

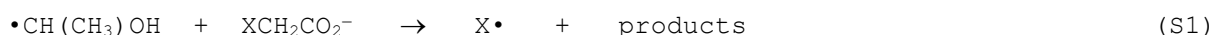
Electronic Supplementary Information

Proton-Coupled Electron Transfer is the Dominant Mechanism of Reduction of Haloacetates by the α -Hydroxyethyl Radical in Aqueous Media

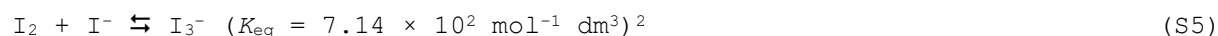
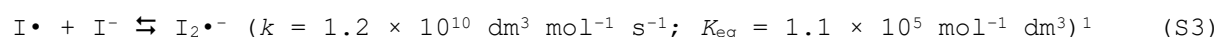
by Iva Džeba, Marija Bonifačić, Ivana Nikšić-Franjić, and Ivan Ljubić

Details of the procedure used to detect the presence of halogen atoms

For the reaction of the $\cdot\text{EtOH}$ radical with XAc^- , $\text{X} = \text{I}$ or Br , we designed an experimental procedure to detect whether halogen atoms, $\text{I}\cdot$ or $\text{Br}\cdot$, may be formed in the system as transient species:



This has been tested by irradiating the solutions which additionally contained 1 mmol dm^{-3} of potassium iodide, KI. This amount of iodide ions cannot appreciably interfere with any of the primary or secondary reactions but, provided halogen atoms are formed, should efficiently scavenge them and end up converted into a stable product, the triiodide ion I_3^- . The relevant reactions and the corresponding rate constants are:



As a much stronger oxidant, bromine atom is expected to convert the iodides to $\text{I}\cdot$ either directly or after the intermediate equilibration and formation of the $\text{BrI}\cdot^-$ ion:



We note that under the present reaction conditions the abstraction of H-atom from ethanol by $\text{Br}\cdot$ or $\text{I}\cdot$ is slower than the reaction with I^- . For

example, for the more reactive $\text{Br}\cdot$ the rate constant for the abstraction is:



After irradiation, the concentration of KI was increased to 0.3 mol dm^{-3} in order to push the equilibrium (S5) to the side of I_3^- . The latter ion is a strongly absorbing species with $\epsilon = 2.54 \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$ at 350 nm .² No such absorption was observed in the case of BrAc^- . For IAc^- , which is somewhat less stable and undergoes a slow hydrolysis in aqueous solutions, some traces of I_3^- were always present but in concentrations identical to the ones measured for the non-irradiated blind samples. Therefore, we conclude that the formation of transient halogen atoms does not take place in these systems.

- (1) Neta, P., Huie, R.E., Ross, A.B., J. Phys. Chem. Ref. Data, 17 (1988) 1027.
- (2) Picardi, G., Guidelli, R., J. Phys. Chem. 72 (1968) 2782; Buxton, G.V., Sellers, J. Chem. Soc., Faraday Trans. 1, 81 (1985) 449; Štefanić, I., Asmus, K.-D., Bonifačić, M., Phys. Chem. Chem. Phys. 5 (2003) 2783.
- (3) Merenyi, G., Lind, J., J. Am. Chem. Soc. 116 (1994) 7872.

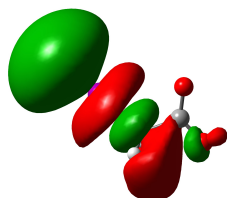


Figure S1. The lowest unoccupied molecular orbital (LUMO) of iodoacetate.

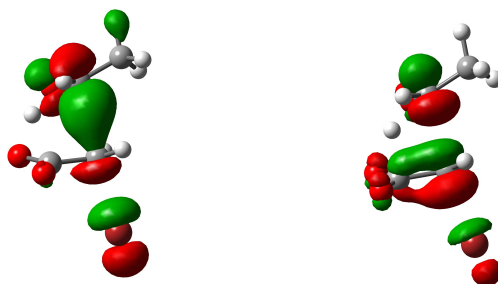


Figure S2. The SOMO and LUMO of the PCET transition state in the reaction of $\cdot\text{EtOH}$ with BrAc^- .

Cartesian coordinates (Å), final SCF energies (a.u.), and harmonic frequencies (cm⁻¹) calculated at the M06-2X-D3-PCM/6-311+G(2d,p) level of theory. The atoms are referenced by their atomic numbers.

•EtOH

1	-1.305175	-0.992398	-0.693189
1	1.979329	0.170388	0.038554
6	-1.225643	-0.163111	0.014179
8	1.163426	-0.340321	0.015967
1	-1.387230	-0.574934	1.019511
6	0.091413	0.505538	-0.105181
1	-2.028501	0.544080	-0.191267
1	0.239550	1.520873	0.244670

E = -154.362934925

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

•EtOH/HCO₃⁻

1	-3.450931	1.005164	-0.781387
1	-3.984000	-0.473047	0.017623
6	-3.355099	0.413084	0.140282
1	-3.757212	1.007896	0.960608
6	-1.945410	0.028732	0.412570
8	-1.385055	-0.814101	-0.489852
1	-1.267840	0.730111	0.892009
1	-0.402041	-0.886285	-0.298317
8	1.178492	1.094267	-0.392958
8	1.126948	-1.061968	0.086908
6	1.848759	-0.038398	0.033293
1	1.825005	1.809980	-0.391915
8	3.048055	0.080012	0.306466

E = -418.938458575

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

•EtOH/HPO₄²⁻

1	4.227889	-0.009155	-0.718274
1	3.975136	-0.119410	1.022576
6	3.612964	-0.486438	0.058296
1	3.792089	-1.560919	0.010226
6	2.165859	-0.183007	-0.115828
8	1.800831	1.104061	0.031805
1	1.568722	-0.773805	-0.810679

8	-1.278272	-1.188985	-1.070341
8	-0.602894	1.201078	-0.517027
1	0.773925	1.180726	-0.213023
15	-1.403591	-0.050051	-0.078689
1	0.287262	-0.731982	1.122959
8	-0.644425	-0.548506	1.316895
8	-2.805753	0.280101	0.377634

E = -797.644940773

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

FAC⁻ (eclipsed conformation)

8	-0.616863	1.311315	0.000003
1	0.755568	-1.317615	-0.889108
6	-0.639658	0.067419	-0.000028
6	0.693288	-0.689373	-0.000006
9	1.798011	0.156861	0.000009
8	-1.635011	-0.691914	0.000014
1	0.755543	-1.317617	0.889096

E = -327.855073859

105.8463 262.7451 495.1927
 593.1317 686.0227 927.6169
 1036.6502 1077.3070 1273.0502
 1360.5630 1455.4764 1474.1223
 1655.3948 3089.2400 3145.0552

FAC⁻ (staggered conformation)

1	1.031152	0.898221	1.187269
6	0.814476	-0.000390	0.611820
9	1.677373	0.000103	-0.495711
1	1.030998	-0.899621	1.186356
6	-0.630741	0.000017	0.078116
8	-1.141575	-1.122369	-0.128412
8	-1.141039	1.122708	-0.128069

E = -327.848559705

-84.9123 267.3109 433.4769
 636.8626 813.7486 946.4977
 1024.3254 1041.2587 1249.4446
 1366.6292 1464.0805 1499.3384
 1644.3319 3096.9759 3163.2114

FAC⁻/H₂O

8	0.198472	-1.038343	0.000618
1	-1.814727	1.138135	-0.889251
6	-0.113285	0.163490	0.000293

6	-1.592639	0.547477	-0.000060
9	-2.429410	-0.560286	-0.000451
8	0.656780	1.159800	0.000236
1	-1.815189	1.137877	0.889194
1	2.507680	-1.051425	-0.000093
8	3.013303	-0.229542	-0.000473
1	2.274029	0.416866	-0.000228

E = -404.298474858

28.9128 73.8205 95.1034
 198.5679 272.1866 320.4150
 347.1844 509.3912 589.4140
 693.0072 740.1513 936.1450
 1038.7818 1088.3077 1270.5083
 1356.6465 1461.7189 1475.3765
 1648.5608 1687.4598 3091.8095
 3147.3917 3470.0590 3868.9169

ClAc⁻ (eclipsed conformation)

8	0.953376	1.327206	-0.000004
1	-0.171139	-1.436413	0.885091
6	1.078091	0.092175	0.000015
6	-0.175730	-0.806421	-0.000001
17	-1.750066	0.071030	0.000000
8	2.131527	-0.583358	-0.000004
1	-0.171130	-1.436393	-0.885108

E = -688.217083960

56.9779 229.8545 420.3686
 574.9004 666.3335 768.1635
 926.0936 952.8297 1194.6180
 1269.6683 1412.8968 1440.5621
 1661.6833 3127.4851 3190.8179

ClAc⁻ (staggered conformation)

1	0.362429	0.897405	1.472095
6	0.258129	-0.000117	0.871335
17	1.659259	0.000015	-0.276827
1	0.362409	-0.897795	1.471866
6	-1.049929	0.000006	0.055605
8	-1.511405	-1.122586	-0.237541
8	-1.511276	1.122686	-0.237403

E = -688.214296511

-27.9269 204.9672 432.5499
 602.5477 700.5693 844.2617
 933.2466 948.0987 1152.9253
 1270.6316 1419.6443 1469.5687
 1649.9503 3135.1476 3210.0717

ClAc⁻/H₂O

8	0.547725	-0.955271	0.000126
1	-1.214922	1.450539	-0.885087
6	0.358148	0.269505	0.000057
6	-1.070415	0.837290	-0.000043
17	-2.375885	-0.398308	-0.000032
8	1.223009	1.183721	0.000063
1	-1.215008	1.450648	0.884910

1	2.803231	-1.203116	-0.000048
8	3.418736	-0.459409	-0.000103
1	2.774591	0.280077	-0.000015

E = -764.660237442

43.3573 62.2989 63.6729
 197.1796 214.9340 332.8326
 357.7823 437.5893 574.0604
 671.9821 724.5372 779.6272
 936.8040 954.4247 1196.6286
 1271.4593 1419.0797 1441.5229
 1652.6315 1688.8242 3129.4165
 3191.8028 3506.3144 3860.5371

BrAc⁻ (eclipsed conformation)

8	1.478945	1.330754	0.000001
1	0.436873	-1.471283	0.886034
6	1.638875	0.100667	0.000000
6	0.420058	-0.844458	0.000003
35	-1.335588	0.032027	-0.000001
8	2.710833	-0.545210	-0.000002
1	0.436873	-1.471289	-0.886024

E = -2802.18521788

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

BrAc⁻ (staggered conformation)

1	-0.293474	0.899111	1.574636
6	-0.357691	-0.000235	0.972405
35	1.273067	0.000013	-0.132266
1	-0.293495	-0.899871	1.574203
6	-1.584439	0.000014	0.042149
8	-2.019964	-1.122504	-0.288080
8	-2.019735	1.122706	-0.287778

E = -2802.18348683

20.8801 165.8472 432.4985
 535.9951 667.2088 824.3875
 918.0141 930.8875 1123.9123
 1233.0333 1409.6374 1464.1925
 1650.5996 3143.0438 3222.9211

BrAc⁻/H₂O

8	-1.121895	-0.905330	0.000002
1	0.475072	1.620905	0.885920
6	-1.013974	0.328676	0.000001
6	0.367286	1.002931	0.000000
35	1.897162	-0.216879	0.000000
8	-1.937789	1.183858	0.000000
1	0.475071	1.620905	-0.885920
1	-3.368812	-1.301536	-0.000002
8	-4.024954	-0.593664	-0.000001
1	-3.424784	0.181940	-0.000002

E = -2878.62825376

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

IAc⁻ (eclipsed conformation)

