

Energetics and Dynamics of the Non-Natural Fluorescent 4AP:DAP Base pair

Mohit Chawla,¹ Ida Autiero,¹ Romina Oliva,² Luigi Cavallo¹

¹King Abdullah University of Science and Technology (KAUST), Physical Sciences and Engineering Division, Kaust Catalysis Center, Thuwal 23955-6900, Saudi Arabia. ²Department of Sciences and Technologies, University Parthenope of Naples, Centro Direzionale Isola C4, I-80143, Naples, Italy

Email: luigi.cavallo@kaust.edu.sa

Table S1: Population of the first 10 clusters (on 2000 total snapshot, each from 100 ps of the last 200 ns of simulation).

Cluster	4AP (63 clusters)	AT (71 clusters)
1	635	773
2	459	426
3	189	131
4	126	103
5	100	78
6	65	73
7	55	60
8	50	33
9	36	31
10	33	23

Table S2: Average interaction energy of the central, top (at 5' direction) and bottom (3' direction) H-bonded base pairs of the modified 4AP and natural/un-modified AT duplex. The single point interaction energies have been calculated at RIMP2/aug-cc-pVTZ level of theory for the three most populated clusters derived from the MD simulations.

	4AP-duplex	AT-duplex
AT along the 5' direction	-9.99	-11.90
Central pair	-13.03	-12.33
AT along the 3' direction	-11.90	-11.44

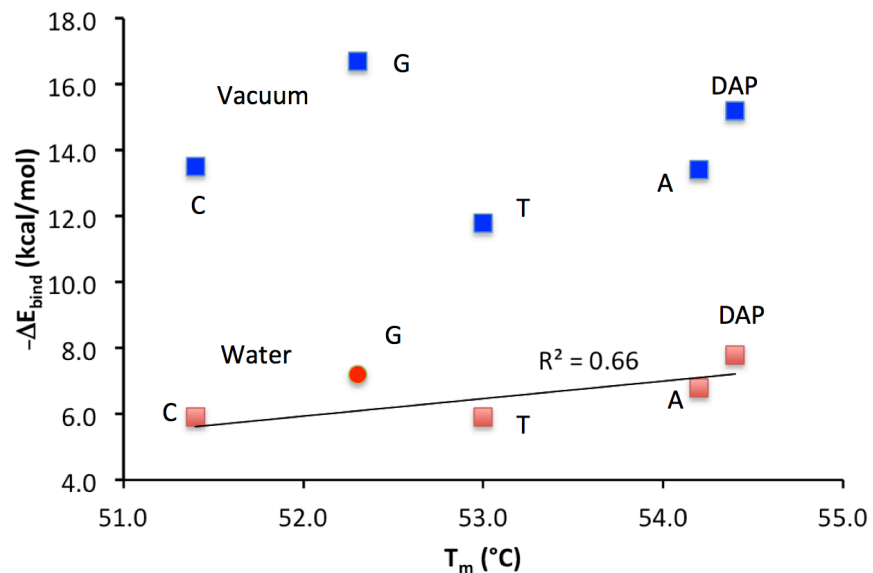


Figure S1: Plot between the experimental temperature, T_m , and the calculated H-bonding energies in vacuo and in water for all the studied base pairs in cWW orientation.

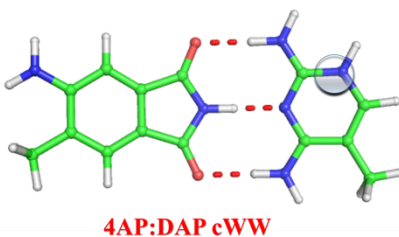


Figure S2: Base pair structure of 4AP:DAP cWW geometry with the protonated N5 atom, shown by circle.

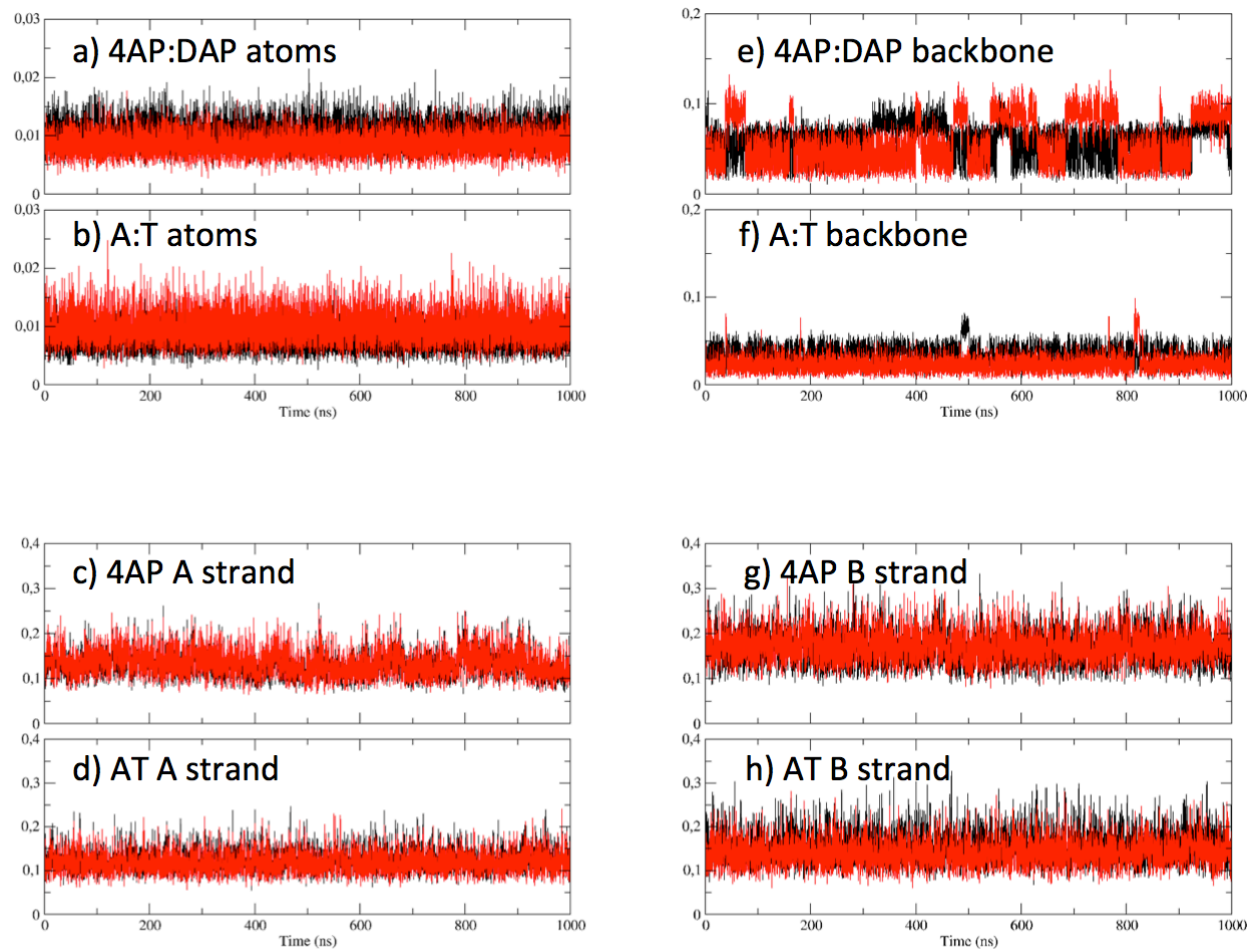


Figure S3: Root mean square deviation (RMSD) computed considering separately the base atoms (left panels) and the backbone atoms (right panels) of each residue in the central position (4AP: a,e and AT: b, f) and the whole strands A and B (4AP: c, g and AT: d, h), always excluding the capping pairs. Black lines refer to the strand containing 4AP or A, while red lines refer to the strand containing DAP or T.

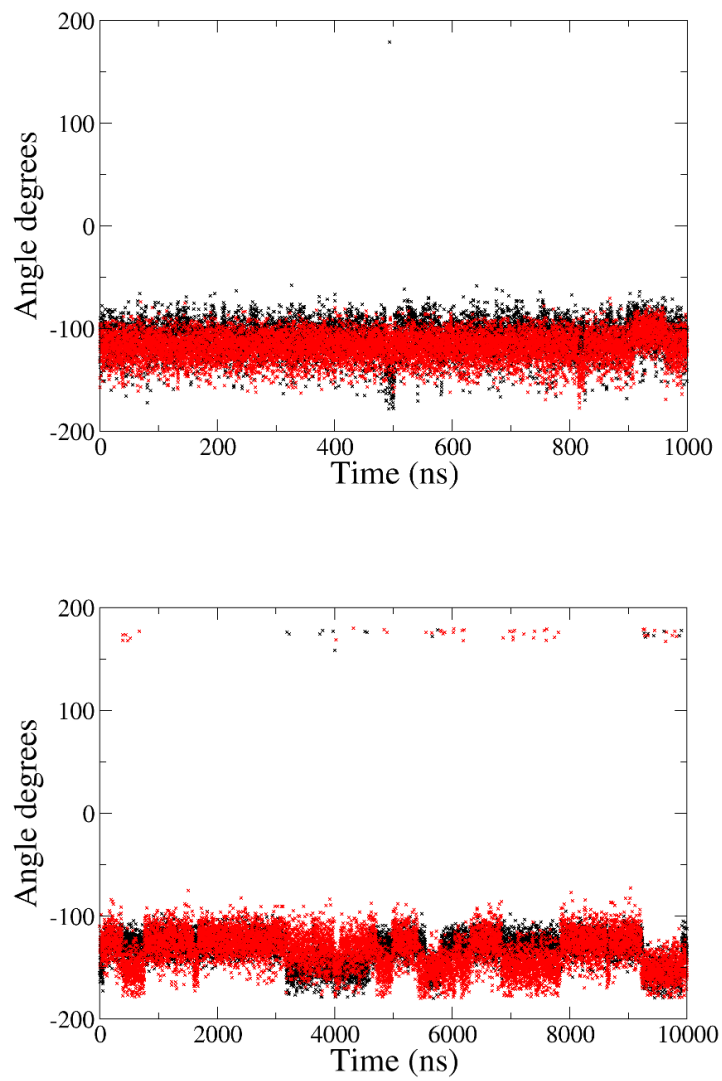


Figure S4: Distribution of the χ angles of the central bases in the 4AP (top) and AT (bottom) duplexes.

