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Stability of pyruvic acid clusters upon slow electron attachment

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ESI: Electronic Supplementary Information

I) Mass spectra

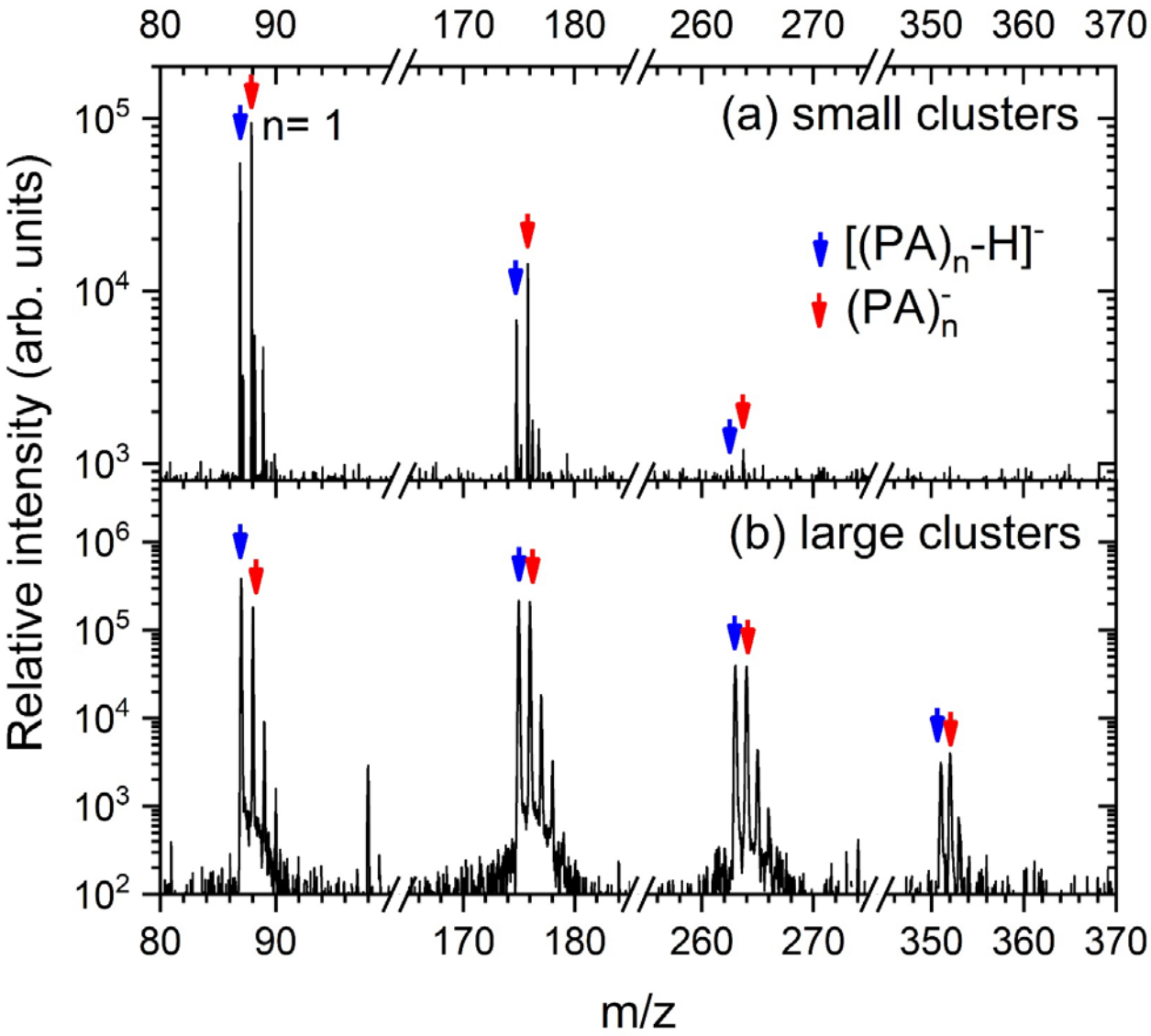

Figure S1: Detailed region around $(PA)_n^-$ clusters of the mass spectra shown in Fig. 1.

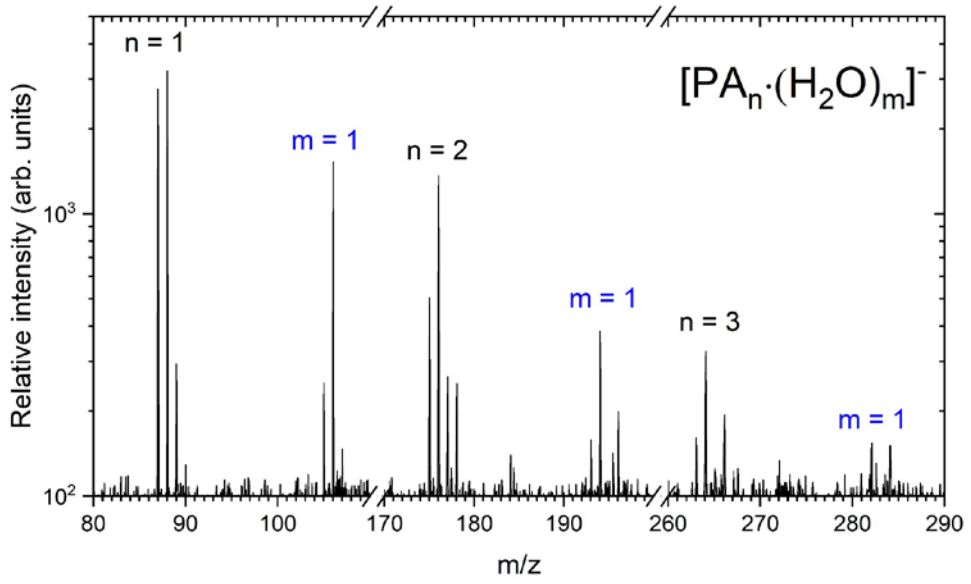

Figure S2: Detailed region around $[(PA)_n \cdot (H_2O)_m]^-$ clusters of the mass spectra shown in Fig. 4.