8	1.856018	1.332050	0.000095
1	0.881694	-1.499871	0.884894
6	2.044362	0.105386	0.000009
6	0.847696	-0.871041	0.000201
53	-1.113763	0.019551	-0.000024
8	3.133192	-0.512316	-0.000181
1	0.881724	-1.500295	-0.884187

E = -239.357099184

28.7460 164.4122 336.5668
550.6090 651.1833 657.1170
881.7156 909.8751 1147.0723
1198.0653 1396.5538 1425.1379
1656.6973 3132.8232 3199.7061

IAc⁻ (staggered conformation)

1	-0.759302	0.897681	1.623829
6	-0.793942	-0.000834	1.017317
53	1.064754	0.000046	-0.082639
1	-0.759282	-0.900432	1.622149
6	-1.972385	0.000050	0.028616
8	-2.394936	-1.121998	-0.321905
8	-2.394490	1.122626	-0.320808

E = -239.356982346

39.1487 147.1226 433.0031
491.7805 662.3895 812.2352
871.0346 926.6536 1102.8020
1187.9423 1397.5086 1458.0489
1645.0380 3140.9585 3220.6305

IAc⁻/H₂O

8	-1.545810	-0.875133	-0.000396
1	-0.059856	1.723275	0.884182
6	-1.491210	0.362714	-0.000158
6	-0.139700	1.098072	-0.000116
53	1.610828	-0.148258	0.000049
8	-2.455969	1.172557	0.000042
1	-0.059758	1.723160	-0.884490
8	-4.470674	-0.681654	0.000254
1	-3.881094	0.103237	0.000232
1	-3.808068	-1.382861	-0.000079

E = -315.800219948

13.1377 42.8326 51.0456
152.4122 182.4659 305.0276
316.4280 360.7779 552.9211
658.4011 669.0223 734.9274
879.2010 923.9534 1154.2759
1200.2879 1400.6435 1429.7457
1645.0941 1685.1742 3133.4190
3199.3833 3476.2684 3872.3112

TSF-PCET

1	-2.141943	1.859202	0.080472
1	0.091003	-1.192389	-1.288899
6	-2.275519	0.995705	0.731210
8	-1.851816	-0.397208	-1.174256
1	-3.341232	0.896159	0.964137
6	-1.828550	-0.257060	0.041469
1	-1.742640	1.135523	1.671261
1	-1.592570	-1.117031	0.688154
8	1.268513	-0.933771	1.467891
1	0.689732	1.530503	0.752475
6	0.901638	-0.536708	0.341214
6	0.841975	0.840113	-0.069065
9	2.288675	1.359565	-0.592209
8	0.751409	-1.500700	-0.649726
1	0.257463	1.053078	-0.957955

E = -482.198281206

-423.4921 52.8248 78.6037
106.5133 134.3990 158.6158
179.1911 188.9566 240.8019
278.9060 422.4589 456.4984
514.6736 564.9918 637.1659
788.3776 880.5281 913.9822
982.8339 1053.4813 1123.9407
1130.7179 1220.1736 1234.3688
1292.3717 1372.2673 1413.6784
1452.9321 1464.2675 1467.6263
1597.5405 1716.0674 3012.3051
3047.6468 3122.2832 3137.5746
3166.0124 3225.1202 3763.9178

TSF-HAT

1	-2.847341	1.082565	-0.839157
1	-0.712664	-1.572347	-0.365093
6	-2.844931	0.749955	0.200787
8	-1.649062	-1.253473	-0.360385
1	-3.780422	0.212080	0.385122
6	-1.664779	-0.136220	0.463088
1	-2.821183	1.625111	0.850515
1	-1.492506	-0.371833	1.518602
8	2.551330	-0.222264	0.642807
1	-0.548484	0.502921	0.121724
6	1.504758	-0.458449	0.018866
6	0.681541	0.690022	-0.496950
9	1.169031	1.932817	-0.192451
8	0.999450	-1.596732	-0.220567
1	0.408045	0.634055	-1.549248

E = -482.200070769

-1687.1450 56.1710 76.8296
 124.3962 157.5404 191.9551
 225.0400 235.0739 280.4346
 433.5927 502.9836 528.1227
 689.1297 716.3467 771.5491
 878.9372 929.1340 955.9610
 1008.6568 1094.3400 1127.4230
 1159.1623 1183.9472 1309.4640
 1340.6440 1391.8582 1401.2554
 1433.9811 1464.3197 1475.4016
 1484.7963 1527.3318 1645.1805
 3040.3626 3047.3195 3106.3924
 3141.2418 3142.7608 3284.6955

TSF-FRS

1	1.912763	-0.660137	-1.659185
1	2.211994	1.604008	1.014833
6	1.801488	-1.087315	-0.661253
8	2.297295	1.036518	0.238114
1	2.757291	-1.533645	-0.371137
6	1.456623	-0.019960	0.320524
1	1.034312	-1.856422	-0.681009
1	1.190727	-0.321181	1.332346
8	-1.356549	-1.339425	-0.694589
1	0.026114	0.871839	-1.177428
6	-1.074923	-0.559384	0.234942
6	-0.286154	0.701174	-0.156136
9	-1.912765	1.553850	-0.600901
8	-1.332798	-0.671122	1.451058
1	-0.164105	1.496019	0.564562

E = -482.174089269

-435.6329 27.0953 110.5477
 161.9976 167.2319 201.6419
 210.8553 247.0831 278.2869
 410.6394 448.4325 475.4541
 488.9759 662.0091 806.2683
 881.0839 914.0207 951.5718
 989.3727 1061.5951 1088.9354
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 1484.5816 1653.4053 3055.2037
 3122.4334 3137.2701 3162.2710
 3187.1588 3283.6014 3843.4635

TSF-FRS/H₂O

1	-0.636003	2.975196	-0.799245
1	-1.895471	-0.358795	-0.366145
6	-0.872245	2.653142	0.215686
8	-1.704421	0.595012	-0.590689
1	-1.867240	3.028230	0.470206
6	-0.892830	1.159589	0.299870
1	-0.151391	3.078189	0.910352
1	-0.894936	0.708558	1.293397
8	0.957911	-1.078248	1.445948
1	1.344486	1.362368	0.586525
6	0.802916	-0.796248	0.246628
6	0.946675	0.665778	-0.136371
9	2.802341	0.316028	-0.582685

8	0.482054	-1.583906	-0.685924
1	0.829816	0.975277	-1.164730
1	-2.563506	-2.460720	-0.595535
8	-2.013263	-1.951949	0.008578
1	-1.072165	-2.093387	-0.268839

E = -558.625973589

-287.4278 46.1955 80.0811
115.8370 143.2369 160.5255
173.7625 192.3171 213.7581
247.5250 250.0902 281.7350
340.5919 412.2597 459.5676
482.2584 512.5089 669.8515
689.9980 814.1270 917.4237
932.2033 963.2433 979.4327
1037.6875 1065.5570 1079.4937
1116.0040 1160.6594 1271.7646
1358.2973 1390.9442 1412.4046
1454.7718 1471.7189 1480.8589
1540.2778 1610.6730 1660.0563
3057.6845 3060.0590 3112.9702
3130.3714 3170.8295 3173.5914
3280.7291 3294.8210 3905.5002

TSF-XA

8	-2.263374	0.951555	-0.904521
1	-1.119087	-1.301249	-1.472080
6	-2.136488	0.041333	-0.042937
6	-1.289464	-1.131592	-0.417515
9	0.337710	-0.584475	0.041938
8	-2.630067	0.042413	1.116253
1	-1.362338	-2.012635	0.205735
1	2.928285	1.996796	0.274190
1	1.774688	1.542164	-0.991481
6	1.994211	1.459975	0.074265
1	1.194156	1.931757	0.641664
6	2.115900	0.037220	0.455269
8	2.932477	-0.683611	-0.334277
1	2.066905	-0.255823	1.496054
1	3.060766	-1.565210	0.034330

E = -482.156552533

-1235.7893 33.1360 48.7034
55.1429 118.0993 144.2371
195.4968 238.6974 289.6998
405.3177 423.3662 452.9145
464.9513 657.9321 778.5327
817.6286 836.0866 939.7882
964.9426 1021.7886 1029.4060
1042.0399 1085.1805 1230.2310
1292.6516 1367.5110 1391.7322
1461.2029 1465.6962 1467.8198
1499.5424 1587.1568 3035.6539
3111.4455 3164.0342 3165.2452
3203.1744 3266.6692 3864.9156

TSF-OA

6	2.640583	-0.378384	-0.576801
6	1.571948	-0.576154	0.443242

8	1.308803	0.474013	1.284095
1	2.428487	0.517293	-1.164374
1	2.672883	-1.233595	-1.253016
1	3.626598	-0.267642	-0.111558
1	1.580022	-1.511878	0.992350
1	1.007697	1.212278	0.721798
8	-0.324159	1.536147	-0.709799
1	-2.453810	1.076568	0.595789
6	-1.894998	0.150229	0.476796
6	-0.702533	0.343341	-0.408864
9	-2.799483	-0.804755	-0.066857
1	-1.610395	-0.256746	1.452349
8	0.047089	-0.701118	-0.604028

E = -482.174667209

-885.6404 28.6495 62.2234
95.2977 175.4365 205.3500
222.7168 294.3312 376.7275
454.5175 469.6485 537.7951
576.7785 707.5428 849.3554
886.6360 919.1339 954.4448
1013.3588 1049.5447 1101.7739
1167.0256 1218.9843 1254.5614
1343.3113 1351.7975 1393.1664
1449.7704 1468.0748 1470.7109
1475.5520 1505.1926 3026.1716
3042.7706 3099.0416 3135.7281
3146.9160 3171.7207 3633.7908

TSF-PCET/HCO₃⁻

8	2.719064	-0.358961	0.999619
1	2.009507	-0.573410	-1.527597
6	1.580604	-0.608790	0.574159
6	1.297981	-0.950233	-0.805260
9	1.629886	-2.584014	-0.978270
8	0.563427	-0.700138	1.458202
1	0.258851	-0.970512	-1.102476
1	2.031209	3.311926	-0.780472
1	2.614418	1.991367	0.253463
6	2.066139	2.223860	-0.661414
1	2.591259	1.799124	-1.516028
6	0.665004	1.704556	-0.563731
8	-0.052016	1.945149	0.419689
1	0.207097	1.301249	-1.477966
1	-1.614247	1.318923	0.195147
8	-1.754077	-0.967056	0.297294
8	-3.879162	-0.638450	-0.320174
6	-2.744238	-0.247598	-0.016559
1	-0.319264	-0.730275	0.991178
8	-2.552329	1.104076	-0.028878

E = -746.776737709

-516.8933 20.8814 49.5048
69.3531 82.6729 110.5310
113.2656 141.8140 146.5954
159.1518 174.0183 180.6434
207.3969 214.0957 222.9263
354.8452 479.7223 522.0545
623.7010 635.1571 687.2667

691.4125 779.5383 846.2575
 913.8681 923.7289 943.6928
 949.7763 992.5142 1031.2484
 1033.1834 1086.5768 1125.1619
 1167.9102 1240.7476 1351.9514
 1360.3699 1366.6807 1403.4251
 1421.3615 1457.3180 1463.4366
 1470.6650 1579.0838 1675.7621
 1689.4572 3022.0882 3040.6177
 3066.2896 3111.2759 3154.6015
 3169.5454 3271.3221 3304.1978

TSF-PCET/HPO₄²⁻

8	-2.953327	-0.625096	-1.100755
1	-2.308082	-0.405311	1.415341
6	-1.782429	-0.796367	-0.690107
6	-1.521716	-0.768791	0.771953
9	-1.745650	-2.459602	1.173584
8	-0.783203	-1.036362	-1.449529
1	-0.499333	-0.697229	1.112575
1	-2.691911	3.193268	0.624318
1	-3.264402	1.648406	-0.030969
6	-2.601189	2.103748	0.709750
1	-2.928819	1.811777	1.708183
6	-1.182159	1.688303	0.449952
8	-0.641850	1.964525	-0.664941
1	-0.533891	1.485395	1.308913
8	1.662062	0.168603	1.507457
8	1.821065	1.216527	-0.805563
1	0.847210	1.477755	-0.716292
15	2.246637	-0.022058	0.132764
1	0.594966	-1.155790	-0.864028
8	1.573452	-1.294243	-0.575396
8	3.736866	-0.175497	0.018598