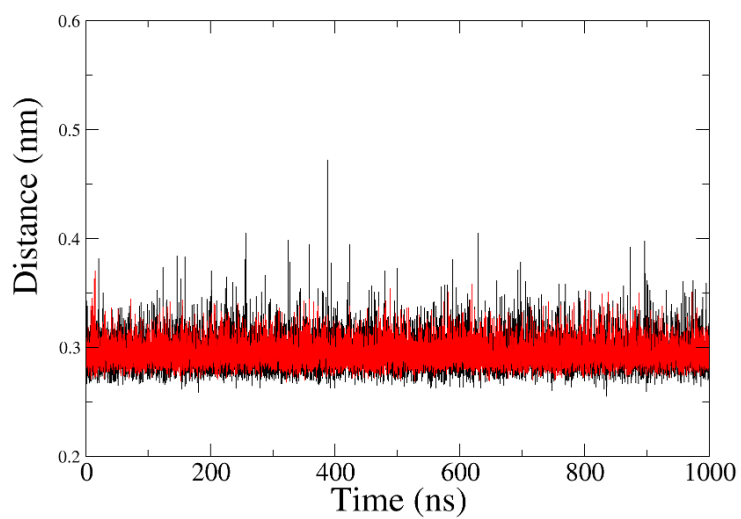
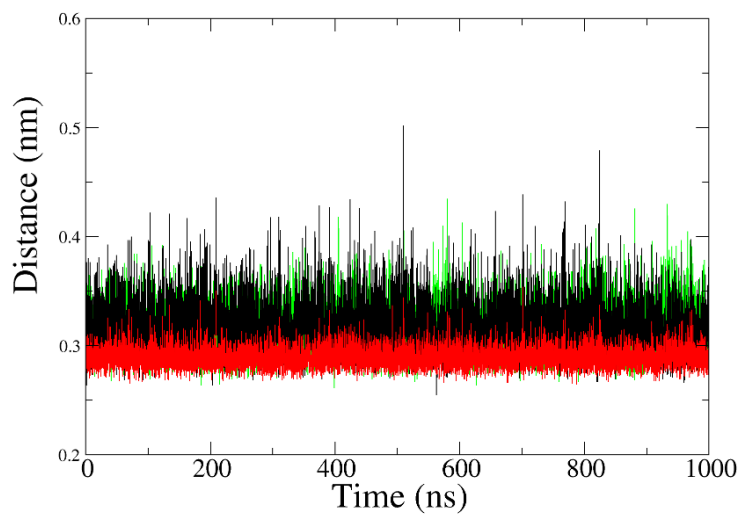


Figure S5: Evolution of the distances between atoms involved into the base pair H-bonds in position 7A-7B with time (4AP: top panel and AT: bottom panel).

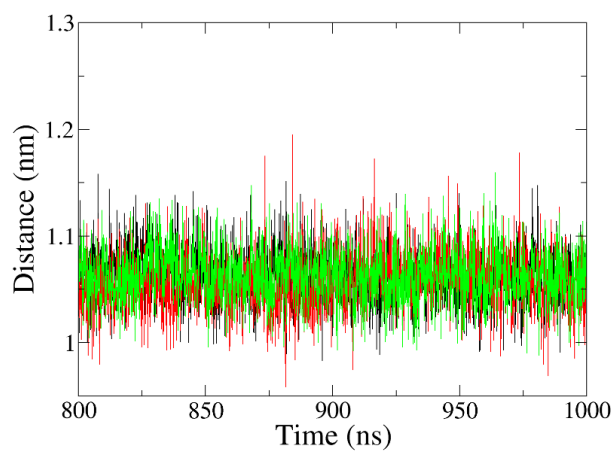
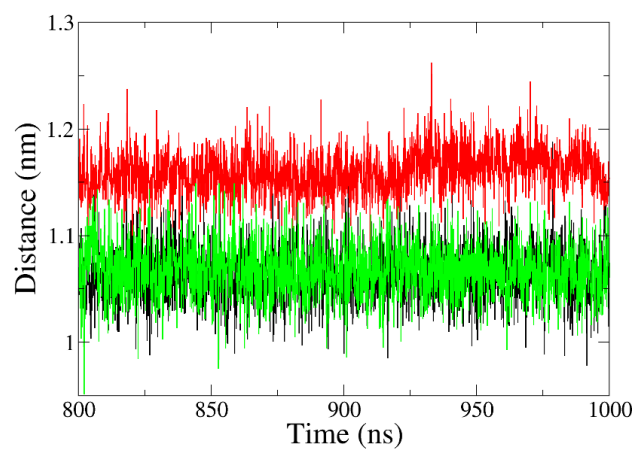


Figure S6: Evolution of the C1'-C1' distances between the central and the neighboring base pairs (4AP: top panel and AT: bottom panel). Red line, central 4AP-DAP or A-T pair. Black lines and green lines, A6-T8 and A8-T6 pairs both in the 4AP and AT duplexes.

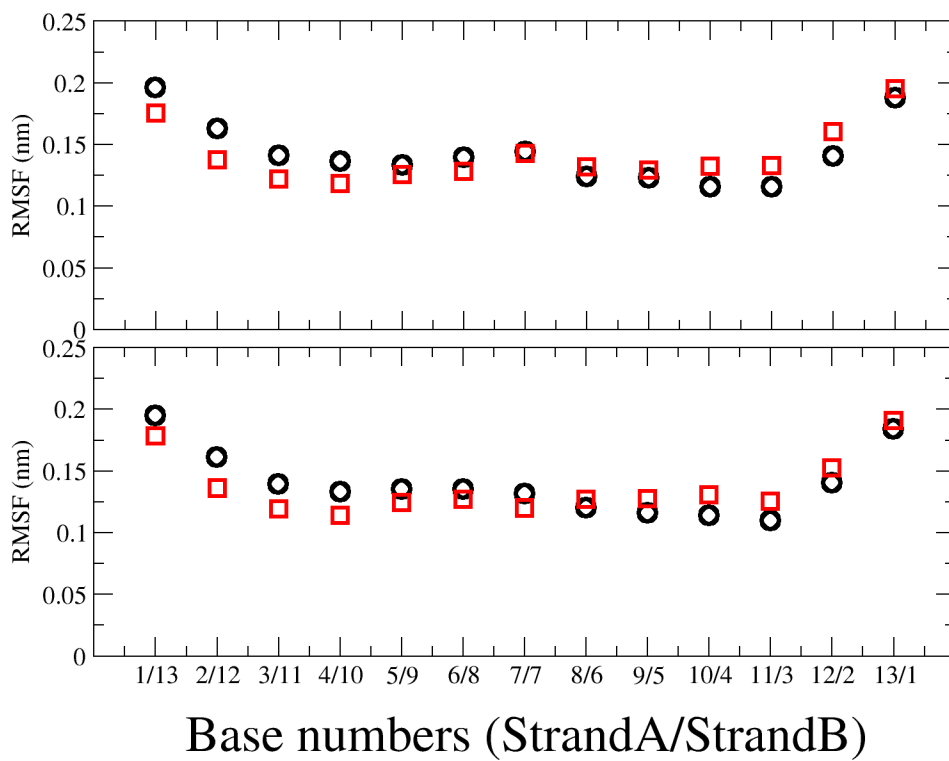


Figure S7: Root mean square fluctuation (RMSF) computed per residues (strand A in black and strand B in red) considering all the atoms and plotted as interacting pairs. 4AP: top panel and AT: bottom panel.

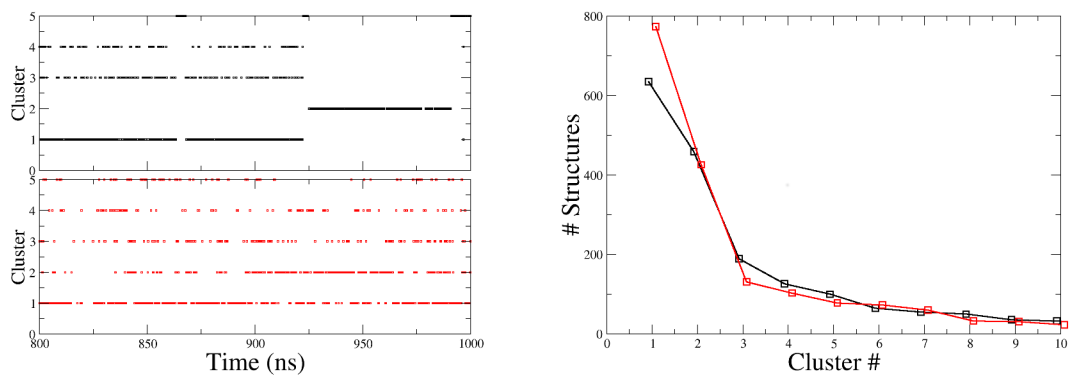


Figure S8: Left: cluster distribution among simulation time, 4AP (top panel) and AT (bottom panel). Right: Cluster size distribution for 4AP (black) and AT (red).

XYZ coordinates of the QM optimized base pairing geometries:

In Water optimized coordinates for the studied base pairs:

4AP:DAP cWW

38

4ap-dap SCF Done: -1022.65594492 A.U.

C	5.891892	-1.680813	0.053548
C	2.337101	0.694803	-0.008798
N	5.940921	1.172799	0.110934
C	3.546805	1.337188	0.062166
N	0.115448	0.148738	-0.116033
C	4.720662	0.554248	0.087309
C	4.634472	-0.862400	0.038122
C	3.387319	-1.474201	-0.030660
C	2.242553	-0.696546	-0.054376
C	0.950153	1.243208	-0.045130
O	0.581116	2.404924	-0.018675
C	0.814768	-1.053167	-0.120086
O	0.282454	-2.151769	-0.167623
H	3.612639	2.417463	0.100150
H	3.321404	-2.554624	-0.066289
H	5.665128	-2.742715	-0.008210
H	6.751942	0.655032	0.406559
H	5.964666	2.154545	0.342781
H	-0.925371	0.209090	-0.142141
C	-5.686515	-1.982985	0.208334
C	-4.833406	-0.754745	0.115344
N	-2.777870	-2.004478	-0.110988
C	-3.426675	-0.823768	-0.035726
N	-4.631760	1.650006	0.086733
N	-2.686461	0.291330	-0.122209
C	-3.312591	1.478998	-0.061958
N	-2.544447	2.591780	-0.191004
C	-5.349527	0.520804	0.169695
H	-6.421618	0.651037	0.289709
H	-5.416522	-2.605136	1.066679
H	-3.270775	-2.867408	0.036950
H	-1.765968	-2.042329	-0.147825
H	-2.977860	3.474634	0.032677
H	-1.538990	2.529303	-0.106722
H	6.544194	-1.422821	-0.784914
H	6.468251	-1.516178	0.968925
H	-5.597090	-2.608941	-0.683872
H	-6.735462	-1.711148	0.317188

4AP:A cWW

39

4ap-A SCF Done: -1114.92906481 A.U.

