Supporting Information

Ionization of Carboxylic Acid Clusters in the Gas Phase and on Free Ar_N and $(H_2O)_N$ Nanoparticles: Valeric Acid as a Model for Small Carboxylic Acids

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Table S1 – Reaction energies (in eV) of dimerization and hydration of carboxylic acids and their ions. Calculated at the B3LYP+D2/def2TZVP level of theory.

reaction	1	2	3	4	5	6	7	8
$2\ CA \rightarrow (CA)_2$	-0.71	-0.77	-0.76	-0.76	-0.76	-0.76	-0.77	-0.77
$CA + 2\ H_2O \rightarrow CA.2H_2O$	-0.93	-0.92	-0.88	-0.89	-0.89	-0.89	-0.89	-0.89
$CA^+ + 2\ H_2O \rightarrow CA^+.2H_2O$	-2.71	-1.88	-1.73	-1.69	-1.65	-1.63	-1.62	-1.60
$CAH^+ + 2\ H_2O \rightarrow CAH^+.2H_2O$	-2.10	-1.86	-1.76	-1.73	-1.72	-1.71	-1.70	-1.70

Cartesian coordinates of calculated structures (in Å) along with electronic energy corrected for ZPE (in Hartree)

Valeric acid, B3LYP+D2/def2TZVP

VA
E = -347.043344
C -3.345629 0.312893 -0.000005
C -2.101306 -0.571667 -0.000001
H -3.361265 0.957988 -0.883082
H -4.260765 -0.284156 -0.000009
H -3.361271 0.957986 0.883074
H -2.114527 -1.227793 0.877430
H -2.114521 -1.227791 -0.877434
C -0.811877 0.244000 0.000004
C 0.425472 -0.643186 0.000008
H -0.786890 0.900652 -0.873885
H -0.786896 0.900650 0.873896
C 1.720433 0.128423 0.000015
H 0.434607 -1.305712 0.871834
H 0.434613 -1.305711 -0.871818
O 2.790740 -0.705709 -0.000012
O 1.835142 1.326103 -0.000002
H 3.587297 -0.152041 -0.000026

VA+
E = -346.686694
C -3.212321 0.373888 -0.225368
C -2.058987 -0.491844 0.295217
H -3.257292 0.380750 -1.314113
H -4.130610 -0.091350 0.166173
H -3.162657 1.396846 0.148153
H -2.036662 -0.504232 1.384858

H -2.124579 -1.516601 -0.070149
C -0.736390 0.169792 -0.256401
C 0.391274 -0.694603 0.313184
H -0.755285 0.144480 -1.345216
H -0.664582 1.199838 0.085687
C 1.755167 -0.030771 0.005175
H 0.381993 -0.757879 1.407875
H 0.383576 -1.700975 -0.099784
O 1.841439 1.248881 0.236721
O 2.633007 -0.761850 -0.388769
H 2.738073 1.594102 0.062052

VA+, h-trans
E = -346.716983
C 3.181054 0.284332 -0.140547
C 1.802384 -0.217667 -0.556410
C 0.860252 -0.278310 0.711481
C -0.447317 -0.796616 0.323873
C -1.556118 0.024493 0.019134
O -2.725867 -0.420325 -0.353042
O -1.441525 1.312811 0.109439
H 3.640735 -0.387762 0.586562
H 3.827810 0.333800 -1.019274
H 3.121292 1.282613 0.297330
H 1.350689 0.449577 -1.292903
H 1.866949 -1.214300 -0.996951
H 1.331525 -0.955935 1.427026
H 0.793142 0.723065 1.136184
H -0.588952 -1.863647 0.188298
H -2.265207 1.784031 -0.115179
H -2.780381 -1.388719 -0.407462

VA, h-trans TS
E = -346.645253 -346.645253
C 0.485647 -0.730893 0.538315
H 1.502601 -1.573717 0.003553
C 1.567370 0.137367 0.043918
O 1.640137 1.411943 0.025716
O 2.429189 -0.675757 -0.392229
C -0.818234 -0.814355 -0.170234
C -1.740226 0.336644 0.370698
C -3.098156 0.252576 -0.324685
H 2.466434 1.751915 -0.374154
H 0.528771 -0.928606 1.610881
H -1.290248 -1.774517 0.039069
H -0.703496 -0.700066 -1.249629
H -1.262482 1.299313 0.177167
H -1.851521 0.226130 1.450941
H -3.584775 -0.703493 -0.123889
H -3.740809 1.050772 0.054730
H -2.997493 0.374745 -1.404641

CH2C(OH)2+
E = -228.778642
H 1.678406 -0.904568 -0.000011
O 0.715348 -1.075193 -0.000017
C -0.003594 -0.007376 -0.000003
C -1.417446 -0.156160 -0.000007
H -2.060858 0.714222 0.000088
H -1.836132 -1.154007 -0.000044
O 0.621883 1.126871 0.000016
H 0.046975 1.912147 0.000041

C3H6
E = -117.883111
C 1.275250 0.221570 0.000004
H 1.283350 1.307081 -0.000032
H 2.234792 -0.281392 0.000031
C 0.134451 -0.456423 -0.000011
H 0.168476 -1.543219 -0.000012
C -1.229065 0.162827 -0.000002
H -1.801676 -0.151559 0.879255
H -1.166691 1.253543 -0.000456
H -1.802067 -0.152297 -0.878733

CH2CHC(OH)2+
E = -267.527361
H 1.471826 1.585877 0.000150
O 0.549562 1.265046 0.000011
C 0.453153 -0.017147 -0.000089
C -0.835357 -0.650654 -0.000157
H -0.841954 -1.733939 -0.000408
C -1.969967 0.062400 0.000178
O 1.565544 -0.675817 0.000017
H 1.458449 -1.642988 -0.000098
H -2.931268 -0.436595 0.000104
H -1.964875 1.146222 0.000435

C2H5
E = -79.136317
C 0.692579 0.000012 -0.002115
H 1.103181 -0.886915 -0.493756
H 1.091416 -0.000722 1.025765
H 1.103169 0.887605 -0.492539
C -0.792530 0.000002 -0.017450
H -1.348989 -0.926661 0.038944
H -1.349071 0.926609 0.038977

VAA+.H2O
E = -693.786552
C -5.207735 -1.765640 0.620877
C -3.689786 -1.614128 0.603515
C -3.225304 -0.997046 -0.760138
C -1.765268 -0.892847 -0.793952
C -1.057012 0.300602 -0.511455
O 0.262974 0.239584 -0.618149
C 1.184588 0.968170 0.240131
O 0.776727 1.573951 1.172426
O -1.695646 1.366865 -0.222415
C 2.573015 0.709927 -0.216698
C 3.048437 -0.693563 0.223340
C 4.493875 -0.939221 -0.203859
C 4.982679 -2.320226 0.225482
H -5.542864 -2.430770 -0.177906
H -5.529391 -2.187668 1.574923
H -5.698989 -0.798699 0.491861
H -3.205244 -2.583352 0.740384
H -3.699402 -0.023135 -0.881789
H -1.156142 -1.768063 -0.982889
H 2.616408 0.784703 -1.305255
H 3.208404 1.475887 0.227879
H 2.964080 -0.777402 1.310415
H 2.397523 -1.452745 -0.217931
H 4.569048 -0.836595 -1.291020
H 5.132804 -0.165168 0.231980
H 6.016319 -2.481345 -0.084746
H 4.935088 -2.429588 1.311989
H 4.369405 -3.107288 -0.221328
H -1.178088 2.258507 -0.100341
H -3.358650 -0.960510 1.413379
H -3.563394 -1.669156 -1.553680
O -0.600470 3.622713 -0.032527

H -0.102678 3.796166 0.777403
H -1.147851 4.395138 -0.221467

(VA)2+
E = -693.775213
C 6.644806 -0.110608 0.779638
C 5.609839 -0.285190 -0.330400
C 4.205661 0.075996 0.162374
C 3.181975 -0.103053 -0.976417
C 1.806941 0.281669 -0.518553
O 1.633201 1.535892 -0.212973
O 0.912341 -0.569462 -0.430658
O -0.912333 0.569463 0.430629
C -1.806937 -0.281666 0.518507
C -3.181963 0.103047 0.976404
C -4.205671 -0.075994 -0.162369
C -5.609840 0.285187 0.330437
C -6.644829 0.110613 -0.779582
O -1.633190 -1.535893 0.212945
H 6.416630 -0.756340 1.631137
H 7.641383 -0.367795 0.415868
H 6.669070 0.923281 1.132333
H 5.864608 0.349674 -1.184148
H 5.612868 -1.318997 -0.687880
H 3.935810 -0.566422 1.005157
H 4.184150 1.110171 0.511338
H 3.427525 0.557305 -1.814454
H 3.164977 -1.133566 -1.328208
H 0.719702 1.687870 0.095112
H -0.719689 -1.687870 -0.095137
H -3.164961 1.133558 1.328203
H -3.427495 -0.557319 1.814441
H -3.935837 0.566430 -1.005152
H -4.184167 -1.110167 -0.511340
H -5.864592 -0.349684 1.184185
H -5.612862 1.318992 0.687924
H -7.641398 0.367797 -0.415790
H -6.416670 0.756351 -1.631081
H -6.669099 -0.923274 -1.132284

(VA)2+, h-trans
E = -693.806968
C -6.125124 -0.038001 -0.605753
C -4.695146 -0.556081 -0.725145
C -3.956982 -0.426893 0.649424
C -2.598486 -0.968001 0.552180
C -1.438788 -0.171703 0.390506
O -0.289976 -0.760355 0.277763
O -1.555946 1.126372 0.362284
O 1.087907 1.435593 0.062033
C 2.261948 1.789734 -0.067364
C 3.421916 0.851727 -0.163784
C 3.050895 -0.624440 -0.086124
C 4.279915 -1.525236 -0.193640
C 3.913730 -3.004729 -0.116910
O 2.599445 3.060362 -0.133668
H -6.137356 1.011379 -0.302841
H -6.634672 -0.121724 -1.567526
H -6.688475 -0.614636 0.131130
H -4.690241 -1.603318 -1.035301
H -4.141806 0.013200 -1.475426
H -3.951978 0.621246 0.948914
H -4.527487 -1.007647 1.379933
H -2.429565 -2.037707 0.535186
H 0.461641 -0.101087 0.175715
H 3.942582 1.082092 -1.099428
H 2.539451 -0.826888 0.860872
H 2.352918 -0.872107 -0.892896
H 4.794607 -1.316541 -1.136668
H 4.980044 -1.271960 0.608490
H 4.802085 -3.633111 -0.195234
H 3.420595 -3.234751 0.831509
H 3.233672 -3.279703 -0.927800
H -0.684141 1.575092 0.250817
H 1.819454 3.636340 -0.067285
H 4.123957 1.127791 0.630192

VAH+.[VA-H]
E = -693.774490
C -6.227163 -0.490090 1.232016
C -5.349950 -0.679591 -0.003106
C -3.913707 -0.230750 0.258897
C -3.040413 -0.433140 -1.011704
C -1.666840 0.010572 -0.729739
O -1.357364 1.238220 -0.917974
O -0.831352 -0.841485 -0.245641
O 1.057690 0.983909 -0.031310
C 2.123371 1.566103 0.202945
O 2.427366 2.764106 0.050939
C 3.369225 0.816482 0.796824
C 3.700484 -0.381702 -0.088406
C 4.843343 -1.181591 0.565285
C 5.184295 -2.408447 -0.281686
H -6.257289 0.560508 1.531709
H -7.249881 -0.813537 1.032274
H -5.846527 -1.073335 2.074347
H -5.347911 -1.731515 -0.304052
H -5.756381 -0.108248 -0.842987
H -3.898024 0.824883 0.541800
H -3.487452 -0.806326 1.084675
H -3.026886 -1.489002 -1.281971
H -3.444476 0.162371 -1.830430
H 0.050183 -0.434066 -0.035932
H 3.028118 0.539601 1.800746
H 4.221366 1.487554 0.893779
H 2.819228 -1.014120 -0.208727
H 4.014126 -0.047746 -1.080189
H 5.719651 -0.537292 0.669722
H 4.543519 -1.488436 1.570875
H 5.994053 -2.970501 0.188915
H 4.321852 -3.071988 -0.378674
H 5.507515 -2.114524 -1.282634
H -0.411360 1.440635 -0.639323

CO2
E = -188.658348
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.159696
O 0.000000 0.000000 -1.159696

C4H9
E = -157.748588
C -1.930976 0.165714 -0.060076
C -0.563109 -0.506345 0.068121
C 0.575978 0.449297 0.029127
C 1.976405 -0.043106 -0.049385
H -2.011255 0.698540 -1.010991
H -2.739632 -0.566943 -0.008398
H -2.078665 0.891414 0.744493
H -0.533053 -1.085214 1.007878
H -0.437377 -1.255877 -0.725783
H 0.388145 1.492196 0.259660

H 2.292864 -0.524142 0.891367
H 2.084707 -0.806098 -0.830391
H 2.684477 0.762762 -0.254560

VAH+
E = -347.353524
C 3.355269 0.323778 0.000000
C 2.128824 -0.583492 0.000000
C 0.826284 0.220752 0.000000
C -0.396128 -0.697367 -0.000000
C -1.699645 0.001181 0.000000
O -1.832057 1.277855 -0.000000
O -2.770952 -0.697209 -0.000000
H 3.367850 0.964168 0.885597
H 4.271112 -0.267959 0.000000
H 3.367850 0.964168 -0.885597
H 2.141600 -1.234487 -0.879220
H 2.141600 -1.234487 0.879220
H 0.810702 0.864107 0.888392
H 0.810702 0.864107 -0.888392
H -0.404024 -1.365892 -0.870063
H -0.404025 -1.365892 0.870063
H -3.593078 -0.167145 -0.000000
H -0.973847 1.745037 -0.000000

C4H9+
E = -157.483605
C -1.933376 -0.154036 0.141038
C -0.559040 0.458415 -0.128273
C 0.594936 -0.376930 -0.130124
C 1.947639 0.060078 0.110932
H -2.064981 -0.283871 1.216294
H -2.712928 0.512880 -0.222970
H -2.039916 -1.122641 -0.349880
H -0.461425 0.625002 -1.250438
H -0.382098 1.445364 0.304965
H 0.442994 -1.428681 -0.378782
H 2.665411 -0.407027 -0.572088
H 2.066213 1.138865 0.197915
H 2.185778 -0.405056 1.093538

[VA-OH].H2O
E = -347.565599
C -3.700123 -0.681576 0.000340
C -2.643117 0.421082 0.000472
C -1.224672 -0.142944 -0.000221
C -0.171862 0.968260 -0.000127
C 1.254061 0.477044 -0.000681
O 1.654295 -0.634839 -0.001080
H -3.595179 -1.317759 0.883440
H -4.709505 -0.264206 0.000861
H -3.595769 -1.316983 -0.883389
H -2.777386 1.062588 -0.877115
H -2.776821 1.061836 0.878695
H -1.075732 -0.780020 0.875847
H -1.076317 -0.779327 -0.876895
H -0.277114 1.623293 -0.871677
H -0.276619 1.622664 0.871959
H 3.785427 -0.618407 0.000318
O 4.685622 -0.269061 0.001070
H 4.569952 0.686318 -0.000654

[VA-H].H2O
E = -422.855794
C -3.542031 -0.898841 0.097131
C -2.264516 -0.212285 0.572667
C -1.595924 0.586868 -0.572000
C -0.346026 1.250656 -0.134150
C 0.927287 0.578548 -0.034145
O 0.904130 -0.708733 -0.425148
O 1.944939 1.136930 0.373956
H -3.325157 -1.593710 -0.718693
H -4.010168 -1.461892 0.907857
H -4.265826 -0.165275 -0.269246
H -2.486062 0.464930 1.402355
H -1.550480 -0.952868 0.939371
H -1.380408 -0.113315 -1.383945
H -2.306250 1.332448 -0.939740
H -0.348572 2.277711 0.206347
H 1.812049 -1.084049 -0.323316
H 3.364230 -0.154061 0.363612
O 3.548454 -1.089865 0.145924
H 4.243725 -1.086252 -0.519483

[VA-OH]+
E = -270.872803
C 2.868792 -0.470480 0.000021
C 1.682245 0.491923 0.000014
C 0.365608 -0.286190 -0.000057
C -0.821866 0.743543 -0.000036
C -2.068910 0.060825 0.000106
O -3.009975 -0.540158 -0.000017
H 2.856086 -1.108677 -0.886279
H 3.804155 0.090473 0.000066
H 2.856034 -1.108733 0.886278
H 1.719884 1.138794 0.881544
H 1.719941 1.138860 -0.881463
H 0.287737 -0.917980 -0.886357
H 0.287681 -0.918057 0.886183
H -0.803432 1.384461 0.891812
H -0.803501 1.384397 -0.891939

CH2C(OH)2
E = -229.087346
H 1.716655 -0.649111 -0.000044
O 0.831648 -1.034781 -0.000029
C -0.074665 -0.036851 0.000003
C -1.389883 -0.244901 0.000001
H -2.076383 0.588933 0.000025
H -1.776203 -1.251656 -0.000026
O 0.547920 1.175456 0.000025
H -0.113327 1.876944 0.000049

[VA].C3H7+
E = -464.632066
C 4.749850 0.119827 -0.511576
C 3.312418 -0.369508 -0.658602
C 2.535207 -0.164316 0.689227
C 1.170620 -0.680529 0.567329
C 0.037073 0.124772 0.318201
O -1.110730 -0.458131 0.194877
C -2.350509 0.305864 -0.048858
C -3.497475 -0.672642 -0.130707
C -4.806442 0.078348 -0.383391
O 0.194782 1.422219 0.227174
H 5.275017 -0.439530 0.265466
H 5.285672 -0.016542 -1.452897
H 4.778813 1.180320 -0.252239
H 2.796709 0.181611 -1.448098
H 3.290547 -1.428541 -0.924009
H 3.069238 -0.728382 1.458772
H 2.548302 0.895554 0.943261

H 0.977888 -1.745970 0.600433
H -2.475741 1.002398 0.785710
H -2.220030 0.850932 -0.988689
H -3.551180 -1.233696 0.804532
H -5.633956 -0.628197 -0.442654
H -5.022606 0.781643 0.424474
H -4.770408 0.632983 -1.324197
H -3.300284 -1.382320 -0.936838
H -0.624846 1.914128 0.060825

[VA].(OH)2CCH2+
E = -575.875719
C -5.178247 -0.858103 -0.000446
C -4.168618 0.285756 0.000071
C -2.725455 -0.221201 -0.000249
C -1.722216 0.931806 0.000090
C -0.269655 0.563994 0.000335
O 0.075836 -0.743040 0.000550
O 0.634574 1.375204 0.000389
O 3.127879 0.967763 -0.000476
C 3.554885 -0.234675 -0.000237
C 4.960591 -0.466849 -0.000379
H 5.629199 0.381810 -0.000706
O 2.781470 -1.279171 0.000341
H -5.054686 -1.488107 0.884380
H -6.199416 -0.474888 -0.000257
H -5.054705 -1.487288 -0.885856
H -4.319729 0.920784 -0.877975
H -4.319585 0.919872 0.878800
H -2.578003 -0.850089 0.886857
H -2.578066 -0.849379 -0.887857
H -1.867918 1.579534 -0.870368
H -1.868307 1.579494 0.870505
H 2.097460 1.098417 -0.000066
H 1.812417 -1.084196 0.000428
H 5.330265 -1.482092 -0.000044
H -0.694701 -1.334286 0.000624

(VA)2
E = -694.114694
C -6.756576 0.777502 -0.000174
C -5.733420 -0.356060 -0.000054
C -4.297630 0.161829 -0.000089
C -3.281959 -0.972682 0.000023
C -1.844714 -0.519904 -0.000055
O -1.514023 0.658939 -0.000115
O -0.988682 -1.521949 0.000339
H -6.631596 1.410302 -0.883349
H -7.779343 0.393526 -0.000150
H -6.631617 1.410470 0.882883
H -5.888088 -0.993548 0.877404
H -5.888068 -0.993716 -0.877392
H -4.132563 0.797491 -0.874187
H -4.132581 0.797658 0.873892
H -3.417850 -1.621849 0.871255
H -3.417836 -1.622012 -0.871087
H -0.041945 -1.186191 0.000468
H 0.041951 1.186130 0.000373
O 0.988672 1.521933 0.000364
C 1.844716 0.519898 0.000107
O 1.514029 -0.658947 0.000003
C 3.281957 0.972683 0.000090
C 4.297631 -0.161824 -0.000082
H 3.417790 1.622022 -0.871021
H 3.417884 1.621842 0.871322
C 5.733418 0.356072 -0.000110
H 4.132625 -0.797660 0.873902
H 4.132526 -0.797481 -0.874177
C 6.756579 -0.777485 -0.000284
H 5.888024 0.993734 -0.877452
H 5.888123 0.993555 0.877345
H 7.779344 -0.393504 -0.000303
H 6.631663 -1.410460 0.882775
H 6.631563 -1.410280 -0.883457