E = -1125.48226148

-587.1625 37.5693 49.5984
 86.6251 92.6525 102.9654
 124.3030 129.4716 149.2780
 158.5171 180.7954 181.7881
 199.7481 206.7934 244.8841
 372.1250 376.3344 378.8976
 486.5225 495.1586 500.7640
 517.6609 523.9343 679.7609
 773.7280 783.7229 852.7605
 887.4709 926.5156 973.9711
 983.1407 994.6322 1033.5122
 1044.5818 1072.9170 1099.0973
 1115.3393 1140.8201 1188.6795
 1260.5309 1347.3159 1374.9747
 1387.0450 1410.9949 1459.2329
 1466.6424 1470.7726 1536.1536
 1581.7886 2514.8544 2795.6216
 3016.7997 3066.6257 3080.7331
 3133.3197 3177.6172 3295.8718

TSF-HAT/HCO₃⁻

1	-2.906997	2.286347	1.132422
1	0.465176	1.508075	0.199182
6	-2.654542	2.392596	0.075215

8	-0.349197	1.957227	0.549989
1	-2.504774	3.455971	-0.133519
6	-1.417753	1.601891	-0.244240
1	-3.497547	2.039865	-0.520362
1	-1.168958	1.560544	-1.310109
8	-0.358819	-2.237845	-0.841839
1	-1.718411	0.350587	0.029468
6	-0.655630	-1.621486	0.197292
6	-2.002617	-0.988738	0.309198
9	-2.905458	-1.357298	-0.657333
8	0.096751	-1.391675	1.191318
1	-2.467351	-0.987940	1.291447
8	1.774080	0.941708	-0.595420
1	1.627241	-0.931270	0.754537
6	2.797515	0.317036	-0.194622
8	2.598163	-0.755551	0.619976
8	3.978885	0.576849	-0.472041

E = -746.774952904

-1605.3285 34.9028 39.9833
56.3275 65.3251 68.6516
82.4567 108.3404 143.8829
151.1232 161.0314 199.3162
208.3562 238.2126 280.6704
450.4210 510.6186 552.1461
636.8351 681.7357 693.3899
711.8651 837.9110 862.9465
887.6966 935.9936 941.4621
974.0456 995.9563 1033.8490
1098.4620 1119.4725 1166.1111
1194.1884 1298.3707 1335.0366
1342.4861 1363.5458 1391.4945
1400.4936 1432.6652 1448.6134
1469.8229 1486.2788 1521.4273
1629.4485 1662.0159 3042.8252
3047.4037 3108.6213 3134.7108
3138.3751 3164.6426 3171.5601

TSF-HAT/HPO₄²⁻

1	3.295740	2.430945	-0.719199
1	-0.288955	1.724190	-0.626554
6	2.789278	2.501116	0.246413
8	0.660310	2.109208	-0.780652
1	2.591146	3.557643	0.449564
6	1.507623	1.710654	0.218482
1	3.460225	2.120181	1.017672
1	1.023336	1.623394	1.197792
8	1.200627	-2.462435	0.715998
1	1.896286	0.487971	-0.025899
6	1.323658	-1.727908	-0.283089
6	2.468159	-0.772558	-0.343820
9	3.434696	-0.951782	0.617078
8	0.533610	-1.643699	-1.269428
1	2.922550	-0.612180	-1.318107
8	-2.118340	-1.185815	-0.733679
1	-1.157172	-1.343414	-0.858063
8	-1.815997	-0.142814	1.574951
8	-3.913226	0.286512	0.167224
15	-2.403179	0.141675	0.200870
8	-1.689490	1.312088	-0.513399

E = -1125.47615667

-1597.7984 50.4188 65.8407
76.0339 97.0339 106.4222
117.9265 131.0832 139.7217
152.7346 176.5881 213.3539
223.5314 239.5074 283.4418
368.2578 395.9643 460.6864
506.9264 516.4784 523.6268
549.1295 551.9916 700.3890
706.8966 750.7808 784.4918
895.3616 938.2318 959.4518
966.5564 997.2716 1049.3395
1103.8425 1115.6527 1118.2205
1120.0365 1168.1605 1213.2620
1221.0768 1303.4337 1362.7824
1389.5176 1408.9925 1436.4989
1451.3760 1469.9061 1486.1657
1580.4159 1620.3234 2408.5317
3041.4967 3050.9015 3105.7664
3134.9820 3157.9825 3452.4787

TSC1-PCET

1	2.059869	-2.134853	0.057403
1	0.805874	1.081629	-1.124451
6	2.576259	-1.339059	0.601743
8	2.019205	0.264101	-1.121440
1	3.650759	-1.467391	0.414508
6	2.111512	0.003274	0.134925
1	2.405228	-1.468188	1.671135
1	2.137198	0.832775	0.850828
8	-0.918461	1.540534	1.272302
1	-0.463728	-1.049223	1.157914
6	-0.478077	0.941661	0.302353
6	-0.559720	-0.545468	0.205560
17	-2.409683	-0.957645	-0.286211
8	-0.040539	1.585306	-0.778491
1	-0.012075	-0.996761	-0.608194

E = -842.572880631

-771.2322 53.8020 68.7410
103.2392 130.2162 168.6892
192.3808 204.7096 293.9280
345.1730 461.6003 479.2475
605.2505 666.5320 715.2702
872.4743 922.1258 948.8801
997.3734 1018.7134 1068.4027
1119.7083 1142.6359 1187.0654
1342.7886 1386.4339 1434.2781
1456.7061 1467.3214 1483.7410
1558.4945 1700.8713 2296.4251
3002.7941 3044.3808 3069.8186
3132.3037 3178.9000 3278.8331

TSC1-PCET/H₂O

1	-1.078615	2.690771	-0.985198
1	-2.459597	-0.979946	-0.259939
6	-1.452789	2.540948	0.033329
8	-2.476724	0.422022	-0.512455

1	-2.375487	3.134605	0.120410
6	-1.697750	1.085797	0.300289
1	-0.724553	2.957233	0.732653
1	-1.609003	0.740610	1.336650
8	0.383821	-0.972997	1.490726
1	1.349993	1.334912	0.812210
6	0.503856	-0.579263	0.345886
6	1.320706	0.632468	-0.011975
17	3.053722	0.099162	-0.288878
8	0.075821	-1.245287	-0.720399
1	0.995188	1.093998	-0.936312
1	-2.799388	-2.488932	-0.761565
8	-2.296281	-2.013913	-0.093648
1	-0.749040	-1.767291	-0.466957

E = -919.013119280

-127.4249 51.7363 68.2093
77.0073 113.0878 122.7590
148.9163 173.8763 190.5988
221.8485 277.6019 301.4071
377.6749 427.9495 454.9088
528.5696 624.7013 637.2183
657.1962 723.7888 824.7592
923.2811 938.5977 952.7375
1012.0003 1114.1037 1142.7017
1191.7001 1246.5194 1253.3540
1330.2014 1378.8953 1427.5388
1453.7820 1459.7022 1483.8985
1497.4495 1700.3552 1726.7701
2070.7907 2935.3328 2970.8996
3031.1386 3045.2482 3112.1347
3159.1717 3240.5553 3908.8088

TSC1-HAT

1	-2.675314	1.547293	-0.808413
1	-1.327956	-1.591434	-0.401320
6	-2.752224	1.207155	0.226174
8	-2.145651	-1.034999	-0.383983
1	-3.796488	0.940847	0.417899
6	-1.856175	0.027985	0.456739
1	-2.482492	2.029473	0.889218
1	-1.740611	-0.264910	1.505857
8	2.170592	-1.166272	0.664719
1	-0.622589	0.358284	0.123067
6	1.114015	-1.093621	0.022443
6	0.616355	0.240903	-0.486258
17	1.575666	1.672027	-0.100842
8	0.324861	-2.047190	-0.254942
1	0.328883	0.249154	-1.532939

E = -842.564518221

-1623.8233 50.0573 74.3818
102.7218 139.2180 188.4981
203.2772 225.2262 235.6920
431.8311 432.7873 513.8622
681.0435 707.3591 771.2704
820.0829 879.0522 930.9395
966.8527 970.5294 1092.4622
1155.8692 1186.4520 1230.0363

1339.5823 1374.3513 1394.5225
1410.9811 1461.5795 1472.3624
1484.4460 1509.9465 1648.0571
3041.4956 3045.4801 3107.6723
3142.4909 3176.2471 3293.2086

TSC1-FRS

1	-2.271637	-0.387830	-1.820964
1	-2.159897	-1.718403	1.408358
6	-2.357760	0.355609	-1.026846
8	-2.314196	-1.464779	0.489639
1	-3.413622	0.632414	-0.934873
6	-1.885013	-0.213015	0.259105
1	-1.778650	1.239417	-1.285462
1	-1.770343	0.424800	1.130472
8	0.532479	1.790422	-0.752942
1	0.041944	-0.794259	-0.985155
6	0.500695	1.057738	0.257100
6	0.275676	-0.430595	0.004284
17	2.433192	-0.979160	-0.286310
8	0.602729	1.391827	1.457280
1	0.218257	-1.108604	0.841212

E = -842.562216173

-441.1000 35.5861 94.2979
117.3949 138.2196 165.7534
180.7381 205.3372 230.8336
351.1105 443.1470 463.9186
494.9454 659.6354 794.5413
855.1253 916.8733 952.5320
969.1948 1024.4770 1045.6526
1082.9142 1100.7477 1246.6006
1297.2826 1356.7863 1391.3402
1447.8981 1461.6112 1472.3154
1498.5635 1650.0122 3040.9997
3114.8040 3165.5164 3175.4771
3188.5943 3313.9401 3851.1696

TSC1-FRS/H₂O

1	-0.778768	2.998229	-0.706312
1	-2.304856	-0.252068	-0.563211
6	-1.177357	2.670214	0.255274
8	-2.053678	0.701297	-0.737284
1	-2.151050	3.151650	0.395736
6	-1.356958	1.194549	0.272125
1	-0.515163	2.996504	1.054325
1	-1.421510	0.666196	1.220703
8	0.415328	-1.143503	1.593091
1	1.025029	1.255064	0.761862
6	0.408926	-0.868763	0.381222
6	0.791989	0.539081	-0.009784
17	2.968224	0.148577	-0.375675
8	0.072940	-1.632999	-0.568689
1	0.644090	0.874884	-1.024368
1	-2.983636	-2.332696	-0.806645
8	-2.490635	-1.812045	-0.164550
1	-1.525183	-1.996067	-0.319196

E = -919.014993290

-367.6711 38.7051 78.4520
 103.5076 114.1107 127.7447
 143.4752 161.8392 191.3526
 217.7729 237.5040 257.2298
 352.7659 361.9225 457.2171
 476.2029 518.8165 664.5156
 722.7018 798.3104 851.2169
 943.0347 960.3118 969.4586
 999.6034 1038.7656 1057.6259
 1066.5800 1123.4798 1269.1083
 1361.1540 1393.0868 1420.0166
 1455.6799 1466.8856 1483.8011
 1558.1076 1611.2490 1661.2918
 2992.1196 3043.8535 3112.6513
 3149.7770 3169.2156 3197.5564
 3202.0477 3324.0042 3905.3593