C	6.897176	1.200043	0.021937
C	3.002153	-0.559682	-0.001917
N	6.481198	-1.624527	0.033512
C	4.091672	-1.394029	-0.008320
N	0.893794	0.338134	0.000236
C	5.377660	-0.814725	-0.006937
C	5.522928	0.597953	0.004335
C	4.391270	1.406952	0.007408
C	3.134389	0.827469	0.003992
C	1.546501	-0.873938	-0.003807
O	1.006154	-1.969539	-0.007319
C	1.782755	1.419658	0.004778
O	1.445279	2.587234	0.008006
H	3.979546	-2.471095	-0.015990
H	4.502472	2.484248	0.014419
H	6.845089	2.285956	0.053077
H	7.373570	-1.254891	-0.250227
H	6.350436	-2.602764	-0.176728
H	-0.139740	0.416297	-0.002151
C	-2.661417	1.477955	-0.018103
N	-1.974137	0.327336	-0.008027
C	-2.638780	-0.848204	0.004491
N	-1.951529	-1.995898	0.013806
C	-4.626135	0.473477	-0.004654
H	-2.451566	-2.870153	0.022153
H	-0.935898	-2.002017	0.007283
H	7.467764	0.861353	0.890646
H	7.471726	0.919860	-0.866147
N	-3.977699	1.646662	-0.017619
C	-4.046203	-0.793826	0.007083
N	-5.018250	-1.775124	0.018524
N	-5.980492	0.254962	-0.000453
C	-7.017167	1.271140	-0.009986
H	-7.986383	0.779941	-0.003701
H	-6.929226	1.906963	0.869171
H	-6.931200	1.888171	-0.902634
H	-2.055213	2.377677	-0.027825
C	-6.148073	-1.109381	0.013633
H	-7.135404	-1.547096	0.019707

4AP:G cWW

40

4ap-G SCF Done: -1190.21161477 A.U.

C	-6.239816	2.245673	0.015261
C	-3.448947	-0.994405	0.008430
N	-7.048589	-0.490596	0.087451
C	-4.786490	-1.290132	0.067360
N	-1.156860	-1.056384	-0.072387
C	-5.708991	-0.221543	0.073562

C	-5.246615	1.121105	0.018031
C	-3.881630	1.376818	-0.039139
C	-2.986933	0.319831	-0.044122
C	-2.261677	-1.898361	-0.008433
O	-2.223324	-3.109568	0.024642
C	-1.520806	0.282883	-0.096035
O	-0.725836	1.214792	-0.150414
H	-5.138528	-2.313346	0.110285
H	-3.528317	2.399643	-0.080528
H	-5.737196	3.207753	-0.052800
H	-7.698258	0.228940	0.357531
H	-7.340072	-1.429317	0.315000
H	-0.175225	-1.365723	-0.097372
C	2.864466	1.690867	-0.008461
N	2.033523	0.605283	-0.069795
C	2.440411	-0.733729	-0.080847
C	4.611287	0.322586	0.032694
H	-6.931595	2.163308	-0.827185
H	-6.845148	2.250282	0.926679
N	4.177331	1.596765	0.048605
C	3.855862	-0.847772	-0.026442
O	1.596661	-1.639321	-0.133234
H	1.021906	0.777597	-0.119032
N	2.272516	2.905935	-0.048003
H	1.285675	2.991728	0.142277
H	2.853156	3.702193	0.166214
N	4.682027	-1.957193	-0.017341
N	5.915104	-0.085620	0.078444
C	5.891643	-1.465307	0.044859
H	6.807335	-2.036766	0.069808
C	7.081739	0.774997	0.146663
H	7.045490	1.389785	1.044313
H	7.971891	0.152419	0.172741
H	7.122496	1.425874	-0.724997

4AP:C cWW

37

4ap-C SCF Done: -1042.52532844 A.U.

C	6.105001	-1.432056	-0.140596
C	2.347425	0.592664	0.056980
N	5.893432	1.408949	0.029417
C	3.493614	1.346900	0.097913
N	0.177325	-0.152053	0.031433
C	4.734561	0.679471	0.038207
C	4.777840	-0.736721	-0.064270
C	3.591658	-1.461851	-0.100394
C	2.380129	-0.795695	-0.039485
C	0.918874	1.007603	0.099986
O	0.465911	2.139416	0.175996
C	0.991750	-1.292216	-0.057677

O	0.583469	-2.432936	-0.133406
H	3.458442	2.426469	0.174816
H	3.624653	-2.541572	-0.177410
H	5.975667	-2.507345	-0.239978
H	6.760338	0.958479	0.272082
H	5.837343	2.378261	0.304266
H	-0.855725	-0.150875	0.049643
C	-5.786939	-1.832513	0.063485
C	-3.537171	-0.847448	0.122809
N	-2.731840	0.245969	0.067514
C	-3.244355	1.467794	-0.082536
N	-2.405635	2.508688	-0.119475
C	-5.445196	0.589050	-0.153005
H	-6.522135	0.653459	-0.234579
H	-5.656614	-2.345476	1.014113
H	-2.768252	3.442472	-0.225357
H	-1.403447	2.378255	-0.006734
H	6.689603	-1.079057	-0.994169
H	6.706641	-1.250644	0.755167
H	-5.527295	-2.523653	-0.735616
H	-6.820596	-1.516409	-0.045018
N	-4.929444	-0.653713	0.006303
C	-4.650896	1.681328	-0.203917
O	-3.114263	-1.993398	0.268144
H	-5.064197	2.670241	-0.328445

4AP:U cWW

36

4ap-U SCF Done: -1062.40916369 A.U.

C	6.376600	-0.469198	0.001958
C	2.181607	0.349503	-0.006905
N	5.321923	2.183362	-0.045195
C	3.049832	1.411967	-0.005812
N	0.337090	-1.006175	-0.006544
C	4.434601	1.143063	0.000901
C	4.900687	-0.198973	0.005500
C	3.985306	-1.245945	0.006051
C	2.628823	-0.970444	-0.000410
C	0.694501	0.322869	-0.009984
O	-0.081349	1.266978	-0.014399
C	1.452713	-1.858767	-0.000268
O	1.390138	-3.070789	0.004426
H	2.693214	2.434399	-0.008282
H	4.340534	-2.269071	0.010131
H	6.575734	-1.538237	-0.014529
H	6.276473	2.031385	0.235734
H	4.970783	3.108756	0.150989
H	-0.639656	-1.311403	-0.006899
C	-5.069945	-2.197663	0.004060
C	-3.281253	-0.550736	-0.002510
N	-2.921677	0.768371	-0.003170

C	-3.778079	1.872462	0.002048
C	-5.544414	0.228726	0.008684
H	-6.583175	-0.073036	0.013201
H	-4.687937	-2.706769	0.886002
H	6.860584	-0.019326	-0.868920
H	6.864137	-0.053173	0.888765
H	-4.695437	-2.705227	-0.881971
H	-6.155152	-2.221113	0.008639
N	-4.640028	-0.799561	0.003417
C	-5.178254	1.524311	0.008410
O	-2.466152	-1.470436	-0.006866
H	-5.914178	2.312225	0.012718
O	-3.316370	3.006472	0.000897
H	-1.913580	0.963758	-0.007934

4AP:U1 cWW

36

4ap-U1 SCF Done: -1062.41029550 A.U.

C	-5.238974	-2.584131	-0.010847
C	-2.791768	0.922725	0.018469
N	-6.317826	0.051185	0.174670
C	-4.152573	1.079684	0.079353
N	-0.520102	1.221640	-0.060797
C	-4.961223	-0.076934	0.066996
C	-4.364931	-1.364496	-0.007675
C	-2.980918	-1.478906	-0.068999
C	-2.198121	-0.336453	-0.055097
C	-1.704067	1.944321	0.013638
O	-1.791614	3.152831	0.062767
C	-0.741911	-0.149295	-0.103689
O	0.145570	-0.990117	-0.167185
H	-4.607110	2.060980	0.135353
H	-2.525523	-2.459816	-0.125719
H	-4.640190	-3.491276	-0.048315
H	-6.913618	-0.713663	-0.095657
H	-6.718314	0.966633	0.035170
H	0.424067	1.624573	-0.083616
C	6.179140	-1.711529	0.146997
C	3.822045	-1.125002	0.005771
N	2.878843	-0.124971	-0.060311
C	3.113806	1.240890	-0.064138
C	5.441623	0.643240	0.066631
H	6.496579	0.877227	0.119570
H	6.134967	-2.355652	-0.728348
H	-5.864867	-2.626463	0.884427
H	-5.912860	-2.594095	-0.872739
H	6.039390	-2.321899	1.036432
H	7.144273	-1.216432	0.189869
N	5.138234	-0.687678	0.071231
C	4.501875	1.608274	0.002049
O	3.531463	-2.308915	0.006855

H	4.769772	2.652378	0.001185
O	2.173617	2.039622	-0.121058
H	1.903087	-0.445419	-0.108934

4AP:T cWW

39

4ap-T SCF Done: -1101.74670844 A.U.

C	-6.699738	0.203284	-0.099315
C	-2.466741	-0.368900	0.032693
N	-5.495894	-2.381803	-0.012981
C	-3.272629	-1.479400	0.051201
N	-0.703181	1.091035	0.031520
C	-4.670070	-1.291319	0.013790
C	-5.211690	0.020738	-0.045503
C	-4.358240	1.118591	-0.059747
C	-2.988691	0.922194	-0.020121
C	-0.983924	-0.255746	0.065119
O	-0.155108	-1.152737	0.110680
C	-1.865552	1.876702	-0.020552
O	-1.873066	3.089849	-0.056016
H	-2.858603	-2.478967	0.095711
H	-4.770990	2.118875	-0.103074
H	-6.960637	1.257103	-0.164823
H	-6.464875	-2.274685	0.237686
H	-5.098426	-3.277875	0.226181
H	0.254843	1.453126	0.050640
C	4.610904	2.616131	0.021832
C	2.924537	0.871106	0.052837
N	2.647656	-0.468236	0.041872
C	3.568204	-1.513160	-0.011685
C	5.227943	0.222044	-0.042300
H	6.243688	0.593768	-0.073177
H	4.234476	3.089232	0.926085
H	-7.131609	-0.308842	-0.963154
H	-7.187619	-0.205401	0.790754
H	4.176764	3.117043	-0.840683
H	5.692450	2.700898	-0.012130
N	4.260006	1.196566	0.011189
C	4.958641	-1.098426	-0.057184
O	2.051806	1.738177	0.097388
O	3.179368	-2.674827	-0.016893
H	1.655298	-0.729125	0.074478
C	6.020482	-2.149437	-0.118381
H	5.961793	-2.812246	0.746350
H	5.896854	-2.775273	-1.003593
H	7.011865	-1.700669	-0.145832

4AP:T1 cWW

39

4ap-T1 SCF Done: -1101.74763167 A.U.