VA.2H2O
E = -499.959946
C 4.346303 0.076207 0.970602
C 3.405395 -0.094499 -0.220005
C 1.937519 -0.001303 0.186749
C 0.995091 -0.179902 -1.013597
C -0.443812 -0.093062 -0.577471
O -0.860963 1.152455 -0.431502
O -1.121895 -1.082465 -0.348616
O -3.336108 1.395302 0.486000
H 4.162421 -0.696148 1.722823
H 5.392934 0.008405 0.664796
H 4.194619 1.048828 1.447132
H 3.617326 0.671390 -0.973565
H 3.584807 -1.062759 -0.699128
H 1.716347 -0.769013 0.935031
H 1.745250 0.969027 0.653243
H 1.198685 0.599781 -1.750893
H 1.155368 -1.157521 -1.469119
H -1.804668 1.209946 -0.089492
H -3.947802 1.843836 -0.105979
H -3.658527 0.465122 0.577554
H -2.783293 -1.317793 0.169701
O -3.712885 -1.251751 0.486877
H -3.761646 -1.766068 1.298164

VA+.2H2O
E = -499.661525
C -4.286391 0.699724 0.289411
C -3.002106 -0.046195 0.638422
C -2.172718 -0.333203 -0.655779
C -0.960081 -1.091920 -0.332541
C 0.325763 -0.503484 -0.197667
O 1.304369 -1.298037 0.135442
O 0.471727 0.755179 -0.407257
O 2.699433 1.851296 0.050251
O 3.905743 -0.619248 0.288045
H -4.910813 0.107088 -0.382849
H -4.859491 0.905323 1.195441
H -4.065408 1.651823 -0.198371
H -2.389830 0.544383 1.323784
H -3.230736 -0.992844 1.133187
H -2.804732 -0.925826 -1.323463
H -1.933412 0.615329 -1.137020
H -1.014478 -2.151141 -0.113856
H 1.401495 1.166173 -0.245401
H 2.220024 -0.911367 0.183359
H 3.505383 1.313959 0.019558
H 2.893986 2.747807 -0.245462
H 4.433013 -1.118225 -0.350660
H 4.278018 -0.815547 1.158829

VAH+.2H2O
E = -500.300313
C 4.955208 -0.123793 -0.065841
C 3.679259 0.711276 -0.017068
C 2.422580 -0.160602 -0.009250

C 1.150615 0.684058 0.038664
C -0.139621 -0.070351 0.051336
O -1.225145 0.529735 0.096943
O -0.163890 -1.380849 0.017779
O -5.530264 0.607726 -0.057606
O -3.296814 -0.690659 -0.053561
H 4.982346 -0.742408 -0.966693
H 5.838356 0.516293 -0.070584
H 5.022421 -0.784626 0.802353
H 3.677201 1.342178 0.876926
H 3.637436 1.383828 -0.879133
H 2.425552 -0.785228 -0.911168
H 2.464637 -0.826964 0.861166
H 1.136848 1.328372 0.923887
H 1.096681 1.365888 -0.816498
H -2.224854 -0.099262 0.056193
H 0.730591 -1.758977 -0.021575
H -4.152035 -0.158714 -0.038927
H -3.405754 -1.504677 0.453080
H -5.818384 1.292701 0.555692
H -6.090379 0.660447 -0.840203

H2O
E = -76.441875
O -0.000000 0.000000 0.116869
H 0.000000 0.765123 -0.467477
H -0.000000 -0.765123 -0.467477

OH
E = -75.759758
O 0.000000 0.000000 0.108530
H 0.000000 0.000000 -0.868242

(H2O)2
E = -152.890614
O 1.480245 0.008995 -0.121234
H 0.532126 -0.014873 0.088636
H 1.934259 -0.054527 0.724128
O -1.380348 -0.008696 0.120273
H -1.619571 0.799436 -0.347138
H -1.645993 -0.732431 -0.457939

OH.H2O
E = -152.209752
O -1.594318 -0.000009 0.017181
O 1.250952 0.000192 -0.083990
H -0.612522 0.001299 -0.070637
H 1.681923 0.769540 0.303236
H 1.677526 -0.772297 0.301866

H3O+
E = -76.703807
O 0.000010 0.000005 -0.069697
H -0.043148 -0.946742 0.185851
H 0.841450 0.436005 0.185949
H -0.798379 0.510694 0.185774

H3O+.H2O
E = -153.205710
O -1.199797 -0.031005 0.046405
O 1.199842 -0.031291 -0.046469
H -1.718085 0.709283 0.397397
H -1.677845 -0.473229 -0.672418
H 1.717510 0.708822 -0.398807
H 1.677532 -0.470967 0.674183
H 0.000534 0.024460 0.000157

VA, S=3
E = -346.890668
C -3.371700 0.292187 0.107411
C -2.116458 -0.513550 -0.219298
H -3.355139 1.258117 -0.405407
H -4.277424 -0.237307 -0.197364
H -3.438036 0.486653 1.181699
H -2.159399 -1.486414 0.282659
H -2.077555 -0.719821 -1.294119
C -0.838256 0.207294 0.198835
C 0.413996 -0.606653 -0.127027
H -0.786849 1.177019 -0.307114
H -0.867356 0.414148 1.273223
C 1.685991 0.078726 0.273084
H 0.390155 -1.568750 0.392278
H 0.450345 -0.814946 -1.207688
O 2.831499 -0.680862 0.042668
O 1.905572 1.304630 -0.240735
H 3.583248 -0.246862 0.468343

VA, h-trans, S=3
E = -346.909572
C 2.260622 -0.748383 0.667735
C 1.798201 -0.006646 -0.538497
C 0.924350 1.199036 -0.406341
C -0.364345 0.986648 0.410413
C -1.312577 0.017984 -0.227804
O -0.876141 -1.276143 -0.437820
O -2.557036 0.031392 0.338970
H 0.027196 -1.229553 -0.795425
H 2.811483 -1.652537 0.402197
H 2.928137 -0.122707 1.282777
H 2.337089 -0.145734 -1.468869
H 1.496628 1.996912 0.095512
H 0.660116 1.578922 -1.396027
H -0.110209 0.638833 1.424243
H -0.883018 1.939919 0.521641
H -3.063079 -0.707548 -0.022282
H 1.423569 -1.030333 1.313996

VAA+
E = -617.320915
C 5.336323 -1.306559 -0.561200
C 3.828765 -1.299462 -0.328763
C 3.453544 -0.159297 0.690256
C 2.015405 -0.181582 0.946431
C 1.097834 0.660578 0.283613
O 1.509139 1.533835 -0.572965
O -0.185404 0.510292 0.588471
C -1.224521 1.319681 0.001846
C -2.548694 0.890392 0.495507
C -2.999393 -0.406792 -0.222854
C -4.385502 -0.834552 0.256156
C -4.853366 -2.107294 -0.445033
O -0.939650 2.160391 -0.800721
H 5.874737 -1.498553 0.369075
H 5.593742 -2.091940 -1.274782
H 5.675424 -0.351108 -0.966635
H 3.493714 -2.258417 0.071489
H 3.778148 0.794716 0.274981
H 1.582376 -0.908724 1.622614
H -2.497021 0.711397 1.571451
H -3.250551 1.698449 0.290098
H -3.016636 -0.232060 -1.302049
H -2.276885 -1.203542 -0.026533

H -4.358330 -0.990457 1.339056
H -5.094573 -0.022585 0.069842
H -5.844223 -2.400251 -0.094627
H -4.907888 -1.958990 -1.526468
H -4.167364 -2.935733 -0.249850
H 0.729996 2.045193 -0.934296
H 3.294034 -1.120672 -1.263831
H 3.996255 -0.363536 1.616430

[VA-OH]
E = -271.119081
C 2.770320 -0.532246 -0.000000
C 1.638247 0.492914 0.000000
C 0.262124 -0.166986 -0.000000
C -0.866800 0.865429 0.000000
C -2.259995 0.273291 -0.000000
O -2.573761 -0.863701 -0.000000
H 2.710576 -1.174249 -0.883307
H 3.748504 -0.045487 0.000000
H 2.710576 -1.174250 0.883306
H 1.727577 1.142243 0.877761
H 1.727577 1.142244 -0.877759
H 0.158602 -0.813524 -0.875972
H 0.158602 -0.813526 0.875970
H -0.807647 1.525870 0.871814
H -0.807647 1.525872 -0.871813

[VA-H]
E = -346.398016
C -3.308814 0.323512 -0.000483
C -2.079055 -0.580321 -0.003108
C -0.778025 0.220690 0.003853
C 0.441231 -0.623056 0.002187
C 1.785825 -0.104470 -0.000093
O 1.837887 1.260205 -0.001394
O 2.793460 -0.787704 -0.000809
H -3.313841 0.973123 -0.880409
H -4.231748 -0.260336 -0.005316
H -3.317072 0.963608 0.886359
H -2.098975 -1.238661 0.871074
H -2.095584 -1.228914 -0.884591
H -0.748789 0.901690 -0.858671
H -0.752883 0.891969 0.874308
H 0.365287 -1.702869 0.003584
H 2.775853 1.502262 -0.002846

VAA+, no h-trans
E = -617.280853
C -6.024482 -1.090659 -0.204196
C -4.520442 -1.167414 0.048679
C -3.844106 0.162180 -0.289640
C -2.315770 0.032684 -0.015089
C -1.645881 1.257066 -0.315609
O -1.291722 2.279733 -0.593856
O 0.697680 -0.016842 -0.464666
C 1.240798 0.158399 0.662327
C 2.658849 -0.118036 0.992503
C 3.571338 -0.196350 -0.236685
C 5.002925 -0.555300 0.163087
C 5.929795 -0.624208 -1.046970
O 0.370157 0.593975 1.468826
H -6.233909 -0.866222 -1.252611
H -6.497976 -2.042617 0.039365
H -6.485574 -0.315205 0.411804
H -4.326398 -1.413727 1.096944
H -4.076111 -1.962244 -0.557959
H -4.003609 0.416025 -1.339292
H -4.255360 0.966777 0.322858
H -2.089849 -0.190018 1.034311
H -1.837021 -0.739624 -0.627957
H 2.991344 0.644108 1.703264
H 2.668870 -1.069706 1.538927
H 3.186392 -0.943682 -0.935389
H 3.563630 0.763973 -0.759521
H 5.372944 0.188865 0.875708
H 4.998350 -1.517081 0.686076
H 6.946629 -0.881328 -0.745380
H 5.586587 -1.380466 -1.757807
H 5.963997 0.337068 -1.566204

VAA.H2O
E = -694.079919
C 5.860795 0.896557 -0.561706
C 4.631675 0.977231 0.340555
C 3.427657 0.257036 -0.260315
C 2.204582 0.341844 0.643148
C 1.000044 -0.371360 0.098284
O 0.963255 -1.041936 -0.893290
O -0.109702 -0.109914 0.873785
C -1.166257 -1.023668 0.982599
C -2.460819 -0.301133 1.198871
C -2.830281 0.622398 0.028234
C -4.195893 1.270397 0.237180
C -4.570108 2.196722 -0.917752
O -0.984263 -2.201705 0.953165
H 5.655386 1.349162 -1.535798
H 6.714759 1.415130 -0.120108
H 6.146985 -0.144990 -0.732168
H 4.861836 0.541513 1.318998
H 4.373357 2.026530 0.520824
H 3.187486 0.686558 -1.236942
H 3.672558 -0.792874 -0.439919
H 2.411937 -0.092481 1.628037
H 1.921380 1.381523 0.835616
H -3.230936 -1.057071 1.354538
H -2.369667 0.292299 2.114710
H -2.066639 1.398635 -0.070516
H -2.822604 0.042778 -0.897701
H -4.953416 0.486485 0.341637
H -4.194368 1.831172 1.178663
H -5.552144 2.649876 -0.763355
H -3.837230 3.002112 -1.020458
H -4.593500 1.644942 -1.861202
H -0.718415 -1.636405 -1.756417
O -1.640853 -1.852661 -1.963498
H -1.842623 -2.571306 -1.354326

Valeric acid, M062X/def2TZVP

VA
E = -346.861923
C -3.333624 0.318166 0.000017
C -2.097337 -0.571293 0.000005
H -3.347971 0.962540 -0.880832
H -4.250889 -0.270750 0.000033
H -3.347946 0.962549 0.880860
H -2.115329 -1.227530 0.875289
H -2.115354 -1.227539 -0.875272
C -0.804626 0.234922 -0.000018
C 0.427271 -0.653452 -0.000032
H -0.774940 0.892380 -0.872228

H -0.774915 0.892389 0.872185
C 1.713884 0.124943 -0.000059
H 0.444917 -1.314149 0.871334
H 0.444894 -1.314155 -0.871393
O 2.789348 -0.688415 0.000042
O 1.814441 1.319163 0.000014
H 3.573810 -0.121436 0.000097

VA+
E = -346.490215
C -3.206788 0.367908 -0.241532
C -2.046714 -0.474844 0.288476
H -3.232813 0.372945 -1.329927
H -4.135430 -0.078106 0.124800
H -3.157384 1.393959 0.119630
H -2.044711 -0.486163 1.378365
H -2.115166 -1.503377 -0.065150
C -0.720495 0.164681 -0.232109
C 0.390251 -0.696418 0.354577
H -0.714922 0.138212 -1.321508
H -0.641771 1.195661 0.106098
C 1.754708 -0.020466 0.003620
H 0.420934 -0.718233 1.450302
H 0.388783 -1.712437 -0.031355
O 1.849444 1.245925 0.235305
O 2.584371 -0.776668 -0.422811
H 2.736195 1.598317 0.030590

VA+, h-trans
E = -346.533299
C 3.157346 0.291250 -0.146847
C 1.772136 -0.190375 -0.553859
C 0.859314 -0.325946 0.709401
C -0.454396 -0.829371 0.308239
C -1.545186 0.024767 0.019924
O -2.717229 -0.373939 -0.368690
O -1.394939 1.299069 0.146340
H 3.634350 -0.414733 0.532810
H 3.788135 0.390243 -1.029307
H 3.107749 1.262712 0.344841
H 1.309157 0.513485 -1.247874
H 1.833135 -1.157306 -1.055521
H 1.329609 -1.034780 1.392486
H 0.781757 0.647308 1.193175
H -0.613323 -1.890128 0.150130
H -2.203879 1.796823 -0.070841
H -2.804623 -1.336614 -0.452253

CH2C(OH)2+
E = -228.673930
H 1.661814 -0.913569 -0.000017
O 0.699158 -1.078358 -0.000017
C -0.003094 -0.007225 -0.000002
C -1.417962 -0.137570 -0.000001
H -2.052564 0.736737 0.000083
H -1.843390 -1.130370 -0.000052
O 0.636139 1.111919 0.000012
H 0.078102 1.907482 0.000038

C3H6
E = -117.803716
C 1.272272 0.221497 0.000001
H 1.281397 1.305813 -0.000019
H 2.231210 -0.279775 0.000035
C 0.134552 -0.455972 -0.000012
H 0.169929 -1.541919 -0.000001
C -1.227327 0.162463 -0.000000
H -1.797028 -0.150977 0.877501
H -1.165178 1.250431 -0.000328
H -1.797314 -0.151508 -0.877119

CH2CHC(OH)2+
E = -267.402428
H 1.450010 1.585264 0.000136
O 0.531532 1.256555 0.000054
C 0.451800 -0.019535 0.000008
C -0.834018 -0.664063 -0.000129
H -0.843902 -1.746401 -0.000377
C -1.953597 0.063323 0.000097
O 1.566591 -0.658789 -0.000044
H 1.475778 -1.626508 -0.000172
H -2.922489 -0.419311 0.000111
H -1.929492 1.146482 0.000363

C2H5
E = -79.074992
C 0.692234 0.000009 -0.000560
H 1.102122 -0.883709 -0.491612
H 1.083731 -0.000628 1.025597
H 1.102100 0.884314 -0.490552
C -0.791713 0.000000 -0.024259
H -1.345518 -0.923674 0.052738
H -1.345560 0.923646 0.052745

VAA+.H2O
E = -693.420532
C -5.144016 -1.776643 0.677166
C -3.631746 -1.619806 0.607774
C -3.204826 -1.032594 -0.767091
C -1.742913 -0.928910 -0.835814
C -1.042059 0.266085 -0.528302
O 0.276024 0.208736 -0.659070
C 1.180318 0.988652 0.116616
O 0.776240 1.666139 0.999783
O -1.680645 1.305672 -0.202794
C 2.575662 0.716866 -0.314940
C 3.055629 -0.643638 0.223189
C 4.504723 -0.911385 -0.167833
C 4.995196 -2.252588 0.360119
H -5.502860 -2.455603 -0.096733
H -5.438253 -2.182021 1.644255
H -5.644371 -0.816715 0.546703
H -3.141764 -2.584182 0.753376
H -3.671828 -0.056616 -0.897008
H -1.129304 -1.789488 -1.068111
H 2.619124 0.722205 -1.405149
H 3.195757 1.521195 0.077644
H 2.958447 -0.653517 1.311865
H 2.415322 -1.437803 -0.168358
H 4.594348 -0.883638 -1.257043
H 5.135238 -0.106555 0.218468
H 6.031205 -2.429038 0.074943
H 4.937387 -2.289126 1.448942
H 4.395147 -3.073106 -0.036465
H -1.209466 2.243046 -0.034497
H -3.279942 -0.954027 1.398380
H -3.558437 -1.704660 -1.551379
O -0.792975 3.577494 0.101451
H -0.191719 3.719805 0.843412
H -1.418992 4.309289 0.056491

(VA)2+

E = -693.394972
C 6.544381 -0.311505 0.734080
C 5.513270 -0.225316 -0.383305
C 4.118120 0.065836 0.162174
C 3.094023 0.150968 -0.983247
C 1.734276 0.439590 -0.439019
O 1.561813 1.605216 0.093473
O 0.844791 -0.425081 -0.487242
O -0.844790 0.425087 0.487231
C -1.734273 -0.439585 0.439008
C -3.094018 -0.150967 0.983243
C -4.118122 -0.065837 -0.162171
C -5.513271 0.225309 0.383317
C -6.544389 0.311496 -0.734061
O -1.561810 -1.605209 -0.093486
H 6.295946 -1.108745 1.436009
H 7.534966 -0.517317 0.331449
H 6.597338 0.624681 1.291336
H 5.793251 0.560261 -1.089766
H 5.493450 -1.162089 -0.945845
H 3.822374 -0.723211 0.858566
H 4.121059 1.007134 0.714811
H 3.345043 0.974973 -1.656208
H 3.055744 -0.777143 -1.549948
H 0.659377 1.699268 0.447529
H -0.659374 -1.699261 -0.447542
H -3.055739 0.777144 1.549945
H -3.345031 -0.974972 1.656206
H -3.822384 0.723211 -0.858564
H -4.121062 -1.007135 -0.714809
H -5.793244 -0.560271 1.089778
H -5.493451 1.162080 0.945859
H -7.534972 0.517303 -0.331424
H -6.295961 1.108739 -1.435991
H -6.597345 -0.624689 -1.291319

(VA)2+, h-trans
E = -693.440474
C 6.067975 0.018506 0.645176
C 4.641098 -0.502314 0.741313
C 3.966367 -0.513120 -0.658855
C 2.606386 -1.058467 -0.560572
C 1.456896 -0.244022 -0.403226
O 0.303940 -0.804110 -0.285339
O 1.598471 1.044619 -0.384271
O -1.045769 1.391915 -0.080349
C -2.201439 1.790687 0.050942
C -3.396335 0.902779 0.160378
C -3.081780 -0.582650 0.094166
C -4.339771 -1.437186 0.212999
C -4.029204 -2.925838 0.147523
O -2.481755 3.068495 0.107084
H 6.089160 1.034133 0.248953
H 6.533599 0.030247 1.629675
H 6.671948 -0.613708 -0.006152
H 4.631025 -1.513794 1.151215
H 4.050653 0.125321 1.412020
H 3.953313 0.502818 -1.053869
H 4.561720 -1.142893 -1.322288
H 2.423072 -2.124720 -0.535798
H -0.433163 -0.130871 -0.185836
H -3.899221 1.168265 1.095285
H -2.582124 -0.811853 -0.852651
H -2.391041 -0.849475 0.900614
H -4.844162 -1.203217 1.154130
H -5.033876 -1.166294 -0.586805
H -4.937516 -3.520055 0.233487
H -3.549924 -3.184245 -0.798237
H -3.359315 -3.221680 0.956648
H 0.740070 1.511590 -0.275368
H -1.678418 3.606911 0.032082
H -4.086061 1.205922 -0.633150