II) Electron energy dependencies

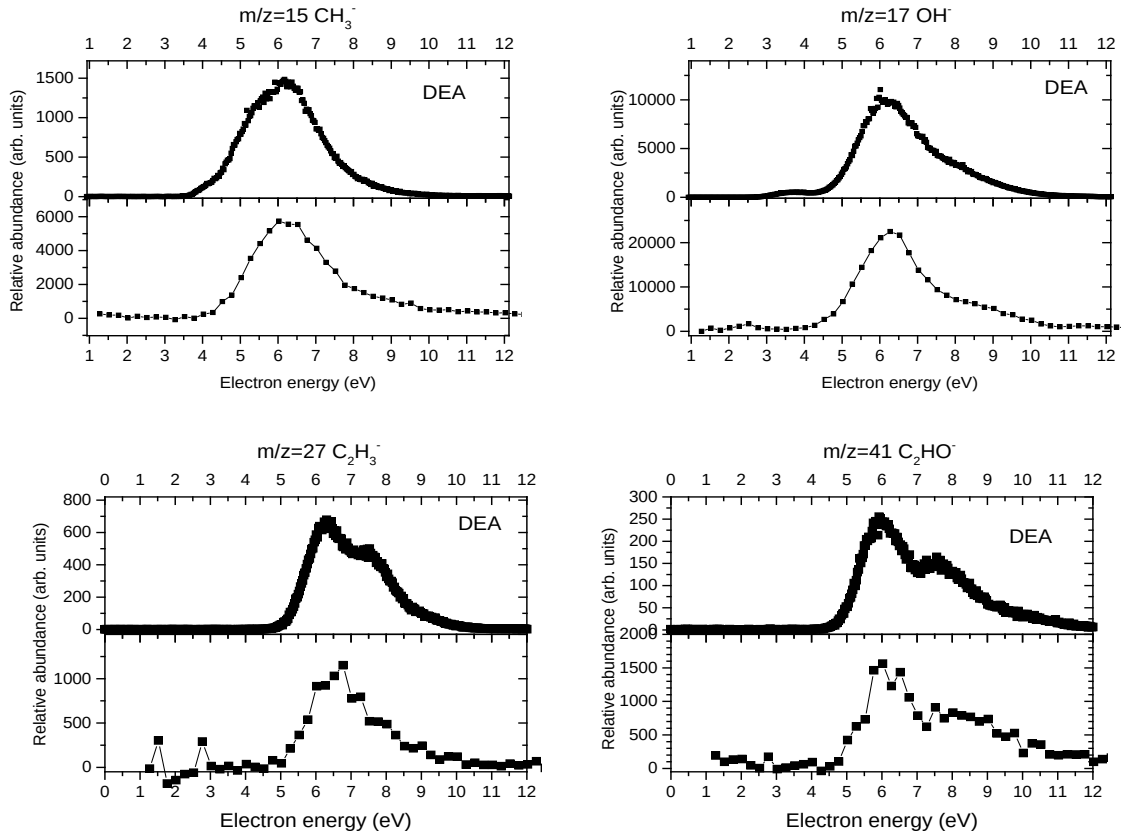

Figure S3: Monomer fragments of the DEA of pyruvic acid molecule in the gas phase (top panel in each figure) in comparison with the same fragment from the attachment of large $(PA)_N$ clusters (small and intermediate clusters show the same behavior with somewhat worse signal-to-noise ratio). There is no significant difference between these fragments from isolated molecules and clusters. There are isolated molecules present in the cluster beam as well, and the above fragments may come from these isolated molecules also in the cluster experiments.