C	5.618264	-2.433855	0.002163
C	2.984706	0.934456	-0.009492
N	6.556905	0.259777	-0.091550
C	4.336106	1.166910	-0.030620
N	0.698351	1.106595	0.019329
C	5.206798	0.056237	-0.023520
C	4.679859	-1.263221	0.004954
C	3.303243	-1.454509	0.027324
C	2.459580	-0.356497	0.019593
C	1.842213	1.894571	-0.008819
O	1.863885	3.106904	-0.028315
C	0.994487	-0.250590	0.036886
O	0.154544	-1.140707	0.061166
H	4.736708	2.172785	-0.051172
H	2.901478	-2.459906	0.048861
H	5.068920	-3.372457	0.003595
H	7.185408	-0.478262	0.178976
H	6.903386	1.191865	0.079060
H	-0.267097	1.456055	0.027968
C	-5.839429	-2.192794	-0.056079
C	-3.515934	-1.487643	-0.002314
N	-2.628102	-0.435972	0.023260
C	-2.937169	0.911762	0.025614
C	-5.223034	0.198725	-0.023697
H	-6.291741	0.368100	-0.043386
H	-5.736316	-2.822804	0.824772
H	6.267051	-2.421037	-0.877597
H	6.270789	-2.428748	0.880399
H	-5.699170	-2.808040	-0.942220
H	-6.828818	-1.746451	-0.073158
N	-4.848155	-1.118979	-0.026512
C	-4.348610	1.226770	0.001189
O	-3.158412	-2.655008	-0.003649
O	-2.041011	1.761942	0.047687
H	-1.634819	-0.699296	0.041119
C	-4.771176	2.661647	0.003809
H	-4.398538	3.176064	0.890877
H	-4.365455	3.189075	-0.860821
H	-5.856249	2.746255	-0.016029

GC cWW

35

GC-gd3bj SCF Done: -1016.62215935 A.U.

C	5.155458	-1.894665	0.000585
N	4.352581	-0.675116	0.000338
C	2.956951	-0.803008	0.000301
O	2.473491	-1.944051	0.000481
N	2.202187	0.317819	0.000058

C	2.767904	1.529138	-0.000129
N	1.967997	2.595184	-0.000354
C	4.187459	1.682370	-0.000099
C	4.929624	0.553570	0.000138
C	-5.528310	-1.490702	0.000024
N	-0.686722	-0.019946	-0.000162
C	-1.209896	-1.288997	-0.000182
N	-0.332556	-2.301573	-0.000343
N	-2.511730	-1.533692	-0.000139
C	-3.256001	-0.415486	-0.000107
C	-2.827511	0.910978	-0.000105
C	-1.428794	1.164195	-0.000125
O	-0.851197	2.261394	-0.000168
N	-3.913232	1.770684	-0.000207
C	-4.956210	0.983159	0.000133
N	-4.623336	-0.357139	-0.000094
H	4.931387	-2.489866	0.883083
H	2.366533	3.520616	-0.000480
H	4.650195	2.657204	-0.000255
H	6.011168	0.572076	0.000181
H	-5.366254	-2.104326	-0.884616
H	0.679550	-2.154058	0.000012
H	-0.704568	-3.237000	-0.000025
H	-5.988684	1.298700	0.000206
H	-5.368229	-2.102708	0.886159
H	-6.550154	-1.120857	-0.001449
H	6.205715	-1.617767	0.000579
H	4.931458	-2.490174	-0.881724
H	0.950357	2.482635	-0.000315
H	0.342807	0.089915	-0.000139

Coordinates of the In Gas Phase optimized structures:

4AP:DAP cWW

38

4ap-nos SCF Done: -1022.63628875 A.U.

C	5.885520	-1.676183	0.019104
C	2.328391	0.693506	-0.008526
N	5.945371	1.169951	0.000738
C	3.541554	1.336118	0.016220
N	0.103458	0.145818	-0.046880
C	4.709102	0.553559	0.030059
C	4.625526	-0.859786	0.016289
C	3.376318	-1.474023	-0.006483
C	2.234751	-0.695352	-0.019281
C	0.938715	1.243975	-0.023233
O	0.578885	2.404863	-0.014611
C	0.797899	-1.055489	-0.042230
O	0.277096	-2.156167	-0.053238

H	3.598335	2.416558	0.023646
H	3.303074	-2.553217	-0.015956
H	5.659687	-2.739306	-0.021487
H	6.732994	0.646890	0.341497
H	5.967430	2.142907	0.254511
H	-0.943169	0.207586	-0.055631
C	-5.677968	-1.982867	0.071346
C	-4.823578	-0.752651	0.041829
N	-2.763282	-2.006110	-0.047090
C	-3.412858	-0.821027	-0.014664
N	-4.624133	1.649687	0.039493
N	-2.667227	0.291391	-0.043503
C	-3.298593	1.479142	-0.018070
N	-2.530221	2.591799	-0.062932
C	-5.342840	0.525549	0.066812
H	-6.420203	0.656707	0.112524
H	-5.468970	-2.608426	0.944824
H	-3.281508	-2.860434	0.013133
H	-1.751176	-2.060076	-0.056460
H	-2.997648	3.475248	0.010530
H	-1.521133	2.555153	-0.041185
H	6.520236	-1.432329	-0.836680
H	6.479136	-1.502132	0.922362
H	-5.531385	-2.605223	-0.816631
H	-6.732942	-1.714054	0.109974

4AP:A cWW

39

4ap-A SCF Done: -1114.90713383 A.U.

C	6.888976	1.187073	0.026878
C	2.988519	-0.555790	-0.001834
N	6.476528	-1.629402	0.061774
C	4.078107	-1.392891	0.000648
N	0.881878	0.344658	-0.010717
C	5.359053	-0.816191	0.004300
C	5.510986	0.591351	0.008268
C	4.381207	1.405170	0.002839
C	3.126137	0.827684	-0.001942
C	1.529808	-0.868357	-0.007830
O	0.997131	-1.965588	-0.010062
C	1.769336	1.430250	-0.007655
O	1.445018	2.594128	-0.009926
H	3.953436	-2.467682	0.001314
H	4.487806	2.481696	0.004894
H	6.842035	2.273069	0.062625
H	7.342635	-1.247206	-0.275991
H	6.339156	-2.593338	-0.190509
H	-0.153042	0.424077	-0.013584
C	-2.656303	1.482411	-0.013989
N	-1.965918	0.332035	-0.012964
C	-2.625268	-0.843729	-0.004925

N	-1.941715	-1.994763	-0.004171
C	-4.612788	0.471742	0.000094
H	-2.457932	-2.855510	0.004796
H	-0.924973	-2.012557	-0.006794
H	7.459267	0.843955	0.893869
H	7.461613	0.913878	-0.865486
N	-3.972510	1.646433	-0.007954
C	-4.032387	-0.794356	0.002099
N	-4.998910	-1.779866	0.011388
N	-5.967935	0.248923	0.008339
C	-6.997243	1.268286	0.010112
H	-7.970927	0.784845	0.015791
H	-6.902261	1.900057	0.891728
H	-6.910056	1.895064	-0.875854
H	-2.051464	2.381571	-0.020267
C	-6.128332	-1.119878	0.014841
H	-7.111244	-1.563001	0.022087

4AP:G cWW

40

4ap-G SCF Done: -1190.18115095 A.U.

C	-6.199382	2.264649	0.091903
C	-3.439354	-0.996998	-0.006449
N	-7.043071	-0.453966	0.096985
C	-4.781031	-1.279472	0.051344
N	-1.141946	-1.075515	-0.101918
C	-5.686238	-0.204303	0.089097
C	-5.214776	1.131642	0.063632
C	-3.846322	1.375777	0.005984
C	-2.966310	0.309820	-0.028712
C	-2.261136	-1.917237	-0.051901
O	-2.246121	-3.121007	-0.046933
C	-1.493269	0.259163	-0.089878
O	-0.708584	1.201074	-0.125386
H	-5.132251	-2.302736	0.066714
H	-3.478495	2.392810	-0.013604
H	-5.690282	3.223908	0.031516
H	-7.650207	0.267093	0.444575
H	-7.330216	-1.384654	0.346868
H	-0.161243	-1.401250	-0.133477
C	2.833248	1.666167	-0.087807
N	2.022444	0.573005	-0.149803
C	2.438036	-0.772141	-0.110787
C	4.589542	0.328067	0.039010
H	-6.902653	2.202565	-0.742467
H	-6.789925	2.265890	1.013763
N	4.139465	1.601077	0.013340
C	3.859657	-0.859459	-0.015478
O	1.597646	-1.668325	-0.155456
H	1.010883	0.733347	-0.202662

N	2.211803	2.875858	-0.176905
H	1.222412	2.924077	0.000048
H	2.768543	3.672267	0.076517
N	4.704875	-1.948431	0.046996
N	5.899179	-0.050417	0.135976
C	5.899178	-1.435272	0.134279
H	6.821188	-1.989873	0.200993
C	7.038457	0.839365	0.212564
H	6.938940	1.510397	1.064287
H	7.940195	0.243417	0.328974
H	7.118530	1.438934	-0.693344

4AP:C cWW

37

4ap-C SCF Done: -1042.49511838 A.U.

C	6.139296	-1.351702	-0.063450
C	2.323894	0.565435	0.022039
N	5.858775	1.481245	-0.019444
C	3.450776	1.352752	0.040610
N	0.173962	-0.231831	0.010175
C	4.703334	0.718730	0.018403
C	4.790308	-0.693622	-0.025659
C	3.624464	-1.454725	-0.040815
C	2.397787	-0.820015	-0.016788
C	0.882657	0.944608	0.037682
O	0.418594	2.074269	0.066766
C	1.015573	-1.363888	-0.026356
O	0.653173	-2.511206	-0.059417
H	3.374935	2.431733	0.069669
H	3.680184	-2.534563	-0.073393
H	6.042056	-2.432684	-0.133635
H	6.703093	1.049016	0.313758
H	5.764448	2.440816	0.267492
H	-0.856072	-0.252248	0.019043
C	-5.776095	-1.824245	0.030610
C	-3.524234	-0.843174	0.052224
N	-2.728158	0.263466	0.025291
C	-3.243136	1.482431	-0.035639
N	-2.400601	2.525567	-0.054099
C	-5.450495	0.609845	-0.059927
H	-6.528814	0.679752	-0.091647
H	-5.597291	-2.389703	0.942951
H	-2.760448	3.459913	-0.094360
H	-1.391802	2.377749	-0.006834
H	6.726190	-1.008000	-0.919037
H	6.722617	-1.133987	0.837276
H	-5.536762	-2.469463	-0.812121
H	-6.818530	-1.518913	-0.019054
N	-4.934688	-0.636170	0.004699

C	-4.657065	1.705138	-0.082462
O	-3.108641	-1.985266	0.113178
H	-5.076225	2.696866	-0.133498

4AP:U cWW

36

4ap-U SCF Done: -1062.38344179 A.U.