TSC1-XA

8	-2.634629	-0.272720	-1.363511
1	-1.761868	-1.887342	0.446084
6	-2.432687	0.121338	-0.187734
6	-1.742973	-0.844605	0.739401
17	0.325131	-0.419090	0.502270
8	-2.729851	1.245977	0.286888
1	-1.858733	-0.657306	1.800127
1	3.529580	1.785247	-0.241224
1	1.952158	1.649805	-1.039803
6	2.491447	1.463850	-0.109893
1	2.041254	2.050502	0.688399
6	2.451238	0.014693	0.225244
8	2.890650	-0.770547	-0.788830
1	2.775282	-0.287682	1.216891
1	2.983587	-1.682027	-0.487561

E = -842.556726357

-543.5576 -16.0401 50.2627
 55.6130 101.4324 157.2062
 215.9913 232.6833 245.9041
 406.2052 414.6971 439.7901
 460.0650 653.5666 773.3337
 779.8579 902.4794 942.5969
 953.9054 1009.7028 1023.2311
 1057.0198 1102.9512 1223.4402
 1292.4034 1375.0215 1391.1310
 1459.6926 1463.3468 1469.1135
 1482.1577 1603.6960 3047.6533
 3119.9639 3148.7180 3157.1701
 3170.1647 3247.9954 3858.5553

TSC1-OA

6	-2.996583	-0.884767	0.245853
6	-2.218598	-0.022229	-0.677565
8	-1.992469	1.266778	-0.335520
1	-2.581879	-0.819864	1.253464
1	-2.946508	-1.922567	-0.083685
1	-4.050384	-0.583223	0.279487
1	-2.342063	-0.138405	-1.746668
1	-1.648041	1.272223	0.576385
8	-0.055050	0.308645	1.496155

1	1.675654	1.658201	0.116277
6	1.377804	0.729448	-0.354171
6	0.250574	0.034051	0.289142
17	3.036662	-0.323271	-0.106181
1	1.317179	0.780209	-1.434026
8	-0.393282	-0.811672	-0.432599

E = -842.542534103

-1313.1800 46.3697 56.1847
78.6869 161.8784 173.7210
196.5465 236.6255 289.5292
370.6031 450.4259 458.4644
561.4086 636.1258 776.2511
787.1161 909.9904 923.3269
957.1661 1025.2248 1059.7955
1092.6559 1103.9977 1187.7204
1241.7229 1357.8335 1394.5403
1451.4209 1461.8178 1468.5190
1471.4498 1530.1563 3021.4987
3100.9444 3144.4614 3156.5982
3204.4735 3244.3225 3668.4033

TSCL-PCET/HCO₃⁻

8	2.255730	0.603516	1.364538
1	1.960963	0.252209	-1.204521
6	1.268056	0.006418	0.905266
6	1.233822	-0.243135	-0.581355
17	2.208521	-2.174602	-0.654276
8	0.279573	-0.426677	1.569001
1	0.323047	-0.601353	-1.033687
1	0.932677	3.846922	-0.998703
1	1.940657	2.732853	-0.057039
6	1.275549	2.808770	-0.920377
1	1.828901	2.561857	-1.825243
6	0.111135	1.902355	-0.741743
8	-0.616582	2.074149	0.332273
1	-0.383801	1.474096	-1.611878
1	-1.443701	1.411792	0.313006
8	-1.699671	-1.404762	0.286829
8	-3.708579	-1.129025	-0.581734
6	-2.721920	-0.598579	-0.061028
1	-0.951192	-0.924543	0.778361
8	-2.604502	0.652728	0.173819

E = -1107.15415418

-426.8610 28.0623 51.6003
78.0312 91.3643 117.9242
126.7385 144.5244 149.1512
162.7189 179.4015 199.9832
205.4885 233.5657 287.8507
348.0711 466.5119 483.8325
647.4541 675.6313 708.4690
785.3767 791.2887 848.1063
941.3559 957.4860 967.3500
1025.2760 1039.2992 1061.5224
1077.4275 1123.8096 1145.6913
1190.4511 1254.3104 1329.3516
1362.2971 1387.3662 1393.9939
1446.3107 1466.5221 1470.2294

1495.2594 1572.7267 1639.8412
1663.5986 2119.7419 2770.6433
3029.4742 3099.0138 3127.4093
3155.1598 3205.8363 3324.6088

TSC1-PCET/HPO₄²⁻

8	2.905484	0.306429	1.185885
1	2.206421	-0.077626	-1.260149
6	1.780621	-0.145044	0.893170
6	1.522830	-0.519809	-0.548898
17	2.042991	-2.432725	-0.672674
8	0.843623	-0.380755	1.714561
1	0.487230	-0.566928	-0.861224
1	1.879105	3.808326	-1.039907
1	2.618653	2.598214	0.021050
6	1.992601	2.727698	-0.868439
1	2.525987	2.307574	-1.723911
6	0.666552	2.060904	-0.674665
8	-0.097979	2.446605	0.300572
1	0.202780	1.555624	-1.526273
8	-1.629683	-0.348749	-1.449482
8	-2.244578	1.199741	0.471633
1	-1.317871	1.685259	0.361970
15	-2.319078	-0.284918	-0.110262
1	-0.573798	-0.830193	1.172188
8	-1.497344	-1.175578	0.956630
8	-3.748122	-0.746776	-0.037470

E = -1485.86398052

-580.1912 50.0048 54.2198
77.8480 88.5345 98.5094
103.8841 126.5208 133.5835
151.8332 168.3904 174.4014
193.3772 199.6877 225.6908
315.4926 366.6623 384.0895
474.4372 490.0351 502.8036
507.1984 523.7608 659.8763
685.9331 782.3239 848.3825
899.4652 924.2245 947.1653
961.2350 975.7147 1011.9831
1067.9826 1096.6683 1113.0866
1139.3715 1164.3459 1183.4274
1246.1237 1309.9655 1375.2235
1383.8747 1438.7551 1455.0119
1458.4628 1475.9560 1495.1310
1614.9508 2153.7718 2853.0226
2974.4451 3045.4793 3067.5210
3111.8518 3157.5496 3266.5171

TSC1-HAT/HCO₃⁻

1	2.232137	2.784496	-1.206946
1	-0.958812	1.520643	-0.164375
6	2.029907	2.788408	-0.133897
8	-0.223975	2.084840	-0.531455
1	1.760938	3.807515	0.158646
6	0.919612	1.828082	0.187211
1	2.942148	2.506873	0.393461
1	0.736303	1.687303	1.258528
8	0.334793	-2.095027	0.631487
1	1.366569	0.657722	-0.163029

6	0.530810	-1.408996	-0.384652
6	1.800431	-0.624975	-0.538847
17	3.131215	-0.982378	0.568240
8	-0.279341	-1.211389	-1.339780
1	2.165190	-0.495235	-1.550831
8	-2.124120	0.767181	0.663507
1	-1.828148	-0.986433	-0.813641
6	-3.081284	0.028165	0.292762
8	-2.803658	-0.948156	-0.613830
8	-4.259180	0.096732	0.676653

E = -1107.14013885

-1525.5624 26.9107 41.5041
59.1085 74.8434 80.5511
86.0842 99.5533 137.0921
144.9760 157.1817 185.8505
206.8063 226.5319 242.1654
438.1284 452.4991 540.6079
638.4653 680.3413 683.5016
705.4741 805.2160 847.0378
868.6938 902.1934 928.8501
941.9963 956.3932 992.6924
1036.4018 1099.3290 1161.3226
1198.5890 1227.4498 1333.5968
1343.9189 1360.8103 1385.6694
1397.4819 1404.6741 1426.3295
1468.5755 1483.6409 1528.0555
1632.9405 1661.2741 3039.6394
3044.6218 3103.5854 3110.4647
3136.6478 3140.2458 3197.9661

TSC1-HAT/HPO₄²⁻

1	-2.785521	2.754875	0.845680
1	0.724088	1.749000	0.602447
6	-2.328693	2.741348	-0.146794
8	-0.190238	2.210124	0.786651
1	-2.047695	3.766355	-0.405411
6	-1.118668	1.843182	-0.145694
1	-3.070626	2.391637	-0.865384
1	-0.698026	1.666117	-1.143083
8	-1.049311	-2.304764	-0.515829
1	-1.597544	0.682627	0.157488
6	-1.129637	-1.546699	0.467137
6	-2.236275	-0.537379	0.553756
17	-3.595852	-0.710111	-0.567081
8	-0.315012	-1.468051	1.433450
1	-2.592790	-0.301768	1.549669
8	2.326244	-1.284437	0.690804
1	1.366595	-1.345921	0.889569
8	2.032447	-0.241006	-1.620682
8	4.194152	0.049480	-0.277577
15	2.677522	0.009879	-0.266355
8	2.070194	1.233414	0.457469

E = -1485.84129851

-1492.7931 27.1043 50.6751
64.4757 93.9529 103.2965
121.8274 123.4093 128.0747
153.5205 169.8821 198.2769

218.0519 236.2954 248.1613
 366.8801 394.3642 435.1516
 461.3217 512.2054 526.4336
 536.3073 551.4374 671.3812
 707.7165 734.4729 784.4402
 804.8886 889.8705 939.5719
 953.8822 961.8129 984.6291
 1048.8203 1105.3272 1119.1493
 1134.1596 1168.2694 1210.4049
 1214.7818 1224.7220 1344.4476
 1383.5563 1397.7762 1410.0975
 1431.4342 1470.9849 1485.0843
 1580.4194 1622.9567 2334.3026
 3035.5741 3043.3053 3106.9815
 3138.9456 3192.6064 3453.2897

TSBr-PCET

1	2.476340	-2.388424	-0.241427
1	1.950985	0.918617	-1.107899
6	2.903078	-1.708127	0.497692
8	2.628244	0.122015	-1.027513
1	3.994260	-1.800066	0.443635
6	2.497635	-0.311699	0.210166
1	2.587740	-2.005876	1.496502
1	2.512767	0.428174	1.009162
8	-0.080368	1.841343	1.250526
1	0.112905	-0.797895	1.182781
6	0.275371	1.225525	0.242024
6	0.132892	-0.281254	0.234812
35	-2.159172	-0.476973	-0.129861
8	0.791433	1.741035	-0.809423
1	0.367690	-0.842278	-0.654480

E = -2956.54687507

-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

TSBr-PCET/H₂O

1	-1.858257	2.720314	-0.979375
1	-3.020098	-0.967951	-0.332647
6	-2.237031	2.526389	0.029679
8	-3.114228	0.354696	-0.570036
1	-3.198334	3.056446	0.113075
6	-2.383385	1.055411	0.268491
1	-1.547232	2.976229	0.746725
1	-2.285670	0.692435	1.296669
8	-0.231527	-0.987151	1.554987
1	0.716647	1.324692	0.903823
6	-0.065185	-0.616111	0.409604

6	0.719558	0.624099	0.078637
35	2.628477	0.098225	-0.163527
8	-0.462306	-1.281987	-0.658464
1	0.421087	1.073852	-0.859419
1	-3.241647	-2.537267	-0.836892
8	-2.797708	-2.027579	-0.152618
1	-1.340778	-1.779175	-0.437940

E = -3032.98327089

-209.2647 49.7963 56.7233
68.4617 103.5196 112.1833
128.8684 161.5978 169.4739
186.5643 260.4073 328.1836
389.3887 419.3602 442.7196
523.9061 617.4760 636.0121
668.4322 737.9247 894.9654
922.0555 935.5810 976.6038
1011.8101 1112.6904 1116.5203
1141.1097 1202.6898 1302.8619
1333.5666 1377.7335 1403.0852
1454.0436 1458.2558 1478.0383
1533.7781 1592.8104 1737.2201
1779.3808 2538.4690 2967.7088
3044.9425 3046.2748 3112.6409
3168.7446 3254.7873 3905.9631

