.089552
H	0.999737	-0.093180	2.487216
H	0.663017	1.369021	0.451646
O	-2.383038	-1.075745	-0.136073
O	-4.065481	-2.487179	-0.526543
C	-3.628758	-1.395169	-0.218919
H	-2.173323	-0.008917	0.162741
O	-4.459300	-0.363998	0.079602
H	-5.365354	-0.683804	-0.010885

E(UM062X) = -509.446137226
E(PMP2) = -792.21160945

E(UMP2) = -792.20818999786
E(CASSCF)= -7606.52113311
E(CASPT2)= -7608.4878998722

Frequencies:
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726.3545 742.3550 825.7813 839.5953 895.4486 963.7280 993.3149
1001.4342 1042.0324 1086.4818 1119.3297 1207.4474 1219.9267
1294.3211 1364.1789 1386.3845 1394.0551 1432.4297 1451.6784
1459.6613 1465.4221 1470.0565 1477.4970 1500.3387 1634.8051
1806.6653 2982.8459 3024.7993 3061.2455 3106.0361 3108.7291
3147.4812 3153.7500 3208.1839 3314.6096 3857.7563

TS αHab/HCO_3^-

H	2.036815	2.511539	0.881188
H	0.438499	1.193934	2.578983
O	3.052280	-0.080649	0.027764
C	1.497317	3.112688	0.143835
H	2.234628	3.625386	-0.482192
H	0.909758	3.865192	0.673430
O	3.495286	-2.243294	0.437034
H	1.992719	0.844650	-0.777632
C	0.001160	0.374001	2.000957
C	2.813032	-1.318501	-0.004871
H	-1.761549	1.604263	1.466122
H	-0.443109	-0.335245	2.705743
C	-1.009047	0.942889	1.044880
C	0.598501	2.234023	-0.692612
O	1.245036	1.191099	-1.339720
H	0.807486	-0.131888	1.464126
H	-0.255097	1.717398	0.111948
O	1.625613	-1.698219	-0.610435
H	1.153022	-0.909331	-0.915874
H	-0.024667	2.776901	-1.406252
I	-1.996981	-0.494055	-0.176790

E(UM062X) = -509.448826594
E(PMP2) = -792.22684777
E(UMP2) = -792.22109392280

Frequencies:
-1559.1887 35.7951 44.6047 48.5004 60.2582 79.7630 89.4270
97.4985 112.5041 148.8873 214.5559 218.2436 230.6922 266.3414
332.7347 448.0418 481.6672 581.1281 602.3123 614.9792 686.1118
818.5110 840.7374 878.1925 917.4424 930.8804 985.9752 991.2907
1065.2684 1094.3513 1107.3746 1164.5669 1184.5640 1242.3005
1287.7774 1337.4068 1350.1619 1393.1901 1399.9264 1420.5346

1455.5425 1464.8121 1466.5613 1477.8341 1486.7455 1493.9662
1729.9609 3042.0703 3044.3717 3068.6352 3107.6223 3108.6868
3116.8265 3130.0187 3139.8510 3171.4560 3769.2836

TS βHab/HCO_3^-

H	−1.001881	1.212145	−1.367933
H	−0.975245	2.561775	0.744124
I	−2.779271	−0.321143	0.015180
C	−0.385409	1.653817	0.646067
C	−0.759965	0.743165	−0.419809
H	−0.129928	1.197471	1.600127
H	−0.113572	−0.121154	−0.533344
H	2.720139	2.644116	1.870429
H	4.010706	2.092529	0.783268
C	2.949528	1.984908	1.030920
H	2.776832	0.949809	1.335781
C	2.089440	2.332015	−0.157593
H	2.102738	3.382493	−0.451069
H	0.843143	2.140093	0.265526
O	2.214177	1.524810	−1.259093
H	2.221734	0.571071	−0.964559
O	2.871051	−2.792735	0.526481
H	1.917421	−2.928067	0.557015
C	3.083666	−1.566038	−0.074777
O	2.037922	−0.953464	−0.422717
O	4.260065	−1.224722	−0.193766

E(UM062X) = −509.450171744
E(PMP2) = −792.22345737
E(UMP2) = −792.21581947206

Frequencies:
−1380.3910 25.2835 30.5526 42.6905 48.5363 64.0794 82.5071
100.5600 123.5468 142.4577 172.8458 192.2983 208.0945 245.2465
420.3657 448.6133 519.7478 521.7498 600.0536 633.4258 673.4269
757.3585 839.1780 870.6819 918.7495 950.7585 1009.3971
1023.5075 1044.6603 1091.7670 1107.7597 1166.8303 1181.4375
1219.7687 1232.8932 1260.0650 1347.9507 1363.9222 1386.1469
1395.6598 1429.8909 1457.9128 1467.1826 1483.6468 1491.9923
1508.2233 1722.9736 3046.3464 3060.2729 3115.9953 3123.8975
3125.3932 3145.2358 3155.4655 3203.6350 3240.7961 3870.9246