C	-6.389591	0.376974	-0.003540
C	-2.176567	-0.324662	-0.006821
N	-5.279306	-2.242989	-0.052700
C	-3.018496	-1.410353	-0.006591
N	-0.365313	1.075663	-0.004397
C	-4.403441	-1.175300	-0.000190
C	-4.905822	0.149102	0.002625
C	-4.018538	1.221658	0.004383
C	-2.658082	0.979301	-0.000513
C	-0.688161	-0.262990	-0.008350
O	0.098075	-1.193830	-0.011326
C	-1.500786	1.906712	0.001045
O	-1.481624	3.112845	0.006491
H	-2.625424	-2.418290	-0.011952
H	-4.393099	2.236488	0.007480
H	-6.619871	1.439420	-0.036072
H	-6.213269	-2.093135	0.286656
H	-4.902328	-3.143609	0.188772
H	0.604090	1.397479	-0.004139
C	5.021056	2.213095	0.003740
C	3.271045	0.528238	-0.001068
N	2.939070	-0.795987	-0.001852
C	3.821963	-1.890619	0.001239
C	5.558682	-0.203473	0.004964
H	6.588083	0.123892	0.007422
H	4.626628	2.714808	0.884811
H	-6.861830	-0.098406	-0.867089
H	-6.866318	-0.033560	0.892533
H	4.628626	2.715730	-0.877655
H	6.105751	2.268639	0.005030
N	4.630568	0.806907	0.002451
C	5.221526	-1.503230	0.004410
O	2.451492	1.440060	-0.003072
H	5.967033	-2.280107	0.006571
O	3.400180	-3.028271	0.001219
H	1.933070	-1.007663	-0.005381

4AP:U1 cWW

36

4ap-U1 SCF Done: -1062.38495620 A.U.

C	-5.181677	-2.636434	0.006719
C	-2.829509	0.932746	0.006481

N	-6.344933	-0.039315	0.076134
C	-4.197313	1.051601	0.017065
N	-0.561884	1.288668	-0.008995
C	-4.967355	-0.124018	0.011970
C	-4.339437	-1.393565	-0.001274
C	-2.950234	-1.472237	-0.013737
C	-2.203936	-0.308581	-0.009432
C	-1.769951	1.988689	0.005566
O	-1.899895	3.187541	0.014461
C	-0.743745	-0.084898	-0.018913
O	0.149732	-0.915554	-0.032575
H	-4.669792	2.024933	0.030322
H	-2.460566	-2.436693	-0.024433
H	-4.558678	-3.527663	0.027865
H	-6.874596	-0.824718	-0.259306
H	-6.750688	0.850815	-0.157228
H	0.372948	1.708791	-0.014379
C	6.225324	-1.683327	0.027397
C	3.855473	-1.141406	-0.000398
N	2.893688	-0.153895	-0.013065
C	3.105153	1.218386	-0.013375
C	5.452189	0.663377	0.012513
H	6.503224	0.913703	0.023222
H	6.149250	-2.319203	-0.852153
H	-5.842070	-2.664321	0.877259
H	-5.816325	-2.702075	-0.883053
H	6.130630	-2.313183	0.909487
H	7.188213	-1.180544	0.035898
N	5.173555	-0.672930	0.012842
C	4.495661	1.610348	0.000004
O	3.605025	-2.327096	-0.000492
H	4.734983	2.659750	0.000198
O	2.163770	2.006490	-0.024294
H	1.917581	-0.482410	-0.022417

4AP:T cWW

39

4ap-T SCF Done: -1101.72219975 A.U.

C	-6.713675	0.110978	0.018843
C	-2.467230	-0.344235	-0.015897
N	-5.453440	-2.439596	-0.059963
C	-3.244802	-1.476970	-0.019614
N	-0.739603	1.158440	-0.012817
C	-4.640836	-1.322917	-0.002979
C	-5.219050	-0.030048	0.014149
C	-4.395405	1.092226	0.019429
C	-3.023297	0.929490	0.004075
C	-0.985013	-0.196361	-0.025508
O	-0.146299	-1.080297	-0.039958
C	-1.921010	1.922187	0.005927
O	-1.972169	3.127322	0.020634

H	-2.794128	-2.460391	-0.035802
H	-4.828061	2.083517	0.033274
H	-7.005978	1.158331	-0.004697
H	-6.391644	-2.348057	0.288462
H	-5.022263	-3.318379	0.171247
H	0.210755	1.535465	-0.017302
C	4.564120	2.624667	0.000058
C	2.915670	0.846901	-0.013095
N	2.664434	-0.496450	-0.012411
C	3.609848	-1.529527	0.002922
C	5.241272	0.242455	0.014000
H	6.248140	0.634853	0.023295
H	4.134233	3.107459	0.875273
H	-7.162963	-0.385450	-0.845069
H	-7.159652	-0.332673	0.914953
H	4.154002	3.102914	-0.887055
H	5.644000	2.739496	0.011880
N	4.251193	1.199460	0.000267
C	4.999234	-1.079963	0.016072
O	2.039094	1.706170	-0.024531
O	3.260667	-2.693766	0.004534
H	1.673968	-0.771122	-0.023547
C	6.073512	-2.118795	0.031337
H	5.975420	-2.762066	0.906802
H	5.992810	-2.769717	-0.840219
H	7.062897	-1.663113	0.039225

4AP:T1 cWW

39

4ap-T1 SCF Done: -1101.71908511 A.U.

C	5.492715	-2.562815	-0.055109
C	3.061584	0.955018	0.017582
N	6.599120	0.060398	0.000131
C	4.425867	1.101450	0.045331
N	0.786573	1.267125	-0.008117
C	5.222252	-0.056509	0.025975
C	4.623608	-1.338802	-0.023185
C	3.236703	-1.446157	-0.048001
C	2.465370	-0.298368	-0.028379
C	1.978692	1.988834	0.034471
O	2.084071	3.188174	0.071594
C	1.000347	-0.109330	-0.044144
O	0.140086	-0.970461	-0.072811
H	4.875276	2.085124	0.081224
H	2.768931	-2.420880	-0.085083
H	4.889618	-3.465060	-0.126686
H	7.136322	-0.724436	0.325173
H	6.976979	0.949832	0.278991
H	-0.154065	1.665942	-0.013205

C	-5.957482	-2.122837	0.078102
C	-3.604853	-1.525578	0.026037
N	-2.681971	-0.499916	-0.011598
C	-2.932915	0.861905	-0.034659
C	-5.245567	0.242146	0.013612
H	-6.304945	0.456329	0.025688
H	-5.841047	-2.734589	0.970412
H	6.176243	-2.544601	-0.907816
H	6.104774	-2.649903	0.848596
H	-5.870170	-2.773293	-0.789834
H	-6.932932	-1.644703	0.083640
N	-4.929171	-1.089384	0.038505
C	-4.333785	1.235075	-0.023784
O	-3.307739	-2.698860	0.042321
O	-2.007892	1.668891	-0.065864
H	-1.694354	-0.760735	-0.037762
C	-4.685461	2.689228	-0.051996
H	-4.257227	3.210304	0.805420
H	-4.280674	3.170369	-0.943431
H	-5.765218	2.831219	-0.040816

Optimized structures of the 4AP base pairing with DAP and natural bases in tWW geometries:

In Water optimized structures:

4AP:DAP tWW

38

4ap-dap-trans SCF Done: -1022.65589980 A.U.

C	6.081622	1.172406	0.158392
C	2.245604	-0.705094	-0.046876
N	5.751231	-1.663652	0.102955
C	3.359921	-1.504628	-0.028220
N	0.115486	0.133409	-0.107708
C	4.626964	-0.886626	0.035391
C	4.728176	0.529265	0.079615
C	3.572721	1.303297	0.057348
C	2.335232	0.686654	-0.005674
C	0.799022	-1.062122	-0.110707
O	0.280220	-2.165655	-0.155138
C	0.966767	1.232376	-0.041247
O	0.583566	2.391148	-0.019372
H	3.282332	-2.584270	-0.062138
H	3.650249	2.383006	0.090921
H	5.994760	2.255288	0.210287
H	6.644006	-1.262060	-0.131518
H	5.659926	-2.641699	-0.127837
H	-0.924692	0.203840	-0.135253
C	-5.705685	-1.951133	0.200493
C	-4.841288	-0.730687	0.110438
N	-2.796696	-1.998805	-0.112146

C	-3.435050	-0.811940	-0.037303
N	-4.618502	1.672250	0.084176
N	-2.684762	0.296390	-0.121288
C	-3.300340	1.489850	-0.061830
N	-2.522113	2.595264	-0.187997
C	-5.346208	0.549462	0.164729
H	-6.417389	0.688919	0.282548
H	-5.444005	-2.575921	1.059497
H	-3.296853	-2.857426	0.036592
H	-1.785530	-2.045273	-0.144558
H	-2.948657	3.482513	0.031179
H	-1.516568	2.524464	-0.106486
H	6.631982	0.832525	1.039589
H	6.694676	0.929238	-0.714676
H	-5.619310	-2.577713	-0.691584
H	-6.752457	-1.669857	0.306270

4AP:A tWW

39

4ap-A-trans SCF Done: -1114.92928601 A.U.