III) Theoretical calculations

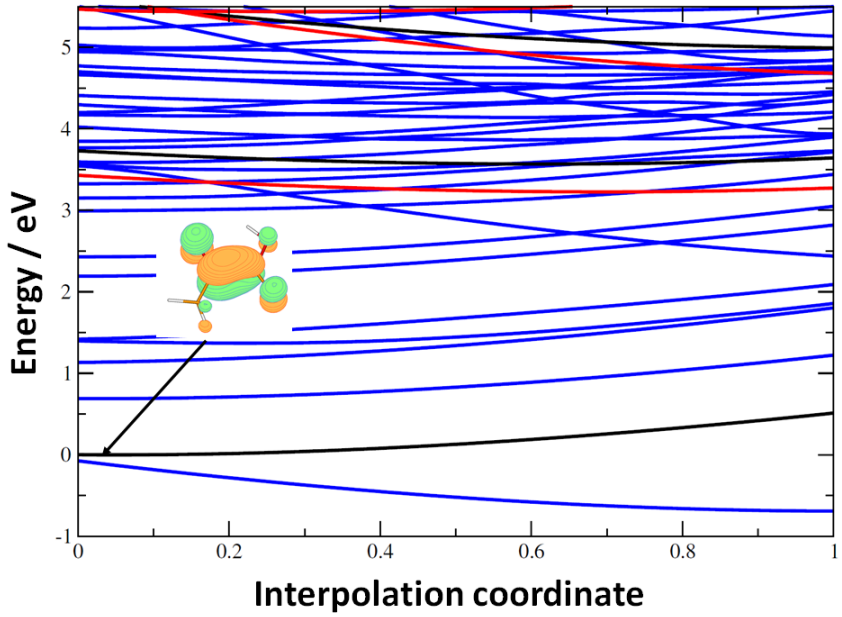

Figure S4: Interpolation between minimum of the neutral molecule (left) and of the anion (right). Singlet and triplet electronic states of the neutral molecule (black and red, respectively) and electronic states of the anion (blue) are shown. The ground electronic state was calculated at the CCSD/aug-cc-pVDZ level, excited states at the TD-BHandHLYP/aug-cc-pVDZ level, anionic states were shifted by –0.3 eV based on benchmarking against EOM-CCSD values in the neutral molecule minimum. The singly occupied molecular orbital of the anionic ground state is also shown.

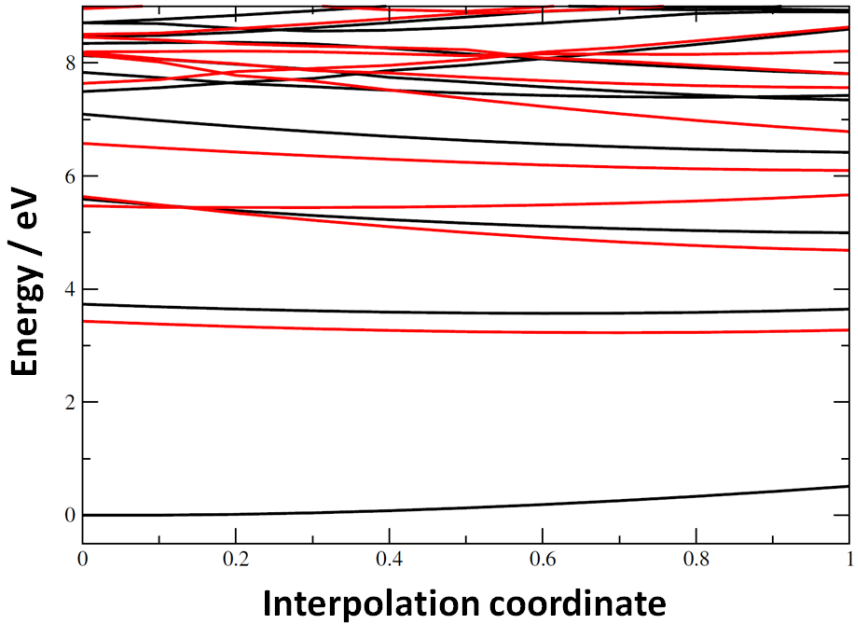

Figure S5: Interpolation between minimum of the neutral molecule (left) and of the anion (right). Singlet and triplet electronic states of the neutral molecule (black and red, respectively) are shown. The ground electronic state was calculated at the CCSD/aug-cc-pVDZ level, excited states at the TD-BHandHLYP/aug-cc-pVDZ level.