TS SN2(O)/HCO_3^-

H	−1.304519	4.562196	−0.511272
C	−1.750264	2.482274	−0.438162
C	−1.016272	3.673991	0.051442
O	−1.676553	1.367125	0.293301

H	-1.219064	3.845371	1.112333
H	-2.055313	2.376429	-1.475620
H	0.072398	3.553563	-0.056305
H	0.079932	0.315069	-0.750288
H	-0.276515	-1.721292	0.617379
I	2.814005	-0.410511	-0.116103
C	-0.269025	-0.788469	1.179358
C	0.164501	0.353507	0.323908
H	-1.285791	-0.597387	1.537986
H	0.379930	-0.893029	2.047496
H	0.584463	1.242947	0.764029
O	-2.787906	-0.412670	-0.916412
O	-4.152459	-2.184140	-0.778217
C	-3.570157	-1.210705	-0.314858
H	-2.226423	0.565085	-0.198704
O	-3.745624	-0.895665	1.010210
H	-4.343711	-1.552675	1.385243

E(UM062X) = -509.445962886
E(PMP2) = -792.20815790
E(UMP2) = -792.20601648821

Frequencies:
-467.6685 17.6195 39.7063 46.8820 55.6051 74.9213 85.4769
99.9037 119.7172 141.7700 154.7925 168.2912 199.5512 259.7566
295.3250 309.7471 474.4411 518.3753 518.7837 588.4326 708.3259
816.3973 834.0086 907.9629 926.3833 969.0950 990.1298
1019.1745 1032.4397 1077.1335 1106.2416 1162.9575 1194.7940
1226.6161 1298.4495 1374.7847 1388.8170 1395.9341 1421.4600
1457.3818 1463.9762 1469.3645 1474.7187 1483.5996 1588.7424
1632.1751 1874.0993 2992.1397 3063.0134 3083.7544 3138.8441
3147.8391 3169.4014 3176.4872 3222.5834 3344.5363 3864.6865

vdW αHab/HCO_3^-

H	1.921501	2.335181	1.068475
H	0.350145	0.675190	2.843990
O	3.119153	-0.042463	-0.002108
C	1.471856	3.015627	0.338005
H	2.285891	3.629312	-0.075824
H	0.787134	3.682128	0.865476
O	3.453091	-2.209227	0.477078
H	2.151623	0.898600	-0.834049
C	0.037463	0.103490	1.964590
C	2.827843	-1.271230	-0.016505
H	-2.090039	0.506588	2.224581
H	-0.027153	-0.949035	2.244455
C	-1.298360	0.634910	1.491227
C	0.747265	2.257933	-0.723039
O	1.420038	1.286798	-1.401255

H	0.802545	0.216385	1.195833
H	-1.242961	1.671971	1.171219
O	1.656318	-1.617665	-0.666859
H	1.216126	-0.816612	-0.988203
H	-0.017231	2.741643	-1.320204
I	-2.000807	-0.422175	-0.263703

E(UM062X) = -509.480295535
E(PMP2) = 792.25321899
E(UMP2) = -792.25118575723

Frequencies:
30.7161 37.7974 42.3701 49.1533 62.1371 84.4723 91.0585
93.6106 116.7831 123.8149 165.8318 210.8933 235.6872 268.2633
295.8548 441.1299 513.8158 587.7620 591.2644 617.3199 688.8964
752.1723 840.0359 928.6310 964.8540 976.2306 991.8819
1013.3893 1023.2862 1081.5731 1112.3468 1237.8917 1249.4264
1264.7486 1294.0645 1351.1781 1368.6510 1405.9720 1414.6774
1457.0963 1471.4993 1478.0963 1483.3265 1487.1572 1500.5189
1728.7926 2956.4897 2993.6264 3058.9584 3074.1018 3127.5693
3134.5309 3139.2385 3161.5963 3192.5736 3206.7032 3773.1974

•EtOH/HPO_4^{2-}

H	1.664577	-1.445740	-0.533260
C	2.634881	-1.070032	-0.198693
H	3.292591	-1.029166	-1.080271
H	3.066073	-1.783864	0.505947
H	0.987541	0.861922	-0.691841
C	2.490952	0.278236	0.438200
O	1.852334	1.253624	-0.242280
H	3.292991	0.643291	1.075091
O	-0.240708	0.288782	-1.156175
O	-2.417835	-0.909382	-0.509840
P	-1.297354	0.006682	-0.049375
H	0.389482	-0.517591	1.286554
O	-1.727236	1.277269	0.675144
O	-0.465048	-0.920083	1.075821