TSBr-HAT

1	2.301555	-2.277763	-0.794983
1	2.323913	1.141468	-0.419089
6	2.512208	-1.986948	0.235978
8	2.849733	0.304212	-0.398438
1	3.576612	-2.157715	0.425312
6	2.163374	-0.545518	0.454196
1	1.938840	-2.626347	0.907518
1	2.182468	-0.221188	1.500370
8	-1.046760	2.165146	0.670194
1	0.904343	-0.363588	0.133721
6	-0.115467	1.666606	0.024862
6	-0.192944	0.240255	-0.473698
35	-1.766444	-0.781386	-0.049121
8	0.989311	2.217972	-0.266778
1	0.056505	0.108626	-1.521459

E = -2956.53255459

-1602.2622 45.4745 72.8122
87.7931 129.8705 180.1307
194.9520 204.6658 224.0392
378.3271 431.8190 507.8832
676.7194 705.0943 757.4355
774.4475 877.8181 930.1227
955.5020 958.7811 1091.1728
1155.8888 1186.3484 1202.6468
1337.4965 1365.5210 1393.7122
1409.6879 1458.4459 1469.6843
1483.7191 1504.7427 1647.6474
3041.7108 3045.4533 3108.6972
3143.1527 3181.9997 3297.4918

TSBr-FRS

1	-2.665986	-0.697272	-1.845671
1	-2.474755	-1.904994	1.435678
6	-2.927486	0.033773	-1.078662
8	-2.636044	-1.710308	0.503954
1	-4.019790	0.115475	-1.048360
6	-2.425458	-0.409124	0.243517
1	-2.505518	1.002771	-1.336790
1	-2.441805	0.264855	1.093961
8	-0.308520	1.939384	-0.794236
1	-0.337098	-0.690756	-0.909257
6	-0.256656	1.258745	0.251180
6	-0.185567	-0.253483	0.066311
35	2.149506	-0.459532	-0.125026
8	-0.283719	1.659584	1.435175
1	-0.190490	-0.895194	0.933125

E = -2956.53809027

-391.0070 38.5908 97.9849
 102.6868 135.3824 146.6952
 174.0942 190.7844 221.6937
 341.1720 443.6585 463.5628
 496.5738 659.1468 792.1900
 836.2432 918.7875 955.1702
 959.9674 1016.0609 1042.9070
 1075.8714 1088.2024 1245.2195
 1301.7172 1358.3782 1394.0788
 1447.9556 1460.6093 1472.0103
 1500.7948 1649.5085 3037.4846
 3111.5300 3168.9403 3179.9385
 3191.3773 3315.4495 3846.8170

TSBr-FRS/H₂O

1	-1.274149	3.002351	-0.677913
1	-2.881739	-0.210512	-0.637252
6	-1.737739	2.682135	0.257184
8	-2.610361	0.738237	-0.793330
1	-2.701783	3.195683	0.343751
6	-1.958138	1.213302	0.256358
1	-1.112411	2.985756	1.094204
1	-2.069616	0.674233	1.193731
8	-0.270571	-1.168362	1.649746
1	0.441834	1.213916	0.865801
6	-0.202253	-0.888759	0.440741
6	0.266926	0.500170	0.076722
35	2.542789	0.064532	-0.195860
8	-0.523635	-1.634459	-0.529311
1	0.145269	0.852590	-0.935847
1	-3.565405	-2.297473	-0.908205
8	-3.103058	-1.778928	-0.242154
1	-2.131392	-1.968158	-0.348796

E = -3032.99082955

-336.6408 49.3506 76.4618
 96.5912 104.4880 123.6424
 131.7743 152.7999 185.2773
 209.7867 232.1930 258.0919
 348.5207 356.4965 454.7532
 472.5681 517.8304 662.5598
 722.2773 793.4028 830.1511

941.2015 942.2643 960.4414
 1006.8357 1029.6827 1041.9201
 1052.5608 1119.3874 1263.0947
 1360.9223 1392.2045 1417.3960
 1453.6561 1465.2552 1483.0538
 1554.2345 1613.3545 1661.1665
 3020.5886 3038.7313 3107.0562
 3155.7854 3168.3892 3193.3491
 3198.7205 3322.8563 3906.4046

TSBr-XA

8	-2.902794	1.131944	-0.844915
1	-1.803250	-1.098167	-1.541038
6	-2.706415	0.216389	-0.007632
6	-1.884354	-0.957582	-0.469915
35	0.269887	-0.376747	0.003953
8	-3.116919	0.186456	1.179435
1	-1.962701	-1.864503	0.117476
1	3.602525	1.970172	0.219844
1	2.407600	1.707230	-1.063335
6	2.590000	1.611691	0.007633
1	1.878135	2.230541	0.549739
6	2.470283	0.187759	0.428021
8	3.256213	-0.639274	-0.303869
1	2.447154	-0.022801	1.493423
1	3.275423	-1.518889	0.091680

E = -2956.53408792

-374.5618 12.9944 48.9044
 53.3051 89.7943 120.2440
 208.7854 223.0807 232.6242
 398.0013 434.4218 438.3088
 458.4139 652.9095 737.8400
 772.3412 906.3952 940.8331
 951.4899 978.3308 1023.2663
 1056.5945 1104.9256 1224.3743
 1293.5977 1373.8895 1391.4554
 1458.9113 1462.4243 1469.5616
 1480.9477 1603.2807 3047.3311
 3122.7426 3148.2822 3154.6964
 3172.1833 3248.9604 3856.6982

TSBr-OA

6	-3.616030	-0.982498	0.173605
6	-2.996981	0.059945	-0.671343
8	-2.725248	1.266543	-0.171917
1	-3.099234	-1.036990	1.132842
1	-3.547882	-1.950798	-0.320103
1	-4.675249	-0.758564	0.352768
1	-3.128495	0.067546	-1.744218
1	-2.385707	1.151336	0.737025
8	-0.784116	0.107400	1.474289
1	0.875599	1.769777	0.379656
6	0.619816	0.923500	-0.242709
6	-0.435430	0.031620	0.253588
35	2.563794	-0.157277	-0.056157
1	0.628114	1.104150	-1.308899
8	-0.969159	-0.753589	-0.595175

E = -2956.51693014

-1781.7749 28.5326 56.5307
 95.5177 111.2782 160.8892
 187.0376 215.6209 228.3564
 324.8947 457.5984 464.3672
 575.5306 645.8045 719.6608
 791.2395 806.0073 857.7828
 963.2398 1006.7803 1020.3143
 1045.6889 1094.1666 1131.3556
 1267.0289 1369.1511 1399.7521
 1450.5634 1465.2711 1469.9527
 1484.2887 1534.1394 3016.7515
 3107.6267 3158.2166 3175.6058
 3226.0691 3272.8921 3611.2071

TSBr-PCET/HCO₃⁻

1	2.442845	1.504313	2.509182
1	2.364706	1.038671	-0.346384
6	1.537273	1.062966	2.075036
8	1.821577	1.925675	-0.186458
1	0.765533	1.043814	2.844072
6	1.085684	1.869428	0.901832
1	1.776050	0.036232	1.789123
1	0.484193	2.756879	1.075088
8	1.447302	-1.536729	-0.392095
1	0.947444	-0.806614	-0.884199
6	2.767230	-1.278840	-0.255262
8	3.477686	-2.193743	0.172324
8	3.173694	-0.109469	-0.567661
8	-1.325179	1.940211	-1.413605
1	-1.391170	1.274159	1.110603
35	-2.796270	-0.763778	0.300398
6	-0.957795	0.540585	0.448866
6	-0.749265	0.920741	-1.000257
1	-0.330056	-0.223641	0.878867
8	-0.006189	0.151445	-1.676454

E = -3221.12828918

-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

TSBr-PCET/HPO₄²⁻

8	2.092395	1.768853	1.277305
1	1.736953	0.956387	-1.129096

6	1.273773	0.868641	1.013147
6	1.276816	0.305033	-0.398125
35	2.588463	-1.306461	-0.356624
8	0.466721	0.335605	1.828285
1	0.352956	-0.159651	-0.723182
1	-0.308328	4.426790	-1.273385
1	0.762785	3.764401	-0.031927
6	0.243509	3.524412	-0.966537
1	0.999020	3.321407	-1.729040
6	-0.662053	2.349301	-0.778382
8	-1.608277	2.417923	0.124110
1	-0.788692	1.642532	-1.602438
8	-1.591753	-0.924604	-1.384684
8	-2.973915	0.388853	0.301176
1	-2.334040	1.250288	0.189527
15	-2.372897	-1.026386	-0.098145
1	-0.655857	-0.702312	1.291954
8	-1.355230	-1.395787	1.106659
8	-3.474920	-2.048625	-0.035226

E = -3599.83659128

-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

TSBr-HAT/HCO₃⁻

1	-1.287394	3.161604	1.277278
1	1.662481	1.486683	0.109808
6	-1.144965	3.114455	0.195680
8	1.023540	2.146094	0.498586
1	-0.767759	4.084046	-0.141612
6	-0.180468	2.015181	-0.151602
1	-2.112179	2.936111	-0.275692
1	-0.074149	1.828471	-1.226420
8	-0.093048	-1.980453	-0.432455
1	-0.746506	0.927533	0.252515
6	-0.148729	-1.224129	0.549937
6	-1.304182	-0.283380	0.729113
35	-2.869543	-0.553021	-0.358259
8	0.732475	-1.076136	1.449498
1	-1.590477	-0.056054	1.748748
8	2.670580	0.572416	-0.753999
1	2.272374	-1.053686	0.836042
6	3.566267	-0.239015	-0.380593

8	3.233670	-1.134076	0.589547
8	4.726541	-0.310050	-0.813280

E = -3221.10822486

-1492.2167 37.2943 45.7028
65.4480 78.2025 89.8559
101.6564 106.5791 136.2359
149.3252 157.6454 176.4306
202.1892 215.0459 235.2930
388.4520 450.2750 537.7599
639.5750 682.2340 685.0418
698.0937 747.1544 848.3507
869.2708 910.5852 936.2196
943.4062 954.0866 988.6855
1036.4866 1098.6802 1159.3108
1195.8707 1199.6419 1331.6044
1346.9350 1360.8853 1383.8537
1396.8350 1399.0195 1419.7761
1469.1066 1484.8556 1530.1665
1632.6367 1663.0004 3040.0274
3045.8585 3094.5569 3112.2870
3139.3893 3155.8999 3201.0541

TSBr-HAT/HPO₄²⁻

1	-2.014559	3.002999	0.982881
1	1.411089	1.776497	0.540599
6	-1.601593	2.975429	-0.028403
8	0.534295	2.278758	0.796527
1	-1.256405	3.981558	-0.282704
6	-0.460735	1.992056	-0.093724
1	-2.396561	2.693816	-0.719551
1	-0.099310	1.805229	-1.112725
8	-0.768922	-2.241045	-0.245473
1	-1.006474	0.873937	0.220495
6	-0.718119	-1.392572	0.661619
6	-1.722631	-0.278156	0.723914
35	-3.291559	-0.415126	-0.388673
8	0.160810	-1.300269	1.568411
1	-2.004512	0.058209	1.714854
8	2.808687	-1.260192	0.802803
1	1.849626	-1.274898	1.009102
8	2.399277	-0.503768	-1.601410
8	4.679618	-0.215362	-0.464928
15	3.170040	-0.132891	-0.343908
8	2.709928	1.219987	0.247671

E = -3599.80925643

-1439.5279 28.7025 43.8971
72.5817 83.8294 107.1360
110.5080 120.5334 131.7537
151.8679 166.7319 183.9878
203.2741 222.9522 239.8318
368.6665 378.0125 402.6859
459.3963 516.3689 525.4881
530.5263 551.6596 675.3307
707.6567 731.9519 742.2719
785.4683 890.3186 937.7385
946.4647 957.7303 973.8932
1047.7431 1101.4060 1110.6163