VAH+.[VA-H]
E = -693.399689
C -6.198057 -0.543980 1.226785
C -5.323438 -0.713260 -0.008131
C -3.896450 -0.240422 0.247402
C -3.024834 -0.420752 -1.019950
C -1.661755 0.047835 -0.726496
O -1.378608 1.278799 -0.900034
O -0.813734 -0.783862 -0.249909
O 1.053888 1.057420 -0.000485
C 2.154641 1.551483 0.239962
O 2.430828 2.780745 0.038653
C 3.346348 0.803892 0.798355
C 3.656771 -0.427106 -0.058168
C 4.832322 -1.207695 0.526006
C 5.149321 -2.444930 -0.303689
H -6.250022 0.502585 1.529964
H -7.213234 -0.885777 1.031499
H -5.806877 -1.120292 2.066339
H -5.305247 -1.762713 -0.312316
H -5.744209 -0.149412 -0.844318
H -3.898672 0.813485 0.535334
H -3.457359 -0.809042 1.070644
H -2.982493 -1.472660 -1.298477
H -3.429701 0.172970 -1.838361
H 0.056947 -0.365286 -0.032246
H 3.056293 0.528550 1.817416
H 4.206975 1.470620 0.863692
H 2.773763 -1.067998 -0.108964
H 3.891438 -0.115372 -1.078895
H 5.708029 -0.556108 0.573718
H 4.598671 -1.496378 1.554010
H 5.990130 -2.990300 0.122138
H 4.295271 -3.122784 -0.340387
H 5.409964 -2.173462 -1.327479
H -0.447876 1.504155 -0.621573

CO2
E = -188.584965
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.154580
O 0.000000 0.000000 -1.154580

C4H9
E = -157.636049
C -1.924531 0.165839 -0.066114
C -0.564243 -0.507383 0.076694
C 0.573267 0.449974 0.024451
C 1.972686 -0.043641 -0.053054
H -1.994216 0.693959 -1.018107
H -2.736424 -0.559833 -0.019120
H -2.078533 0.894981 0.731203
H -0.535677 -1.070553 1.022523
H -0.436161 -1.264137 -0.706407
H 0.390968 1.480350 0.305348
H 2.289702 -0.516370 0.887327
H 2.078981 -0.806333 -0.830162
H 2.678286 0.759200 -0.264465

VAH+
E = -347.168755
C 3.345562 0.325514 0.000000
C 2.124343 -0.582504 0.000000
C 0.821412 0.216677 0.000000
C -0.395868 -0.701063 -0.000000
C -1.696573 0.000582 0.000000
O -1.820293 1.271734 -0.000000
O -2.767955 -0.687255 -0.000000
H 3.360210 0.965121 0.883557
H 4.261361 -0.262428 0.000000
H 3.360210 0.965122 -0.883557
H 2.140554 -1.233822 -0.877284
H 2.140554 -1.233822 0.877284
H 0.807587 0.859376 0.888012
H 0.807587 0.859376 -0.888012
H -0.411219 -1.367677 -0.870127
H -0.411219 -1.367677 0.870127
H -3.582580 -0.148129 -0.000000
H -0.960314 1.733493 -0.000000

C4H9+
E = -157.372656
C -1.965584 -0.091533 0.062279
C -0.566795 0.402749 -0.021577
C 0.566769 -0.402542 -0.021483
C 1.965625 0.091393 0.062266
H -2.332690 0.189920 1.054198
H -2.604363 0.406481 -0.665636
H -2.033258 -1.172006 -0.043221
H -0.000063 0.000120 -1.132116
H -0.399154 1.478999 -0.023525
H 0.398836 -1.478762 -0.023777
H 2.604083 -0.406470 -0.666040
H 2.033526 1.171905 -0.042726
H 2.332993 -0.190593 1.053935

[VA-OH].H2O
E = -347.372178
C -3.702763 -0.495653 0.000063
C -2.559950 0.511507 0.000153
C -1.195426 -0.166724 -0.000089
C -0.055302 0.846328 -0.000137
C 1.315342 0.213334 -0.000067
O 1.593010 -0.927812 -0.000103
O 4.527821 0.050576 0.000178
H -3.654727 -1.137776 0.881149
H -4.672022 0.002622 0.000299
H -3.654944 -1.137374 -0.881326
H -2.640913 1.161966 -0.875513
H -2.640734 1.161611 0.876096
H -1.099438 -0.814554 0.874567
H -1.099638 -0.814346 -0.874918
H -0.091204 1.504878 -0.872181
H -0.091256 1.505094 0.871737
H 3.912371 -0.689240 0.000147
H 3.954442 0.822253 -0.000193

[VA-H].H2O
E = -422.638189
C -3.959576 -0.614829 0.001153
C -2.849592 0.426740 -0.001940
C -1.463871 -0.208343 -0.002766
C -0.360515 0.780153 -0.005355
C 1.035099 0.406117 -0.003002
O 1.236738 -0.915440 -0.003165
O 1.945575 1.221699 -0.000378
H -3.890587 -1.254016 0.883245
H -4.944128 -0.147683 0.001793
H -3.893058 -1.256790 -0.879145
H -2.948099 1.072430 -0.878575
H -2.945639 1.074873 0.873119
H -1.348702 -0.871699 0.864288
H -1.351211 -0.874464 -0.868080
H -0.558653 1.843309 -0.005424
H 2.205304 -1.083840 0.002380
H 3.621337 0.265148 0.047391
O 3.947134 -0.651191 0.083078
H 4.608597 -0.746842 -0.605819

[VA-OH]+
E = -270.721173
C 2.865560 -0.470717 0.000140
C 1.683066 0.489906 0.000022
C 0.364287 -0.278993 -0.000326
C -0.815023 0.741684 -0.000078
C -2.068810 0.052159 0.000300
O -3.009846 -0.535233 0.000007
H 2.854734 -1.108709 -0.884007
H 3.801439 0.085076 0.000404
H 2.854384 -1.108950 0.884109
H 1.724475 1.137221 0.879560
H 1.724843 1.137489 -0.879301
H 0.287133 -0.912650 -0.884749
H 0.286861 -0.912996 0.883809
H -0.814955 1.380543 -0.891659
H -0.814630 1.380608 0.891433

[VA].(OH)2CCH2+
E = -575.586266
C -5.175939 -0.839144 -0.001809
C -4.162264 0.295961 -0.000171
C -2.723845 -0.217464 -0.000281
C -1.716633 0.926219 0.001015
C -0.271539 0.540038 0.001301
O 0.054097 -0.759372 0.000647
O 0.637345 1.343020 0.002138
O 3.091157 0.955238 -0.002796
C 3.556449 -0.222376 -0.000644
C 4.968444 -0.414417 -0.001503
H 5.608994 0.453058 -0.003856
O 2.818553 -1.288106 0.002401
H -5.059745 -1.470543 0.880404
H -6.193097 -0.451306 -0.001344
H -5.059611 -1.468103 -0.885739
H -4.311145 0.932509 -0.875874
H -4.311669 0.930470 0.876914
H -2.582925 -0.847776 0.885919
H -2.582378 -0.846196 -0.887497
H -1.850197 1.576153 -0.868511
H -1.850955 1.574852 0.871399
H 2.045995 1.070538 -0.000806
H 1.851491 -1.120565 0.002191
H 5.365081 -1.417208 0.000231
H -0.727092 -1.335020 -0.000007

(VA)2
E = -693.749929
C -6.705077 0.807743 0.000273
C -5.705810 -0.341566 0.000403
C -4.262662 0.147083 0.000007
C -3.268173 -1.000610 0.000128

C -1.831496 -0.557139 -0.000170
O -1.498564 0.615311 -0.000577
O -0.978648 -1.554707 -0.000099
H -6.571312 1.437878 -0.880864
H -7.732982 0.445038 0.000584
H -6.570958 1.438383 0.880995
H -5.873462 -0.976001 0.875847
H -5.873785 -0.976481 -0.874632
H -4.084405 0.780221 -0.872523
H -4.084084 0.780676 0.872142
H -3.403533 -1.648304 0.870954
H -3.403798 -1.648711 -0.870356
H -0.041465 -1.209966 -0.000350
H 0.041429 1.209933 -0.000314
O 0.978636 1.554662 -0.000067
C 1.831496 0.557102 -0.000170
O 1.498595 -0.615356 -0.000506
C 3.268155 1.000607 0.000126
C 4.262662 -0.147070 -0.000029
H 3.403755 1.648733 -0.870342
H 3.403515 1.648284 0.870967
C 5.705800 0.341607 0.000364
H 4.084102 -0.780686 0.872092
H 4.084408 -0.780190 -0.872573
C 6.705088 -0.807684 0.000194
H 5.873755 0.976547 -0.874657
H 5.873450 0.976023 0.875822
H 7.732987 -0.444959 0.000503
H 6.570990 -1.438349 0.880901
H 6.571326 -1.437798 -0.880958

VA.2H2O
E = -499.700931
C 4.338908 0.057442 0.972687
C 3.402303 -0.131414 -0.213393
C 1.936838 0.001774 0.180710
C 0.997119 -0.194987 -1.013157
C -0.436633 -0.067745 -0.579538
O -0.813693 1.181918 -0.408570
O -1.151448 -1.028760 -0.373259
O -3.302011 1.381798 0.476335
H 4.141014 -0.686515 1.746512
H 5.383446 -0.037736 0.675832
H 4.205491 1.044203 1.419724
H 3.633475 0.604751 -0.988554
H 3.566941 -1.115051 -0.662279
H 1.696473 -0.736386 0.951500
H 1.759711 0.987833 0.617511
H 1.206826 0.560194 -1.772280
H 1.132955 -1.186075 -1.443549
H -1.755886 1.241377 -0.079673
H -3.940634 1.867706 -0.050697
H -3.650097 0.470023 0.584295
H -2.835725 -1.342998 0.162421
O -3.751606 -1.262395 0.493138
H -3.825126 -1.842229 1.254225

VA+.2H2O
E = -499.401917
C -4.223737 0.741267 0.291686
C -2.937656 0.003827 0.636096
C -2.175481 -0.403695 -0.653794
C -0.958448 -1.152678 -0.312481
C 0.316297 -0.535862 -0.188005
O 1.307873 -1.296232 0.160231
O 0.434313 0.713753 -0.421786
O 2.623844 1.850915 0.000276
O 3.907503 -0.560717 0.296305
H -4.889466 0.111008 -0.298575
H -4.750869 1.030365 1.199833
H -4.015725 1.645644 -0.280891
H -2.287347 0.636051 1.244307
H -3.157030 -0.891509 1.220601
H -2.831648 -1.034684 -1.256209
H -1.932577 0.494911 -1.221099
H -0.992241 -2.207242 -0.072872
H 1.356777 1.150568 -0.270313
H 2.208483 -0.887057 0.202295
H 3.463992 1.372558 -0.009282
H 2.770142 2.780408 -0.203193
H 4.448111 -1.046333 -0.339777
H 4.295282 -0.733595 1.163955

VAH+.2H2O
E = -500.040230
C 4.936798 0.149942 0.037711
C 3.672449 -0.696928 0.018896
C 2.407811 0.158860 0.001759
C 1.147586 -0.696885 -0.015451
C -0.147582 0.047131 -0.036063
O -1.226573 -0.547838 -0.067617
O -0.169597 1.355233 -0.023046
O -5.495129 -0.583749 0.027402
O -3.278963 0.684149 0.070825
H 4.968278 0.788408 0.921888
H 5.825482 -0.478703 0.049533
H 4.993164 0.790483 -0.843726
H 3.671520 -1.348752 -0.858332
H 3.646710 -1.350599 0.894359
H 2.414768 0.803698 0.888431
H 2.437947 0.805050 -0.883225
H 1.126852 -1.361786 -0.883648
H 1.100595 -1.356032 0.856392
H -2.259499 0.105342 -0.027102
H 0.724199 1.731288 0.006782
H -4.142729 0.163149 0.031839
H -3.350678 1.512541 -0.416088
H -5.813788 -1.213062 -0.627184
H -6.083101 -0.626102 0.788454

H2O
E = -76.404574
O 0.000000 0.000000 0.116372
H 0.000000 0.763889 -0.465487
H -0.000000 -0.763889 -0.465487

OH
E = -75.723446
O 0.000000 0.000000 0.108140
H 0.000000 0.000000 -0.865120

(H2O)2
E = -152.815423
O 1.507176 0.007649 -0.120830
H 0.556002 -0.016754 0.051292
H 1.928767 -0.046725 0.738955
O -1.383828 -0.007065 0.109195
H -1.715498 0.795352 -0.303247
H -1.756055 -0.736548 -0.393919

OH.H2O
E = -152.135839

O -1.616652 0.000036 0.012109
O 1.253650 -0.000203 -0.055147
H -0.638237 -0.001426 -0.041453
H 1.768993 0.771718 0.192435
H 1.773259 -0.768963 0.193322

H3O
E = -76.666210
O -0.000017 -0.000003 -0.068292
H 0.489412 -0.811049 0.182105
H 0.457901 0.829252 0.182213
H -0.947179 -0.018182 0.182017

H3O.H2O
E = -153.129954
O -1.192813 -0.028432 0.042650
O 1.192844 -0.028661 -0.042710
H -1.715492 0.697891 0.410324
H -1.676648 -0.481755 -0.662533
H 1.715116 0.697500 -0.411337
H 1.676321 -0.479988 0.664026
H 0.000453 0.023095 0.000005

VA, S=3
E = -346.702087
C 3.349043 0.291587 -0.108849
C 2.102114 -0.523544 0.207433
H 3.335510 1.244368 0.423612
H 4.257303 -0.239043 0.177059
H 3.410128 0.510098 -1.176579
H 2.146456 -1.484506 -0.313556
H 2.072352 -0.754299 1.276147
C 0.819897 0.198762 -0.185478
C -0.426722 -0.620905 0.129392
H 0.769378 1.158617 0.338053
H 0.838610 0.429166 -1.254642
C -1.693269 0.070796 -0.268951
H -0.405801 -1.575912 -0.399997
H -0.473236 -0.842485 1.204569
O -2.831314 -0.663372 -0.041222
O -1.828082 1.323475 0.234237
H -3.581909 -0.227009 -0.460064

VA, h-trans, S=3
E = -346.724698
C 3.251620 0.439865 -0.114376
C 2.112701 -0.462811 0.346773
H 3.000219 1.489660 0.044608
H 4.172484 0.225721 0.427436
H 3.447189 0.301351 -1.178892
H 2.410089 -1.514710 0.218567
H 1.946048 -0.342830 1.422518
C 0.839249 -0.211862 -0.379515
C -0.447990 -0.810952 0.070507
H -0.726427 1.713836 0.081322
H 0.891660 0.144799 -1.404107
C -1.620727 0.063683 -0.255534
H -0.626457 -1.784611 -0.403358
H -0.421853 -0.992453 1.155614
O -2.821197 -0.530631 -0.027613
O -1.603033 1.344388 0.243805
H -3.508220 0.141649 -0.100368

VAA+
E = -616.991980
C -5.303264 1.283234 -0.592373
C -3.802141 1.265045 -0.341913
C -3.444654 0.175655 0.717202
C -2.004681 0.202985 0.980716
C -1.094550 -0.636923 0.301724
O -1.511691 -1.491236 -0.555477
O 0.188230 -0.500757 0.595059
C 1.195127 -1.301029 -0.008729
C 2.537831 -0.908339 0.469751
C 2.988240 0.399689 -0.213771
C 4.389984 0.795396 0.238177
C 4.855544 2.081111 -0.431422
O 0.889470 -2.123666 -0.818136
H -5.849991 1.518560 0.320801
H -5.548161 2.039261 -1.337206
H -5.651669 0.318683 -0.961856
H -3.461196 2.237690 0.016323
H -3.760614 -0.797314 0.341417
H -1.564761 0.918867 1.663466
H 2.504928 -0.771210 1.551753
H 3.216706 -1.723470 0.224344
H 2.973544 0.261487 -1.297793
H 2.283596 1.200177 0.024894
H 4.396736 0.915573 1.324647
H 5.083506 -0.017019 0.007830
H 5.857211 2.350418 -0.100253
H 4.880849 1.970538 -1.516380
H 4.189853 2.911791 -0.192192
H -0.732694 -1.999534 -0.927710
H -3.262559 1.047183 -1.265531
H -3.987972 0.402651 1.635708

[VA-OH]
E = -270.963494
C 2.755880 -0.534409 -0.000000
C 1.631651 0.493633 0.000000
C 0.254037 -0.157593 -0.000000
C -0.868724 0.874118 0.000000
C -2.255818 0.265342 -0.000000
O -2.541391 -0.872606 -0.000001
H 2.695381 -1.175591 -0.881103
H 3.734911 -0.055334 0.000000
H 2.695381 -1.175592 0.881102
H 1.724965 1.142615 0.875647
H 1.724965 1.142616 -0.875645
H 0.146342 -0.804432 -0.874200
H 0.146342 -0.804433 0.874199
H -0.819655 1.532225 0.871648
H -0.819655 1.532226 -0.871647

n = 1, B3LYP+D2/def2TZVP

CA
E = -189.815863
H -0.104215 1.494945 0.000002
C -0.136940 0.397172 -0.000001
O -1.134578 -0.264092 0.000000
O 1.117432 -0.088315 0.000000
H 1.063024 -1.058725 -0.000000

CA+
E = -189.405899
H 0.208674 1.495227 0.000001
C 0.086321 0.396625 -0.000001
O -1.090570 -0.082077 0.000001
O 1.144791 -0.269396 0.000000

H -1.160365 -1.063195 -0.000002

CA+, h-trans
E = -189.413746
C 0.003878 -0.419180 0.000004
O 1.080657 0.225090 -0.000003
O -1.157480 0.005444 -0.000004
H -1.311947 0.983612 0.000020
H 1.903263 -0.312807 0.000011

CAA+.H2O
E = -379.271033
H -2.186327 -1.610188 0.053732
C -1.269253 -1.016676 0.008517
O -1.651487 0.358565 0.030102
C -0.771440 1.333983 -0.008082
O 0.420819 1.345666 -0.033313
O -0.150537 -1.390532 -0.052540
O 2.345915 -0.255253 0.106944
H 1.539867 0.408420 0.029009
H 2.042290 -1.164426 -0.081883
H 3.130650 -0.005221 -0.413008

(CA)2+
E = -379.282793
H 2.569345 -1.318492 -0.000261
C 1.787396 -0.549093 -0.000093
O 0.606807 -0.918015 -0.000052
O 2.226557 0.658977 0.000166
O -0.606793 0.917994 -0.000184
C -1.787388 0.549098 -0.000042
O -2.226574 -0.658961 0.000139
H -2.569326 1.318509 0.000065
H 1.508930 1.321991 0.000313
H -1.508971 -1.322000 0.000134

H
E = -0.502154
H 0.000000 0.000000 0.000000

CAH+
E = -190.097786
H -0.045402 1.514089 -0.000113
C -0.004362 0.424590 0.000002
O 1.146179 -0.093104 0.000009
O -1.046508 -0.303646 -0.000133
H -1.891155 0.187852 0.000811
H 1.165356 -1.075481 0.000282

[CA-OH]+
E = -113.580234
C 0.000000 0.000000 -0.514430
O 0.000000 0.000000 0.587286
H 0.000000 0.000000 -1.611707

CA.2H2O
E = -342.733757
H -2.732781 -0.519043 0.008202
C -1.650080 -0.334022 0.004385
O -0.846205 -1.244005 0.030635
O -1.392000 0.950721 -0.031409
O 1.174354 1.522003 -0.079559
O 1.896583 -1.044842 0.077385
H -0.400726 1.153014 -0.040228
H 0.939779 -1.265501 0.076444
H 2.289897 -1.524912 -0.657566
H 1.634449 0.646917 -0.047209
H 1.508004 2.042642 0.657631

CA+.2H2O
E = -342.397077
C 2.082182 0.619476 -0.070604
O 0.903026 0.585907 -0.244047
O 2.869611 -0.373022 0.242681
H 3.793174 -0.081711 0.326681
H -0.314876 -0.374892 -0.150300
O -1.173112 -0.914383 -0.081850
H -1.224214 -1.602632 -0.762551
H -2.064232 -0.334160 -0.002665
O -3.275275 0.350714 0.132290
H -3.482801 1.174887 -0.326280
H -3.794139 0.307927 0.946149

CAH+.2H2O
E = -343.058783
H 2.775712 -1.391166 0.054038
C 2.037482 -0.583103 0.014808
O 2.483722 0.650219 0.098653
O 0.849656 -0.816284 -0.105023
O -1.022884 0.807226 -0.049102
O -3.295555 -0.225704 0.061939
H -3.585301 -1.013258 -0.414155
H -3.851038 -0.122399 0.844495
H -1.954573 0.343940 -0.014605
H -0.992256 1.514940 -0.708586
H -0.185497 0.154610 -0.096511
H 3.448549 0.688292 0.194740