E(UM062X) = -797.612744371
E(PMP2) = -796.57067228
E(UMP2) = -796.56870596661

Frequencies:
57.8985 79.0781 107.2017 123.0731 152.1021 214.4437 267.9403
341.9489 373.4849 438.7101 467.1753 495.4718 511.3373 543.5315
643.5397 737.4536 925.7620 945.0213 1030.3613 1041.6354
1070.0481 1115.0823 1144.6975 1198.9949 1265.4365 1370.1716
1412.9328 1459.9392 1489.1830 1557.5620 2172.8109 2987.1578
3087.3630 3133.2652 3151.7349 3773.6687

vdW FRS/HPO_4^{2-}

C	-1.963407	0.330156	-0.390657
H	-2.028693	0.765450	-1.383751
H	-1.726682	1.102889	0.334279
C	-1.022135	-0.852607	-0.324373
H	-0.989997	-1.279100	0.679572
H	-1.317113	-1.634440	-1.025636
H	-0.019816	-0.502727	-0.589568
H	0.512135	0.946250	1.370523
H	2.244443	-0.168110	-0.273327
C	0.836108	1.935018	1.020047
O	1.822109	1.061642	-1.029526
H	1.775454	2.160398	1.551491
C	1.011071	1.949535	-0.471356
H	0.091633	2.669594	1.339322
H	0.877824	2.904763	-0.988724
I	-4.012599	-0.247580	0.080338
O	5.215881	-1.720284	-0.138273
O	2.791821	-0.957965	0.104403
P	4.348946	-0.529332	0.173666
O	4.627146	0.229252	1.450874
O	4.449492	0.505580	-1.097306
H	3.592939	0.978366	-1.200413

E(UM062X) = -888.158882483
E(PMP2) = -1170.5031163
E(UMP2) = -1170.5008761671

Frequencies:
12.8965 25.0025 40.0967 49.4869 52.9591 63.8977 79.3213
108.3095 117.6219 145.0848 186.5150 235.6622 260.5567 269.4324
296.0731 341.2729 391.1085 439.5527 477.2979 487.2102 488.2857
520.4240 538.6214 684.6724 748.8395 800.7974 853.4700 921.8586
978.5131 1001.9524 1009.1506 1054.3906 1077.8278 1081.8642
1122.9680 1181.4593 1206.5644 1229.4395 1256.7997 1289.3247
1367.6213 1398.8947 1403.0427 1457.2827 1462.1972 1466.7035
1487.1436 1490.8518 1493.2852 2456.2301 2962.1066 3032.0232
3051.1182 3059.9359 3107.2885 3134.2860 3146.1712 3147.6915
3215.3206 3424.9644

vdW αHab/HPO_4^{2-}

H	0.745437	2.584672	1.248905
H	-0.198242	0.632950	2.745218
C	0.361231	3.202474	0.430635
H	1.133528	3.955084	0.208832
H	-0.526930	3.732077	0.781364

H	1.744176	1.352092	-0.580491
C	-0.491758	0.049633	1.866187
H	-2.632991	0.330125	2.183341
H	-0.487207	-1.006308	2.141595
C	-1.868873	0.499897	1.429313
C	0.036174	2.363627	-0.762303
O	1.010759	1.587799	-1.291740
H	0.251858	0.212789	1.084127
H	-1.882821	1.535927	1.101919
H	-0.690015	2.715788	-1.488771
I	-2.560156	-0.607749	-0.300614
O	2.723503	0.811316	0.314959
O	3.224241	-1.512848	1.302944
P	3.075043	-0.680398	0.040191
H	1.216547	-0.560530	-1.155444
O	4.196302	-0.838574	-0.980472
O	1.678772	-1.267914	-0.686179

E(UM062X) = -888.161647740
E(PMP2) = -1170.5053270
E(UMP2) = -1170.5032526257

Frequencies:
26.1605 44.9989 51.9254 72.6315 73.0943 81.3249 90.6559
112.3681 126.4687 132.0509 167.8038 214.7111 262.0328 266.2858
297.4761 324.3037 366.2785 416.7345 449.0828 499.1784 508.9753
512.1703 540.6747 585.5869 735.1401 748.6260 927.7662 939.9592
974.5540 1011.4087 1018.4951 1037.9608 1058.9338 1080.7520
1112.1477 1141.9954 1194.4592 1247.0981 1259.7939 1263.0553
1372.8042 1407.3762 1419.5962 1455.6704 1468.0673 1476.3166
1485.4545 1495.9095 1547.9832 2221.7637 2983.0430 3053.2703
3069.8266 3123.6322 3128.4381 3138.4862 3156.8554 3164.0261
3207.6065 3805.6021

TS FRS/HPO_4^{2-}

C	1.779601	0.172759	0.114659
H	1.611058	0.094919	1.180548
H	1.740147	1.189862	-0.249876
C	1.136873	-0.883763	-0.742926
H	1.421777	-0.770998	-1.789881
H	1.423713	-1.883542	-0.413456
H	0.047835	-0.800336	-0.657285
H	-0.574214	1.399687	-1.547852
H	-2.474762	-0.325480	-0.518410
C	-0.773065	2.061834	-0.694245
O	-1.530325	0.252856	0.719460
H	-1.757995	2.518836	-0.876647
C	-0.756679	1.287844	0.590773
H	-0.027917	2.860850	-0.693686

H	-0.372542	1.777238	1.490734
I	4.103333	-0.170894	0.045244
O	-5.675020	-1.281752	-0.289571
O	-3.289039	-0.705162	-0.953925
P	-4.579895	-0.280328	-0.058283
O	-4.877559	1.184989	-0.257350
O	-4.007740	-0.511237	1.459686
H	-3.098254	-0.148316	1.516138