Cartesian coordinates (in Å) along with zero-point corrected energies (in Hartree) for molecules and ions calculated at the B3LYP/aug-cc-pVDZ level of theory

```
PA
E = -342.394085
C 1.355357 1.375636 0.000000
C -0.000000 0.738740 0.000000
O -1.059858 1.337125 0.000000
C -0.039888 -0.814107 0.000000
O 0.956789 -1.493556 0.000000
O -1.282798 -1.314126 0.000000
H 1.918582 1.026462 0.879238
H 1.257365 2.466740 0.000000
H 1.918582 1.026462 -0.879238
H -1.900406 -0.556819 0.000000

CHO2-
E = -189.221106
C -0.000002 0.318829 -0.000000
O -0.000002 -0.210890 1.141308
O -0.000002 -0.210890 -1.141308
H 0.000055 1.461274 -0.000000

COCH3
E = -153.163676
C 0.244937 -0.432762 -0.000020
C -1.171065 0.099430 -0.000057
H -1.690656 -0.297002 -0.884784
H -1.688813 -0.293009 0.887546
H -1.179235 1.201970 -0.002278
O 1.264433 0.173504 -0.000003

CH3COO
E = -228.518211
C 0.041061 -1.353586 0.000000
C 0.000000 0.208479 0.000000
O -1.157447 0.710972 0.000000
O 1.115302 0.797414 0.000000
H 1.076353 -1.729610 0.000000
H -0.492777 -1.733418 0.887867
H -0.492777 -1.733418 -0.887867

HCO
E = -113.859087
H -0.873221 1.224885 -0.000000
C 0.062373 0.586931 0.000000
O 0.062373 -0.593309 -0.000000

CH3COCO-
E = -266.539328
C -1.286753 -1.053745 -0.029480
C -0.396991 0.195569 -0.026838
C 0.953401 -0.053113 0.336191
O 2.067793 -0.155325 -0.159419
O -0.947804 1.346573 -0.033691
H -0.699189 -1.987974 0.001164
H -1.885941 -1.025251 -0.957036
H -1.992729 -1.049024 0.821522

CH2COCHO-
E = -266.572175
C 1.565087 -0.792441 -0.000100
C 0.524120 0.141629 0.000044
C -0.832959 -0.549690 0.000168
O -1.927545 -0.005466 -0.000168
O 0.587107 1.406251 0.000066
H 1.359060 -1.864412 0.000075
H 2.607753 -0.465263 -0.000387
H -0.780794 -1.673590 0.000450

OH
E = -75.740616
O 0.000000 0.000000 0.108809
H 0.000000 0.000000 -0.870468

(PA)2
E = -684.806119
C -4.145043 -1.165532 0.000172
C -3.447701 0.168552 0.000096
O -4.006554 1.240334 0.000022
C -1.896128 0.102579 0.000049
O -1.324056 -0.988020 -0.000041
O -1.310679 1.272520 -0.000116
H -3.831786 -1.746978 -0.880391
H -5.228910 -1.008738 0.000594
H -3.831070 -1.747354 0.880219
H -0.311594 1.165606 -0.000311
H 0.311600 -1.165607 -0.000384
O 1.310688 -1.272527 -0.000290
C 1.896134 -0.102582 -0.000098
O 1.324052 0.988012 -0.000118
C 3.447702 -0.168548 0.000097
O 4.006557 -1.240328 0.000155
C 4.145032 1.165540 0.000144
H 5.228900 1.008753 -0.000165
H 3.831150 1.747390 -0.879918
H 3.831674 1.746952 0.880694

CH3COOH
E = -229.066956
C 0.000000 0.156101 -0.000000
O 0.178520 1.353612 -0.000000
O -1.243791 -0.397939 -0.000000
H -1.882299 0.333615 -0.000000
C 1.072432 -0.901852 0.000000
H 2.055629 -0.420817 0.000000
H 0.957121 -1.541840 0.886726
H 0.957121 -1.541840 -0.886726

CO2
E = -188.602775 in
O 0.000000 0.000000 1.167441
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 -1.167441

CH3-
E = -39.819720
C 0.000000 0.000053 -0.127775
H 0.904685 0.522134 0.255590
H -0.904677 0.522147 0.255590
H -0.000008 -1.044602 0.255472

COCOOH
E = -302.446785
C -0.474921 0.117709 -0.029600
C 0.972502 -0.081364 -0.406669
O 1.972187 -0.066478 0.215647
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O -0.973313 1.214555 0.046863
O -1.114516 -1.064757 0.041947
H -2.060351 -0.884633 0.181957

OH-
E = -75.808427
O 0.000000 0.000000 0.107740
H 0.000000 0.000000 -0.861918

CH3COCO
E = -266.495772
C 1.389927 -0.983282 -0.030896
C 0.444906 0.195588 -0.002391
O 0.783743 1.378383 -0.030934
C -0.959796 -0.112210 0.268766
O -2.054057 -0.230291 -0.131552
H 1.955160 -1.026521 0.912862
H 2.101422 -0.824480 -0.853273
H 0.855712 -1.934305 -0.172568

CH2CH-
E = -77.905102
C 0.763810 -0.194205 0.000000
C -0.581120 0.025464 0.000000
H -1.304750 -0.810972 -0.000001
H -1.083356 1.025170 0.000001
H 1.291967 0.798246 -0.000001

C2OH-
E = -152.013767
C -0.004428 0.029728 0.000008
C -1.267055 -0.127031 -0.000002
H -2.146589 0.498239 -0.000006
O 1.221936 0.010697 -0.000003

H2
E = -1.164099 in
H 0.000000 0.000000 0.380357