(CA)2
E = -379.657997
H -2.982712 0.201641 -0.000539
C -1.887549 0.146983 -0.000312
O -1.462099 -1.090236 -0.000017
O -1.196127 1.149706 -0.000381
O 1.196095 -1.149696 0.000006
C 1.887559 -0.147002 0.000228
H 2.982726 -0.201725 0.000329
O 1.462117 1.090226 0.000414
H 0.457566 1.126476 0.000306
H -0.457525 -1.126276 0.000230

CAA+
E = -302.787336
C -1.127697 0.317562 0.000166
O 0.000262 1.070385 -0.000015
C 1.127404 0.317621 -0.000148
O 1.088439 -0.887170 0.000261
O -1.088513 -0.886997 -0.000267
H -2.051554 0.909907 0.000632
H 2.051803 0.909252 -0.000572

[CA-OH]
E = -113.891304
H -0.865229 1.220297 0.000000
C 0.061802 0.582490 -0.000000
O 0.061802 -0.589405 0.000000

OH
E = -75.759757
O 0.000000 0.000000 0.108525
H 0.000000 0.000000 -0.868203

n = 2, B3LYP+D2/def2TZVP

CA
E = -229.131440
C -0.090862 0.128767 0.000227
O -0.789799 -1.033890 -0.000027
H -1.731927 -0.802798 -0.000151
O -0.624345 1.206415 -0.000058
C 1.390611 -0.125101 -0.000039
H 1.662403 -0.711790 -0.880288
H 1.662705 -0.711675 0.880191
H 1.921478 0.824066 -0.000195

CA+
E = -228.749344
H 1.514371 -0.919204 -0.905119
C 1.354851 -0.319404 -0.000013
C -0.090231 0.056771 0.000014
O -0.343847 1.278975 0.000001
O -0.994617 -0.855181 0.000020
H 1.514214 -0.919939 0.904637
H 2.009970 0.553116 0.000442
H -1.918561 -0.528525 -0.000137

CA+, h-trans
E = -228.778645
H -1.837045 -1.152552 0.000716
C -1.417793 -0.154942 -0.000018
C -0.003635 -0.007358 0.000005
O 0.623008 1.126276 -0.000073
O 0.714382 -1.075803 -0.000046
H -2.060292 0.716025 -0.000726
H 1.677555 -0.905840 0.000146
H 0.049237 1.912384 0.000898

CAA+.H2O
E = -457.940110
C 2.363653 -1.174097 -0.379138
H 3.299055 -0.724496 -0.054453
H 2.304848 -2.215114 -0.051667
H 2.288502 -1.169372 -1.469690
C 1.231037 -0.410919 0.196623
O 1.202499 0.521502 0.918868
O -0.017164 -1.043703 -0.238950
C -1.223076 -0.552609 -0.029499
C -2.275973 -1.505202 0.055252
H -2.050155 -2.559783 -0.011237
O -1.505884 0.678596 0.059854
H -0.783504 1.441123 -0.084463
O -0.002298 2.595140 -0.387308
H 0.686700 2.808712 0.256468
H -0.446441 3.414745 -0.642091
H -3.290073 -1.151134 0.177990

(CA)2+
E = -457.939864
H 3.213133 1.626056 -0.001311
C 3.258561 0.539957 -0.000710
C 1.890623 -0.055186 0.000062
O 1.829800 -1.352171 0.000631
O 0.887034 0.679400 0.000056
O -0.887042 -0.679414 0.000044
C -1.890623 0.055183 0.000014
C -3.258569 -0.539941 -0.000689
H -3.213159 -1.626039 -0.001461
O -1.829784 1.352167 0.000614
H 3.784890 0.174550 -0.886927
H 3.785501 0.175531 0.885541
H 0.905845 -1.665079 0.001152
H -0.905826 1.665065 0.001297
H -3.785413 -0.175634 0.885667
H -3.784985 -0.174386 -0.886795

CH3
E = -39.829965
C -0.000000 0.000000 -0.000436
H 0.000000 1.080511 0.000873
H 0.935750 -0.540255 0.000873
H -0.935750 -0.540255 0.000873

CAH+
E = -229.431966
H -1.869250 0.745299 -0.502755
C -1.412958 -0.111215 -0.004655
C 0.057419 -0.007129 -0.011146
O 0.745612 -1.080780 -0.002757
O 0.705337 1.102495 0.002885
H -1.736542 -0.119232 1.045082
H -1.725386 -1.048753 -0.463513
H 1.714186 -0.938503 0.024003
H 0.142635 1.897543 -0.009033

CH3+
E = -39.464733
C 0.000000 -0.000000 -0.000026
H 0.000000 1.093677 0.000051
H 0.947152 -0.546839 0.000051
H -0.947152 -0.546839 0.000051

[CA-OH]+
E = -152.945867
H 1.555008 -1.043298 -0.028834
C 1.210464 -0.000056 0.000002
C -0.216124 -0.000274 0.000081
O -1.328705 0.000098 -0.000024
H 1.554477 0.497335 0.917136
H 1.554113 0.547154 -0.888608

CA.2H2O
E = -382.049104
C 1.178241 -0.093762 -0.001480
O 0.740038 1.151704 0.032252
O 0.463119 -1.081764 -0.026156
C 2.681426 -0.173930 -0.005038
H 3.073197 0.372276 -0.865881
H 2.998318 -1.213578 -0.041556
H -0.264149 1.210770 0.042212
O -1.896065 1.393144 0.080556
O -2.264339 -1.250820 -0.080704
H -1.283169 -1.321184 -0.077693
H -2.578049 -1.775004 0.662236
H -2.235872 0.465454 0.046409
H -2.283238 1.859182 -0.666844
H 3.072932 0.310120 0.892643

CA+.2H2O
E = -381.731434
C 1.254227 -0.036098 0.002577
O 0.750866 1.134739 0.077420
O 0.564278 -1.130004 -0.069343

H -0.435354 -1.061717 -0.037550
H -0.283733 1.237972 0.037202
O -1.721652 1.485387 -0.095965
H -2.121642 2.337521 0.114160
H -2.335222 0.769241 0.123560
O -2.086758 -1.263607 0.053497
H -2.372864 -1.823848 0.788533
H -2.477679 -1.644922 -0.745344
C 2.674815 -0.164829 -0.002002
H 3.117495 -1.148362 -0.064418
H 3.280877 0.727557 0.055526

CAH+.2H2O
E = -382.384102
C -1.193027 -0.016885 -0.011689
O -0.676050 1.136297 0.052705
O -0.517618 -1.108619 -0.073932
C -2.667743 -0.141937 0.008739
H -3.133654 0.799696 -0.272355
H -2.982666 -0.959495 -0.639501
H 0.362446 1.231307 0.030640
H 0.484774 -1.056275 -0.040419
O 2.128366 -1.282162 0.049696
O 1.798980 1.474939 -0.078090
H 2.198281 2.326244 0.137074
H 2.409894 0.757408 0.143402
H 2.514841 -1.658144 -0.753903
H 2.407144 -1.855646 0.777384
H -2.965856 -0.395801 1.032361

(CA)2
E = -458.291021
C 1.911886 -0.057986 -0.000035
O 1.244733 -1.084706 -0.000114
O 1.398071 1.154254 0.000220
H 0.393121 1.119746 0.000328
C -1.911890 0.057984 -0.000107
O -1.244717 1.084690 -0.000129
O -1.398080 -1.154261 0.000213
H -0.393128 -1.119767 0.000275
C -3.413916 0.064650 -0.000053
H -3.778112 -0.470350 -0.879865
H -3.778100 -0.470279 0.879809
C 3.413914 -0.064628 -0.000084
H 3.778130 0.470226 0.879810
H 3.778060 0.470459 -0.879864
H 3.782250 -1.087600 -0.000233
H -3.782238 1.087628 -0.000093

CA, S=3
E = -228.979607
C -0.037485 0.058729 -0.310654
O -0.912705 -0.937325 0.114474
H -1.778216 -0.783715 -0.287709
O -0.538016 1.246901 0.081838
C 1.393375 -0.204195 0.036538
H 1.708954 -1.131538 -0.445030
H 1.515710 -0.300894 1.124458
H 2.023979 0.612332 -0.317527

CA, h-trans, S=3
E = -228.985824
H -1.749645 -0.305865 1.080660
C -1.441065 -0.141832 0.048638
C -0.017791 -0.018420 -0.281479
O 0.631561 1.151702 0.114465
O 0.733315 -1.109253 0.052587
H -2.202811 -0.082375 -0.717401
H 1.664216 -0.895042 -0.096529
H 0.122369 1.905200 -0.206099

CAA+
E = -381.468989
C 2.366691 -0.817896 0.000099
C 1.219189 0.109494 -0.000023
O -0.028495 -0.661933 -0.000117
C -1.213273 -0.092747 -0.000108
O -1.393138 1.179252 0.000059
O 1.168554 1.296654 -0.000016
C -2.344611 -0.946512 0.000035
H 3.289191 -0.241454 0.000284
H 2.311722 -1.463251 0.881559
H 2.312055 -1.462898 -0.881655
H -2.203214 -2.018308 0.000019
H -0.521941 1.662391 0.000041
H -3.331156 -0.502303 0.000330

[CA-OH]
E = -153.207353
H -1.176519 1.193099 -0.000001
C -1.167126 0.098083 0.000001
C 0.246817 -0.430682 -0.000000
O 1.258117 0.173352 -0.000001
H -1.683278 -0.292159 0.879919
H -1.683280 -0.292161 -0.879915

n = 3, B3LYP+D2/def2TZVP

CA
E = -268.435337
C -0.561286 0.107580 0.000216
O -1.676433 -0.664638 -0.000078
H -2.440332 -0.066906 -0.000222
O -0.606493 1.309818 -0.000016
C 0.689003 -0.736624 0.000047
H 0.637822 -1.395703 -0.871895
H 0.637997 -1.395741 0.871969
C 1.966906 0.093244 -0.000066
H 2.009680 0.736239 0.880096
H 2.009498 0.736284 -0.880206
H 2.841007 -0.560809 -0.000173

CA+
E = -268.064080
H -2.794798 -0.090723 0.072013
C -1.825111 0.221396 -0.340300
C -0.781975 -0.517111 0.497368
C 0.619477 -0.073311 0.060527
O 0.912135 1.180096 0.117040
O 1.347901 -0.986523 -0.309445
H -1.810919 -0.083866 -1.388658
H -1.718457 1.301402 -0.260638
H -0.778144 -0.249009 1.565626
H -0.875666 -1.601149 0.417024
H 1.823349 1.388921 -0.171699

CA+, h-trans
E = -268.104342
H -2.607832 -0.274917 -0.870365

C -2.016116 0.044756 0.000056
C -0.733278 -0.663397 -0.000099
C 0.530573 -0.020126 0.000014
O 0.585540 1.271897 -0.000024
O 1.672384 -0.646675 -0.000086
H -1.911655 1.127289 0.000695
H -2.608061 -0.275888 0.869921
H -0.718575 -1.748422 -0.000243
H 1.497914 1.618612 0.000189
H 1.597745 -1.615849 0.000863

CAA+.H2O
E = -536.567673
C 2.267277 -1.158207 -0.430384
C 3.647648 -0.747215 0.070940
H 2.051041 -2.211087 -0.220798
H 2.171713 -1.052222 -1.516669
C 1.172539 -0.356501 0.182503
O 1.198414 0.506788 0.989580
O -0.100544 -0.831097 -0.346049
C -1.269190 -0.257623 -0.104398
C -2.386096 -1.131472 -0.039643
H -2.164419 -2.186379 -0.144300
O -1.436482 0.998339 0.023583
H -0.635982 1.654446 -0.106241
O 0.341054 2.714861 -0.387576
H 1.007387 2.831429 0.302802
H 0.037390 3.588988 -0.663956
C -3.770536 -0.680715 0.146540
H 3.857711 0.294910 -0.172625
H 3.722081 -0.868748 1.151929
H 4.405078 -1.371782 -0.401952
H -4.196989 -1.166231 1.034904
H -3.857794 0.399464 0.239444
H -4.386608 -1.033524 -0.692195

(CA)2+
E = -536.552408
H 5.172479 -0.516346 0.381028
C 4.186754 -0.109452 0.610280
C 3.240826 -0.464243 -0.549823
C 1.867583 0.091714 -0.309880
O 1.775868 1.386498 -0.233190
O 0.896786 -0.670463 -0.185420
O -0.896784 0.670464 0.185417
C -1.867581 -0.091714 0.309867
C -3.240823 0.464242 0.549826
C -4.186763 0.109452 -0.610267
H -5.172486 0.516347 -0.381003
O -1.775864 -1.386498 0.233184
H 3.844689 -0.551593 1.547348
H 4.269976 0.970073 0.730380
H 3.588242 -0.010454 -1.484014
H 3.162153 -1.541147 -0.690274
H 0.855347 1.661721 -0.063699
H -0.855342 -1.661720 0.063695
H -3.162149 1.541145 0.690279
H -3.588229 0.010450 1.484020
H -3.844709 0.551595 -1.547338
H -4.269987 -0.970072 -0.730368

C2H5
E = -79.136317
C -0.692952 0.000001 -0.002155
C 0.792903 0.000000 -0.017377
H 1.348366 0.927147 0.038995
H -1.102667 0.887484 -0.493327
H -1.102664 -0.887488 -0.493312
H -1.091129 -0.000011 1.025863
H 1.348384 -0.927142 0.038970

CAH+
E = -268.741500
H 2.834678 -0.574655 0.000000
C 1.959847 0.074033 0.000000
C 0.696920 -0.784570 -0.000000
C -0.568875 -0.015860 -0.000000
O -0.637091 1.265532 0.000000
O -1.671879 -0.661348 -0.000000
H 2.023013 0.698897 0.895254
H 2.023013 0.698897 -0.895253
H 0.646559 -1.450343 -0.870130
H 0.646559 -1.450343 0.870130
H -2.468696 -0.093709 -0.000000
H 0.239281 1.696167 0.000000

C2H5+
E = -78.834984
C -0.688838 0.000010 0.063079
C 0.689205 -0.000001 0.063036
H 1.243658 0.936098 0.077751
H -1.244155 0.935563 0.077522
H -0.001453 -0.000615 -1.067993
H -1.244406 -0.935391 0.078712
H 1.244153 -0.935708 0.077314

[CA-OH]+
E = -192.257403
H 2.557545 0.026762 0.000034
C 1.586541 -0.467976 0.000001
C 0.521418 0.672410 -0.000068
C -0.802907 0.137827 0.000244
O -1.820457 -0.317571 -0.000105
H 1.494743 -1.082459 -0.894025
H 1.494569 -1.082334 0.894089
H 0.593253 1.312618 0.890570
H 0.593241 1.312413 -0.890887

CA.2H2O
E = -421.351460
C 0.693920 -0.147155 -0.331153
O 0.291770 1.110274 -0.274996
O -0.039750 -1.115623 -0.212211
C 2.184557 -0.272688 -0.524729
H 2.489736 0.399531 -1.329896
H 2.399290 -1.300089 -0.816684
H -0.695459 1.197506 -0.103819
O -2.295220 1.427940 0.192606
O -2.743575 -1.206819 0.152736
H -1.775139 -1.303126 0.006326
H -2.951002 -1.708648 0.946614
H -2.656630 0.508530 0.234289
H -2.783812 1.887675 -0.497082
C 2.936671 0.093760 0.763813
H 2.645884 -0.569442 1.581612
H 2.717441 1.121932 1.055232
H 4.013007 -0.003549 0.610730

CA+.2H2O
E = -421.051807
C -0.734173 -0.276208 0.012128
O -0.402112 0.958927 -0.075807

O 0.121753 -1.254311 0.085882
H 1.092120 -1.030105 0.037817
H 0.601232 1.199084 -0.032722
O 2.015247 1.635500 0.108801
H 2.311426 2.525720 -0.112896
H 2.710108 0.995012 -0.104663
O 2.787152 -1.012208 -0.077353
H 3.136604 -1.511857 -0.827996
H 3.232097 -1.358107 0.708822
C -2.111953 -0.633837 0.030994
H -2.317816 -1.694645 0.101490
C -3.213408 0.336512 -0.035117
H -3.859338 0.104257 -0.892425
H -2.867835 1.365681 -0.104861
H -3.857712 0.222895 0.847218

CAH+.2H2O
E = -421.689864
O -4.360020 -0.463791 0.006992
H -4.635292 -1.167076 -0.591745
H -4.937920 -0.489632 0.778326
O -2.100438 0.739785 0.062425
H -2.978834 0.234051 0.024710
H -2.148733 1.543447 -0.470803
H -1.102665 0.124229 -0.030374
O -0.091145 -0.584746 -0.062423
C 1.027046 -0.058374 -0.024027
O 1.090481 1.254901 -0.015371
H 2.005779 1.577358 0.020863
C 2.269812 -0.894790 0.008636
H 2.165592 -1.551313 0.877806
H 2.211285 -1.553351 -0.863127
C 3.587353 -0.123779 0.042884
H 3.713965 0.500764 -0.846158
H 3.669039 0.498064 0.939189
H 4.421490 -0.824074 0.063373

(CA)2
E = -536.898577
C 1.889583 0.314867 -0.000016
O 1.432323 -0.820768 -0.000123
O 1.149465 1.404934 0.000181
H 0.171489 1.175765 0.000194
C -1.889586 -0.314873 -0.000124
O -1.432311 0.820755 -0.000193
O -1.149471 -1.404944 0.000183
H -0.171498 -1.175771 0.000187
C -3.369081 -0.607023 0.000047
H -3.570302 -1.237882 -0.871063
H -3.570186 -1.237699 0.871319
C 3.369075 0.607032 0.000046
H 3.570221 1.237713 0.871304
H 3.570243 1.237889 -0.871079
C 4.241582 -0.641750 -0.000069
H 4.041965 -1.254337 -0.880419
H 4.041944 -1.254517 0.880151
C -4.241579 0.641765 -0.000022
H -4.041885 1.254536 0.880183
H -4.042007 1.254345 -0.880387
H 5.296861 -0.362897 -0.000028
H -5.296860 0.362922 0.000082

CA, S=3
E = -268.282409
C -0.515984 0.033851 -0.264486
O -1.691295 -0.668384 -0.005456
H -2.418079 -0.245539 -0.482683
O -0.708497 1.301995 0.146906
C 0.721902 -0.661391 0.221418
H 0.718788 -1.658835 -0.224994
H 0.645867 -0.785970 1.312098
C 2.004818 0.091212 -0.134847
H 2.011475 1.086412 0.315133
H 2.099274 0.205800 -1.216830
H 2.876591 -0.452786 0.233167

CA, h-trans, S=3
E = -268.295972
H -2.936241 -0.403991 0.348271
C -2.109153 0.006122 -0.236676
C -0.820858 -0.078517 0.500742
C 0.476904 0.006640 -0.179247
O 1.139020 1.191153 0.004600
O 1.360530 -1.060555 -0.036691
H -2.052653 -0.512754 -1.198073
H -2.362295 1.054133 -0.463693
H -0.827874 -0.010373 1.589721
H 2.031325 1.102337 -0.357130
H 0.869978 -1.879608 -0.171282

CAA+
E = -460.100235
C 3.704701 -0.183586 -0.001085
C 2.339150 -0.864172 0.000112
C 1.216249 0.103887 0.000599
O -0.046011 -0.606725 0.001109
C -1.215812 0.013340 0.000093
O -1.326173 1.297602 -0.000505
O 1.223133 1.297014 0.000765
C -2.369943 -0.804830 -0.000145
C -3.739265 -0.281820 -0.000520
H 2.198988 -1.514836 0.871380
H 2.197729 -1.514935 -0.870906
H -2.187174 -1.872817 -0.000007
H -0.422590 1.720582 -0.000060
H 3.829474 0.439446 -0.887077
H 3.828715 0.444250 0.881622
H 4.483681 -0.945172 0.001319
H -4.279829 -0.679841 0.870191
H -3.786867 0.804819 -0.001535
H -4.280185 -0.681540 -0.870196

[CA-OH]
E = -192.511010
H 2.446666 -0.317821 0.000000
C 1.380538 -0.555224 0.000000
C 0.553318 0.733043 0.000000
C -0.944560 0.502864 -0.000000
O -1.528773 -0.521384 -0.000000
H 1.155397 -1.156245 -0.882284
H 1.155396 -1.156246 0.882284
H 0.768470 1.358639 0.871823
H 0.768471 1.358640 -0.871822

n = 4, B3LYP+D2/def2TZVP

CA
E = -307.739216
H -3.527949 0.516174 0.000129

C -2.719382 -0.218069 0.000070
C -1.354677 0.466874 -0.000009
C -0.219353 -0.549510 -0.000097
C 1.151440 0.077821 -0.000195
O 1.394060 1.256227 0.000048
O 2.125240 -0.866800 0.000087
H -2.838376 -0.852021 0.883590
H -2.838488 -0.852002 -0.883448
H -1.254990 1.114977 -0.873644
H -1.254878 1.114956 0.873628
H -0.282254 -1.209067 0.871843
H -0.282362 -1.209043 -0.872046
H 2.976724 -0.402084 0.000254