E(UM062X) = -888.155418781
E(PMP2) = -1170.4940503
E(UMP2) = -1170.4914145906

Frequencies:
-532.6378 17.7884 26.4001 48.5709 60.1888 67.3264 88.9318
98.6018 119.6032 152.7816 166.5943 211.7452 230.1044 237.7890
283.3768318.9739 347.8902 377.1477 472.4367 477.6759 487.6528
503.2402 565.3679 682.7584 750.4100 808.4758 831.3246 882.9151
918.2159 933.6193 966.1490 1004.0608 1045.4677 1080.3426
1104.3706 1114.73821157.8475 1205.6228 1226.0964 1231.6740
1327.0261 1384.8326 1393.0200 1442.5928 1454.8903 1457.7239
1476.4262 1485.4155 1492.0005 2979.4844 3027.7983 3045.8458
3054.2004 3090.4505 3120.1881 3122.1155 3147.1123 3189.9853
3282.3181 3503.6054

TS PCET/HPO_4^{2-}

H	-2.082615	3.883951	-1.764766
C	-2.008530	2.327974	-0.281823
C	-1.505903	3.600954	-0.882864
O	-1.436854	1.834101	0.749340
H	-1.546807	4.427106	-0.161213
H	-2.856918	1.805033	-0.737995
H	-0.450441	3.498155	-1.175608
H	0.145922	0.046289	0.056830
H	0.934111	-0.397527	2.405022
I	2.951278	-0.370287	-0.265061
C	0.905773	0.636091	2.056933
C	0.829520	0.708589	0.566228
H	0.011291	1.113786	2.475316
H	1.783035	1.158846	2.442056
H	0.982705	1.668488	0.094858
H	-1.902122	0.378777	1.125146
O	-1.680423	-0.879703	-1.238456
H	-1.741968	0.045974	-1.510799
O	-2.787774	-2.729072	0.072111
P	-2.800135	-1.237098	-0.076794
O	-4.074919	-0.517633	-0.433642

O	-2.147162	-0.593795	1.250704

E(UM062X) = -888.143385680
E(PMP2) = -1170.4836397
E(UMP2) = -1170.4789360030

Frequencies:
-2293.3359 27.5876 36.9127 51.8279 57.3352 71.9069 82.9353
99.0366 109.9218 140.1000 145.5904 156.3505 189.7851 223.0787
239.3978 290.0306 338.8679 353.3812 401.7040 454.0696 488.7631
494.9653 498.5857 516.8268 637.1939 755.4370 785.7883 863.1512
874.4235 915.4406 974.9192 984.8936 993.3912 1018.0523
1045.6899 1089.7037 1094.1764 1125.3911 1216.1220 1231.5959
1359.5827 1383.5410 1386.9039 1430.5612 1451.1861 1466.7830
1471.2979 1475.5501 1480.1517 2715.2993 2981.6041 3025.8382
3030.8394 3062.5185 3107.8430 3136.1443 3144.7403 3203.7594
3309.1065 3791.0245

TS αHab/HPO_4^{2-}

H	1.102567	3.000983	0.964318
H	-0.172978	1.164368	2.579693
C	0.463968	3.443376	0.195670
H	1.080469	4.112170	-0.413965
H	-0.312192	4.037393	0.683225
H	1.546861	1.315565	-0.641010
C	-0.542426	0.309141	2.004350
H	-2.409180	1.371732	1.458422
H	-0.941752	-0.423711	2.713208
C	-1.585781	0.797683	1.040579
C	-0.156352	2.358540	-0.656775
O	0.742169	1.503690	-1.260416
H	0.300887	-0.140013	1.474574
H	-0.897355	1.681658	0.121922
H	-0.869251	2.736495	-1.395770
I	-2.410035	-0.701627	-0.229475
O	2.676506	0.809791	0.170476
O	3.172474	-1.425887	1.351180
P	2.922154	-0.718641	0.027127
H	0.916837	-0.608985	-0.921982
O	3.915120	-1.055721	-1.080551
O	1.428505	-1.298653	-0.476978

E(UM062X) = -888.129642425
E(PMP2) = -1170.4785507
E(UMP2) = -1170.4728980819

Frequencies:
-1484.9865 27.6352 33.0364 50.6069 54.5582 70.3090 97.6588
100.7864 117.4682 146.9129 201.5749 222.7612 250.0941 266.6125

322.0898 344.6962 374.6749 433.6093 447.5156 477.3021 501.0308
510.6611 535.1101 579.9901 734.7340 825.1796 878.3070 922.6528
943.8807 989.1061 1021.2961 1052.4280 1067.2095 1097.4448
1109.8218 1132.2551 1166.2317 1173.8455 1209.5915 1245.5365
1340.0648 1390.8403 1400.9399 1422.5520 1449.1711 1465.3178
1467.2868 1482.9946 1490.3363 1541.4032 2447.8966 3034.9160
3044.1565 3072.3396 3099.2133 3114.9778 3130.2369 3139.0732
3162.4598 3794.5029