1120.4930 1164.5661 1192.1272
 1206.0035 1215.4378 1343.7636
 1380.0255 1393.7749 1406.4589
 1424.4774 1470.6759 1483.6815
 1580.8276 1623.0185 2312.4282
 3034.3953 3044.7439 3108.7841
 3139.8272 3194.1861 3479.6418

TSI-PCET

1	2.796723	-2.473127	-0.207853
1	2.417239	0.834723	-1.139506
6	3.281079	-1.801256	0.502944
8	3.061896	0.006431	-1.059039
1	4.363567	-1.957911	0.423385
6	2.948161	-0.391194	0.191309
1	2.976301	-2.056999	1.516555
1	3.016830	0.364616	0.971929
8	0.529754	1.932447	1.243353
1	0.523995	-0.710737	1.235152
6	0.803945	1.266025	0.240297
6	0.547369	-0.221543	0.272324
53	-1.917844	-0.294007	-0.079292
8	1.322599	1.722466	-0.839228
1	0.753751	-0.821135	-0.599095

E = -393.722198281

-370.8355 67.0310 87.4537
 90.2000 124.2386 133.3348
 166.5205 210.1042 280.7872
 353.9295 438.2198 470.7941
 660.9621 755.3294 804.5720
 885.1395 925.8683 951.8969
 985.9402 995.9315 1036.5718
 1066.5343 1122.3079 1200.8439
 1335.9950 1390.0040 1429.3417
 1446.5701 1459.9798 1487.8084
 1504.9156 1676.5852 2265.9173
 3030.3262 3103.4582 3133.0500
 3159.5513 3197.1312 3315.2215

TSI-PCET/H₂O

1	-2.427273	2.730057	-0.981951
1	-3.495218	-0.951007	-0.378707
6	-2.811061	2.514973	0.020706
8	-3.614876	0.325111	-0.612561
1	-3.788751	3.014993	0.098506
6	-2.914582	1.039725	0.243850
1	-2.142352	2.976973	0.749516
1	-2.808891	0.662356	1.264787
8	-0.742495	-0.979195	1.591644
1	0.227334	1.323045	0.957963
6	-0.543535	-0.617480	0.447158
6	0.239799	0.624005	0.131186
53	2.346285	0.073674	-0.113885
8	-0.921863	-1.287282	-0.622788
1	-0.046175	1.076038	-0.809927
1	-3.653366	-2.555821	-0.880035
8	-3.247883	-2.030385	-0.183866
1	-1.825216	-1.774706	-0.421066

E = -470.157697059

-441.8221 44.4474 53.8320
70.8417 99.7029 105.3715
116.6945 154.8196 165.7041
174.4162 252.3066 336.9717
368.4028 419.1970 444.0101
525.4529 600.0617 633.4874
668.2856 737.3483 856.0704
877.2541 939.4029 979.0949
1007.3397 1018.8102 1099.3014
1119.7792 1151.9577 1296.5976
1332.2846 1378.7649 1389.1898
1453.2421 1456.3234 1467.9901
1510.2116 1552.2174 1728.8102
1758.3705 2350.7962 2968.1145
3047.5687 3060.9798 3116.2824
3166.3018 3252.7489 3904.3697

TSI-HAT

1	2.213491	-2.530406	-0.823791
1	2.896000	0.806045	-0.395777
6	2.472811	-2.306262	0.212854
8	3.259830	-0.114079	-0.374581
1	3.481466	-2.687941	0.399875
6	2.413766	-0.828558	0.457568
1	1.780833	-2.831788	0.871449
1	2.484724	-0.532896	1.510091
8	-0.232857	2.453670	0.639635
1	1.214668	-0.405976	0.133886
6	0.595902	1.778634	0.014316
6	0.253177	0.386693	-0.477719
53	-1.651207	-0.411264	-0.027612
8	1.790419	2.109008	-0.259043
1	0.489695	0.208130	-1.522496

E = -393.705702166

-1567.4174 47.6503 73.6419
81.0426 127.7604 166.4216
184.0802 200.8159 228.1899
355.2328 431.5811 504.0915
675.1356 703.3760 720.3700
783.6622 878.3522 926.0227
940.1223 950.3081 1092.1969
1155.4006 1171.4023 1187.1266
1337.9727 1358.4960 1394.7559
1405.2784 1457.1707 1469.1302
1484.4543 1498.5676 1641.6041
3040.9370 3044.2487 3107.6979
3141.8407 3171.6788 3283.9977

TSI-FRS

1	-3.011797	-1.004101	-1.829515
1	-2.885067	-1.811253	1.571198
6	-3.323991	-0.195242	-1.166632
8	-3.020784	-1.733108	0.618654
1	-4.418512	-0.143821	-1.189320
6	-2.860884	-0.458808	0.216052
1	-2.917330	0.749665	-1.522435
1	-2.948666	0.305082	0.981689

8	-0.904749	1.968738	-0.820811
1	-0.718946	-0.653521	-0.883157
6	-0.782059	1.315514	0.237427
6	-0.594055	-0.188680	0.083578
53	1.903794	-0.288471	-0.075401
8	-0.828778	1.742304	1.412418
1	-0.600348	-0.813263	0.963184

E = -393.713191129

-407.4005 36.1874 89.7854
98.5923 119.0292 131.8608
171.2939 205.1739 218.1618
332.8472 442.4803 459.3551
490.1503 658.9378 791.6300
827.3981 919.5782 940.5386
951.0970 1011.8157 1026.9607
1059.8414 1085.4718 1242.1426
1301.2928 1355.6909 1391.7753
1444.4356 1461.8667 1472.5539
1497.4922 1643.4725 3034.1444
3109.5473 3162.8448 3177.1583
3192.0139 3312.7837 3847.9436

TSI-FRS/H₂O

1	-1.720166	3.002776	-0.669915
1	-3.342153	-0.204365	-0.675631
6	-2.213071	2.683643	0.250573
8	-3.068995	0.744534	-0.823195
1	-3.176622	3.202512	0.308679
6	-2.438554	1.216097	0.242102
1	-1.610919	2.983468	1.105790
1	-2.566812	0.672902	1.174511
8	-0.788468	-1.162856	1.678729
1	-0.038259	1.210711	0.907228
6	-0.681334	-0.885796	0.471182
6	-0.181856	0.492610	0.115284
53	2.259731	0.040170	-0.130249
8	-0.989604	-1.632438	-0.504176
1	-0.295217	0.847965	-0.897457
1	-4.004303	-2.296576	-0.971677
8	-3.569331	-1.778044	-0.287460
1	-2.591233	-1.957321	-0.364346

E = -470.165980102

-331.2003 40.5686 71.7584
91.2723 98.2394 110.3862
126.9088 148.4376 185.6200
207.6424 229.5108 260.2006
341.9531 358.4438 456.8462
472.4586 522.1226 661.6287
726.3778 792.0598 824.3493
921.6532 939.0578 959.5768
997.3661 1014.7308 1036.3830
1047.2291 1118.4863 1256.6059
1357.1481 1391.5086 1415.0774
1450.5179 1464.7707 1482.3295
1553.0751 1611.3096 1659.8376
3016.7034 3036.2812 3104.3985
3156.3799 3165.5780 3174.3286

3195.9796 3316.8771 3906.7995

TSI-XA

8	-3.111690	1.190436	-0.851658
1	-2.064956	-1.076310	-1.536110
6	-2.926567	0.279349	-0.006560
6	-2.147813	-0.921604	-0.466753
53	0.253784	-0.313910	0.006185
8	-3.322778	0.272172	1.185988
1	-2.211722	-1.815832	0.142013
1	3.754588	1.988706	0.207069
1	2.551424	1.785301	-1.079728
6	2.726941	1.679887	-0.008789
1	2.043201	2.330218	0.532681
6	2.550424	0.256006	0.414725
8	3.350635	-0.581559	-0.305838
1	2.566814	0.073327	1.486675
1	3.362863	-1.458394	0.095932

E = -393.713694850

-292.9971 16.5580 37.2504
45.4704 76.1908 102.7245
200.9296 219.9578 245.5052
406.7932 430.4919 436.3596
457.6130 652.1758 656.6450
753.6175 905.2278 923.1761
944.3500 957.5836 1013.6383
1056.9726 1116.3534 1215.9370
1291.9415 1368.9245 1392.4552
1454.4322 1458.5349 1469.9680
1478.4518 1600.2631 3050.1484
3125.0228 3140.1510 3144.4653
3171.3207 3247.8655 3856.9771

TSI-OA

6	-4.080890	-1.077378	0.240705
6	-3.620528	0.026205	-0.623230
8	-3.322726	1.213677	-0.128812
1	-3.478067	-1.119620	1.148182
1	-4.000271	-2.024671	-0.289613
1	-5.132129	-0.924697	0.517727
1	-3.823074	0.037453	-1.685778
1	-2.866955	1.080797	0.735402
8	-1.319409	0.251123	1.377449
1	0.315275	1.883795	0.209394
6	0.095480	0.992993	-0.362685
6	-0.949031	0.107219	0.164035
53	2.243766	-0.115264	-0.012103
1	0.134873	1.100602	-1.438324
8	-1.450298	-0.742165	-0.632199

E = -393.693175134

-3811.2518 39.1006 52.1201
87.6175 115.2777 147.2059
189.3785 220.7377 240.2750
312.4639 460.2038 475.9498
617.3605 646.7140 651.9353
734.4544 806.6635 820.2387
965.0490 990.7788 1016.3597

1041.2590 1070.4419 1123.2060
 1287.1080 1377.7368 1405.1817
 1448.8973 1468.7276 1476.6903
 1494.2895 1522.9725 3010.6627
 3111.6498 3163.4054 3173.7304
 3187.7048 3271.1011 3332.5321

TSI-PCET/HCO₃⁻

8	0.434911	2.025423	1.490854
1	0.731027	1.431155	-1.024120
6	0.043958	0.938685	1.031567
6	0.399411	0.615754	-0.399903
53	2.527141	-0.498504	-0.198218
8	-0.620354	0.059990	1.658864
1	-0.118964	-0.198870	-0.881864
1	-2.189915	3.810183	-1.303078
1	-0.806236	3.495392	-0.242146
6	-1.349598	3.130126	-1.117913
1	-0.690909	3.155579	-1.984911
6	-1.844255	1.753446	-0.863899
8	-2.645931	1.590405	0.163916
1	-1.921560	1.032314	-1.674633
1	-2.970279	0.594107	0.207473
8	-1.602338	-1.866422	0.289300
8	-3.386629	-2.805705	-0.607220
6	-2.899280	-1.800607	-0.077842
1	-1.291557	-1.052131	0.809733
8	-3.527350	-0.712622	0.150167

E = -658.304425912

-386.4351 25.7826 47.2392
 68.6089 87.0867 98.0628
 120.0689 124.4014 139.6528
 145.5978 174.2504 190.3488
 209.2371 214.5927 278.9807
 320.4663 460.5613 479.3440
 647.7125 670.9819 701.7546
 734.5198 787.6393 847.3390
 901.8476 938.4718 963.0318
 1019.1083 1032.7653 1043.1163
 1056.2974 1115.4304 1132.2667
 1157.4598 1244.5373 1330.5298
 1368.8316 1385.1732 1388.5546
 1441.4555 1462.6679 1466.1263
 1486.7891 1581.7532 1634.7063
 1664.8408 2232.5520 2785.6625
 3019.7044 3085.6457 3137.6759
 3153.1851 3197.5699 3308.9435

TSI-PCET/HPO₄²⁻

8	1.288582	2.331953	1.353106
1	1.173396	1.431742	-1.044563
6	0.707596	1.262160	1.089927
6	0.874506	0.693009	-0.311431
53	2.628862	-0.692671	-0.253069
8	0.016945	0.575541	1.895302
1	0.071031	0.041317	-0.639673
1	-1.703216	4.314506	-1.442082
1	-0.627932	4.006547	-0.075946
6	-0.977532	3.595344	-1.029358