H 0.000000 0.000000 -0.380357

COOH
E = -189.108449
C -0.000000 0.442884 -0.000000
O -1.064771 -0.355012 -0.000000
O 1.161133 0.184127 0.000000
H -0.770895 -1.290222 0.000000

(PA)2-
E = -684.865227
C -4.102404 -1.176111 0.000308
C -3.399868 0.171551 0.000384
O -4.031002 1.240507 0.000369
C -1.914437 0.108314 0.000165
O -1.316612 -0.997225 -0.000033
O -1.281059 1.276701 0.000162
H -3.808161 -1.768520 -0.881345
H -5.187105 -1.007624 0.001326
H -3.806520 -1.769546 0.880697
H -0.283789 1.127189 -0.000045
H 0.283820 -1.127476 -0.000350
O 1.281110 -1.276806 -0.000414
C 1.914451 -0.108362 -0.000256
O 1.316512 0.997129 -0.000088
C 3.399872 -0.171486 -0.000299
O 4.031101 -1.240408 -0.000352
C 4.102347 1.176217 0.000035
H 5.187059 1.007789 -0.000882
H 3.806543 1.769759 -0.880310
H 3.807983 1.768500 0.881733

(PA)2-, transferred H+
E = -684.873167
C 4.061283 -1.192413 0.206955
C 3.363029 0.155728 0.041005
C 1.936510 0.124867 -0.038482
O 1.246284 1.249270 -0.182572
O 4.027768 1.225241 -0.019563
O 1.322852 -1.062352 0.037218
O -1.374041 1.089755 -0.307228
C -1.879400 -0.054140 -0.157829
C -3.412843 -0.087817 -0.101530
C -4.002876 0.332630 1.230672
O -1.283371 -1.152264 -0.006673
O -4.100337 -0.410990 -1.054897
H 3.739727 -1.700054 1.131489
H 5.143720 -1.011667 0.240428
H 3.821916 -1.874230 -0.625620
H 0.248268 1.115888 -0.238061
H 0.311537 -1.020956 0.001242
H -5.099094 0.283518 1.194015
H -3.611198 -0.328596 2.020286
H -3.662341 1.353686 1.461185

[PA-H]-
E = -341.865942
C -1.462122 -1.069760 0.004058
C -0.655086 0.224502 -0.000756
O -1.210585 1.317490 -0.004645
C 0.869376 0.014093 -0.000088
O 1.379392 -0.091598 -1.143429
O 1.380551 -0.081271 1.143582
H -1.181659 -1.663991 -0.879841
H -2.540319 -0.851968 0.000530
H -1.185901 -1.654012 0.895959

[PA-H]-
E = -341.723128
C 1.409701 1.268974 0.000000
C -0.000000 0.759965 0.000000
O -1.005180 1.432952 0.000000
C -0.181462 -0.770937 0.000000
O 0.756746 -1.595273 0.000000
O -1.334108 -1.295483 0.000000
H 1.937777 0.874843 0.883353
H 1.415343 2.364728 0.000000
H 1.937777 0.874843 -0.883353

[PA+H]-
E = -342.985423
C 1.704689 -0.950726 0.006758
C 0.687674 0.176303 -0.007061
C -0.648277 -0.092274 -0.066653
O -1.546343 0.981518 -0.005346
O 1.113103 1.418922 0.022925
O -1.285213 -1.328631 -0.076165
H 1.223018 -1.941400 -0.013627
H 2.336189 -0.867485 0.911613
H 2.380359 -0.860482 -0.863942
H -0.908363 1.725707 0.062981
H -1.748090 -1.430626 0.773396
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[PA+H]
E = -342.951728
C 1.763061 -0.881187 0.000015
C 0.717127 0.206103 -0.000024
C -0.670378 -0.107523 -0.000024
O -1.567290 0.883165 0.000003
O 1.005720 1.434677 0.000005
O -1.166727 -1.352786 0.000015
H 2.402913 -0.765928 0.887746
H 2.402388 -0.766585 -0.888189
H 1.314859 -1.882785 0.000438
H -1.018194 1.699498 0.000032
H -2.134446 -1.309008 -0.000017

(PA)3
E = -1027.214380
C 4.039780 2.176727 0.687680
C 3.355026 1.107760 -0.118645
O 3.898020 0.122730 -0.564303
C 1.833828 1.312777 -0.336632
O 1.224326 2.156227 0.319998
O 1.317516 0.520298 -1.240665
O -1.312803 0.807158 -1.301154
C -1.883846 1.244862 -0.311224
C -3.328695 0.820366 0.012264
O -3.628338 -0.348876 -0.140183
O -1.391195 2.080995 0.572546
C -4.272262 1.874525 0.505617
O -1.630870 -2.261833 -0.422313
C -0.573738 -1.911979 0.292897
C 0.558416 -2.970113 0.258963
C 1.934955 -2.441074 0.556639
O -0.463041 -0.880426 0.936732
O 0.298814 -4.130955 0.032164
H 3.895464 3.155247 0.203979
H 5.104955 1.939290 0.778770
H 3.564427 2.248546 1.677553
H 0.327247 0.665461 -1.309501
H -0.397565 2.184964 0.435288
H -5.273200 1.450255 0.639396
H -3.884082 2.278194 1.453453
H -4.292669 2.713108 -0.208558
H -2.321971 -1.556419 -0.372337
H 2.643657 -3.274525 0.609986
H 2.237135 -1.736399 -0.234094
H 1.916390 -1.873366 1.498129

(PA)3-
E = -1027.300199
C 5.140332 -0.173420 0.819013
C 4.099398 0.491528 -0.058417
O 4.349836 1.434443 -0.786136
C 2.697904 -0.137989 0.008652
O 2.632462 -1.329418 -0.404056