CA+
E = -307.375301
H -3.347444 0.592829 -0.457377
C -2.642858 -0.059056 0.078299
C -1.242163 0.355158 -0.427777
C -0.256058 -0.537883 0.358703
C 1.183459 -0.088882 0.050676
O 1.943992 -0.990143 -0.248881
O 1.459746 1.170508 0.161387
H -2.755461 0.110244 1.149259
H -2.871364 -1.097867 -0.158710
H -1.159427 0.172931 -1.499244
H -1.040368 1.405319 -0.225140
H -0.325710 -0.427300 1.449062
H -0.382614 -1.589411 0.103681
H 2.398206 1.374310 -0.020982

CA+, h-trans
E = -307.409992
H -3.400267 0.449347 -0.299854
C -2.491886 -0.103571 -0.538725
C -1.440023 0.197279 0.573176
C -0.220971 -0.583674 0.348323
C 1.038756 -0.026470 0.021365
O 2.119314 -0.724946 -0.193176
O 1.162048 1.258515 -0.077584
H -2.728038 -1.167597 -0.577559
H -2.124771 0.220004 -1.512762
H -1.229966 1.264424 0.623773
H -1.877292 -0.123237 1.527648
H -0.269062 -1.667232 0.392832
H 2.068794 1.539355 -0.303051
H 1.994452 -1.685003 -0.109785

C2H4
E = -78.574653
C -0.000011 -0.662753 0.000000
H 0.924371 -1.230528 0.000000
C -0.000011 0.662720 -0.000000
H -0.923956 -1.230068 0.000000
H -0.923906 1.230203 -0.000000
H 0.923623 1.230593 -0.000000

CH3
E = -39.829966
C 0.000021 0.000122 0.000503
H -1.064701 0.184923 -0.001005
H 0.692679 0.829004 -0.001006
H 0.371895 -1.014659 -0.001004

CAA+.H2O
E = -615.176993
C 2.293769 -0.817871 -0.299328
C 3.602620 -0.428188 0.383783
H 2.091643 -1.890147 -0.197012
H 2.327872 -0.631736 -1.379085
C 1.112698 -0.090668 0.237938
O 1.017039 0.701824 1.110260
O -0.075330 -0.539598 -0.478498
C -1.278146 -0.003119 -0.335206
C -2.375669 -0.892646 -0.455205
H -2.122039 -1.938253 -0.583698
O -1.483254 1.241363 -0.146670
H -0.682735 1.904030 -0.144067
O 0.326123 2.982638 -0.248486
H 0.899177 3.058699 0.526032
H 0.056665 3.871738 -0.511699
C -3.786098 -0.487978 -0.392150
H 3.767117 0.644801 0.259135
H 3.515634 -0.611578 1.456876
C 4.775084 -1.214423 -0.197425
C -4.523494 -1.214061 0.762161
H -3.884197 0.592678 -0.299575
H -4.263068 -0.795666 -1.333521
H 5.707189 -0.931418 0.292805
H 4.633044 -2.289126 -0.057913
H 4.884290 -1.023051 -1.268055
H -5.577594 -0.937932 0.734697
H -4.444896 -2.297308 0.657053
H -4.109297 -0.921832 1.727770

(CA)2+
E = -615.164449
H 6.253689 -0.179816 1.041051
C 5.599553 -0.342360 0.182713
C 4.171038 0.071229 0.534158
C 3.246635 -0.159129 -0.680990
C 1.842945 0.259618 -0.367457
O 0.936285 -0.583560 -0.301038
O 1.654691 1.529963 -0.156405
O -0.936298 0.583569 0.301072
C -1.842949 -0.259614 0.367534
O -1.654704 -1.529954 0.156440
C -3.246652 0.159141 0.680996
C -4.171006 -0.071245 -0.534184
C -5.599538 0.342344 -0.182805
H -6.253639 0.179778 -1.041165
H 5.981768 0.246298 -0.654179
H 5.648203 -1.399356 -0.087955
H 3.807428 -0.514783 1.381991
H 4.133983 1.124499 0.816367
H 3.574480 0.453670 -1.527043
H 3.248239 -1.206953 -0.978679
H 0.720966 1.708414 0.063595
H -0.720981 -1.708404 -0.063573
H -3.248268 1.206973 0.978660
H -3.574530 -0.453638 1.527050
H -3.807366 0.514749 -1.382015
H -4.133936 -1.124522 -0.816369
H -5.981782 -0.246297 0.654086
H -5.648204 1.399345 0.087839

C3H7
E = -118.445293
C 1.289046 -0.199084 0.002288
C 0.000001 0.540630 -0.041375
C -1.289044 -0.199088 0.002294
H 1.295467 -1.026111 -0.719106

H 2.142639 0.448752 -0.208618
H 1.462315 -0.657543 0.990516
H -0.000005 1.615006 0.095235
H -2.142601 0.448832 -0.208517
H -1.295532 -1.026007 -0.719218
H -1.462304 -0.657681 0.990466

CAH+
E = -308.047906
H 3.522250 0.540144 0.000000
C 2.737387 -0.215730 0.000000
C 1.360779 0.449048 0.000000
C 0.246952 -0.600049 -0.000000
C -1.127133 -0.051472 -0.000000
O -2.111920 -0.866806 -0.000000
O -1.403776 1.201792 0.000000
H 2.864337 -0.840881 -0.886187
H 2.864337 -0.840882 0.886187
H 1.267755 1.084700 0.888178
H 1.267755 1.084700 -0.888177
H 0.313460 -1.265156 -0.870199
H 0.313460 -1.265157 0.870198
H -2.989320 -0.434073 -0.000000
H -0.606374 1.765939 0.000000

C3H7+
E = -118.174489
C -1.274460 -0.198012 0.021686
C 0.000030 0.457493 0.000099
C 1.274361 -0.198217 -0.021620
H -1.239604 -1.271742 0.198636
H -2.017552 0.336808 0.623892
H -1.633398 -0.023388 -1.022919
H 0.000053 1.548305 -0.000088
H 2.016640 0.335565 -0.625867
H 1.239070 -1.272236 -0.196383
H 1.635205 -0.020898 1.021739

[CA-OH]+
E = -231.566326
H 3.044676 -0.803244 0.000121
C 2.329588 0.020686 0.000033
C 0.917019 -0.556221 -0.000036
C -0.103824 0.639757 -0.000072
C -1.443521 0.158787 0.000172
O -2.469451 -0.280278 -0.000045
H 2.509181 0.628956 0.888760
H 2.509299 0.628875 -0.888724
H 0.739411 -1.167053 -0.885891
H 0.739295 -1.167013 0.885821
H 0.009143 1.271918 0.891433
H 0.009037 1.271728 -0.891745

CA.2H2O
E = -460.655761
H 4.479079 0.076994 1.277190
C 3.916229 -0.047788 0.349329
C 2.413308 0.032655 0.603338
C 1.612942 -0.147490 -0.696896
C 0.132444 -0.077034 -0.428310
O -0.561232 -1.074110 -0.303390
O -0.306736 1.163038 -0.303101
O -2.873492 1.373794 0.320287
O -3.233039 -1.273035 0.212561
H 4.233350 0.732742 -0.347903
H 4.185850 -1.014962 -0.083960
H 2.112950 -0.741251 1.315455
H 2.156880 0.997955 1.046516
H 1.890994 0.639182 -1.402100
H 1.834171 -1.120165 -1.137484
H -1.284688 1.209095 -0.073541
H -3.414871 1.836526 -0.326669
H -3.199449 0.440769 0.349980
H -2.271986 -1.329212 0.007346
H -3.375834 -1.807223 0.999545

CA+.2H2O
E = -460.355961
H -4.575333 0.789598 0.441324
C -3.735908 0.128538 0.657608
C -2.693675 0.247780 -0.481739
C -1.577131 -0.688296 -0.282942
C -0.213468 -0.303143 -0.164105
O 0.105732 0.936896 -0.247357
O 0.649724 -1.260747 0.025525
O 2.483543 1.658316 0.182010
O 3.319921 -0.971578 0.122759
H -3.298296 0.420017 1.613257
H -4.110563 -0.893126 0.739479
H -3.196023 -0.024702 -1.420460
H -2.336444 1.272327 -0.577427
H -1.772299 -1.750190 -0.191959
H 1.093155 1.194202 -0.101750
H 1.614148 -1.015835 0.069271
H 3.203493 1.023079 0.050998
H 2.788764 2.546686 -0.034534
H 3.749609 -1.477978 -0.580082
H 3.689515 -1.296446 0.955451

CAH+.2H2O
E = -460.995315
H 5.167938 0.001636 0.071725
C 4.274837 -0.622495 0.039719
C 3.014054 0.240743 0.027139
C 1.753761 -0.623562 -0.016982
C 0.450467 0.110073 -0.035173
O 0.405629 1.421601 -0.006807
O -0.624103 -0.506042 -0.080318
O -2.719981 0.670940 0.062814
O -4.915088 -0.675490 0.021999
H 4.324821 -1.245046 -0.856323
H 4.284573 -1.278103 0.913229
H 3.001278 0.868924 0.925482
H 3.040573 0.902136 -0.846585
H 1.751199 -1.273122 -0.898448
H 1.710042 -1.300963 0.842290
H -1.652569 0.111437 -0.041552
H 1.292713 1.815785 0.032926
H -3.563357 0.116851 0.030753
H -2.835006 1.482759 -0.446478
H -5.169528 -1.371210 -0.594247
H -5.483039 -0.747710 0.797511

(CA)2
E = -615.506400
H -6.384995 1.037560 0.000107
C -5.738961 0.157154 0.000137
C -4.265119 0.555602 -0.000028
C -3.357105 -0.667952 0.000003
C -1.884291 -0.348972 -0.000196
O -1.123834 -1.425212 0.000116
O -1.447168 0.794689 -0.000279

O 1.447164 -0.794684 -0.000151
C 1.884292 0.348975 -0.000032
C 3.357108 0.667951 0.000073
C 4.265122 -0.555603 -0.000001
C 5.738966 -0.157157 0.000100
H 6.384999 -1.037563 0.000045
O 1.123826 1.425210 0.000122
H -5.982445 -0.440389 0.883587
H -5.982596 -0.440559 -0.883157
H -4.038423 1.170721 -0.873831
H -4.038273 1.170887 0.873620
H -3.552399 -1.301914 0.871313
H -3.552546 -1.302071 -0.871157
H -0.150298 -1.177658 0.000140
H 0.150288 1.177651 0.000062
H 3.552514 1.302072 -0.871095
H 3.552439 1.301911 0.871375
H 4.038314 -1.170886 0.873657
H 4.038389 -1.170723 -0.873793
H 5.982563 0.440554 -0.883206
H 5.982487 0.440388 0.883538

CA, S=3
E = -307.586530
H -3.559248 0.465315 0.173308
C -2.735675 -0.189254 -0.120475
C -1.387910 0.400950 0.285874
C -0.229606 -0.512916 -0.117596
C 1.114905 0.030027 0.264837
O 1.437302 1.248487 -0.210820
O 2.172959 -0.827526 -0.029871
H -2.890954 -1.162837 0.353614
H -2.786369 -0.333284 -1.203335
H -1.255798 1.380753 -0.182510
H -1.357996 0.560885 1.367240
H -0.329746 -1.490410 0.362643
H -0.248301 -0.676053 -1.206545
H 2.976035 -0.484893 0.385266

CA, h-trans, S=3
E = -307.602163
H -3.544456 0.505029 -0.504244
C -2.812799 -0.117198 0.015009
C -1.421240 0.339014 -0.234368
C -0.276906 -0.505050 0.201613
C 1.064826 -0.007739 -0.242861
O 2.155325 -0.834706 -0.014797
O 1.333446 1.267255 0.161685
H -3.063855 -0.091036 1.088545
H -2.955473 -1.157500 -0.304268
H -1.224808 1.361087 -0.528611
H -0.265098 -0.591617 1.311822
H 2.242187 1.481253 -0.084523
H 1.983946 -1.686828 -0.430745
H -0.405901 -1.534943 -0.159438

CAA+
E = -538.710427
C 4.818583 -0.893777 0.068772
C 3.674999 0.114496 0.146077
C 2.328271 -0.578508 -0.058913
C 1.175800 0.349990 0.003719
O -0.057812 -0.379781 -0.197690
C -1.246788 0.206410 -0.195654
O -1.397485 1.474197 -0.010872
O 1.142316 1.529552 0.184893
C -2.368345 -0.625991 -0.408963
C -3.755825 -0.152134 -0.425120
C -4.577730 -0.817414 0.715307
H 2.155486 -1.361216 0.690061
H 2.278536 -1.092166 -1.026971
H -2.152729 -1.680542 -0.536697
H -0.509135 1.908476 0.122017
H 3.797960 0.889868 -0.613154
H 3.674920 0.617854 1.115301
H -3.810683 0.933507 -0.360839
H -4.205074 -0.468047 -1.376638
H 5.776504 -0.394247 0.215740
H 4.717071 -1.662945 0.838627
H 4.841362 -1.388090 -0.905761
H -5.613427 -0.489450 0.627851
H -4.546759 -1.905011 0.637501
H -4.193975 -0.518171 1.690963

[CA-OH]
E = -231.814983
H 2.892748 -0.986590 0.000000
C 2.259538 -0.096285 0.000001
C 0.780346 -0.475686 -0.000000
C -0.115120 0.766422 0.000000
C -1.600066 0.470771 -0.000000
O -2.138150 -0.578836 -0.000001
H 2.510381 0.496886 0.883942
H 2.510381 0.496887 -0.883940
H 0.543632 -1.084573 -0.875762
H 0.543631 -1.084574 0.875761
H 0.078122 1.400656 0.871921
H 0.078123 1.400656 -0.871919

n = 6, B3LYP+D2/def2TZVP

CA
E = -386.347461
C -2.728310 0.524886 0.000005
C -1.523315 -0.411797 -0.000012
C -0.193468 0.335172 -0.000033
C 0.995784 -0.616100 -0.000052
C 2.329340 0.086510 -0.000083
O 2.506587 1.276540 0.000031
O 3.354132 -0.802712 0.000074
H -2.672853 1.178305 -0.877089
C -4.056292 -0.229074 0.000024
H -2.672828 1.178306 0.877096
H -1.575777 -1.067234 0.877611
H -1.575803 -1.067236 -0.877632
H -0.133535 0.989222 -0.873917
H -0.133508 0.989223 0.873849
H 0.969993 -1.277987 0.871821
H 0.969967 -1.277987 -0.871923
H 4.178371 -0.291280 0.000164
H -4.906704 0.456854 0.000036
H -4.137768 -0.869199 -0.883304
H -4.137743 -0.869199 0.883354

CA+
E = -385.997035
C -2.621855 0.515495 -0.319059
C -1.477511 -0.419385 0.188081
C -0.149350 0.247305 -0.276067

C 0.949806 -0.691298 0.252665
C 2.341567 -0.067954 0.022201
O 3.233339 -0.800129 -0.328284
O 2.440143 1.214675 0.272616
H -2.568562 0.596564 -1.404708
C -3.939350 -0.134157 0.130514
H -2.506261 1.508981 0.113719
H -1.514758 -0.496273 1.274745
H -1.581091 -1.414956 -0.243078
H -0.124204 0.311477 -1.362913
H -0.053066 1.243698 0.148851
H 0.895863 -0.836046 1.337326
H 0.920849 -1.663883 -0.233021
H 3.354353 1.532370 0.149429
H -4.741139 0.525685 -0.234255
H -4.076484 -1.123137 -0.306869
H -4.013200 -0.200887 1.216106

CA+, h-trans
E = -386.022722
C 2.623997 0.025006 0.410999
C 1.279815 -0.244950 -0.266833
C 0.196223 -0.604650 0.826432
C -1.066022 -0.893110 0.156158
C -2.076856 0.069658 -0.049970
O -1.913996 1.276381 0.398466
O -3.204147 -0.160380 -0.669465
H 2.928340 -0.863320 0.970953
C 3.685896 0.387058 -0.626248
H 2.507344 0.838068 1.132607
H 0.947286 0.636917 -0.818964
H 1.368446 -1.073092 -0.973393
H 0.553897 -1.488602 1.357435
H 0.113804 0.236737 1.513856
H -1.236431 -1.870203 -0.282996
H -2.675189 1.855631 0.210186
H -3.297314 -1.072671 -0.989431
H 4.641761 0.578047 -0.133948
H 3.829863 -0.425827 -1.341791
H 3.405016 1.286233 -1.179751

C4H8
E = -157.191121
C -0.533256 0.395901 -0.000089
C 0.533237 -0.395837 -0.000046
C 1.954142 0.078914 0.000039
H -0.380328 1.473590 -0.000032
C -1.954136 -0.078954 0.000025
H 0.380291 -1.473527 -0.000081
H 2.494125 -0.288912 -0.879269
H 2.003240 1.170438 0.000553
H 2.494294 -0.289762 0.878887
H -2.494457 0.289426 -0.878822
H -2.003098 -1.170473 -0.000145
H -2.493985 0.289079 0.879337

CAA+.H2O
E = -772.396019
C -5.249445 -1.542039 0.004892
C -3.735007 -1.359606 0.095404
C -3.187747 -0.671904 -1.202285
C -1.733083 -0.542634 -1.111496
C -1.080082 0.630046 -0.663194
O -1.766257 1.653763 -0.329159
O 0.245913 0.605297 -0.668174
C 1.074467 1.258098 0.332133
C 2.501759 1.080199 -0.034392
C 2.982760 -0.353495 0.286455
C 4.463198 -0.518579 -0.044685
C 4.971983 -1.925154 0.262684
O 0.576656 1.753776 1.285960
O -0.728928 3.895669 0.160775
H -5.484898 -2.151733 -0.872232
C -5.804041 -2.199829 1.266697
H -5.720230 -0.566605 -0.148729
H -3.246626 -2.328501 0.226591
H -3.671415 0.299030 -1.309262
H -1.090046 -1.386795 -1.326833
H 2.628723 1.276533 -1.101073
H 3.077267 1.804862 0.541469
H 2.814569 -0.559928 1.346990
H 2.391687 -1.071467 -0.287646
H 4.625863 -0.294294 -1.104582
H 5.046491 0.212625 0.524949
C 6.454009 -2.086343 -0.067691
H 4.801851 -2.144542 1.321774
H 4.383547 -2.652229 -0.306923
H -1.279061 2.535010 -0.083337
H -3.480533 -0.740744 0.959476
H -3.452737 -1.309295 -2.049227
H -0.305022 3.994250 1.023562
H -1.269437 4.678975 -0.000774
H 6.800722 -3.096427 0.157706
H 6.638823 -1.893698 -1.127905
H 7.059036 -1.383999 0.511754
H -6.885923 -2.324747 1.191140
H -5.359568 -3.186192 1.421023
H -5.594788 -1.590699 2.149749

(CA)2+
E = -772.385540
C 6.692385 0.142254 0.688122
C 5.634499 -0.206608 -0.361637
C 4.229225 0.171633 0.112825
C 3.196211 -0.187737 -0.972271
C 1.812755 0.219686 -0.551005
O 0.930401 -0.627765 -0.383383
O 1.622617 1.496935 -0.371371
O -0.930387 0.627749 0.383318
C -1.812749 -0.219699 0.550905
O -1.622599 -1.496952 0.371307
C -3.196188 0.187716 0.972231
C -4.229241 -0.171630 -0.112836
C -5.634497 0.206611 0.361680
C -6.692419 -0.142226 -0.688050
H 6.459830 -0.383592 1.619260
C 8.096656 -0.228447 0.214431
H 6.642620 1.213162 0.907036
H 5.858157 0.318828 -1.295601
H 5.673641 -1.278400 -0.580038
H 3.996364 -0.363935 1.037004
H 4.178014 1.241010 0.324516
H 3.410428 0.358167 -1.897098
H 3.202698 -1.256152 -1.181982
H 0.704779 1.661465 -0.081623
H -0.704758 -1.661481 0.081569
H -3.202666 1.256127 1.181963
H -3.410375 -0.358205 1.897054
H -3.996407 0.363954 -1.037014
H -4.178042 -1.241002 -0.324547
H -5.858126 -0.318840 1.295642
H -5.673625 1.278399 0.580101

C -8.096672 0.228474 -0.214306
H -6.459892 0.383634 -1.619186
H -6.642668 -1.213131 -0.906984
H -8.839379 -0.025586 -0.973714
H -8.353323 -0.307463 0.702946
H -8.169977 1.300093 -0.012580
H 8.839336 0.025631 0.973860
H 8.169974 -1.300069 0.012727
H 8.353335 0.307476 -0.702821