1	-0.125101	3.556006	-1.711262
6	-1.574257	2.238829	-0.834082
8	-2.575249	2.102671	0.007187
1	-1.471777	1.497990	-1.631074
8	-1.531191	-1.256742	-1.244876
8	-3.459398	-0.170202	0.016772
1	-3.017910	0.830870	-0.000921
15	-2.482486	-1.415227	-0.084172
1	-1.000608	-0.623733	1.391917
8	-1.629497	-1.390949	1.294993
8	-3.306708	-2.673690	-0.030173

E = -1037.01067884

-187.9782 30.3932 47.5207
60.7627 76.8919 86.0194
98.5042 108.8419 122.7964
133.8657 150.0101 161.7352
174.5292 185.8257 264.4384
267.6779 364.9563 378.3209
461.6872 474.9990 503.1874
506.0707 523.9906 576.1124
665.1427 790.3038 828.6368
856.0338 901.6392 910.7836
934.2833 953.3773 1004.2140
1050.3480 1094.4068 1113.8918
1149.7982 1169.1282 1217.5010
1240.9179 1257.0438 1364.4138
1384.3473 1407.7868 1451.9254
1466.5377 1483.7958 1496.7936
1624.3989 1682.7312 2951.2385
3042.5175 3071.2137 3100.3464
3109.3313 3131.0422 3235.2316

TSI-HAT/HCO₃⁻

1	-0.636561	3.309788	1.292976
1	2.186645	1.449558	0.084991
6	-0.521546	3.233793	0.209722
8	1.593744	2.146364	0.482283
1	-0.095322	4.172667	-0.155195
6	0.368759	2.073123	-0.136017
1	-1.507979	3.104430	-0.237303
1	0.436996	1.857753	-1.208725
8	0.237738	-1.891693	-0.376610
1	-0.252327	1.027869	0.302787
6	0.252189	-1.141689	0.613008
6	-0.848953	-0.141971	0.831925
53	-2.649530	-0.369566	-0.249347
8	1.170531	-1.050374	1.482709
1	-1.054106	0.125151	1.862339
8	3.118107	0.473443	-0.795245
1	2.690023	-1.108442	0.831441
6	3.990220	-0.364498	-0.423786
8	3.642345	-1.231291	0.566247
8	5.139249	-0.484488	-0.875261

E = -658.281342497

-1472.4668 29.9107 43.9157
62.6408 70.9012 84.3240
101.0235 101.9715 135.7100

147.8801 158.1466 173.9232
 189.2772 214.5877 233.3001
 364.5357 450.6363 534.7826
 638.5678 673.6552 682.7518
 687.7298 728.0380 846.3751
 867.5576 901.8011 916.8720
 930.1840 944.7824 976.4064
 1035.6485 1098.4754 1156.7701
 1172.4335 1199.1071 1328.1512
 1344.1075 1358.8055 1380.9909
 1392.1279 1396.8333 1415.6690
 1468.8842 1484.1707 1531.2888
 1626.3329 1661.4932 3037.7623
 3045.6379 3084.9739 3111.8669
 3138.7925 3142.4564 3192.2209

TSI-HAT/HPO₄²⁻

1	-1.439045	3.132626	0.989480
1	1.933042	1.752505	0.524833
6	-1.034097	3.068666	-0.023488
8	1.070819	2.277206	0.792349
1	-0.635495	4.050779	-0.293481
6	0.053036	2.025211	-0.081087
1	-1.847394	2.821822	-0.706499
1	0.391421	1.798743	-1.099986
8	-0.396875	-2.131184	-0.263011
1	-0.547258	0.941293	0.260934
6	-0.298208	-1.325018	0.679501
6	-1.269322	-0.184161	0.814748
53	-3.092377	-0.280720	-0.255513
8	0.609707	-1.300807	1.562341
1	-1.452387	0.161298	1.826233
8	3.250299	-1.301942	0.794188
1	2.290129	-1.300207	0.996944
8	2.848918	-0.545908	-1.610865
8	5.142830	-0.315676	-0.488389
15	3.636636	-0.191001	-0.359640
8	3.217420	1.177829	0.225924

E = -1036.98225389

-1415.2719 33.6538 42.8373
 65.4510 85.1317 104.0041
 108.9877 111.2427 125.9400
 149.1376 166.0821 179.7454
 192.8470 221.3976 238.8250
 352.0788 372.3778 399.6364
 460.2474 516.5965 524.1109
 528.8869 552.6480 672.7968
 687.1299 716.4271 735.0354
 786.2763 886.0629 928.0203
 939.7067 955.6104 967.6256
 1046.6432 1101.4726 1118.1460
 1124.2188 1160.5535 1173.0978
 1209.2361 1215.6772 1337.6307
 1371.2596 1388.0329 1400.4879
 1418.9567 1469.7793 1481.3054
 1576.7399 1614.7960 2282.2794
 3032.6029 3043.8801 3107.8918
 3140.0620 3189.3211 3463.9570

Ac radikal Protonated (PCET)

8	-0.853825	-0.949662	-0.000153
1	1.663260	-1.312696	0.000229
6	-0.015873	0.105232	0.000012
6	1.375196	-0.273263	0.000137
8	-0.418108	1.252281	0.000009
1	2.116709	0.509110	-0.000635
1	-1.760445	-0.609177	0.000670

E = -228.413655202

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

Ac radikal De-protonated (PCET)

8	0.698137	-1.123677	0.000002
1	-1.899915	-0.933323	-0.000021
6	0.125816	-0.000003	-0.000011
6	-1.354003	-0.000075	0.000012
8	0.697988	1.123757	0.000002
1	-1.899956	0.933149	-0.000022

E = -227.947039772

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

Ac radikal Protonated H2O (PCET/H2O)

1	-1.901813	-0.796405	0.021544
8	0.163521	-1.153761	-0.004401
1	2.774463	-0.842692	0.019754
6	0.740812	-0.074672	0.001082
6	2.178001	0.055348	0.013976
8	0.091768	1.092391	-0.004801
1	2.640231	1.029996	0.017064
1	-3.023232	0.067911	0.641381
8	-2.396001	0.030285	-0.088352
1	-0.876827	0.905823	-0.009657

E = -304.855340244

79.1554 139.6987 195.5724
244.6029 329.5463 335.1131
438.6585 536.0270 625.3932
636.6875 763.5556 855.2948
960.6168 1011.6190 1301.0771
1432.6202 1487.8503 1606.1831
1711.6725 3199.6326 3323.9187
3395.5377 3774.9485 3915.5945

Ac radikal De-protonated H2CO3 (PCET/HCO3)

1	0.237914	-1.038954	0.025108
8	1.265274	1.120171	-0.148237
1	0.238691	1.039321	-0.025149
6	1.948450	-0.000045	-0.000022
8	3.164934	-0.000352	-0.000325

8	1.264703	-1.119806	0.148628
8	-1.221501	-1.107953	-0.140440
1	-3.812631	-0.928895	-0.119190
6	-3.276170	0.000127	-0.000240
6	-1.817013	0.000020	0.000014
1	-3.812551	0.929214	0.118557
8	-1.221289	1.107777	0.140644

E = -493.000331147

31.4185 62.8457 118.1676
163.2669 189.6800 275.3819
281.4776 482.3592 605.3509
644.8822 654.0843 692.5932
771.7588 827.2205 1004.8669
1006.7369 1049.9950 1076.4346
1117.0407 1333.0082 1399.6195
1408.2140 1487.6902 1529.9416
1595.9556 1785.1150 2365.0247
2504.4136 3184.2605 3304.2636

Ac radikal De-protonated H2PO4 (PCET/HPO4)

8	1.728153	-1.124040	-0.127208
1	4.286705	-0.934874	0.250121
6	2.300603	0.000766	-0.042821
6	3.752318	0.000429	0.172388
8	1.726451	1.123209	-0.128401
1	4.287043	0.935527	0.250850
8	-1.362547	-0.043075	1.575144
8	-0.837280	-1.233791	-0.612178
1	0.145453	-1.197713	-0.409956
15	-1.607734	-0.003993	0.092994
1	0.120598	1.223522	-0.381654
8	-0.865666	1.285116	-0.537181
8	-3.019274	-0.004136	-0.405385

E = -871.715428024

42.3360 46.9797 100.8042
122.4340 152.2876 195.1196
252.6424 364.6506 372.5911
473.2485 493.6890 497.7093
509.7412 587.7041 666.3910
770.3984 838.1497 861.1072
867.7950 921.1029 998.6354
1004.3468 1083.5835 1204.3172
1308.7284 1373.4036 1404.2682
1477.5029 1559.7842 2954.7981
3046.7626 3175.8649 3293.3281

Acetaldehyde (PCET)

1	-1.151155	-1.237655	-0.001118
6	-1.160899	-0.150210	0.000040
8	1.227771	-0.276354	-0.000002
1	-1.691745	0.226419	0.877444
6	0.227762	0.399118	0.000094
1	-1.691504	0.228052	-0.876941
1	0.311060	1.500564	-0.000172

E = -153.815015184

163.9335 516.8157 780.0132

906.4373 1140.3739 1148.4825
1378.3896 1431.4690 1452.5465
1460.5933 1824.2786 2984.5334
3063.9584 3128.4579 3179.3275

FAC radikal (HAT)

8	-0.612005	1.299967	0.000190
6	-0.611183	0.046703	-0.000077
6	0.692157	-0.641057	0.000527
9	1.819047	0.079398	-0.000323
8	-1.601060	-0.729767	-0.000248
1	0.847244	-1.710056	0.000667

E = -327.195675493

167.4152 262.9381 351.6974
509.1916 707.8616 742.0841
962.2338 1194.2196 1308.9698
1452.7947 1618.7185 3242.1530

ClAc radikal (HAT)

8	-0.988364	1.307443	0.000022
6	-1.060558	0.059475	-0.000007
6	0.202821	-0.725726	0.000044
17	1.740441	0.034468	-0.000015
8	-2.094785	-0.655440	-0.000030
1	0.224115	-1.804471	0.000101

E = -687.558568939

111.3317 220.3258 397.4084
428.5193 686.3367 750.1300
829.3039 1005.1480 1243.4574
1386.4045 1623.1564 3248.5153

BrAc radikal (HAT)

8	-1.529357	1.309222	0.000041
6	-1.628953	0.064085	-0.000144
6	-0.386464	-0.756158	0.000020
35	1.318616	0.015363	0.000001
8	-2.678697	-0.628010	0.000042
1	-0.394637	-1.834952	0.000040

E = -2801.52504614

95.1626 191.3152 370.0179
382.1395 682.6475 748.6119
751.3009 983.2138 1211.7904
1375.3871 1623.4626 3248.9196

IAC radikal (HAT)

8	-1.915984	1.309747	0.000151
6	-2.036702	0.065912	0.000021
6	-0.806689	-0.779009	0.000402
53	1.095423	0.009220	-0.000038
8	-3.101331	-0.603787	-0.000292
1	-0.858530	-1.857763	0.000595

E = -238.697580114

80.4708 168.9793 346.0464
398.0968 674.5124 705.7479

749.5757 969.3881 1176.8354
1363.6779 1617.1787 3234.8911

Ethanol (HAT)

1	-1.288567	-0.854827	-0.885930
1	1.983685	0.085327	-0.000751
6	-1.220240	-0.221976	-0.000057
8	1.150631	-0.395866	0.000109
1	-1.288602	-0.854951	0.885745
6	0.081116	0.547266	0.000045
1	-2.066081	0.466245	-0.000007
1	0.144741	1.186722	-0.885298
1	0.144519	1.186674	0.885450

E = -155.021823243

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

Ethanol - HCO3 (HAT/HCO3)