O 1.765792 0.561836 0.481030
O -0.457122 -0.680593 0.840447
C -0.690215 -1.776342 0.145820
C -2.005237 -2.331749 0.136616
O -2.989884 -1.742147 0.695099
O 0.277408 -2.385778 -0.528151
C -2.246594 -3.642910 -0.578063
O -2.960271 0.809207 0.873390
C -2.433606 1.320613 -0.215545
C -1.986614 2.783281 -0.058148
C -0.563496 3.044414 -0.482963
O -2.264027 0.760881 -1.288752
O -2.755206 3.646981 0.324510
H 4.800304 -0.145782 1.867094
H 6.105820 0.337704 0.714098
H 5.217971 -1.232695 0.532390
H 0.446013 -0.242146 0.657400
H 1.187837 -1.932545 -0.445557
H -2.982474 -4.224098 -0.003330
H -2.679003 -3.444355 -1.573753
H -1.323631 -4.220763 -0.711808
H -2.988349 -0.221033 0.803070
H -0.311136 4.098697 -0.315910
H 0.126963 2.380259 0.061598
H -0.463433 2.778915 -1.546138

[PA2-H]+
E = -684.303985
C -2.324649 1.258684 -0.999872
C -2.522331 0.252688 0.116421
C -1.565409 -0.945233 0.052068
C 1.629221 0.861439 -0.129802
C 1.493368 1.582238 1.188367
O -3.378855 0.379231 0.978889
O -1.868212 -1.868918 -0.712785
O -0.518012 -0.805846 0.778434
C 2.426392 -0.457304 -0.081443
O 1.770022 -1.566584 0.157891
O 3.635378 -0.387264 -0.254772
O 1.215726 1.299000 -1.188177
H -1.270042 1.575830 -1.027563
H -2.995622 2.117319 -0.861516
H -2.530743 0.756630 -1.958056
H 0.757082 -1.372420 0.372206
H 2.479310 1.651026 1.673114
H 1.064741 2.579767 1.027241
H 0.827344 0.979833 1.824295

[PA2+H]+
E = -685.480135
C -2.599201 1.170477 -0.248419
C -1.944054 -0.157886 0.074219
O -2.496604 -0.988949 0.769358
C -0.512212 -0.377583 -0.494034
O -0.429180 0.269140 -1.775140
O -0.296216 -1.734137 -0.635682
O 2.750085 0.948295 -0.175279
C 2.004909 -0.059102 -0.058834
C 0.551899 0.278967 0.459669
O 0.414493 1.703128 0.393365
O 2.271204 -1.271165 -0.269510
C 0.405778 -0.214166 1.900358
H -1.912227 1.984964 0.022456
H -3.547432 1.249680 0.297933
H -2.765634 1.233919 -1.333546
H 0.691411 -1.846203 -0.599169
H -0.095728 1.161890 -1.592945
H 1.233875 0.188815 2.500077
H -0.546273 0.126462 2.330238
H 0.436244 -1.309937 1.921012
H 1.352788 1.955678 0.199283

C5O5H4-
E = -569.134759
C -3.004820 -0.290777 0.179905
C -1.519260 -0.489603 -0.038113
O -1.106785 -1.650711 -0.336872
C -0.698224 0.713150 0.066843

O -1.277775 1.816235 0.309901
C 0.793282 0.748667 -0.194348
O 1.312412 1.787722 -0.584829
C 1.778632 -0.425214 0.125959
O 2.900996 -0.170063 0.521897
O 1.375351 -1.677088 -0.070320
H -3.187435 0.139397 1.176321
H -3.516599 -1.255905 0.070628
H -3.396965 0.442413 -0.541570
H 0.369738 -1.712001 -0.265078

CH3OH
E = -115.693612
C -0.669864 -0.020100 -0.000220
O 0.751973 0.122557 -0.000241
H 1.148126 -0.755949 0.001406
H -1.029642 -0.549822 -0.899496
H -1.086466 0.995498 0.001340
H -1.028620 -0.549586 0.899994

C4O4-
E = -453.390020
C 0.000065 -1.070638 0.000000
C -1.070429 -0.000107 0.000000
C 1.070591 0.000022 -0.000000
C -0.000000 1.070382 -0.000000
O 2.292855 -0.000093 -0.000000
O -0.000435 -2.292937 0.000000
O -2.292779 0.000638 0.000000
O 0.000189 2.292648 -0.000000

C4O3H2-
E = -379.359420
O 0.000218 0.938572 -0.000035
C -1.152911 0.117858 0.000056
C -0.702293 -1.239615 0.000011
C 0.702345 -1.239299 -0.000023
C 1.152487 0.118284 0.000114
H 1.381876 -2.089210 -0.000131
O -2.276523 0.633042 -0.000027
O 2.276561 0.632767 -0.000035
H -1.381682 -2.089207 -0.000045

HCOOH
E = -189.762682
O -1.033971 -0.445666 0.000000
H -0.665446 -1.346360 -0.000000
C -0.000000 0.422926 0.000000
O 1.165081 0.114476 -0.000000
H -0.383430 1.458323 0.000000

C5O4H6-
E = -495.049013
C -1.627689 -0.095470 0.056124
O -1.100332 1.097078 0.210760
C 0.504528 0.967964 0.481527
C 0.779713 -0.466794 -0.015792
C -0.555752 -1.186173 0.117991
O 1.134466 -0.418167 -1.423519
C 1.931707 -1.112688 0.751521
O 1.175606 1.929234 0.047890
O -2.826927 -0.323073 -0.089262
H 2.829160 -0.484493 0.653874
H 2.145205 -2.111538 0.338907
H 1.676114 -1.201216 1.818216
H -0.640913 -1.684767 1.095847
H -0.715825 -1.932781 -0.669905
H 1.448722 0.493179 -1.552118