TS βHab/HPO_4^{2-}

H	−1.612498	1.435491	−1.350947
H	−1.522780	2.629395	0.844848
I	−3.096604	−0.443779	0.029010
C	−0.861977	1.792989	0.632182
C	−1.205570	0.942247	−0.474881
H	−0.480320	1.298429	1.523145
H	−0.490624	0.157607	−0.702458
H	2.160642	3.011213	1.794317
H	3.453316	2.554178	0.675391
C	2.404168	2.375230	0.940524
H	2.286046	1.328895	1.239322
C	1.508331	2.701682	−0.229681
H	1.436191	3.763606	−0.475256
H	0.285078	2.420496	0.226472
O	1.639693	1.941150	−1.344692
H	1.692767	0.929261	−1.095796
O	4.141884	−0.538643	−0.198984
H	4.155332	0.312719	0.249496
O	2.376866	−1.173480	1.540376
P	2.662723	−1.300326	0.048506
O	2.897170	−2.703695	−0.480662
O	1.662675	−0.486456	−0.816349

E(UM062X) = −888.132894244
E(PMP2) = −1170.4751305
E(UMP2) = −1170.4674182179

Frequencies:
−1243.0382 24.0174 48.1477 56.6992 62.4564 68.9101 82.5677
99.2409 109.5466 139.9066 180.5290 182.8857 190.3411 257.8798
304.6008 360.6724 392.1138 425.4650 452.7593 492.6501 509.6481
518.0296 540.2286 649.4877 731.2156 764.2389 880.3365 929.1498
956.0550 1008.9381 1013.2471 1045.5228 1063.4659 1088.5805
1111.5295 1147.9412 1161.7591 1181.9094 1192.7393 1247.7478
1258.6432 1369.4031 1378.3049 1396.0736 1421.5589 1459.3121
1477.1418 1502.3973 1513.6664 1541.3696 2272.1976 3026.6050
3094.6362 3104.4038 3123.9072 3134.8457 3145.8602 3203.8164
3240.1789 3886.7626

•EtOH

C	-1.205020	-0.182158	0.020527
C	0.092692	0.531460	-0.121061
O	1.252893	-0.179494	0.049668
H	-1.256636	-1.046345	-0.650048
H	-2.031865	0.484695	-0.225540
H	-1.362091	-0.551380	1.044138
H	0.204678	1.559966	0.197221
H	1.096737	-1.106796	-0.159912

E(UM062X) = -154.359052630
E(PMP2) = -154.10359239
E(UMP2) = -154.10161698522

Frequencies:
203.0230 358.9520 416.4127 611.6939 928.0855 1021.3523
1070.2386 1207.9916 1304.1138 1394.9384 1442.6511 1464.6353
1480.7705 3002.2161 3073.7605 3145.1418 3212.2064 3862.7012

TS FRS

C	0.749860	0.274581	0.184092
H	0.748651	-0.344326	1.068338
H	0.905210	-0.205995	-0.770392
C	0.783322	1.775953	0.294673
H	0.298070	2.236156	-0.565441
H	0.273673	2.106712	1.198916
H	1.812543	2.142856	0.324011
H	2.743408	-1.886774	-0.851318
H	3.624142	0.236257	-1.431030
C	3.066454	-1.594270	0.151612
O	3.552270	0.683867	-0.577871
H	4.102063	-1.928623	0.283426
C	2.981212	-0.120053	0.336379
H	2.446129	-2.109748	0.884250
H	3.043600	0.305051	1.331919
I	-1.771712	-0.151694	-0.050005

E(UM062X) = -244.888254533
E(PMP2) = -528.01141856
E(UMP2) = -528.00722282976

Frequencies:
-440.9637 59.0816 89.0523 113.8702 151.8087 187.7216 201.3801
237.4540 294.1970 354.5792 456.8983 474.1990 812.2063 852.4042
937.1610 957.9041 976.7599 1023.3817 1051.8526 1072.2278
1088.6646 1193.2651 1227.1688 1334.6189 1399.7650 1408.9576

1452.0059 1461.6696 1467.5062 1474.7903 1482.7085 1487.1437
3041.1139 3072.0859 3107.7378 3138.2102 3160.8368 3166.2879
3199.3421 3202.6249 3316.9522 3832.8996

TS αHab

H	3.339238	-0.120177	-1.931481
H	4.423802	-0.711283	-0.658187
C	3.516439	-0.131906	-0.854744
H	3.690806	0.897519	-0.527693
C	2.332283	-0.728142	-0.139493
H	2.047637	-1.723606	-0.480675
H	1.301846	-0.000608	-0.428552
O	2.433805	-0.757556	1.252944
H	2.840138	0.061749	1.556028
H	1.475917	2.503295	0.139992
C	0.545479	2.015750	0.447654
H	0.170763	1.188181	-1.568790
C	0.231979	0.909126	-0.519961
H	-0.238963	2.777951	0.470661
H	0.674788	1.630525	1.461492
I	-1.489689	-0.242114	-0.031266