1	-2.716768	1.546600	-0.138413
1	-0.338350	-0.968576	-0.484974
6	-3.095602	0.578425	0.193346
8	-1.205145	-0.556641	-0.728822
1	-3.743361	0.175200	-0.586671
6	-1.948976	-0.370268	0.468098
1	-3.692299	0.729204	1.093873
1	-2.331728	-1.331877	0.826107
1	-1.298929	0.038555	1.250559
8	1.263573	-1.106087	-0.011270
1	0.217922	0.793069	-0.637821
6	1.838303	0.014277	0.041719
8	1.096877	1.107641	-0.367098
8	2.987339	0.265489	0.414485

E = -419.595376874

28.4041 56.3014 79.7410
115.5211 150.5949 190.2216
268.4692 433.8457 619.7857
683.3735 693.2618 812.2551
841.9772 898.0888 925.6233
989.3998 1084.5460 1128.3225
1183.2702 1309.0016 1332.2755
1357.7351 1373.5981 1398.9694
1477.8015 1488.2888 1501.3777
1530.3457 1711.0413 3022.6853
3055.8927 3060.5288 3133.5907
3139.8226 3243.8155 3701.7511

Ethanol - HPO4 (HAT/HPO4)

1	3.373948	0.628908	1.349232
1	0.798025	-1.046673	-0.394793
6	3.624328	0.431362	0.305334
8	1.708834	-0.978667	0.049932
1	4.297502	-0.426907	0.269960

6	2.367803	0.149912	-0.492545
1	4.150441	1.299393	-0.094905
1	2.625801	-0.025717	-1.544056
1	1.703668	1.023295	-0.463561
8	-0.590289	0.230670	1.345581
1	0.309428	-0.095663	1.194277
8	-1.506882	1.434386	-0.713913
8	-2.827654	-0.442526	0.401381
15	-1.476112	0.065109	-0.060013
8	-0.667748	-0.971478	-0.869567

E = -798.297208640

24.6752 64.5111 86.1274
 120.5459 147.0614 225.2932
 274.5977 337.5542 381.5233
 438.0961 482.3369 510.5661
 516.4536 537.4782 732.0702
 807.1265 911.2425 950.3038
 1033.8091 1065.4039 1088.9661
 1130.4576 1137.9074 1183.8822
 1269.0425 1308.2976 1376.0927
 1397.6481 1477.8221 1488.9641
 1526.0959 1532.3748 2746.8777
 3010.9916 3037.9875 3058.3311
 3130.7441 3135.3322 3753.1415

Betahidroxy_acid (FRS)

1	-2.565469	-0.798083	1.049383
1	-0.240722	1.603377	0.170598
6	-2.431219	-0.701020	-0.030431
8	-1.173750	1.304378	0.221393
1	-3.266358	-0.125900	-0.433353
6	-1.117739	-0.006546	-0.328203
1	-2.449970	-1.697475	-0.474702
1	-0.994796	0.069010	-1.418148
8	2.441221	-0.834358	-0.035289
1	0.108398	-1.780301	-0.179596
6	1.436699	-0.097190	0.004369
6	0.074556	-0.772317	0.236708
8	1.444033	1.163128	-0.102308
1	-0.056886	-0.873369	1.320792

E = -382.455705757

49.3507 126.3139 222.6046
 250.1119 340.0134 376.2618
 469.3555 494.9400 631.1479
 738.4578 761.6169 872.3929
 922.1960 933.9444 975.9718
 1087.1377 1107.9329 1177.4649
 1236.9055 1293.9666 1334.4898
 1381.7546 1397.4206 1427.4278
 1442.2134 1473.2327 1487.1567
 1492.2909 1626.1195 2993.0453
 3045.6309 3055.0497 3117.3480
 3128.3055 3136.0381 3473.2090

Betahidroxy_acid_Radical (FRS)

1	-2.560543	-0.965330	0.916476
1	-0.438150	1.779588	0.270889

6	-2.399581	-0.721996	-0.135326
8	-1.227920	1.252337	0.444808
1	-3.235740	-0.117690	-0.486469
6	-1.107547	0.050785	-0.299488
1	-2.370356	-1.647481	-0.710373
1	-0.949242	0.286480	-1.356904
8	2.427645	-0.827063	0.129364
1	0.122273	-1.748449	-0.299615
6	1.380356	-0.046686	-0.031661
6	0.080172	-0.778451	0.199720
8	1.515818	1.118509	-0.325127
1	-0.012990	-0.959281	1.274167

E = -382.226065447

38.6763 120.9256 192.2587
 242.6425 282.2750 342.4503
 422.7901 451.3600 475.9504
 549.4757 632.9837 833.1017
 889.7883 921.4872 965.4251
 1067.7929 1106.7155 1114.7495
 1196.0393 1237.3543 1298.1328
 1339.2840 1387.9386 1400.5318
 1429.0024 1445.9197 1480.2557
 1491.8080 1722.9907 3051.8762
 3067.4353 3079.5237 3130.8215
 3143.9915 3153.3511 3837.0640

Betahidroxy_acid_H2O (FRS/H2O)

1	-2.560543	-0.965330	0.916476
1	-0.438150	1.779588	0.270889
6	-2.399581	-0.721996	-0.135326
8	-1.227920	1.252337	0.444808
1	-3.235740	-0.117690	-0.486469
6	-1.107547	0.050785	-0.299488
1	-2.370356	-1.647481	-0.710373
1	-0.949242	0.286480	-1.356904
8	2.427645	-0.827063	0.129364
1	0.122273	-1.748449	-0.299615
6	1.380356	-0.046686	-0.031661
6	0.080172	-0.778451	0.199720
8	1.515818	1.118509	-0.325127
1	-0.012990	-0.959281	1.274167

E = -382.226065447

38.6763 120.9256 192.2587
 242.6425 282.2750 342.4503
 422.7901 451.3600 475.9504
 549.4757 632.9837 833.1017
 889.7883 921.4872 965.4251
 1067.7929 1106.7155 1114.7495
 1196.0393 1237.3543 1298.1328
 1339.2840 1387.9386 1400.5318
 1429.0024 1445.9197 1480.2557
 1491.8080 1722.9907 3051.8762
 3067.4353 3079.5237 3130.8215
 3143.9915 3153.3511 3837.0640

Betahidroxy_acid_H2O_Radical (FRS/H2O)

1	-3.114432	-0.272005	0.766644
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1	-0.078706	1.560028	0.368764
6	-2.777724	-0.031763	-0.243713
8	-0.944471	1.199793	0.627471
1	-3.260004	0.892119	-0.561593
6	-1.273097	0.147679	-0.256210
1	-3.078986	-0.836052	-0.914968
1	-0.937618	0.393341	-1.269555
8	1.579691	-1.239103	-0.925630
1	-0.889170	-1.983970	-0.472488
6	0.887816	-1.027887	0.101220
6	-0.584579	-1.165456	0.181628
8	1.641004	-0.631478	1.021697
1	-0.862716	-1.386491	1.213649
1	1.850266	2.814802	-0.470504
8	1.551226	1.901734	-0.404243
1	2.237262	1.435229	0.088144

E = -458.662310967

40.3850 73.2915 82.5607
 116.3311 147.9494 182.6725
 204.1627 246.4620 259.0586
 303.2079 330.1390 385.0915
 426.8542 476.2917 590.5794
 673.5900 711.6028 869.6879
 899.7717 928.4447 950.9917
 974.8192 1094.5032 1100.6406
 1153.1194 1217.0946 1289.9117
 1335.9390 1372.1520 1403.9003
 1448.9708 1467.2369 1480.7410
 1492.2604 1609.5536 1639.6640
 3049.6002 3066.9208 3085.6379
 3141.8401 3149.4585 3154.8371
 3662.5279 3840.0775 3933.9198

1-FEthanol (XA)

9	0.466211	-1.239087	-0.138195
1	-1.725716	1.180457	0.337427
1	-1.411990	0.284729	-1.165176
6	-1.366672	0.239333	-0.076721
1	-1.998499	-0.572190	0.279716
6	0.053093	0.009136	0.351385
8	0.865344	0.983269	-0.191133
1	0.171229	-0.057340	1.434121
1	1.727795	0.959171	0.238745

E = -254.283982264

239.3347 372.4663 403.3802
 464.8124 580.1712 864.9178
 949.1655 1078.1451 1108.3463
 1190.4026 1300.3143 1383.3673
 1403.0280 1475.7577 1479.8357
 1490.9770 3080.5075 3105.5274
 3163.0068 3170.1126 3865.6576

1-ClEthanol (XA)

17	1.342121	-0.100079	-0.055575
1	-2.247148	-1.014749	0.198721
1	-1.144753	-1.177036	-1.185175
6	-1.202264	-1.113010	-0.098823

1	-0.788232	-2.017424	0.341109
6	-0.454449	0.098174	0.381288
8	-0.957137	1.225311	-0.223056
1	-0.425028	0.184016	1.464852
1	-0.613529	2.013055	0.214934

E = -614.636490214

259.3805 315.4062 357.6993
403.6458 485.5649 601.8333
930.4219 1039.3004 1080.3432
1174.9645 1297.2024 1301.5339
1401.6392 1461.7673 1477.0369
1482.0333 3076.8426 3139.7828
3156.2323 3177.1010 3859.6744

1-BrEthanol (XA)

35	1.016295	-0.029397	-0.024313
1	-2.702762	-1.109380	0.167171
1	-1.560257	-1.223816	-1.187775
6	-1.646052	-1.155000	-0.103961
1	-1.196823	-2.032603	0.354429
6	-0.985630	0.098975	0.388810
8	-1.514115	1.192579	-0.235387
1	-0.963397	0.191236	1.470830
1	-1.244062	1.998967	0.220292

E = -2728.60383049

258.2552 283.7898 286.2110
431.0310 474.9694 535.1076
928.8112 1028.5910 1074.2951
1167.0276 1268.2846 1302.5466
1401.9683 1463.5042 1476.0222
1482.0720 3073.4728 3146.7284
3160.3578 3180.9156 3850.7039

1-IEthanol (XA)

53	0.848428	-0.015627	-0.014742
1	-3.069571	-1.122058	0.141029
1	-1.901290	-1.245721	-1.189588
6	-2.006495	-1.166000	-0.108167
1	-1.565891	-2.040371	0.364997
6	-1.361702	0.095845	0.391596
8	-1.901797	1.184282	-0.240703
1	-1.359415	0.187986	1.474279
1	-1.646941	1.995051	0.215670

E = -165.772694770

238.0552 260.0675 274.1451
423.7593 470.0754 501.8881
925.0948 1014.3233 1066.7667
1146.7961 1248.2620 1300.0735
1400.6642 1456.2343 1474.5999
1482.0290 3066.8127 3140.3103
3153.3001 3178.3030 3851.5999

Ester Radical (OA)

6	1.657855	-0.741117	-0.917964
6	1.167730	-0.312465	0.448505

8	1.415965	1.020034	0.748327
1	1.194439	-0.148473	-1.705061
1	1.432121	-1.794777	-1.078702
1	2.738005	-0.603716	-0.956997
1	1.645242	-0.898194	1.230550
1	1.029050	1.554290	0.041088
8	-0.841129	0.999792	-0.816138
1	-3.286978	0.141450	-0.361841
6	-2.488340	-0.372354	0.148920
6	-1.135214	0.073420	-0.077925
1	-2.691178	-1.199098	0.811215
8	-0.233946	-0.636874	0.619128

E = -382.244577085

93.3346 145.9589 222.3842
247.4408 331.8122 345.0581
430.9530 452.0349 508.9144
520.7506 631.0973 727.1802
770.0601 827.7361 923.2385
989.3486 1027.5426 1095.8870
1106.4013 1174.9019 1300.3976
1343.1269 1402.1464 1419.4503
1457.1655 1465.8383 1484.7151
1494.0496 1701.1326 3081.8687
3143.0858 3160.4825 3172.7767
3197.9944 3322.3977 3816.5219