C	6.616667	-1.650325	-0.002728
C	3.134814	0.831919	-0.004309
N	6.753484	1.200675	-0.047519
C	4.365268	1.438146	-0.004093
N	0.892543	0.349578	-0.002454
C	5.515143	0.620418	0.000251
C	5.384641	-0.793945	0.003595
C	4.118210	-1.368143	0.005098
C	2.997620	-0.555113	0.000798
C	1.765259	1.426632	-0.005601
O	1.442430	2.597192	-0.008822
C	1.560185	-0.869381	0.001546
O	1.006235	-1.959841	0.004996
H	4.464644	2.516563	-0.005705
H	4.018204	-2.446498	0.008019
H	6.355987	-2.706122	-0.018349
H	7.560604	0.668037	0.231803
H	6.816673	2.188536	0.147985
H	-0.141749	0.418669	-0.001426
C	-2.665967	1.475078	0.004489
N	-1.974055	0.327261	0.001379
C	-2.633738	-0.851261	-0.001616
N	-1.941106	-1.995501	-0.004625
C	-4.626472	0.462445	0.001909
H	-0.924855	-1.996353	-0.001573
H	-2.437171	-2.872025	-0.005474
H	7.241389	-1.441264	-0.875094
H	7.234569	-1.473055	0.882641
N	-3.982928	1.638433	0.005111
C	-4.041459	-0.802548	-0.001625

N	-5.009589	-1.787795	-0.004221
N	-5.979926	0.238479	0.001489
C	-7.020629	1.250587	0.004954
H	-7.987885	0.755509	0.001828
H	-6.937008	1.873538	0.893710
H	-6.935236	1.881265	-0.878143
H	-2.063415	2.377308	0.006748
C	-6.142105	-1.126590	-0.002192
H	-7.127646	-1.568315	-0.003324

4AP:G tWW

40

4ap-G-trans SCF Done: -1190.21124393 A.U.

C	-7.196406	-0.455131	0.093481
C	-2.996157	0.324078	-0.026900
N	-6.117908	2.187572	0.044154
C	-3.854503	1.394477	-0.033310
N	-1.161169	-1.046121	-0.040478
C	-5.241191	1.138229	0.002686
C	-5.718721	-0.199130	0.045190
C	-4.812731	-1.254415	0.048556
C	-3.454266	-0.991401	0.012824
C	-1.510785	0.282594	-0.061958
O	-0.727754	1.222944	-0.102397
C	-2.284857	-1.888851	0.005153
O	-2.231620	-3.100797	0.030633
H	-3.489102	2.413233	-0.066874
H	-5.176772	-2.273932	0.080272
H	-7.404693	-1.521325	0.144632
H	-7.080757	2.037277	-0.207906
H	-5.764011	3.104237	-0.185293
H	-0.182354	-1.364298	-0.059310
C	2.879389	1.689759	0.005458
N	2.041730	0.608371	-0.040845
C	2.441048	-0.733254	-0.056610
C	4.619075	0.311791	0.021191
H	-7.653983	0.023238	0.963433
H	-7.702514	-0.058848	-0.791965
N	4.192321	1.588350	0.041974
C	3.856558	-0.854555	-0.024038
O	1.592016	-1.634347	-0.095038
H	1.031209	0.785464	-0.076577
N	2.293871	2.908177	-0.027239
H	1.311130	3.000720	0.180375
H	2.882899	3.701187	0.176026
N	4.676809	-1.968350	-0.026701
N	5.921226	-0.103306	0.046541
C	5.889875	-1.482884	0.015315
H	6.802793	-2.059197	0.026367
C	7.093350	0.751197	0.094503

H	7.073983	1.368648	0.990833
H	7.980446	0.123903	0.108855
H	7.124365	1.399434	-0.779533

4AP:C tWW

37

4ap-C-trans SCF Done: -1042.52560363 A.U.

C	6.033761	1.418104	0.062406
C	2.381364	-0.802779	-0.028951
N	5.963220	-1.431611	-0.065856
C	3.564085	-1.495182	-0.084835
N	0.176923	-0.162830	0.031862
C	4.769730	-0.762969	-0.058493
C	4.742225	0.655152	0.024895
C	3.520977	1.317642	0.076858
C	2.344921	0.586952	0.050445
C	0.974229	-1.298999	-0.042785
O	0.579342	-2.444095	-0.106152
C	0.935210	1.002649	0.087959
O	0.469697	2.131671	0.152133
H	3.584456	-2.575992	-0.149101
H	3.498540	2.398599	0.138622
H	5.851350	2.487146	0.144739
H	6.804075	-0.941124	-0.321854
H	5.953207	-2.407456	-0.322119
H	-0.856152	-0.150864	0.048153
C	-5.795339	-1.811252	0.041321
C	-3.540631	-0.837901	0.105173
N	-2.730201	0.252142	0.062194
C	-3.237413	1.478824	-0.065804
N	-2.393467	2.515439	-0.093343
C	-5.443239	0.612175	-0.135225
H	-6.520349	0.683144	-0.208786
H	-5.543480	-2.489572	-0.771159
H	-1.389859	2.376955	0.001235
H	-2.751896	3.452237	-0.186077
H	6.651916	1.112326	0.910637
H	6.626686	1.250244	-0.841731
H	-5.662210	-2.341297	0.982127
H	-6.828083	-1.488554	-0.055898
N	-4.932601	-0.635656	-0.000281
C	-4.643850	1.701214	-0.173116
O	-3.122610	-1.988081	0.230108
H	-5.052943	2.694081	-0.278628

4AP:U tWW

36

4ap-U-trans SCF Done: -1062.40999522 A.U.

C	-6.461950	-0.007153	0.120129
C	-2.204507	-0.335896	-0.055032
N	-5.114915	-2.516844	-0.069451
C	-2.945633	-1.490541	-0.068731
N	-0.525397	1.220909	-0.058409
C	-4.350663	-1.383312	-0.008263
C	-4.965566	-0.104804	0.065017
C	-4.175681	1.040061	0.077698
C	-2.797815	0.922961	0.016922
C	-0.731383	-0.138577	-0.101074
O	0.146200	-0.987546	-0.162331
C	-1.729506	1.939242	0.014612
O	-1.805012	3.149604	0.063261
H	-2.475466	-2.464500	-0.122860
H	-4.644644	2.014598	0.133919
H	-6.783122	1.031545	0.148217
H	-6.068922	-2.487020	0.250438
H	-4.652888	-3.401521	0.079372
H	0.413876	1.634357	-0.079107
C	6.188102	-1.699459	0.144198
C	3.829674	-1.118206	0.006004
N	2.884316	-0.120141	-0.058258
C	3.115356	1.246598	-0.061479
C	5.444852	0.653845	0.065692
H	6.499320	0.890312	0.117272
H	6.143848	-2.343712	-0.731042
H	-6.923026	-0.482478	-0.749611
H	-6.864940	-0.504715	1.007322
H	6.051068	-2.310113	1.033868
H	7.152221	-1.202286	0.185501
N	5.144772	-0.677886	0.070061
C	4.502822	1.616864	0.002929
O	3.541447	-2.302714	0.006892
H	4.768713	2.661477	0.002219
O	2.172856	2.042500	-0.116440
H	1.909995	-0.442713	-0.105894

4AP:U1 tWW

36

4ap-U1-trans SCF Done: -1062.40943319 A.U.

C	-5.449172	2.236090	-0.002798
C	-2.624987	-0.974577	-0.004963
N	-6.230792	-0.508219	-0.039896
C	-3.960749	-1.284867	-0.002410
N	-0.333276	-1.013941	-0.005397
C	-4.894196	-0.226216	0.002514
C	-4.444554	1.121713	0.003076
C	-3.081107	1.392219	0.002125

C	-2.175150	0.344918	-0.001962
C	-1.429726	-1.867588	-0.006572
O	-1.380655	-3.079083	-0.008554
C	-0.706491	0.325038	-0.002429
O	0.080520	1.262053	-0.000360
H	-4.302958	-2.312330	-0.002150
H	-2.737639	2.419241	0.003188
H	-4.954859	3.204651	-0.023744
H	-6.896898	0.196461	0.229342
H	-6.520068	-1.455990	0.149752
H	0.647020	-1.308114	-0.004193
C	5.076421	-2.180913	0.007176
C	3.279869	-0.542555	0.002045
N	2.913285	0.774436	-0.000419
C	3.764346	1.882521	-0.001661
C	5.539167	0.247799	0.002908
H	6.579418	-0.048798	0.004445
H	4.701325	-2.692907	-0.876054
H	-6.108790	2.172406	-0.872232
H	-6.087462	2.207585	0.885424
H	4.699845	-2.689246	0.891901
H	6.161743	-2.199203	0.008140
N	4.639815	-0.784906	0.003942
C	5.166383	1.541458	0.000155
O	2.469432	-1.466577	0.002615
H	5.898265	2.333144	-0.000662
O	3.297476	3.014479	-0.004057
H	1.903333	0.964294	-0.001141

4AP:T tWW

39

4ap-T-trans SCF Done: -1101.74733969 A.U.

C	-6.700581	0.219556	-0.039815
C	-2.467316	-0.362474	0.009489
N	-5.501323	-2.368521	-0.027518
C	-3.275189	-1.471659	0.019043
N	-0.700388	1.094317	0.008071
C	-4.672587	-1.280223	0.008480
C	-5.212261	0.033629	-0.014890
C	-4.356770	1.130077	-0.021379
C	-2.987239	0.930356	-0.008865
C	-0.983966	-0.251795	0.019991
O	-0.155926	-1.150978	0.035249
C	-1.861630	1.882496	-0.009512
O	-1.867835	3.096249	-0.021574
H	-2.862755	-2.472721	0.036429
H	-4.767974	2.131804	-0.037641
H	-6.960699	1.274858	-0.080049
H	-6.465350	-2.264607	0.242787
H	-5.101777	-3.269703	0.187898

H	0.261664	1.452847	0.015331
C	5.855246	-2.173757	-0.040965
C	3.527956	-1.480402	-0.006886
N	2.634773	-0.432947	0.012130
C	2.936802	0.916584	0.019126
C	5.226515	0.214626	-0.011301
H	6.294490	0.389319	-0.021382
H	5.725754	-2.788972	-0.928756
H	-7.148019	-0.274597	-0.906206
H	-7.174186	-0.205923	0.850102
H	5.747755	-2.804944	0.838515
H	6.842452	-1.722361	-0.049194
N	4.858324	-1.104985	-0.019118
C	4.346863	1.238329	0.007391
O	3.175851	-2.649318	-0.012629
O	2.036341	1.762133	0.034559
H	1.643682	-0.701774	0.021834
C	4.762395	2.675234	0.015991
H	4.361094	3.202289	-0.850914
H	4.380134	3.186174	0.900977
H	5.847162	2.765107	0.005076

4AP:T1 tWW

39

4ap-T1-trans SCF Done: -1101.74699170 A.U.