E(UM062X) = -244.877094369
E(PMP2) = -528.01012684
E(UMP2) = -528.00429788394

Frequencies:
-1611.6687 7.0012 54.3287 94.4901 148.4745 214.3926 220.2350
261.2970 310.1435 373.8255 425.8690 487.5758 580.2041 836.8330
870.9323 919.3484 987.1096 1057.0579 1076.3013 1095.2991
1143.7024 1168.2281 1246.3742 1285.2146 1391.5038 1396.3166
1400.0603 1432.7393 1456.0089 1469.9973 1476.4514 1480.6354
1488.7440 3042.5165 3047.0653 3107.8874 3110.1587 3127.0249
3130.4914 3144.2569 3167.4855 3862.4936

TS βHab

H	0.324824	1.321531	0.405569
H	0.787121	-0.714481	1.806049
I	-1.978850	-0.001453	-0.060871
C	0.958339	-0.712640	0.732333
C	0.260459	0.327507	-0.025900
H	0.949226	-1.707879	0.293381
H	0.486054	0.340765	-1.088317
H	4.082905	-1.929658	-0.245974
H	5.081941	-0.628055	-0.921856
C	4.065615	-0.907484	-0.627158
H	3.431298	-0.887225	-1.519019

C	3.531087	0.027624	0.421448
H	4.014752	-0.022873	1.395498
H	2.285525	-0.383039	0.654007
O	3.421641	1.358947	0.041254
H	3.169300	1.406322	-0.887551

E(UM062X) = -244.878040996
E(PMP2) = -528.00828094
E(UMP2) = -528.00103206751

Frequencies:
-1483.8503 36.1971 50.5104 56.6066 140.2728 167.0211 208.4084
263.9918 362.6666 412.3768 479.6795 521.5004 617.8146 755.0461
877.5804 927.4534 1026.3201 1053.3529 1069.8009 1094.6262
1154.3429 1176.7121 1198.2237 1260.5246 1289.8571 1386.8401
1396.0310 1417.1477 1441.1028 1457.0465 1475.2491 1483.4457
1484.2825 3044.3968 3107.4496 3123.3754 3142.0402 3145.1794
3150.4880 3201.1187 3224.9487 3859.8127

$CH_3CH_2CH(OH)CH_3/HCO_3^-$

C	-1.560890	0.728817	-0.762862
H	-2.314467	0.691549	-1.555804
H	-0.592788	0.520870	-1.234568
C	-1.558534	2.114673	-0.123019
H	-1.292028	2.886216	-0.847898
H	-2.547900	2.354475	0.275738
H	-0.845937	2.171273	0.702442
H	-1.174292	-1.999859	-1.023732
H	-0.037842	-0.940350	0.764394
C	-2.065608	-1.728703	-0.449604
O	-0.798323	-0.492015	1.201780
H	-2.254800	-2.512061	0.286890
C	-1.849163	-0.388521	0.240159
H	-2.915133	-1.681369	-1.134056
H	-2.745751	-0.123842	0.811174
O	1.669514	0.972396	0.562667
H	0.809632	0.738028	0.945035
C	2.183042	-0.149141	-0.072981
O	3.270615	0.017845	-0.631526
O	1.485471	-1.194184	-0.005393

E(RM062X) = -498.199799418
E(MP2) = -497.43156392711

Frequencies:
38.4377 49.1311 76.0758 89.3328 115.2894 149.7043 203.2404
207.2179 244.5798 273.0364 387.9232 472.6059 509.3268 614.1054
649.3535 683.5316 778.6257 830.8207 840.1802 865.6475 939.7423

978.9359 983.1290 1013.1023 1059.8440 1133.2395 1153.6243
1192.0034 1280.1782 1322.2329 1327.8907 1354.6701 1368.1750
1399.6637 1404.4406 1408.7618 1462.7462 1475.5418 1488.6660
1490.9628 1499.4288 1500.3156 1724.1555 3045.0789 3052.6477
3058.8240 3059.6526 3091.7382 3127.3730 3129.5195 3137.6784
3142.5953 3359.2745 3746.2167

•CH_2CH_3

H	1.347514	0.925606	0.056667
H	-1.104446	0.893348	-0.476883
C	-0.694247	0.000243	-0.000657
C	0.793956	0.000004	-0.026192
H	-1.082645	-0.015498	1.027723
H	-1.105016	-0.878560	-0.502849
H	1.346338	-0.926380	0.056439

E(UM062X) = -79.1281384159
E(PMP2) = -78.966746697
E(UMP2) = -78.964565253981

Frequencies:
129.1431 438.3624 806.3249 978.6220 1076.4255 1189.8213
1396.0337 1460.7735 1475.0296 1477.1861 3005.1377 3085.3602
3130.1439 3167.6625 3271.3748

CH_3CHO/HCO_3^-

H	-3.571467	-1.087326	-0.875692
C	-2.545402	0.535330	0.000680
C	-2.945473	-0.898889	0.000608
O	-1.396785	0.929594	-0.001218
H	-2.079934	-1.559096	-0.001304
H	-3.360547	1.275368	0.002571
H	-3.568351	-1.088317	0.878916
O	0.678790	-0.752294	-0.001581
O	2.901132	-0.794716	0.000940
C	1.865305	-0.182829	-0.000008
H	-0.053852	-0.085473	-0.001646
O	1.780746	1.155562	0.000369
H	2.676513	1.518010	0.001399