C5H11
E = -197.051926
C -2.399015 -0.205378 0.143372
C -0.978099 -0.311568 -0.405057
C -0.020422 0.693871 0.271935
C 1.381852 0.596709 -0.215796
H -2.801257 0.799209 -0.016857
H -3.069556 -0.919878 -0.340536
H -2.413252 -0.401555 1.219450
H -0.593939 -1.324622 -0.253241
H -0.977367 -0.132159 -1.484551
H -0.413705 1.703541 0.116164
H -0.050430 0.499716 1.353255
C 2.226967 -0.571319 0.150824
H 1.708868 1.250840 -1.015807
H 3.288341 -0.381413 -0.027119
H 2.093211 -0.836692 1.206349
H 1.961391 -1.470880 -0.428775

CAH+
E = -386.658365
C 2.745298 0.526740 0.000000
C 1.557188 -0.431882 0.000000
C 0.217153 0.305722 0.000000
C -0.957899 -0.672009 -0.000000
C -2.294234 -0.038844 0.000000
O -3.330427 -0.788639 -0.000000
O -2.488670 1.229902 -0.000000
H 2.681898 1.176733 0.878970
C 4.078341 -0.215403 0.000000
H 2.681898 1.176733 -0.878970
H 1.608197 -1.082191 -0.879433
H 1.608197 -1.082191 0.879433
H 0.169274 0.947461 0.888372
H 0.169274 0.947462 -0.888372
H -0.932692 -1.340228 -0.869970
H -0.932692 -1.340229 0.869970
H -4.177195 -0.298974 -0.000000
H -1.653644 1.737514 -0.000000
H 4.915270 0.484442 0.000000
H 4.169951 -0.851294 0.884351
H 4.169951 -0.851293 -0.884351

C5H11+
E = -196.792375
C 1.762679 -0.747797 -0.164710
C 0.963156 0.336269 0.533735
C -0.086658 1.064086 -0.545699
C -1.091269 0.459314 0.228976
H 2.309555 -0.340761 -1.014733
H 2.474160 -1.171490 0.546853
H 1.119970 -1.557623 -0.514532
H 0.483731 -0.075071 1.434954
H 1.530503 1.193702 0.892589
H 0.023815 2.139835 -0.475671
H 0.099080 0.649772 -1.531087
C -1.692978 -0.844752 -0.054784
H -1.453467 1.001314 1.099301
H -1.862232 -1.435913 0.847286
H -2.695330 -0.601813 -0.448830
H -1.159361 -1.404670 -0.821231

[CA-OH]+
E = -310.178009
C 2.219462 -0.602010 0.000041
C 1.059406 0.395019 0.000030
C -0.283288 -0.333537 0.000126
C -1.432808 0.739431 0.000105
C -2.702780 0.100759 -0.000213
O -3.661938 -0.471464 -0.000030
H 2.139055 -1.248011 -0.879378
C 3.569584 0.112651 -0.000109
H 2.139163 -1.247851 0.879586
H 1.127126 1.040674 0.881639
H 1.127044 1.040549 -0.881677
H -0.385217 -0.961953 -0.886031
H -0.385150 -0.961872 0.886351
H -1.390989 1.379046 0.891948
H -1.390881 1.379194 -0.891635
H 4.386073 -0.610652 -0.000093
H 3.675861 0.744272 -0.885421
H 3.675970 0.744435 0.885074

CA.2H2O
E = -539.264060
C -3.806978 0.079266 -0.814470
C -2.823166 -0.084377 0.341065
C -1.367469 0.004000 -0.105195
C -0.393781 -0.169884 1.070759
C 1.033144 -0.088222 0.596143
O 1.703130 -1.080190 0.354686
O 1.448597 1.155636 0.432190
O 3.899599 1.388418 -0.550819
O 4.270262 -1.259302 -0.548603
H -3.606807 -0.691241 -1.566659
C -5.262240 -0.008703 -0.359650
H -3.628802 1.043491 -1.302270
H -3.018578 0.686286 1.095679
H -2.996011 -1.049844 0.830423
H -1.167005 -0.768112 -0.854565
H -1.185532 0.971358 -0.581569
H -0.576342 0.614127 1.808949
H -0.543660 -1.144686 1.535728
H 2.383040 1.209313 0.065171
H 4.527649 1.838432 0.022610
H 4.217388 0.456997 -0.646094
H 3.349283 -1.321705 -0.206459
H 4.296233 -1.777452 -1.358496
H -5.952006 0.110190 -1.198576
H -5.463090 -0.976273 0.109379
H -5.485517 0.770148 0.375218

CA+.2H2O
E = -538.966420
C -3.801337 0.328532 -0.261306
C -2.498646 -0.247244 0.291460
C -1.569968 -0.726761 -0.871340
C -0.344249 -1.317471 -0.326164
C 0.877007 -0.606536 -0.190538
O 0.952670 0.607973 -0.603161
O 1.874433 -1.246428 0.354335
O 3.045657 1.953516 -0.159945

O 4.398307 -0.330235 0.590731
H -4.307424 -0.438179 -0.855341
C -4.717336 0.812420 0.860637
H -3.569556 1.154991 -0.939758
H -1.972739 0.510259 0.878613
H -2.712375 -1.088511 0.955874
H -2.119153 -1.480318 -1.441677
H -1.350908 0.124603 -1.516121
H -0.345304 -2.325105 0.070268
H 1.830566 1.117827 -0.439360
H 2.751043 -0.779540 0.405544
H 3.886064 1.486404 -0.037798
H 3.204494 2.799886 -0.592925
H 5.016919 -0.882289 0.093345
H 4.700929 -0.344204 1.509166
H -5.644028 1.221248 0.453459
H -4.976879 -0.008297 1.534071
H -4.233014 1.594969 1.450469

CAH+.2H2O
E = -539.604817
C 4.352263 0.360133 0.045924
C 3.100869 -0.512402 -0.002332
C 1.812621 0.310142 -0.000738
C 0.573501 -0.582083 -0.048421
C -0.743653 0.123638 -0.053023
O -0.817036 1.431472 -0.010369
O -1.806609 -0.516855 -0.100371
O -3.920633 0.629102 0.061967
O -6.112854 -0.744789 0.061148
H 4.318006 0.986953 0.943228
C 5.633095 -0.470495 0.043598
H 4.348999 1.039711 -0.812805
H 3.124686 -1.139377 -0.899864
H 3.093519 -1.191721 0.856539
H 1.795082 0.929425 0.904633
H 1.825399 0.982078 -0.867676
H 0.580694 -1.222508 -0.936537
H 0.548278 -1.269451 0.803667
H -2.821413 0.072540 -0.054312
H 0.063166 1.842012 0.029478
H -4.757149 0.070053 0.045854
H -4.060466 1.444246 -0.435004
H -6.381548 -1.431285 -0.559196
H -6.669253 -0.823734 0.844165
H 6.516529 0.169037 0.078519
H 5.664516 -1.138100 0.908655
H 5.695838 -1.084914 -0.858386

(CA)2
E = -772.722967
C -6.772002 0.714691 -0.000092
C -5.729027 -0.399540 0.000013
C -4.298091 0.129010 0.000001
C -3.274145 -0.998018 0.000107
C -1.840348 -0.534503 0.000083
O -0.976732 -1.530012 0.000268
O -1.518563 0.646829 -0.000073
O 1.518555 -0.646824 -0.000068
C 1.840347 0.534507 0.000077
C 3.274147 0.998017 0.000082
C 4.298095 -0.129010 -0.000068
C 5.729031 0.399539 -0.000064
C 6.772007 -0.714692 -0.000213
O 0.976720 1.530009 0.000250
H -6.614667 1.351192 -0.877318
C -8.201996 0.178680 -0.000082
H -6.614704 1.351322 0.877047
H -5.883735 -1.038545 0.877648
H -5.883700 -1.038676 -0.877533
H -4.137050 0.765608 -0.873999
H -4.137086 0.765741 0.873912
H -3.405168 -1.648261 0.871279
H -3.405144 -1.648396 -0.870969
H -0.032647 -1.186775 0.000260
H 0.032632 1.186769 0.000217
H 3.405132 1.648418 -0.870978
H 3.405186 1.648238 0.871269
H 4.137102 -0.765764 0.873828
H 4.137041 -0.765584 -0.874083
H 5.883692 1.038698 -0.877594
H 5.883753 1.038520 0.877587
C 8.202002 -0.178681 -0.000209
H 6.614721 -1.351347 0.876910
H 6.614660 -1.351169 -0.877455
H 8.934043 -0.989746 -0.000316
H 8.383084 0.440757 -0.883445
H 8.383145 0.440579 0.883140
H -8.934037 0.989745 -0.000157
H -8.383091 -0.440735 -0.883333
H -8.383127 -0.440605 0.883252

CA, S=3
E = -386.194762
C -2.752573 0.480177 0.216170
C -1.535863 -0.379160 -0.116080
C -0.215911 0.294165 0.244430
C 0.988677 -0.585011 -0.092153
C 2.301073 0.053185 0.252456
O 2.558983 1.253012 -0.303394
O 3.404570 -0.763743 0.013120
H -2.671537 1.434929 -0.314378
C -4.068716 -0.202850 -0.148329
H -2.742158 0.717480 1.285383
H -1.612226 -1.335509 0.414981
H -1.542481 -0.618119 -1.185825
H -0.135381 1.245550 -0.291314
H -0.203462 0.532235 1.312493
H 0.937081 -1.530004 0.455739
H 0.984571 -0.825057 -1.166710
H 4.186972 -0.351516 0.403825
H -4.928016 0.426134 0.096105
H -4.105451 -0.425250 -1.218709
H -4.176464 -1.148064 0.391636

CA, h-trans, S=3
E = -386.213439
C 2.782080 -1.126932 0.143578
C 2.032712 0.147566 0.543273
C 1.257936 0.747013 -0.578811
C 0.081205 1.635556 -0.336068
C -1.063013 0.987945 0.470697
C -1.672482 -0.194478 -0.218112
O -2.854713 -0.593532 0.341886
O -0.858008 -1.277693 -0.487502
H -0.014384 -0.932210 -0.830755
H 1.367785 -0.061887 1.386300
H 1.725012 0.758406 -1.558957
H 0.409328 2.523957 0.227217
H -0.316721 1.994198 -1.287808
H -0.693682 0.682451 1.462442
H -1.849948 1.725101 0.636831

H -3.108657 -1.436781 -0.054416
H 3.394526 -1.498181 0.968076
H 2.078512 -1.915063 -0.137090
H 3.438062 -0.937536 -0.710458
H 2.761312 0.887326 0.916196

CAA+
E = -695.930826
C -5.756334 -2.262085 0.876665
C -5.358339 -1.046743 0.041103
C -3.840310 -0.970687 -0.123115
C -3.453289 0.294861 -0.975909
C -2.004591 0.322024 -1.154894
C -1.137980 1.054557 -0.318761
O 0.163278 0.960051 -0.569337
C 1.155518 1.671997 0.192940
O 0.815894 2.380102 1.096600
O -1.607329 1.782866 0.638466
C 2.511415 1.324725 -0.278967
C 2.929484 -0.066461 0.261634
C 4.344275 -0.418660 -0.190625
C 4.791158 -1.782500 0.331379
C 6.207293 -2.133201 -0.119801
H -5.823317 -1.099070 -0.947279
H -5.715452 -0.128866 0.516328
H -3.467136 -1.869768 -0.619066
H -3.818133 1.181862 -0.458344
H -1.525120 -0.290944 -1.908239
H 2.526431 1.310376 -1.370646
H 3.191903 2.092353 0.088782
H 2.879771 -0.056187 1.353750
H 2.226291 -0.823213 -0.096101
H 4.388494 -0.412018 -1.285027
H 5.039051 0.352137 0.158530
H 4.739191 -1.782669 1.424914
H 4.089994 -2.548123 -0.017078
H -0.855245 2.236490 1.115760
H -3.356556 -0.901563 0.854143
H -3.948928 0.199216 -1.944151
H 6.510595 -3.109797 0.261384
H 6.272087 -2.160380 -1.210766
H 6.924366 -1.391494 0.241464
H -6.841511 -2.307693 0.987740
H -5.425227 -3.189199 0.402562
H -5.316091 -2.212562 1.875620

[CA-OH]
E = -310.423199
C 2.135736 -0.605098 -0.000000
C 1.017224 0.434530 0.000000
C -0.372583 -0.194426 -0.000000
C -1.478069 0.863538 0.000001
C -2.884579 0.303127 0.000000
O -3.223720 -0.826595 -0.000000
H 2.023148 -1.250892 -0.877240
C 3.523564 0.029884 -0.000000
H 2.023148 -1.250893 0.877238
H 1.126170 1.082247 0.877929
H 1.126170 1.082248 -0.877928
H -0.491319 -0.838153 -0.875879
H -0.491319 -0.838154 0.875878
H -1.403796 1.522291 0.871805
H -1.403796 1.522292 -0.871803
H 4.310652 -0.727972 -0.000001
H 3.661473 0.660207 -0.883394
H 3.661473 0.660206 0.883395

n = 7, B3LYP+D2/def2TZVP

CA
E = -425.651556
C 2.146006 0.311589 0.000017
C 0.892732 -0.558108 0.000040
C -0.394574 0.260216 0.000083
C -1.633677 -0.625081 0.000110
C -2.927144 0.148786 0.000171
O -3.039665 1.346676 -0.000069
O -3.998697 -0.683555 -0.000181
H 2.130600 0.968572 0.877325
C 3.438850 -0.499552 -0.000024
H 2.130555 0.968591 -0.877275
H 0.908816 -1.215214 -0.877559
H 0.908861 -1.215234 0.877624
H -0.418835 0.916548 0.873951
H -0.418882 0.916566 -0.873771
H -1.643791 -1.287391 -0.871772
H -1.643749 -1.287404 0.871981
H -4.793933 -0.128105 -0.000380
C 4.685085 0.383181 -0.000047
H 3.450103 -1.155494 0.877252
H 3.450058 -1.155475 -0.877315
H 5.600272 -0.213862 -0.000077
H 4.701555 1.028383 -0.883194
H 4.701600 1.028364 0.883113

CA+
E = -425.306525
C -2.058960 0.323445 -0.175422
C -0.870302 -0.586400 0.210336
C 0.413321 0.200383 -0.198554
C 1.584303 -0.709556 0.205740
C 2.933630 -0.005983 -0.012688
O 3.872189 -0.654240 -0.400644
O 2.956142 1.274588 0.291833
H -2.054803 0.530008 -1.245676
C -3.352385 -0.459500 0.216326
H -2.018325 1.268080 0.366703
H -0.872139 -0.781874 1.282518
H -0.918687 -1.535359 -0.323333
H 0.409987 0.382258 -1.272490
H 0.458919 1.152250 0.325798
H 1.566830 -0.952544 1.273422
H 1.590953 -1.638310 -0.360370
H 3.849968 1.644879 0.171504
C -4.542470 0.431031 -0.170840
H -3.381414 -1.408654 -0.319072
H -3.346412 -0.663736 1.287144
H -5.449842 -0.125412 0.104789
H -4.535338 1.376035 0.372805
H -4.569174 0.629080 -1.242643

CA+, h-trans
E = -425.327737
C 3.112466 0.159021 -0.664294
C 2.036737 -0.156115 0.377718
C 0.675363 -0.358405 -0.285289
C -0.411860 -0.670670 0.822275
C -1.692197 -0.891458 0.161858
C -2.646641 0.125387 -0.043421

O -3.790915 -0.043137 -0.653104
O -2.412646 1.324599 0.395805
H 2.310852 -1.058852 0.931563
H 1.974005 0.660891 1.102646
H 0.377571 0.540388 -0.829374
H 0.714523 -1.187440 -0.994890
H -0.091475 -1.572919 1.345355
H -0.443763 0.171548 1.512704
H -1.919442 -1.858996 -0.272450
H -3.142218 1.943384 0.209146
H -3.937750 -0.950555 -0.966303
C 4.478958 0.362192 -0.009003
H 3.164486 -0.658855 -1.389185
H 2.827605 1.058655 -1.218267
H 5.236312 0.585719 -0.762865
H 4.450891 1.191842 0.701619
H 4.789943 -0.536208 0.529629

C5H10
E = -196.494408
C -2.517885 -0.272313 -0.053299
C -1.163203 0.339991 -0.238161
C -0.064186 -0.032430 0.408071
C 1.296164 0.565592 0.214323
H -0.130483 -0.848573 1.126597
H -1.090554 1.152199 -0.959180
H -2.896668 -0.685594 -0.994455
H -2.487798 -1.075610 0.686655
H -3.247205 0.474326 0.279383
C 2.321854 -0.467841 -0.269241
H 1.232603 1.391228 -0.500702
H 1.647311 0.990688 1.162272
H 3.313868 -0.020138 -0.369264
H 2.395068 -1.299476 0.437278
H 2.027403 -0.877043 -1.238743

C4H9
E = -157.748591
C -1.976403 -0.043051 0.049768
C -0.575981 0.449235 -0.029848
C 0.563134 -0.506405 -0.068561
C 1.930943 0.165760 0.060522
H 0.533668 -1.084999 -1.008499
H -0.388124 1.492090 -0.260497
H -2.292688 -0.526621 -0.889724
H -2.084713 -0.804072 0.832716
H -2.684544 0.763257 0.252810
H 2.739724 -0.566729 0.008827
H 2.078783 0.891842 -0.743661
H 2.010716 0.698166 1.011701
H 0.437021 -1.256170 0.725050

CAA+.H2O
E = -851.004865
C -5.155725 -1.366461 -0.268848
C -3.652268 -1.132946 -0.142111
C -3.115559 -0.336592 -1.382305
C -1.668922 -0.160580 -1.256523
C -1.068102 0.999012 -0.713193
O -1.797082 1.971494 -0.320595
O 0.258287 1.022345 -0.693826
C 1.044325 1.625428 0.368825
C 2.484133 1.510480 0.026923
C 2.996089 0.072190 0.270505
C 4.487829 -0.035606 -0.032540
C 5.024046 -1.444985 0.201706
O 0.511798 2.039798 1.342749
O -0.848729 4.208997 0.344212
H -5.360716 -1.923167 -1.188862
C -5.712461 -2.133102 0.930216
H -5.668077 -0.403198 -0.359273
H -3.127265 -2.088640 -0.070436
H -3.635115 0.620332 -1.429719
H -0.991235 -0.963357 -1.518640
H 2.630565 1.776520 -1.021932
H 3.025825 2.212026 0.661235
H 2.808363 -0.204152 1.311658
H 2.437970 -0.623185 -0.361501
H 4.669374 0.257554 -1.072227
H 5.037691 0.673330 0.595286
C 6.517098 -1.565081 -0.094971
H 4.836482 -1.737036 1.241108
H 4.471734 -2.153561 -0.426247
H -1.345930 2.848969 -0.004763
H -3.432821 -0.565121 0.765285
H -3.344559 -0.923913 -2.274477
H -0.440746 4.259390 1.218722
H -1.415346 4.982195 0.230924
C 7.044395 -2.978119 0.141860
H 6.700874 -1.269412 -1.133228
H 7.064618 -0.854705 0.533133
H 8.112282 -3.044589 -0.074959
H 6.891285 -3.280079 1.181626
H 6.524619 -3.698330 -0.496164
C -7.216986 -2.368550 0.805731
H -5.192225 -3.092194 1.017332
H -5.498404 -1.573831 1.846638
H -7.599424 -2.916777 1.668744
H -7.754966 -1.419135 0.741316
H -7.446394 -2.947532 -0.092543

(CA)2+
E = -851.000577
C 8.124695 0.218122 0.045520
C 6.712970 -0.368330 -0.150701
C 5.652557 0.692455 0.177849
C 4.245593 0.092671 -0.014146
C 3.205910 1.161810 0.343933
C 1.792949 0.602077 0.241849
O 1.553819 -0.422467 1.009887
O 0.977647 1.117463 -0.512039
O -0.977627 -1.117381 0.511957
C -1.792946 -0.601969 -0.241894
C -3.205889 -1.161738 -0.344023
C -4.245599 -0.092658 0.014151
C -5.652547 -0.692467 -0.177872
C -6.712989 0.368259 0.150779
C -8.124699 -0.218218 -0.045470
O -1.553811 0.422561 -1.009950
H 6.593308 -0.706038 -1.183376
H 6.584387 -1.239074 0.497278
H 5.771209 1.030434 1.210260
H 5.780149 1.561280 -0.472123
H 4.124443 -0.224266 -1.052084
H 4.116169 -0.780449 0.625800
H 3.329928 1.488182 1.381170
H 3.279599 2.026180 -0.312513
H 0.613708 -0.731124 0.881988
H -0.613699 0.731216 -0.882057
H -3.279550 -2.026163 0.312355
H -3.329907 -1.488029 -1.381285
H -4.124445 0.224201 1.052113