C	5.612433	-2.447753	0.013357
C	2.986447	0.926390	-0.018556
N	6.555674	0.242378	-0.136451
C	4.337939	1.155296	-0.061080
N	0.701452	1.103971	0.036587
C	5.206327	0.042841	-0.047572
C	4.676916	-1.274821	0.009152
C	3.300344	-1.462423	0.052348
C	2.458939	-0.362710	0.037937
C	1.846533	1.889195	-0.018246
O	1.869940	3.100909	-0.056573
C	0.994458	-0.254116	0.072160
O	0.153482	-1.141776	0.120873
H	4.740402	2.159761	-0.102980
H	2.896645	-2.466355	0.095250
H	5.060918	-3.384789	0.036404
H	7.186688	-0.492948	0.135545
H	6.906502	1.176343	0.013656
H	-0.260023	1.457018	0.055187
C	-4.619434	2.603344	0.010910
C	-2.924608	0.866657	0.051471
N	-2.640638	-0.471037	0.044993
C	-3.555873	-1.520422	-0.007355
C	-5.224616	0.206074	-0.046381
H	-6.242142	0.572635	-0.080337

H	-4.187502	3.103067	-0.853431
H	6.250339	-2.450424	-0.874419
H	6.275753	-2.430388	0.883303
H	-4.245588	3.081832	0.913378
H	-5.701376	2.682735	-0.023714
N	-4.261597	1.185537	0.005970
C	-4.948458	-1.112998	-0.056610
O	-2.056354	1.738402	0.095321
O	-3.161692	-2.680407	-0.008612
H	-1.646058	-0.726235	0.080233
C	-6.004604	-2.169784	-0.116272
H	-5.875756	-2.798135	-0.998955
H	-5.944193	-2.829241	0.750914
H	-6.998320	-1.726449	-0.147367

iG:C tWW

35

iGC-s SCF Done: -1016.62060201 A.U.

C	-2.850877	1.518275	-0.000498
N	-2.200586	0.349510	-0.000043
C	-2.870841	-0.822083	0.000566
C	-4.936073	0.387370	0.000132
C	5.698920	0.942765	0.001053
N	0.687241	0.219789	-0.000447
C	1.376023	1.451931	0.000116
N	2.724523	1.459239	0.000357
C	3.282361	0.249920	0.000103
C	2.658039	-1.002245	-0.000426
C	1.261001	-1.010948	-0.000732
N	3.591656	-2.026036	-0.000686
C	4.742626	-1.409539	0.000234
N	4.625097	-0.031625	0.000362
H	-6.016060	0.327107	0.000213
H	5.636268	1.575061	-0.883192
H	-1.100297	2.590741	-0.000894
H	5.712918	-1.883165	0.000412
H	5.637198	1.572910	0.886909
H	6.649212	0.415526	-0.000085
H	-0.529991	-2.038606	-0.000957
H	-0.346041	0.280145	-0.000645
C	-4.983568	-2.071699	0.001074
H	-4.717051	-2.649639	-0.881119
H	-4.717061	-2.648934	0.883732
H	-6.051184	-1.871897	0.000988
H	-4.811395	2.505499	-0.000742
N	-4.271433	-0.796880	0.000570
C	-4.278116	1.567340	-0.000391
O	0.682416	2.487781	0.000155
O	-2.305130	-1.926210	0.000786
N	0.495715	-2.096492	-0.001481

N	-2.126418	2.635806	-0.001082
H	0.946412	-2.998152	-0.001138
H	-2.588749	3.531117	-0.001238

iC:G tWW:

35

GiC-s SCF Done: -1016.61053471 A.U.

C	-2.797015	1.569780	0.000200
O	-2.101429	2.602661	0.000390
N	-2.207336	0.334104	0.000123
C	-2.932367	-0.771821	-0.000006
N	-2.310518	-1.952971	-0.000064
C	-4.938016	0.469803	-0.000038
C	5.712624	0.892055	0.000019
N	0.698200	0.223821	0.000028
C	1.418640	1.392689	-0.000029
N	0.712535	2.530202	-0.000081
N	2.743242	1.423197	-0.000065
C	3.296203	0.199226	-0.000074
C	2.658812	-1.041127	-0.000042
C	1.238380	-1.063076	0.000002
O	0.489175	-2.052832	0.000049
N	3.591278	-2.065222	0.000008
C	4.747577	-1.456340	-0.000182
N	4.635831	-0.079776	-0.000134
H	-2.807512	-2.825813	-0.000060
H	-6.018476	0.431269	-0.000119
H	5.652436	1.523962	-0.884582
H	-0.313083	2.539965	0.000390
H	1.226941	3.395580	0.000216
H	5.715516	-1.934465	-0.000252
H	5.654096	1.522043	0.886114
H	6.660867	0.361193	-0.001447
H	-1.283434	-1.972119	0.000147
H	-0.334918	0.280779	0.000210
C	-5.082833	-1.987243	-0.000219
H	-4.865572	-2.576655	-0.891085
H	-4.865679	-2.576777	0.890593
H	-6.137494	-1.732161	-0.000265
H	-4.749234	2.574135	0.000151
C	-4.244877	1.620338	0.000103
N	-4.305973	-0.749824	-0.000089

In gas phase optimized geometries for tWW base pairs:

4AP:DAP tWW

38

4ap-dap-trans SCF Done: -1022.63621005 A.U.

C	6.074840	1.166462	0.111796
C	2.234866	-0.703866	-0.029719
N	5.752867	-1.661990	0.100263
C	3.350863	-1.503810	-0.011947
N	0.103601	0.135221	-0.078701
C	4.612587	-0.885349	0.028613
C	4.718088	0.526332	0.054029
C	3.562667	1.302811	0.032759
C	2.327573	0.685001	-0.009119
C	0.784982	-1.062006	-0.072055
O	0.274008	-2.166644	-0.094486
C	0.952060	1.236042	-0.037774
O	0.582058	2.393921	-0.027934
H	3.262264	-2.582067	-0.027202
H	3.634645	2.381975	0.051136
H	5.991577	2.249721	0.161173
H	6.617112	-1.246959	-0.200963
H	5.655669	-2.627866	-0.162411
H	-0.942284	0.205649	-0.098766
C	-5.689048	-1.955218	0.131600
C	-4.827234	-0.731184	0.075278
N	-2.781336	-2.001092	-0.095218
C	-3.420091	-0.809825	-0.031206
N	-4.609390	1.669531	0.070008
N	-2.667825	0.296368	-0.084464
C	-3.287734	1.489146	-0.036433
N	-2.513519	2.596416	-0.116231
C	-5.335207	0.551093	0.121541
H	-6.409118	0.690545	0.207037
H	-5.456098	-2.583958	0.996904
H	-3.299886	-2.848815	0.027690
H	-1.769842	-2.059848	-0.104499
H	-2.970111	3.479077	0.016347
H	-1.504494	2.550516	-0.080987
H	6.636720	0.830156	0.986882
H	6.675402	0.924856	-0.771182
H	-5.575941	-2.576982	-0.761547
H	-6.740199	-1.679154	0.205970

4AP:A tWW

39

4ap-A-trans SCF Done: -1114.90744929 A.U.

C	6.602852	1.652182	0.004766
C	3.125508	-0.833493	0.005524
N	6.756386	-1.190088	0.050764
C	4.359516	-1.435542	0.004098
N	0.881062	-0.354039	0.004797

C	5.500577	-0.615220	-0.001210
C	5.370262	0.794758	-0.002124
C	4.101470	1.367200	-0.002497
C	2.986589	0.550247	0.001613
C	1.755825	-1.436203	0.006418
O	1.442960	-2.603227	0.007320
C	1.540586	0.864061	0.001465
O	0.997840	1.956608	-0.001547
H	4.450975	-2.513743	0.007750
H	3.992137	2.443406	-0.003948
H	6.341841	2.707639	0.034269
H	7.529972	-0.645427	-0.288257
H	6.812579	-2.164342	-0.192545
H	-0.154493	-0.426031	0.003545
C	-2.661028	-1.479242	-0.001231
N	-1.966241	-0.331686	-0.000119
C	-2.621061	0.846928	0.000321
N	-1.932769	1.994722	0.001525
C	-4.613649	-0.461256	-0.001669
H	-0.915488	2.008048	0.000836
H	-2.445319	2.857726	0.001596
H	7.234126	1.435494	0.870334
H	7.213502	1.491355	-0.889604
N	-3.977853	-1.638501	-0.002183
C	-4.028503	0.802628	-0.000424
N	-4.991452	1.791713	-0.000251
N	-5.967943	-0.233425	-0.002168
C	-7.001048	-1.248896	-0.003905
H	-7.972921	-0.761799	-0.000713
H	-6.913855	-1.875721	-0.889874
H	-6.910865	-1.881360	0.877705
H	-2.059704	-2.380808	-0.001369
C	-6.123329	1.135993	-0.001316
H	-7.104604	1.582778	-0.001436

4AP:G tWW

40

4ap-G-trans SCF Done: -1190.18043676 A.U.

C	7.177032	-0.420935	-0.141995
C	2.972649	0.314321	0.019852
N	6.088872	2.208737	-0.123470
C	3.823627	1.393572	-0.000763
N	1.145173	-1.066958	0.080760
C	5.205792	1.147638	-0.048853
C	5.696648	-0.180621	-0.078394
C	4.800866	-1.245914	-0.053566
C	3.443740	-0.992161	-0.004786
C	1.486287	0.259654	0.074692
O	0.710573	1.208485	0.109746

C	2.278641	-1.909435	0.033868
O	2.251106	-3.112883	0.029155
H	3.441408	2.405495	0.019406
H	5.166026	-2.263907	-0.073740
H	7.396342	-1.484885	-0.192521
H	7.033572	2.044869	0.178004
H	5.731253	3.108283	0.149403
H	0.167007	-1.399283	0.114865
C	-2.845661	1.665892	0.069127
N	-2.028871	0.577417	0.133628
C	-2.438334	-0.770637	0.108418
C	-4.596250	0.318163	-0.034404
H	7.620870	0.058295	-1.018322
H	7.690051	-0.022751	0.739437
N	-4.152054	1.593511	-0.022337
C	-3.860074	-0.865255	0.024161
O	-1.593411	-1.662090	0.154277
H	-1.018291	0.742151	0.182655
N	-2.230388	2.880131	0.145108
H	-1.243818	2.932657	-0.045605
H	-2.794426	3.670233	-0.112335
N	-4.700307	-1.958791	-0.022633
N	-5.904664	-0.067446	-0.118133
C	-5.897751	-1.452220	-0.105196
H	-6.817461	-2.011893	-0.160278
C	-7.048927	0.816038	-0.194297
H	-6.964613	1.472604	-1.058880
H	-7.949616	0.214441	-0.287353
H	-7.118500	1.430786	0.702183

4AP:C tWW

37

4ap-C-trans SCF Done: -1042.49565949 A.U.