C5O3H4-
E = -418.657296
C 0.438001 1.216352 -0.000006
C -0.814893 0.580750 -0.000056
H 0.650602 2.283653 -0.000087
C 1.458834 0.217021 0.000010
C -0.585287 -0.832781 -0.000007
C -2.181818 1.189800 0.000021
H -2.937462 0.390432 0.000010
H -2.352369 1.827037 0.888344
H -2.352384 1.827239 -0.888137
O -1.363809 -1.796203 -0.000021
O 0.808233 -1.041992 0.000032
O 2.693400 0.268793 0.000001

H2O
E = -76.423464
O -0.000000 0.000000 0.117797
H -0.000000 -0.764159 -0.471188
H 0.000000 0.764159 -0.471188

(PA)2.3H2O, iso I
E = -914.115620
C 0.947492 2.927996 1.039591
C 1.048628 2.068169 -0.186544
C -0.295613 1.490459 -0.701140
O -0.118220 0.531495 -1.598815
O 2.078830 1.793910 -0.760892
O -1.370003 1.893123 -0.289571
O -2.060290 -1.339336 -1.684084
O -0.039873 -2.232565 -0.132078
C 0.620459 -1.418925 0.506730
C 2.153107 -1.312220 0.314726
C 2.639647 -1.489940 -1.094589
O 0.149040 -0.578306 1.399850
O 2.857853 -1.120985 1.281149
O -2.344427 -0.910291 1.973926
H 0.192984 3.713354 0.890701
H 1.930376 3.350063 1.273900
H 0.593236 2.296751 1.869786
H -0.959763 0.038638 -1.780646
H -0.841046 -0.731121 1.594322
H 3.734817 -1.498591 -1.108027
H 2.223515 -2.415750 -1.516786
H 2.255472 -0.647928 -1.691469
H -2.938969 -0.453112 1.317905
H -2.617244 -0.622685 2.851971
H -1.474860 -1.835693 -1.063385
H -2.173939 -1.902783 -2.458029
O -3.668779 0.272890 -0.011199
H -3.048228 1.006853 -0.177674
H -3.431720 -0.370709 -0.701508

(PA)2.3H2O, iso II
E = -914.116122
C -4.696785 1.054752 -0.712525
C -4.106248 -0.326066 -0.581465
C -2.702110 -0.380135 0.081969
O -2.289304 -1.597974 0.330716
O -4.646948 -1.338007 -0.965618
O -2.091167 0.655860 0.314373
O 0.051485 -1.872916 1.442405

O 1.808379 0.231317 0.930983
C 2.624287 0.132516 0.022912
C 3.244317 -1.246316 -0.343028
C 4.472831 -1.250558 -1.209145
O 3.058598 1.108543 -0.735464
O 2.703336 -2.245089 0.080001
O -0.057081 2.347551 1.274150
H -4.766834 1.523361 0.281184
H -5.683813 0.985599 -1.182590
H -4.021343 1.689575 -1.305522
H -1.371037 -1.615294 0.757064
H 2.558193 1.993457 -0.563641
H 4.825673 -2.278880 -1.343176
H 4.235585 -0.786529 -2.178552
H 5.252045 -0.622928 -0.749602
H 0.707779 -1.155473 1.337560
H 0.524436 -2.650372 1.119159
H 0.541706 1.603789 1.457433
H -0.855880 1.904123 0.936208
O 1.709533 3.260363 -0.444082
H 2.117948 4.063113 -0.101229
H 0.943136 3.044109 0.163687

(PA)2.3H2O, iso III
E = -914.111613
C -3.716572 1.159955 0.209599
C -3.449788 -0.316154 0.076599
C -2.041610 -0.673516 -0.452220
O -1.614354 -1.852043 -0.091954
O -4.243791 -1.192537 0.330141
O -1.431466 0.132082 -1.160705
O 1.170509 0.196615 -1.112421
C 1.630885 -0.869658 -0.506130
C 3.047348 -0.664289 0.077510
C 3.707102 -1.888550 0.636337
O 1.049804 -1.941259 -0.380754
O 3.541207 0.445956 0.086756
O 2.113855 2.935044 -0.348948
O -0.498258 2.553771 0.400043
H -2.923198 1.633643 0.808658
H -4.700506 1.312597 0.665745
H -3.678351 1.624920 -0.787472
H -0.645087 -1.955431 -0.311951
H 0.185724 0.097674 -1.282784
H 4.704383 -1.635775 1.011084
H 3.073462 -2.298453 1.437638
H 3.759139 -2.666664 -0.140441
H -0.922196 2.190515 -0.388515
H 0.416758 2.783680 0.116967
H 2.707556 3.514095 0.141232
H 2.528125 2.052417 -0.318903
H -0.165532 1.079893 1.304540
O 0.003568 0.168678 1.640520
H -0.133057 0.209703 2.592601

(PA)2.3H2O, iso IV
E = -914.112156
C -4.557238 -0.741024 0.753805
C -3.752510 -0.156306 -0.377424
C -2.213141 -0.172515 -0.171063
O -1.535330 0.178442 -1.232141
O -4.226304 0.318737 -1.383369
O -1.740765 -0.483054 0.920688
O 1.041569 0.088012 -0.945853
C 1.911066 0.784402 -0.417774
C 1.573550 2.138192 0.263762
C 0.107751 2.448048 0.423309
O 3.176802 0.486052 -0.381273
O 2.464953 2.872846 0.620725
O 3.588208 -1.948639 -1.154700
O 1.800927 -3.009196 0.529029
H -4.249472 -1.783631 0.927771
H -5.623274 -0.684578 0.509093
H -4.336912 -0.195310 1.683585
H -0.540644 0.176289 -1.058834
H 3.349516 -0.442901 -0.761027
H -0.000022 3.416421 0.923246
H -0.383689 2.468508 -0.560535