E(RM062X) = -418.828888377
E(MP2) = -418.22157268711

Frequencies:

21.2443 49.5108 60.0709 91.9790 114.7543 178.0904 197.7896
523.1957 530.4541 582.3578 644.0679 777.8230 808.0260 851.3801
913.4094 1027.5492 1150.4326 1151.5693 1204.8418 1354.5651
1381.4231 1434.1039 1444.4894 1456.4755 1458.4088 1803.3588
1842.2827 3037.1898 3066.4795 3133.5555 3182.1507 3267.2599
3843.5898

CH_3CH_2OH/HCO_3^-

H	−2.240207	−1.667814	−0.119185
O	0.881750	−0.890972	0.559579
C	−2.866425	−0.785764	−0.274847
H	−3.542354	−0.686671	0.576945
H	−3.463001	−0.944846	−1.175985
O	2.885857	−0.529604	−0.388856
H	−0.580918	−0.029865	0.831451
C	1.765910	−0.189066	0.001692
C	−2.004549	0.457765	−0.415437
O	−1.233156	0.704248	0.753676
H	−1.343246	0.359560	−1.286015
O	1.449701	1.144899	−0.206462
H	0.554468	1.303255	0.133365
H	−2.627570	1.340199	−0.572512

E(RM062X) = −419.587064249
E(MP2) = −418.97569571277

Frequencies:
37.2366 59.2654 78.4542 107.4913 137.8690 205.8700 277.1865
436.0667 617.7427 680.8942 683.4967 801.8625 841.7166 862.4550
905.2791 981.9580 1092.5122 1122.1013 1148.3912 1306.3467
1329.2698 1358.0866 1389.2670 1413.8793 1463.1698 1485.3419
1490.7611 1516.2510 1720.8187 3026.2760 3058.8145 3105.8737
3136.0563 3140.6867 3360.2475 3719.8674

$CH_3CH_2OC\bullet(H)CH_3/\ HCO_3^-$

H	−2.798549	−2.833419	−0.290673
C	−1.394555	−1.260884	−0.396150
C	−2.712558	−1.798642	0.040655
O	−1.027162	0.015733	−0.038034
H	−2.815627	−1.785588	1.135070
H	−0.524482	−1.902442	−0.447314
H	−3.555162	−1.240055	−0.374951
H	−2.590729	0.996160	−0.960252
H	−0.723266	2.610176	−0.568479
C	−1.406882	2.354446	0.243031
C	−2.060663	1.013473	−0.003754
H	−0.852375	2.343784	1.183244

H	-2.173204	3.128161	0.303811
H	-2.763999	0.765166	0.794246
O	1.492646	0.823984	-0.363294
O	3.575512	0.096051	-0.087204
C	2.387385	-0.075411	-0.013518
H	0.569840	0.492088	-0.226209
O	1.813997	-1.203612	0.433379
H	2.511244	-1.829173	0.671159

E(UM062X) = -497.972561185
E(PMP2) = -497.20052931
E(UMP2) = -497.19859848807

Frequencies:
20.9721 33.6683 58.0731 86.2525 101.2599 106.4563 137.7636
181.7114 245.0934 252.4495 280.7617 376.0318 522.0806 533.5763
583.5291 628.3381 643.3875 806.6548 827.0508 837.9267 860.8060
953.9491 1020.0075 1026.7447 1062.2393 1116.3549 1166.2759
1178.9713 1203.7199 1256.9747 1315.3660 1366.6194 1383.7400
1400.3111 1422.8173 1436.6757 1460.7000 1468.6720 1482.6542
1486.4912 1496.2690 1523.0126 1843.8658 3007.5201 3066.0701
3071.8312 3093.8061 3116.1521 3151.5263 3152.1800 3155.0427
3222.2864 3289.3460 3842.2844

CH_2CH_2I

H	-2.259165	-1.235781	0.925990
H	-2.258558	1.236041	0.925926
I	0.678418	-0.000028	-0.000005
C	-2.243025	0.672974	0.000015
C	-2.243626	-0.672809	0.000014
H	-2.258765	1.236046	-0.925892
H	-2.259759	-1.235791	-0.925946

E(UM062X) = -89.8854092579
E(PMP2) = -373.26650947
E(UMP2) = -373.26474525877

Frequencies:
75.8026 152.6009 287.0528 826.1173 1005.2710 1013.1316
1014.7904 1233.0928 1355.3345 1464.8376 1637.7685 3168.2015
3176.7768 3256.8516 3279.6405

•$CH(I)CH_3$

H	3.404007	0.183135	-0.226947
C	2.466143	-0.324294	0.009992
H	1.450704	1.684405	0.195168
H	2.560707	-0.747342	1.018246

C	1.343170	0.643985	-0.076195
H	2.333282	-1.157799	-0.683177
I	-0.615181	-0.035482	0.001772

E(UM062X) = -89.8761743994
E(PMP2) = -373.25980518
E(UMP2) = -373.25671690348

Frequencies:
150.4451 268.5501 362.2002 561.8681 992.5700 999.4209
1114.1341 1245.9606 1397.7935 1457.5273 1469.3838 3022.9132
3095.9396 3135.9206 3233.2279