H -4.116209 0.780516 -0.625729
H -5.771204 -1.030366 -1.210309
H -5.780104 -1.561348 0.472030
H -6.593321 0.705886 1.183480
H -6.584440 1.239060 -0.497131
C -9.180798 0.840569 0.282368
H -8.235361 -0.558338 -1.077933
H -8.245151 -1.090672 0.601305
C 9.180767 -0.840723 -0.282215
H 8.245182 1.090519 -0.601326
H 8.235352 0.558324 1.077956
H 10.178492 -0.411319 -0.139609
H 9.085863 -1.709932 0.371924
H 9.096564 -1.175486 -1.318170
H -10.178512 0.411147 0.139740
H -9.096590 1.175248 1.318349
H -9.085928 1.709835 -0.371700

C5H11
E = -236.355962
C 1.786222 0.375145 -0.303283
C 0.439789 -0.069188 0.260911
C -0.716983 0.860135 -0.164737
C -2.044308 0.423676 0.347210
C -2.700849 -0.791126 -0.206019
H 1.993795 1.398009 0.029298
C 2.929661 -0.546563 0.115914
H 1.721003 0.411687 -1.396139
H 0.222985 -1.089077 -0.073657
H 0.492426 -0.101987 1.354469
H -0.488289 1.875380 0.174241
H -0.733906 0.883243 -1.263284
H -2.420136 0.849530 1.270350
H -3.762849 -0.834930 0.047810
H -2.602322 -0.827925 -1.297572
H -2.241776 -1.718044 0.175745
H 3.885357 -0.213984 -0.296916
H 3.023459 -0.575762 1.205360
H 2.749064 -1.568612 -0.229687

CAH+
E = -425.962886
C 3.468737 -0.497078 0.000000
C 2.170563 0.307125 0.000000
C 0.931779 -0.583366 -0.000000
C -0.365148 0.227571 -0.000000
C -1.593328 -0.682900 -0.000000
C -2.891605 0.024944 -0.000000
O -3.013508 1.302709 -0.000000
O -3.968982 -0.664411 0.000000
H 2.148628 0.961024 0.879164
H 2.148628 0.961025 -0.879164
H 0.945886 -1.235304 -0.879423
H 0.945886 -1.235304 0.879422
H -0.376989 0.870825 0.888471
H -0.376989 0.870825 -0.888471
H -1.605496 -1.351288 -0.870092
H -1.605496 -1.351288 0.870091
H -4.786268 -0.127011 0.000000
H -2.150571 1.761392 -0.000000
C 4.703856 0.399922 0.000000
H 3.484362 -1.151075 0.877916
H 3.484362 -1.151075 -0.877916
H 5.620450 -0.192263 0.000000
H 4.717204 1.042913 -0.884141
H 4.717204 1.042913 0.884141

C5H11+
E = -236.100799
C 2.590760 0.552631 -0.016096
C 1.303268 -0.076060 -0.555858
C 0.445860 -0.550002 0.760599
C -0.662745 -1.056000 0.042407
C -1.859421 -0.318673 -0.311424
H 3.171802 -0.169946 0.556896
H 3.183784 0.878214 -0.874399
H 2.375440 1.418658 0.609801
H 0.725377 0.648464 -1.128021
H 1.523688 -0.939643 -1.182381
H 1.055189 -1.295661 1.265430
H 0.253335 0.338135 1.355611
H -0.584906 -2.067835 -0.352163
H -2.048441 -0.469177 -1.386009
H -2.658639 -0.953314 0.129700
C -1.976944 1.132740 0.129797
H -2.939026 1.535123 -0.184167
H -1.909194 1.225420 1.214830
H -1.193078 1.743745 -0.321685

[CA-OH]+
E = -349.482804
C 2.931206 0.443448 -0.000020
C 1.626739 -0.354535 0.000017
C 0.399938 0.557022 0.000025
C -0.887013 -0.265577 0.000051
C -2.110966 0.723622 0.000005
C -3.330119 -0.006152 -0.000067
O -4.243082 -0.649934 -0.000006
H 1.597791 -1.005948 -0.879691
H 1.597822 -1.005918 0.879749
H 0.420770 1.205571 0.881705
H 0.420746 1.205550 -0.881671
H -0.944321 -0.899281 -0.886280
H -0.944308 -0.899239 0.886414
H -2.114205 1.364112 0.892025
H -2.114151 1.364122 -0.892004
C 4.156302 -0.467623 -0.000022
H 2.951806 1.095959 -0.878670
H 2.951835 1.095995 0.878602
H 5.077491 0.117208 -0.000049
H 4.163445 -1.109926 0.884363
H 4.163415 -1.109962 -0.884381

CA.2H2O
E = -578.568162
C -3.292724 0.085172 -0.422681
C -2.227905 -0.190825 0.634339
C -0.808827 -0.030559 0.098723
C 0.248360 -0.318727 1.175948
C 1.636669 -0.161550 0.613998
O 2.295789 -1.109382 0.216010
O 2.028888 1.099462 0.561630
O 4.400603 1.480249 -0.560121
O 4.792575 -1.144935 -0.880734
H -3.145720 -0.593280 -1.271116
C -4.715829 -0.071314 0.106636
H -3.161387 1.101109 -0.812890
H -2.373545 0.487837 1.482526
H -2.357070 -1.207306 1.023196
H -0.656953 -0.711309 -0.744707
H -0.669179 0.986470 -0.278000
H 0.112981 0.375099 2.008544

H 0.140265 -1.341574 1.537899
H 2.933928 1.208865 0.137778
H 5.064596 1.873900 0.014274
H 4.718462 0.570522 -0.781431
H 3.899282 -1.259948 -0.483265
H 4.764088 -1.569304 -1.743393
C -5.772155 0.207226 -0.960546
H -4.842870 -1.086879 0.496974
H -4.858795 0.606994 0.954762
H -6.783726 0.090572 -0.564235
H -5.674383 1.226862 -1.344380
H -5.658348 -0.478327 -1.805315

CA+.2H2O
E = -578.270888
C -3.257507 -0.047388 -0.312381
C -1.922265 -0.507099 0.267266
C -0.957683 -0.973851 -0.873009
C 0.302856 -1.450910 -0.297858
C 1.463437 -0.643601 -0.174967
O 1.450180 0.559173 -0.627843
O 2.501271 -1.185494 0.400564
O 3.428924 2.076928 -0.207359
O 4.946492 -0.069688 0.627330
H -3.712552 -0.870790 -0.872432
C -4.219721 0.425267 0.776293
H -3.084605 0.764157 -1.026856
H -1.450699 0.309730 0.819673
H -2.080004 -1.330839 0.968001
H -1.450817 -1.788306 -1.409184
H -0.795981 -0.138285 -1.554328
H 0.374175 -2.441369 0.133776
H 2.283637 1.139947 -0.472202
H 3.338120 -0.650458 0.442782
H 4.300880 1.678911 -0.063315
H 3.528230 2.918050 -0.667402
H 5.610977 -0.588065 0.153489
H 5.238739 -0.031679 1.548415
C -5.556498 0.884653 0.196707
H -4.384218 -0.388919 1.489245
H -3.756322 1.244470 1.335655
H -6.231996 1.219031 0.986353
H -5.413108 1.714206 -0.500745
H -6.045093 0.070426 -0.344769

CAH+.2H2O
E = -578.909155
C 3.750223 0.242257 0.024880
C 2.483930 -0.607018 -0.017539
C 1.210956 0.239081 -0.015574
C -0.044539 -0.630289 -0.057220
C -1.348007 0.099909 -0.060407
O -1.396927 1.408749 -0.023157
O -2.423214 -0.521037 -0.101494
O -4.513864 0.668066 0.062520
O -6.735633 -0.660976 0.086311
H 3.734612 0.873889 0.920479
C 5.024103 -0.599373 0.022773
H 3.762379 0.920341 -0.836155
H 2.493443 -1.237111 -0.913014
H 2.465588 -1.283167 0.843525
H 1.207050 0.861591 0.887729
H 1.233966 0.907739 -0.884839
H -0.051655 -1.273339 -0.943479
H -0.080153 -1.314637 0.796939
H -3.422575 0.086703 -0.055211
H -0.508922 1.802735 0.012087
H -5.361551 0.126871 0.056156
H -4.641209 1.482888 -0.438213
H -7.023714 -1.344908 -0.528109
H -7.288926 -0.722569 0.873050
C 6.286036 0.258643 0.065599
H 5.006551 -1.276983 0.882713
H 5.034410 -1.230455 -0.871993
H 7.185357 -0.359894 0.063421
H 6.332150 0.924821 -0.800273
H 6.304109 0.877813 0.966679

(CA)2
E = -851.331259
C -6.799435 0.370618 -0.000301
C -5.701969 -0.688612 -0.000070
C -4.299872 -0.087498 0.000032
C -3.220103 -1.161166 0.000256
C -1.811510 -0.626033 0.000329
O -0.898888 -1.576937 0.000772
O -1.549435 0.569930 0.000283
O 1.549436 -0.569941 0.000389
C 1.811509 0.626022 0.000466
C 3.220100 1.161160 0.000309
C 4.299873 0.087496 0.000017
C 5.701968 0.688616 -0.000140
C 6.799439 -0.370609 -0.000436
O 0.898879 1.576918 0.000792
H -6.679032 1.016526 -0.877753
C -8.205801 -0.222648 -0.000405
H -6.679234 1.016700 0.877050
H -5.823108 -1.334606 0.877534
H -5.822905 -1.334779 -0.877574
H -4.171438 0.556422 -0.873978
H -4.171640 0.556594 0.873946
H -3.318260 -1.817177 0.871434
H -3.318060 -1.817343 -0.870817
H 0.026731 -1.186843 0.001001
H -0.026731 1.186797 0.000887
H 3.318015 1.817352 -0.870758
H 3.318294 1.817157 0.871492
H 4.171683 -0.556608 0.873927
H 4.171403 -0.556412 -0.873997
H 5.822862 1.334797 -0.877640
H 5.823143 1.334598 0.877468
C 8.205802 0.222664 -0.000593
H 6.679280 -1.016705 0.876912
H 6.679000 -1.016505 -0.877892
C 9.293619 -0.849379 -0.000889
H 8.322115 0.868062 -0.878018
H 8.322396 0.867861 0.876943
C -9.293612 0.849400 -0.000636
H -8.322156 -0.868033 -0.877835
H -8.322358 -0.867859 0.877127
H 10.292924 -0.407499 -0.000998
H 9.205974 -1.488838 0.882246
H 9.205693 -1.488635 -0.884143
H -10.292920 0.407524 -0.000706
H -9.205925 1.488845 0.882505
H -9.205723 1.488668 -0.883884

CA, S=3
E = -425.498874
C 2.166464 0.287446 -0.150157
C 0.904767 -0.518585 0.141682
C -0.374769 0.229787 -0.217111

C -1.626110 -0.596735 0.079352
C -2.900504 0.114726 -0.263788
O -3.107196 1.310772 0.320937
O -4.046090 -0.652479 -0.060330
H 2.129563 1.231660 0.405671
C 3.449761 -0.457476 0.207228
H 2.187840 0.555627 -1.212944
H 0.940535 -1.462421 -0.415098
H 0.883260 -0.786701 1.204139
H -0.415448 1.169136 0.343764
H -0.359923 0.497144 -1.278180
H -1.613556 -1.527990 -0.493769
H -1.648784 -0.865745 1.146886
H -4.801582 -0.192921 -0.451094
C 4.704861 0.360418 -0.089328
H 3.424530 -0.724573 1.269269
H 3.482825 -1.400728 -0.348798
H 5.612939 -0.188090 0.172451
H 4.757933 0.615671 -1.151720
H 4.699333 1.296101 0.477301

CA, h-trans, S=3
E = -425.517758
C 3.535482 -0.948377 0.524257
C 2.448788 -0.414055 -0.405050
C 1.562679 0.632260 0.278954
C 0.541048 1.231128 -0.623096
C -0.746516 1.781843 -0.101508
C -1.617875 0.769011 0.669524
C -2.065997 -0.384654 -0.174350
O -3.059298 -1.123503 0.407202
O -1.095691 -1.200191 -0.724459
H -0.390378 -0.625082 -1.071616
H 1.079164 0.182205 1.151781
H 0.857590 1.507263 -1.624192
H -0.531254 2.612402 0.589877
H -1.333087 2.198748 -0.923046
H -1.063868 0.389093 1.542461
H -2.506500 1.274082 1.051026
H -3.190825 -1.922328 -0.119277
H 2.903781 0.030528 -1.296262
H 2.214741 1.428900 0.677780
H 4.154006 -1.697524 0.024817
H 4.188597 -0.138567 0.862074
H 1.820323 -1.241293 -0.749765
H 3.091959 -1.411808 1.410009

CAA+
E = -774.540009
C -6.785223 -2.967968 -0.146765
C -6.311913 -1.572229 0.251463
C -4.875468 -1.299372 -0.189896
C -4.394998 0.094301 0.205025
C -2.960512 0.356047 -0.246476
C -2.507606 1.780491 0.164421
C -1.133289 2.038478 -0.311458
O -0.757223 2.641974 -1.275156
O -0.177877 1.379012 0.537184
C 1.130601 1.410013 0.304941
O 1.637839 2.024217 -0.711779
C 1.959285 0.742368 1.227725
C 3.408891 0.658110 1.081066
C 3.766693 -0.687718 0.342533
C 5.282231 -0.822322 0.210311
C 5.665952 -2.113490 -0.513740
C 7.182022 -2.253858 -0.648001
H 5.737098 -0.807964 1.205517
H 5.679405 0.038630 -0.336141
H 3.357868 -1.529098 0.906482
H 3.810328 1.485276 0.496009
H 1.448684 0.219908 2.027299
H -2.542507 1.873694 1.251695
H -3.156851 2.528133 -0.290636
H -2.888505 0.256841 -1.332866
H -2.289850 -0.382821 0.200019
H -4.460874 0.211494 1.291937
H -5.056083 0.847923 -0.234914
H -4.802162 -1.414800 -1.277049
H -4.211625 -2.052252 0.250331
H 0.907406 2.448326 -1.246394
H 3.298101 -0.685096 -0.644251
H 3.886475 0.629252 2.062118
H -6.381941 -1.452036 1.337614
H -6.970765 -0.817035 -0.189320
H -7.812895 -3.144524 0.176246
H -6.745409 -3.096293 -1.231904
H -6.152155 -3.736516 0.305371
H 5.260013 -2.969145 0.034674
H 5.202399 -2.123136 -1.505189
H 7.441076 -3.179108 -1.166129
H 7.601386 -1.418463 -1.214322
H 7.659476 -2.269925 0.334922

[CA-OH]
E = -349.727283
C 2.896265 0.420790 -0.000000
C 1.561677 -0.319935 -0.000000
C 0.357612 0.617826 0.000000
C -0.972332 -0.129759 0.000000
C -2.165558 0.828289 0.000001
C -3.518042 0.147657 0.000001
O -3.757613 -1.007301 0.000000
H 1.510480 -0.974725 -0.877485
H 1.510481 -0.974727 0.877484
H 0.408999 1.272338 0.877911
H 0.408999 1.272339 -0.877910
H -1.034539 -0.781246 -0.875919
H -1.034538 -0.781247 0.875919
H -2.148683 1.490886 0.871881
H -2.148684 1.490887 -0.871878
C 4.092839 -0.528052 -0.000001
H 2.942678 1.074977 -0.877355
H 2.942678 1.074976 0.877356
H 5.038563 0.019178 -0.000000
H 4.074853 -1.173063 0.883214
H 4.074853 -1.173062 -0.883217

n = 8, B3LYP+D2/def2TZVP

CA
E = -464.955657
C 4.064322 0.542618 -0.000031
C 2.834669 -0.361745 0.000006
C 1.520342 0.412483 0.000057
C 0.292104 -0.492401 0.000093
C -1.017744 0.289253 0.000145
C -2.231359 -0.630658 0.000188
C -3.546260 0.106233 0.000268
O -4.593866 -0.756093 -0.000327

O -3.692783 1.300442 -0.000151
H 1.485694 1.068530 0.877333
H 1.485633 1.068542 -0.877207
H 0.326726 -1.148816 -0.877471
H 0.326787 -1.148827 0.877647
H -1.060506 0.944653 0.874012
H -1.060569 0.944662 -0.873714
H -2.222740 -1.293021 -0.871673
H -2.222687 -1.293021 0.872046
H -5.404541 -0.223416 -0.000676
H 2.869145 -1.018204 0.877556
H 2.869084 -1.018192 -0.877556
C 5.372649 -0.245124 -0.000082
H 4.026561 1.197536 -0.877221
H 4.026623 1.197524 0.877170
H 6.241172 0.418011 -0.000108
H 5.437266 -0.887359 0.883130
H 5.437204 -0.887346 -0.883308

CA+
E = -464.615317
C -1.459503 0.400063 -0.211721
C -0.286924 -0.535180 0.182727
C 1.018916 0.217403 -0.195033
C 2.172532 -0.713676 0.207982
C 3.536796 -0.046472 0.000861
O 4.468655 -0.696123 -0.399326
O 3.584653 1.232082 0.331012
H -1.428754 0.614772 -1.279825
C -2.754813 -0.361240 0.154231
H -1.400455 1.338895 0.338438
H -0.311598 -0.741221 1.252957
H -0.351391 -1.479394 -0.358262
H 1.035528 0.415701 -1.266474
H 1.079586 1.163072 0.339784
H 2.136979 -0.962521 1.273869
H 2.162752 -1.640506 -0.361538
H 4.487111 1.580565 0.215070
C -3.945305 0.562543 -0.246000
H -2.815594 -1.303769 -0.390441
H -2.790233 -0.571909 1.223380
C -5.239484 -0.181934 0.109304
H -3.873285 1.504939 0.297906
H -3.897836 0.776367 -1.314228
H -6.074730 0.472802 -0.174430
H -5.330979 -1.118297 -0.442234
H -5.306855 -0.386211 1.178428

CA+, h-trans
E = -464.632575
C 3.906904 0.009318 0.376790
C 2.568870 0.114894 -0.360425
C 1.420535 -0.469126 0.463288
C 0.097395 -0.355204 -0.292419
C -1.069725 -0.959725 0.591706
C -2.311682 -0.869080 -0.165160
C -3.205656 0.214220 -0.062888
O -2.950972 1.183693 0.763508
O -4.314848 0.329122 -0.746881
H 1.622428 -1.520137 0.689037
H 1.343857 0.058233 1.418514
H -0.130082 0.690189 -0.510817
H 0.149135 -0.896850 -1.239044
H -0.817999 -2.002052 0.791948
H -1.112531 -0.398381 1.524462
H -2.549868 -1.620866 -0.909669
H -3.641233 1.871585 0.760042
H -4.478856 -0.412118 -1.352251
H 2.638936 -0.410829 -1.318268
H 2.361579 1.165678 -0.588243
C 5.054129 0.591646 -0.446117
H 3.830307 0.532866 1.334741
H 4.107180 -1.041785 0.606083
H 6.000083 0.508391 0.093030
H 5.158773 0.063274 -1.397260
H 4.880243 1.648626 -0.663966

C6H12
E = -235.798600
C 3.171436 0.219244 -0.158551
C 1.793625 -0.365418 -0.221713
C 0.739697 0.094069 0.443423
C -0.643025 -0.476023 0.368613
C -1.672065 0.527240 -0.167526
H 0.865033 0.966169 1.083852
H 1.662664 -1.234200 -0.864276
H 3.512128 0.536551 -1.150161
H 3.200195 1.084979 0.507350
H 3.897243 -0.517102 0.203533
H -0.640249 -1.368757 -0.265489
H -0.966788 -0.796594 1.367339
C -3.084600 -0.052273 -0.192691
H -1.651500 1.428321 0.454600
H -1.374799 0.836363 -1.174203
H -3.807620 0.671666 -0.576255
H -3.126641 -0.941695 -0.828197
H -3.400075 -0.346727 0.812578

C5H11
E = -197.052633
C 2.600507 -0.228732 -0.049123
C 1.286166 0.461131 0.031488
C 0.020410 -0.317766 0.066424
C -1.241476 0.535743 -0.065885
H -0.043548 -0.895421 1.006414
H 1.251506 1.519947 0.262799
H 2.842877 -0.755491 0.889125
H 2.597785 -0.995523 -0.833940
H 3.418312 0.466784 -0.249970
C -2.518874 -0.297722 -0.001753
H -1.247330 1.285813 0.731869
H -1.202167 1.085672 -1.011283
H 0.032974 -1.079250 -0.727275
H -3.410205 0.326889 -0.097789
H -2.537713 -1.039624 -0.805522
H -2.582889 -0.835723 0.948670

CAA+.H2O
E = -929.613570
C 6.995728 -2.664582 0.133675
C 6.466030 -1.240345 -0.012140
C 4.962746 -1.137759 0.229636
C 4.437965 0.287733 0.082736
C 2.934746 0.377396 0.329704
C 2.433724 1.831983 0.176738
C 0.980231 1.923359 0.463588
O 0.405995 2.259590 1.444112
O 0.242173 1.410003 -0.676604
C -1.082517 1.386440 -0.753112
O -1.831366 2.323656 -0.314130
C -1.654440 0.274145 -1.412744
C -3.093229 0.106678 -1.613321