H -0.374798 1.653954 1.011166
H 2.945117 -2.430119 -0.569325
H 4.461075 -2.297305 -0.940057
H 1.443964 -2.229000 1.016469
H 1.042687 -3.401781 0.081667
O 0.830115 -0.808321 1.850628
H 0.725080 -0.942935 2.799374
H -0.076886 -0.671438 1.499855

(PA)2.3H2O-, iso I
E = -914.177831
C -1.654374 3.290013 0.564280
C -0.847823 2.352350 -0.319342
C -1.319828 1.006166 -0.454886
O -0.560429 0.199015 -1.281986
O 0.207754 2.775896 -0.887014
O -2.338425 0.496568 0.128900
O -0.556716 -2.755250 -1.674626
O 1.379106 -1.940988 0.054139
C 1.610683 -0.869859 0.611643
C 2.800724 -0.010283 0.161994
C 2.608504 0.724216 -1.126421
O 0.948705 -0.354411 1.613048
O 3.811502 0.002736 0.843851
O -1.447182 -1.146183 2.073098
H -2.594316 2.832738 0.899330
H -1.867003 4.216277 0.005639
H -1.054461 3.571009 1.447049
H -0.942899 -0.691252 -1.245880
H 0.058819 -0.830960 1.799520
H 3.540244 1.233421 -1.403497
H 2.294957 0.012002 -1.904639
H 1.767477 1.443797 -1.026455
H -1.802112 -1.900223 1.564162
H -1.843801 -0.396965 1.558253
H 0.154623 -2.558071 -1.026573
H -0.226301 -2.419409 -2.515254
O -2.894412 -2.236560 -0.104034
H -2.845272 -1.254845 -0.156374
H -2.226494 -2.539713 -0.741889

(PA)2.3H2O-, iso II
E = -914.195880
C -3.516481 -0.797581 -1.875667
C -3.755111 -0.197329 -0.501712
C -2.471487 0.133705 0.274132
O -2.019945 -0.812936 0.969849
O -4.875183 0.002029 -0.059482
O -2.014925 1.286590 0.073821
O 0.260432 -1.233232 2.265339
O 2.120881 0.419353 1.050296
C 2.428924 -0.104280 -0.041239
C 2.379781 -1.524707 -0.298174
C 2.929377 -2.163475 -1.533495

O 2.847882 0.628885 -1.094779
O 1.853374 -2.369205 0.582619
O 0.259184 2.492152 0.841655
H -2.912826 -0.094334 -2.470506
H -4.473295 -1.005790 -2.373092
H -2.927437 -1.721046 -1.761531
H -0.606126 -1.029974 1.807583
H 2.678020 1.599632 -0.924414
H 3.565608 -3.018873 -1.251753
H 2.108020 -2.560880 -2.155714
H 3.507395 -1.446888 -2.125922
H 0.764399 -0.404877 2.205276
H 1.239620 -1.922554 1.272967
H 0.839775 1.749372 1.090959
H -0.596571 2.056081 0.582533
O 2.166085 3.208650 -0.821335
H 2.729578 3.704746 -0.217028
H 1.331545 3.039098 -0.286292

(PA)2.3H2O-, iso III
E = -914.193317
C -3.724138 0.546266 0.104965
C -3.324873 -0.900890 -0.062056
C -1.816010 -1.145302 -0.292599
O -1.245719 -2.042123 0.367521
O -4.119046 -1.823372 -0.049468
O -1.277881 -0.376546 -1.151622
O 1.274365 -0.251231 -1.089498
C 1.909466 -0.934813 -0.154637
C 3.239004 -0.542749 0.188829
C 4.033840 -1.385079 1.167087
O 1.337551 -1.970748 0.452510
O 3.758915 0.506978 -0.304521
O 2.124628 2.650446 -0.741628
O -0.642601 2.342146 -0.561128
H -3.126720 1.025850 0.897984
H -4.796618 0.610663 0.328384
H -3.485208 1.086419 -0.823579
H 0.325277 -2.008971 0.331443
H 0.272200 -0.424479 -1.131070
H 5.031757 -1.571203 0.740446
H 4.176111 -0.823698 2.105784
H 3.541002 -2.337947 1.395217
H -0.896653 1.438735 -0.819810
H 0.336457 2.383794 -0.650766
H 2.419505 3.115041 0.049006
H 2.642925 1.804947 -0.721335
H -1.313973 2.694118 0.988953
O -1.793699 2.906560 1.829569
H -2.361902 3.645244 1.585919

(PA)2.3H2O-, iso IV
E = -914.176549
C -3.462146 -0.532435 1.521346
C -2.979119 -0.790899 0.099209
C -1.547200 -0.676950 -0.126193
O -1.122074 -0.882957 -1.405213
O -3.789724 -1.117842 -0.800454
O -0.699784 -0.390784 0.778772
O 1.351011 0.553769 -1.208745
C 1.259592 1.282538 -0.208603
C 0.145653 2.321011 -0.048161
C -0.993671 2.263245 -1.029709
O 2.138544 1.307544 0.772706
O 0.224857 3.175421 0.825373
O 3.666651 -0.865790 0.915288
O 2.662540 -1.915355 -1.465114
H -3.596273 -1.491489 2.053036
H -4.444170 -0.039877 1.471399
H -2.751004 0.078429 2.092259
H -0.206565 -0.546699 -1.445877
H 2.786370 0.543415 0.709453
H -1.383964 3.278612 -1.175382
H -0.698953 1.803648 -1.979754
H -1.801420 1.639440 -0.605280
H 3.686731 -1.226351 0.004831
H 2.906434 -1.365347 1.281633
H 2.079773 -2.330849 -0.806570
H 2.270315 -1.022602 -1.544193
O 1.228247 -2.146711 1.097121
H 0.811249 -2.815928 1.648635
H 0.520682 -1.441823 0.970597