$CH_3CH_2CH(OH)CH_3/HPO_4^{2-}$

C	-3.233617	-0.394171	-0.346791
H	-3.424429	-0.684070	-1.384650
H	-4.189129	-0.059273	0.070881
C	-2.715063	-1.599116	0.438050
H	-2.665339	-1.385296	1.508338
H	-3.371367	-2.461160	0.302589
H	-1.710418	-1.877057	0.109608
H	-1.316575	0.551082	1.557619
H	-0.531579	-0.177274	-0.608134
C	-1.912686	1.296899	1.026399
O	-1.093812	0.486181	-1.109175
H	-1.324372	2.214502	0.959118
C	-2.267595	0.794814	-0.370717
H	-2.815238	1.503805	1.607610
H	-2.756955	1.606458	-0.919430
O	2.876732	-0.568387	-1.153248
O	0.676817	-0.968199	0.104120
P	2.014825	-0.189437	0.051068
O	2.763573	-0.149036	1.378460
O	1.526590	1.400636	-0.198285
H	0.657589	1.409723	-0.626197

E(RM062X) = -876.877991136
E(MP2) = -875.68138127444

Frequencies:
33.7108 54.1720 67.9881 98.8674 122.8547 128.6814 207.4334
226.1962 285.2497 296.3478 352.1917 372.6647 386.2455 440.7119
485.8673 505.1422 514.4277 527.2669 599.5695 728.7979 784.6858
807.7670 924.8346 945.7625 965.4488 997.1908 1009.7867
1027.8705 1058.5995 1117.7186 1130.2341 1158.8908 1174.9298
1208.4105 1294.1157 1352.9295 1370.8890 1378.3054 1406.0956
1415.5233 1463.9083 1469.8148 1485.4412 1495.1195 1503.9327
1509.1976 2962.1625 3047.8714 3054.4873 3058.9074 3063.1835
3092.0605 3128.0122 3132.6812 3135.2884 3136.4817 3757.2479

CH_3CHO/HPO_4^{2-}

H	4.279384	−0.672120	1.024450
C	2.844841	0.541743	0.059898
C	3.806425	−0.595619	0.041687
O	1.662156	0.435166	−0.184225
H	3.308600	−1.528104	−0.217051
H	3.256841	1.532067	0.313862
H	4.601966	−0.372601	−0.674335
H	0.294030	−0.979880	−0.672381
O	−1.008335	1.393245	−0.396077
H	−0.058117	1.490975	−0.235309
O	−2.954068	−0.203587	−0.328651
P	−1.527671	−0.078306	0.103319
O	−1.130943	−0.279491	1.538391
O	−0.653213	−1.091894	−0.841754

E(RM062X) = −797.533008203
E(MP2) = −796.49427961198

Frequencies:
24.4492 38.5973 54.5974 94.5818 118.9255 143.3504
162.6986 335.1850 349.2031 428.9921 457.2054 486.5542
501.1787 528.5484 550.0774 783.2948 809.5481 817.7053
914.9530 1065.0952 1084.1436 1145.1056 1149.0435 1150.3055
1266.0588 1378.4598 1433.2760 1453.0756 1456.8354 1816.1330
3021.3249 3067.2931 3134.2281 3184.4138 3774.2950 3786.9383

CH_3CH_2OH/HPO_4^{2-}

H	−2.870029	1.573319	−0.507755
C	−3.485039	0.751339	−0.133604
H	−4.062313	0.345568	−0.967375
H	−4.180827	1.152747	0.607405
H	−1.011108	−0.174248	−0.663321
C	−2.605958	−0.329482	0.478856
O	−1.701313	−0.878563	−0.461308
H	−2.055205	0.082547	1.335093
H	−3.225202	−1.148980	0.853318
O	0.243826	0.793024	−0.707563
O	2.302775	1.085426	0.818502
P	1.485777	0.138222	−0.049900
H	−0.008233	−1.300447	0.683647
O	2.301194	−0.699810	−1.032896
O	0.812548	−0.941949	1.050262

E(RM062X) = −798.266604318
E(MP2) = −797.22686058156

Frequencies:
41.2995 44.0681 56.9782 104.0569 128.8732 221.2014
284.5652 354.3258 365.8555 432.9688 492.7183 502.7665
511.3960 525.7492 726.8328 799.8769 904.6134 951.8183
987.0708 1055.5212 1091.6894 1119.8040 1133.0520 1150.7937
1202.4749 1312.3819 1385.4400 1410.5994 1472.3239 1485.4821
1511.5690 1517.8449 2891.1967 3024.0955 3055.6676 3085.8280
3132.3363 3134.8124 3778.8107

I^-

E(RM062X) = -11.52713145
E(MP2) = -295.06065755006

$I^\bullet$

E(UM062X) = -11.30845567
E(PMP2) = -294.84884460
E(UMP2) = -294.84720689399