C -3.675725 -0.790158 -0.464848
C -5.171142 -1.017106 -0.673587
C -5.770236 -1.881248 0.433851
C -7.267430 -2.120390 0.239386
O -0.918204 4.501735 0.565812
H -5.333274 -1.496795 -1.643970
H -5.685214 -0.051257 -0.706080
H -3.147891 -1.746797 -0.449492
H -3.616019 1.062913 -1.603727
H -0.962719 -0.504210 -1.709480
H 2.625881 2.178278 -0.840807
H 2.946933 2.480238 0.886888
H 2.702724 0.022031 1.337426
H 2.403839 -0.265031 -0.377372
H 4.663784 0.659739 -0.922467
H 4.961020 0.943834 0.786315
H 4.730618 -1.507989 1.234422
H 4.436560 -1.792940 -0.473960
H -1.396714 3.172777 0.088876
H -3.497744 -0.297445 0.493989
H -3.282483 -0.406815 -2.558714
H -0.545605 4.481151 1.457142
H -1.482570 5.281385 0.492954
H 6.698443 -0.868109 -1.016505
H 6.991690 -0.584479 0.691130
C 8.500335 -2.754898 -0.109706
H 6.759996 -3.032975 1.137772
H 6.466813 -3.317038 -0.569404
H -5.250255 -2.844889 0.466734
H -5.602724 -1.400632 1.404075
C -7.861283 -2.986026 1.348198
H -7.782714 -1.154999 0.204505
H -7.430181 -2.597487 -0.732396
H -8.930043 -3.146783 1.193370
H -7.373404 -3.963961 1.380637
H -7.728346 -2.511989 2.324531
H 8.860689 -3.779942 -0.001250
H 8.751098 -2.413173 -1.117828
H 9.046011 -2.127827 0.600840

(CA)2+
E = -929.612982
C 9.174156 0.804619 -0.262558
C 8.102178 -0.255341 0.063133
C 6.699055 0.333903 -0.136544
C 5.637041 -0.730278 0.187771
C 4.230351 -0.135833 -0.006243
C 3.187431 -1.205751 0.340860
C 1.777191 -0.646620 0.228388
O 1.527618 0.355125 1.026025
O 0.973345 -1.132866 -0.556250
O -0.973361 1.132959 0.556402
C -1.777187 0.646750 -0.228281
O -1.527623 -0.355021 -1.025887
C -3.187448 1.205841 -0.340705
C -4.230349 0.135853 0.006240
C -5.637050 0.730288 -0.187726
C -6.699043 -0.333962 0.136433
C -8.102177 0.255273 -0.063196
C -9.174136 -0.804755 0.262337
H -6.579082 -0.672337 1.168587
H -6.564419 -1.202178 -0.513210
H -5.754950 1.070062 -1.219667
H -5.769769 1.597654 0.463268
H -4.111437 -0.187383 1.042699
H -4.096711 -0.734048 -0.637559
H -3.310282 1.536074 -1.376477
H -3.266578 2.066707 0.319949
H -0.589531 -0.676063 -0.895010
H 0.589523 0.676161 0.895157
H 3.266519 -2.066696 -0.319696
H 3.310286 -1.535861 1.376668
H 4.111425 0.187274 -1.042740
H 4.096748 0.734152 0.637449
H 5.754953 -1.069924 1.219753
H 5.769725 -1.597730 -0.463115
H 6.579082 0.672149 -1.168739
H 6.564465 1.202205 0.512989
H 8.223626 -0.592780 1.095722
H 8.237604 -1.125465 -0.584499
H -8.237638 1.125311 0.584546
H -8.223614 0.592843 -1.095744
C -10.572469 -0.215639 0.064513
H -9.030520 -1.672611 -0.385977
H -9.044614 -1.142167 1.293609
C 10.572478 0.215494 -0.064684
H 9.044623 1.141901 -1.293871
H 9.030574 1.672562 0.385646
H -11.323989 -0.977405 0.299200
H -10.737151 0.640914 0.721646
H -10.723067 0.106705 -0.967974
H 11.324013 0.977210 -0.299484
H 10.723088 -0.106721 0.967841
H 10.737127 -0.641148 -0.721710

C6H13
E = -275.660100
C -2.513376 0.529749 0.061568
C -1.295283 -0.382191 -0.091851
C -0.000024 0.343569 -0.158457
C 1.295682 -0.381868 -0.097630
C 2.512821 0.529323 0.068042
C 3.825010 -0.250262 0.099984
H 2.401067 1.109245 0.989407
H 2.529795 1.251123 -0.755244
H 1.434793 -0.988528 -1.010740
H 1.271642 -1.114207 0.722318
H -0.000679 1.389734 -0.448659
H -1.432049 -0.999536 -0.998079
H -1.272218 -1.105266 0.736418
C -3.824865 -0.250541 0.101757
H -2.403014 1.120863 0.975964
H -2.530235 1.241519 -0.770374
H 4.683700 0.415005 0.218085
H 3.832175 -0.962201 0.930602
H 3.960841 -0.817860 -0.825349
H -4.684257 0.415207 0.211704
H -3.959589 -0.828902 -0.817049
H -3.831763 -0.952876 0.940516

CAH+
E = -465.267261
C 4.088795 0.551011 0.000000
C 2.868928 -0.367076 0.000000
C 1.550745 0.402110 0.000000
C 0.336032 -0.520984 -0.000000
C -0.982085 0.255118 -0.000000
C -2.185459 -0.687766 -0.000000
C -3.502026 -0.014806 -0.000000
O -4.560850 -0.732428 0.000000
O -3.657647 1.259308 -0.000000
H 1.510914 1.055026 0.879120

H 1.510914 1.055026 -0.879120
H 0.367424 -1.172342 -0.879402
H 0.367424 -1.172342 0.879401
H -1.011028 0.897837 0.888485
H -1.011028 0.897837 -0.888485
H -2.179795 -1.356286 -0.870072
H -2.179795 -1.356286 0.870072
H -5.391971 -0.216713 0.000000
H -2.806978 1.740429 -0.000000
H 2.907021 -1.021355 0.878159
H 2.907021 -1.021355 -0.878159
C 5.401679 -0.227947 0.000000
H 4.045130 1.204316 -0.877818
H 4.045130 1.204316 0.877818
H 6.261551 0.444540 0.000000
H 5.473190 -0.867822 0.883736
H 5.473190 -0.867822 -0.883736

C6H13+
E = -275.406502
C -2.937126 -0.984837 -0.007973
C -1.803998 -0.122051 -0.569510
C -1.125342 0.629382 0.719900
C -0.127867 1.318009 -0.010766
C 1.214754 0.844216 -0.272992
C 1.646806 -0.506949 0.283779
H -3.686790 -0.372786 0.493567
H -3.409366 -1.499097 -0.848692
H -2.556615 -1.730842 0.689811
H -1.056577 -0.736785 -1.069147
H -2.188386 0.620505 -1.267938
H -1.904437 1.255150 1.148590
H -0.762847 -0.144688 1.389963
H -0.414835 2.253073 -0.489580
H 1.415555 0.950730 -1.351755
H 1.840636 1.669584 0.132717
C 3.100322 -0.811196 -0.073860
H 1.519307 -0.509848 1.369291
H 0.992112 -1.285647 -0.117780
H 3.397474 -1.780257 0.326788
H 3.239461 -0.834981 -1.157345
H 3.770025 -0.053560 0.340046

[CA-OH]+
E = -388.787303
C 3.515242 -0.597003 -0.000013
C 2.304136 0.333336 -0.000008
C 0.981147 -0.431347 0.000061
C -0.222077 0.511169 0.000071
C -1.529316 -0.278762 0.000123
C -2.728034 0.741221 0.000029
C -3.964643 0.041758 -0.000172
O -4.892347 -0.580805 -0.000053
H 0.935203 -1.081647 -0.879611
H 0.935257 -1.081588 0.879778
H -0.184891 1.158973 0.881745
H -0.184938 1.158923 -0.881642
H -1.602648 -0.910787 -0.886224
H -1.602623 -0.910694 0.886542
H -2.714968 1.381468 0.892087
H -2.714833 1.381517 -0.891984
H 2.346396 0.986067 -0.878870
H 2.346451 0.986129 0.878806
C 4.833657 0.173018 -0.000080
H 3.465836 -1.249222 0.878061
H 3.465781 -1.249284 -0.878038
H 5.687160 -0.507221 -0.000083
H 4.910434 0.811702 -0.884111
H 4.910489 0.811765 0.883900

CA.2H2O
E = -617.872267
C -5.202021 0.194166 -0.861330
C -4.121755 -0.075431 0.182798
C -2.706264 0.079453 -0.364692
C -1.628458 -0.190723 0.680774
C -0.216160 -0.031942 0.127198
C 0.854278 -0.314134 1.192859
C 2.235516 -0.158425 0.613412
O 2.626046 1.102649 0.550581
O 2.890559 -1.107520 0.211694
O 4.983658 1.480239 -0.601765
O 5.373694 -1.146090 -0.915328
H -2.568484 -0.603066 -1.211201
H -2.579809 1.093444 -0.761070
H -1.764372 0.491849 1.527410
H -1.752108 -1.205395 1.076042
H -0.073976 -0.716598 -0.714766
H -0.081951 0.983390 -0.256044
H 0.728354 0.383485 2.023767
H 0.751493 -1.335358 1.560891
H 3.525801 1.210799 0.115353
H 5.654317 1.876907 -0.037276
H 5.299475 0.569750 -0.822855
H 4.485451 -1.259923 -0.506341
H 5.334857 -1.574359 -1.775652
H -4.248057 -1.089542 0.579913
H -4.259607 0.606960 1.029791
C -6.613453 0.035835 -0.300026
H -5.072434 1.207480 -1.256617
H -5.061029 -0.488441 -1.706344
H -7.372912 0.232485 -1.060683
H -6.767672 -0.979138 0.077751
H -6.779090 0.728244 0.530516

CA+.2H2O
E = -617.575306
C -2.684034 -0.398609 -0.523378
C -1.356759 -0.680019 0.176396
C -0.309977 -1.252425 -0.836907
C 0.942734 -1.556999 -0.140834
C 2.044829 -0.665255 -0.085706
O 1.985967 0.455613 -0.712301
O 3.079802 -1.047637 0.610814
O 3.848625 2.144066 -0.435021
O 5.438890 0.249016 0.783382
H -3.062667 -1.324652 -0.967752
C -3.724003 0.171974 0.437837
H -2.519717 0.304076 -1.346710
H -0.960395 0.239051 0.615528
H -1.504008 -1.396575 0.988315
H -0.729135 -2.167217 -1.262578
H -0.159776 -0.519871 -1.630211
H 1.048147 -2.467209 0.436012
H 2.774541 1.105954 -0.607435
H 3.879788 -0.457532 0.611627
H 4.732408 1.829241 -0.191518
H 3.925493 2.911862 -1.012556
H 6.158137 -0.288581 0.425010
H 5.675577 0.441183 1.701138
C -5.059732 0.456131 -0.247950
H -3.882415 -0.530841 1.263192

H -3.341168 1.097075 0.883214
C -6.095246 1.027065 0.717963
H -4.896332 1.155783 -1.074211
H -5.437491 -0.470141 -0.692836
H -7.042302 1.223566 0.211456
H -6.288381 0.328938 1.537014
H -5.743462 1.966248 1.153782

CAH+.2H2O
E = -618.213415
C 3.131128 0.367335 0.015491
C 1.883598 -0.509400 -0.026878
C 0.592460 0.308693 -0.019054
C -0.643973 -0.587536 -0.061053
C -1.962697 0.114482 -0.059258
O -2.039712 1.421628 -0.015955
O -3.024532 -0.529364 -0.101785
O -5.139658 0.615256 0.069916
O -7.334966 -0.759101 0.087120
H 3.103233 0.995279 0.913235
C 4.422186 -0.445850 0.007451
H 3.125682 1.048294 -0.843187
H 1.904710 -1.136089 -0.924524
H 1.882093 -1.188707 0.831871
H 0.577186 0.927721 0.886547
H 0.598955 0.980781 -0.885958
H -0.639048 -1.227824 -0.949323
H -0.663072 -1.275199 0.791000
H -4.034476 0.056192 -0.051810
H -1.160186 1.834261 0.019790
H -5.976068 0.057325 0.060901
H -5.284570 1.430863 -0.424669
H -7.610128 -1.444283 -0.531799
H -7.886036 -0.837313 0.873931
C 5.673810 0.427032 0.049978
H 4.426464 -1.127891 0.865287
H 4.449014 -1.074766 -0.889681
C 6.958968 -0.397116 0.041306
H 5.664530 1.108203 -0.807601
H 5.642128 1.054804 0.946868
H 7.842416 0.243634 0.072200
H 6.996289 -1.066194 0.905446
H 7.018947 -1.012295 -0.860781

(CA)2
E = -929.939494
C 9.307049 -0.799487 0.000104
C 8.203821 0.255231 0.000155
C 6.800919 -0.343936 -0.000039
C 5.699065 0.711031 0.000012
C 4.299431 0.104347 -0.000181
C 3.215397 1.173659 -0.000123
C 1.808877 0.633114 -0.000299
O 0.892555 1.580412 -0.000265
O 1.551420 -0.563880 -0.000520
O -0.892559 -1.580436 -0.000221
C -1.808881 -0.633136 -0.000148
O -1.551414 0.563855 -0.000421
C -3.215403 -1.173673 -0.000004
C -4.299430 -0.104355 -0.000008
C -5.699068 -0.711030 0.000157
C -6.800916 0.343944 0.000167
C -8.203822 -0.255215 0.000335
C -9.307043 0.799511 0.000346
H -6.682399 0.990079 -0.877193
H -6.682249 0.990219 0.877404
H -5.817507 -1.357558 0.877724
H -5.817654 -1.357697 -0.877287
H -4.173734 0.540115 -0.874030
H -4.173592 0.540259 0.873888
H -3.310798 -1.830117 0.871164
H -3.310951 -1.830266 -0.871046
H 0.031579 -1.186655 -0.000442
H -0.031589 1.186643 -0.000449
H 3.310935 1.830294 -0.871133
H 3.310795 1.830061 0.871076
H 4.173598 -0.540312 0.873682
H 4.173737 -0.540079 -0.874236
H 5.817643 1.357745 -0.877399
H 5.817502 1.357512 0.877613
H 6.682260 -0.990259 0.877163
H 6.682403 -0.990025 -0.877434
H 8.322186 0.901915 -0.877345
H 8.322043 0.901681 0.877847
H -8.322195 -0.901850 -0.877199
H -8.322044 -0.901710 0.877993
C 10.705729 -0.185952 0.000301
H 9.185687 -1.444200 0.877288
H 9.185831 -1.443965 -0.877272
C -10.705727 0.185985 0.000515
H -9.185673 1.444176 0.877564
H -9.185824 1.444036 -0.876996
H -11.481943 0.955082 0.000521
H -10.852181 -0.442738 -0.882635
H -10.852029 -0.442597 0.883792
H 11.481950 -0.955043 0.000262
H 10.852176 0.442820 -0.882817
H 10.852031 0.442585 0.883610

CA, S=3
E = -464.802976
C 4.083178 0.507546 -0.169530
C 2.845010 -0.336358 0.121231
C 1.538884 0.383935 -0.198568
C 0.302600 -0.460901 0.092929
C -1.000905 0.262793 -0.228083
C -2.226056 -0.602639 0.066677
C -3.523434 0.083822 -0.239405
O -4.645797 -0.717568 -0.038429
O -3.751062 1.259468 0.378146
H 1.486403 1.313180 0.380424
H 1.536084 0.677476 -1.254668
H 0.353326 -1.389997 -0.486979
H 0.304729 -0.754731 1.148756
H -1.056533 1.187004 0.356183
H -1.009486 0.555931 -1.282395
H -2.198972 -1.518903 -0.529608
H -2.225140 -0.898181 1.127412
H -5.418719 -0.268223 -0.406299
H 2.847812 -0.630037 1.177573
H 2.897473 -1.266203 -0.457418
C 5.382996 -0.225467 0.155387
H 4.077115 0.799803 -1.225221
H 4.027301 1.435887 0.409224
H 6.257807 0.393295 -0.058883
H 5.415971 -0.503625 1.212846
H 5.466070 -1.144261 -0.432518

CA, h-trans, S=3
E = -464.821304
C 3.089592 -1.389334 0.852283
C 3.344758 -0.279341 -0.167920

C 2.061472 0.273392 -0.789909
C 1.135976 0.954313 0.225305
C -0.051786 1.597505 -0.400349
C -1.337408 1.772409 0.340913
C -1.963519 0.464897 0.867930
C -2.334836 -0.492716 -0.222409
O -3.143105 -1.509439 0.206190
O -1.326293 -0.968890 -1.038088
H -0.753579 -0.215704 -1.268443
H 0.814134 0.230561 0.977853
H 0.109271 2.173867 -1.306162
H -1.166270 2.421478 1.214852
H -2.066036 2.282571 -0.292897
H -1.266921 -0.028038 1.564411
H -2.866582 0.699521 1.433392
H -3.216889 -2.158427 -0.505121
H 2.315274 0.994302 -1.573835
H 1.724095 1.713132 0.770964
H 3.892995 0.540550 0.309256
H 4.028523 -1.806889 1.223010
H 2.527027 -1.018263 1.711825
H 1.516895 -0.545255 -1.273563
H 3.986962 -0.663233 -0.965970
H 2.510783 -2.200288 0.400552

CAA+
E = -853.148864
C -6.746849 -2.621296 -0.137596
C -6.275204 -1.202216 0.169402
C -4.822371 -0.960039 -0.230888
C -4.357811 0.460194 0.079853
C -2.906232 0.692671 -0.331093
C -2.470639 2.144428 -0.006493
C -1.079037 2.373439 -0.445826
O -0.157133 1.777876 0.481590
C 1.160051 1.798935 0.299054
C 1.952821 1.199360 1.295873
C 3.406928 1.114152 1.210602
C 3.793789 -0.267270 0.554702
C 5.313690 -0.402217 0.485862
C 5.723338 -1.725117 -0.159925
C 7.243218 -1.880431 -0.237733
O -0.667377 2.910910 -1.434072
O 1.705042 2.346023 -0.736713
H 5.730722 -0.338106 1.495363
H 5.728774 0.432603 -0.086818
H 3.365683 -1.080152 1.145315
H 3.829236 1.910375 0.597911
H 1.412782 0.727418 2.107336
H -2.547885 2.315109 1.069163
H -3.102482 2.855166 -0.538623
H -2.790393 0.515149 -1.403650
H -2.254095 -0.009844 0.194494
H -4.467739 0.656569 1.151672
H -5.000442 1.177700 -0.440454
H -4.703844 -1.154625 -1.302531
H -4.177529 -1.676363 0.290721
H 0.994594 2.728798 -1.326501
H 3.362194 -0.315743 -0.447537
H 3.847630 1.137523 2.208600
H -6.394560 -1.004072 1.240706
H -6.918944 -0.485349 -0.352632
C -8.201411 -2.851295 0.265548
H -6.623958 -2.815494 -1.208385
H -6.100153 -3.334580 0.384643
H 5.301783 -2.558496 0.412160
H 5.300216 -1.787430 -1.168317
C 7.650278 -3.202704 -0.884052
H 7.659942 -1.043327 -0.806712
H 7.661785 -1.814185 0.771440
H -8.520728 -3.870483 0.038654
H -8.337651 -2.685020 1.337781
H -8.864303 -2.163167 -0.266217
H 8.736984 -3.297339 -0.931528
H 7.261335 -4.050371 -0.313641
H 7.259444 -3.274307 -1.902584

[CA-OH]
E = -389.031385
C 3.458079 -0.623297 -0.000001
C 2.271050 0.336419 -0.000000
C 0.923010 -0.377865 -0.000000
C -0.262371 0.583587 0.000000
C -1.606772 -0.137614 0.000000
C -2.780858 0.843740 0.000001
C -4.146540 0.190026 0.000001
O -4.408991 -0.959958 0.000000
H 0.858270 -1.031246 -0.877443
H 0.858270 -1.031247 0.877442
H -0.198058 1.236983 0.877873
H -0.198058 1.236984 -0.877871
H -1.681810 -0.787768 -0.875919
H -1.681810 -0.787769 0.875919
H -2.750926 1.505912 0.871862
H -2.750926 1.505913 -0.871860
H 2.335097 0.990421 -0.877611
H 2.335098 0.990420 0.877611
C 4.800776 0.104188 -0.000001
H 3.390562 -1.275701 0.877222
H 3.390562 -1.275699 -0.877225
H 5.637983 -0.598004 -0.000001
H 4.894716 0.742678 -0.883253
H 4.894716 0.742677 0.883252