C	5.988398	1.487195	-0.018659
C	2.394890	-0.826177	0.017276
N	6.004260	-1.357425	0.086150
C	3.598063	-1.487514	0.033360
N	0.172474	-0.234875	-0.001875
C	4.777030	-0.723675	0.016337
C	4.715544	0.690739	-0.013726
C	3.476033	1.323540	-0.030706
C	2.323526	0.560282	-0.014963
C	0.998517	-1.365165	0.026008
O	0.644029	-2.515303	0.051984
C	0.895745	0.943971	-0.025533
O	0.424637	2.071126	-0.048920
H	3.635933	-2.568620	0.059199
H	3.418163	2.403537	-0.053716
H	5.778767	2.554482	-0.009775

H	6.802791	-0.858526	-0.265505
H	6.012317	-2.337661	-0.139165
H	-0.857981	-0.245337	-0.008981
C	-5.782740	-1.804273	-0.022994
C	-3.526173	-0.833989	-0.036602
N	-2.725261	0.269080	-0.017762
C	-3.234774	1.491439	0.022743
N	-2.387581	2.530392	0.035659
C	-5.446499	0.629330	0.038026
H	-6.524725	0.704591	0.058865
H	-5.596681	-2.383740	-0.925027
H	-1.378449	2.377365	0.002857
H	-2.743421	3.466820	0.061173
H	6.606539	1.256543	0.852836
H	6.593213	1.280454	-0.907687
H	-5.555955	-2.438367	0.831602
H	-6.824197	-1.493455	0.010707
N	-4.935997	-0.619937	-0.005096
C	-4.648179	1.721064	0.053431
O	-3.115521	-1.978904	-0.077859
H	-5.063025	2.715334	0.087453

4AP:U tWW

36

4ap-U-trans SCF Done: -1062.38468034 A.U.

C	-6.472928	-0.089926	-0.000253
C	-2.207817	-0.311794	-0.007944
N	-5.074590	-2.569113	-0.058079
C	-2.922033	-1.485675	-0.009782
N	-0.564662	1.283697	-0.004314
C	-4.324528	-1.408820	-0.002037
C	-4.972744	-0.149790	0.004767
C	-4.212004	1.016178	0.008511
C	-2.833164	0.929254	0.001786
C	-0.736206	-0.081051	-0.010534
O	0.150057	-0.919089	-0.015874
C	-1.787010	1.981447	0.004093
O	-1.905960	3.181399	0.011937
H	-2.417683	-2.442845	-0.017979
H	-4.698868	1.982124	0.014474
H	-6.820355	0.940252	-0.028515
H	-6.017713	-2.526685	0.286808
H	-4.597162	-3.420735	0.183820
H	0.366278	1.711854	-0.004854
C	6.233794	-1.670287	0.010223
C	3.862499	-1.134720	0.001487
N	2.897974	-0.149801	-0.003591
C	3.105294	1.223404	-0.004054
C	5.453982	0.674314	0.004025

H	6.504391	0.927411	0.006983
H	6.153073	-2.304900	-0.869821
H	-6.889161	-0.611822	-0.865691
H	-6.900255	-0.554793	0.894185
H	6.147439	-2.301795	0.891972
H	7.195211	-1.164678	0.012411
N	5.178987	-0.662893	0.005080
C	4.494983	1.618811	-0.000253
O	3.614585	-2.321115	0.002778
H	4.731646	2.668812	-0.000897
O	2.161703	2.008542	-0.007456
H	1.923413	-0.481398	-0.007836

4AP:U1 tWW

36

4ap-U1-trans SCF Done: -1062.38364865 A.U.

C	-5.397761	2.292508	-0.008855
C	-2.653166	-0.983878	-0.004482
N	-6.257110	-0.420927	-0.049322
C	-3.998503	-1.258920	-0.002512
N	-0.360920	-1.078562	-0.004231
C	-4.898139	-0.179194	0.001153
C	-4.419100	1.153993	-0.000302
C	-3.048101	1.391510	-0.000266
C	-2.173403	0.321048	-0.002513
C	-1.480554	-1.911875	-0.004396
O	-1.470940	-3.118170	-0.003740
C	-0.697162	0.267434	-0.002231
O	0.095989	1.192773	-0.000079
H	-4.356116	-2.280127	-0.004592
H	-2.672175	2.405716	-0.000452
H	-4.880896	3.248782	-0.043225
H	-6.870348	0.302343	0.283245
H	-6.557497	-1.349475	0.193353
H	0.612161	-1.390240	-0.002262
C	5.024385	-2.200024	0.001048
C	3.269219	-0.520600	0.002846
N	2.932587	0.802194	0.002834
C	3.812141	1.899567	0.001501
C	5.554635	0.218146	-0.000296
H	6.585014	-0.106136	-0.001601
H	4.633839	-2.703038	-0.881027
H	-6.065447	2.237867	-0.872501
H	-6.026774	2.293175	0.887248
H	4.631331	-2.703935	0.881444
H	6.109260	-2.252172	0.002552
N	4.629505	-0.795157	0.001435
C	5.213190	1.516644	-0.000296

O	2.452832	-1.435605	0.004202
H	5.955978	2.296134	-0.001594
O	3.387349	3.035972	0.001990
H	1.925314	1.010365	0.003029

4AP:T tWW

39

4ap-T-trans SCF Done: -1101.72307548 A.U.

C	-6.710685	0.127569	0.002149
C	-2.464997	-0.336597	-0.009003
N	-5.455690	-2.426394	-0.057132
C	-3.245033	-1.467763	-0.010609
N	-0.733687	1.162707	-0.005513
C	-4.640726	-1.310732	-0.001796
C	-5.216341	-0.016769	0.005479
C	-4.390317	1.103862	0.008787
C	-3.018636	0.938111	0.001276
C	-0.982485	-0.190364	-0.012062
O	-0.145422	-1.077163	-0.017825
C	-1.913960	1.928749	0.003457
O	-1.964338	3.133727	0.011673
H	-2.796579	-2.452312	-0.019322
H	-4.820758	2.096202	0.015169
H	-7.000468	1.175475	-0.027423
H	-6.394833	-2.330103	0.287650
H	-5.027518	-3.303884	0.184522
H	0.220416	1.536564	-0.006014
C	5.897892	-2.146843	0.011745
C	3.559964	-1.498668	0.001065
N	2.648101	-0.462951	-0.004536
C	2.928289	0.892522	-0.004434
C	5.235201	0.234653	0.005696
H	6.298547	0.428777	0.009782
H	5.789472	-2.776771	-0.868892
H	-7.156946	-0.371674	-0.861719
H	-7.162078	-0.311041	0.898049
H	5.781449	-2.774711	0.892824
H	6.881981	-1.686908	0.015677
N	4.891371	-1.091643	0.005997
C	4.338779	1.240753	0.000883
O	3.246753	-2.670740	0.001652
O	2.027156	1.729134	-0.008636
H	1.657558	-0.741003	-0.009542
C	4.715716	2.687825	0.000782
H	4.309550	3.194766	-0.875433
H	4.302345	3.196757	0.872466
H	5.798052	2.810304	0.005101

4AP:T1 tWW

39

4ap-T1-trans SCF Done: -1101.72240962 A.U.

C	5.570152	-2.496000	0.002362
C	3.017553	0.932297	-0.012751
N	6.581852	0.161687	-0.104059
C	4.376251	1.129151	-0.036668
N	0.734603	1.159296	0.018685
C	5.212140	-0.000460	-0.026736
C	4.657714	-1.303623	0.004923
C	3.275510	-1.461619	0.030314
C	2.463830	-0.342541	0.020943
C	1.900063	1.926189	-0.012847
O	1.960436	3.130856	-0.034301
C	0.993084	-0.203371	0.040440
O	0.147889	-1.081129	0.069197
H	4.791828	2.127764	-0.063711
H	2.842089	-2.452335	0.054834
H	4.999643	-3.421860	-0.004853
H	7.158553	-0.588714	0.233778
H	6.938879	1.076037	0.114673
H	-0.219897	1.526660	0.029687
C	-4.565543	2.616151	0.006914
C	-2.914072	0.841403	0.030158
N	-2.659648	-0.501125	0.026237
C	-3.602973	-1.535900	-0.003567
C	-5.238056	0.232848	-0.026020
H	-6.245470	0.623493	-0.045413
H	-4.129197	3.103218	-0.862752
H	6.224389	-2.494973	-0.873230
H	6.214009	-2.515674	0.887636
H	-4.163941	3.091717	0.899328
H	-5.645513	2.728952	-0.013661
N	-4.249931	1.191609	0.004056
C	-4.993195	-1.088957	-0.031674
O	-2.039661	1.702928	0.054942
O	-3.252035	-2.699491	-0.004676
H	-1.668365	-0.773774	0.046260
C	-6.064948	-2.129925	-0.065218
H	-5.955061	-2.768104	-0.943005
H	-5.993003	-2.785532	0.803587
H	-7.055167	-1.676287	-0.082328

iG:C tWW

35

iGC SCF Done: -1016.59445327 A.U.

C	-2.814567	1.516884	-0.000473
N	-2.192994	0.336732	-0.000212
C	-2.875638	-0.826535	0.000388
C	-4.924278	0.422647	0.000393

C	5.670674	0.972058	0.001335
N	0.685375	0.193615	-0.000696
C	1.362690	1.442746	-0.000126
N	2.711766	1.454334	0.000285
C	3.269888	0.252423	0.000130
C	2.660472	-1.010086	-0.000431
C	1.267149	-1.028662	-0.000891
N	3.600902	-2.026121	-0.000455
C	4.743449	-1.400267	0.000319
N	4.617226	-0.019929	0.000516
H	-6.003945	0.383035	0.000656
H	5.593690	1.606956	-0.880198
H	-1.027377	2.555181	-0.001056
H	5.715034	-1.867589	0.000568
H	5.595095	1.604259	0.884947
H	6.632757	0.465217	-0.000191
H	-0.508971	-2.089366	-0.001019
H	-0.344016	0.247601	-0.000885
C	-5.011459	-2.037512	0.001224
H	-4.748985	-2.620771	-0.878831
H	-4.748669	-2.620147	0.881598
H	-6.078173	-1.828835	0.001341
H	-4.765839	2.535214	-0.000340
N	-4.285763	-0.773474	0.000642
C	-4.246133	1.590825	-0.000151
O	0.654781	2.461440	-0.000128
O	-2.339914	-1.937483	0.000652
N	0.513001	-2.128773	-0.001693
N	-2.066533	2.616263	-0.001087
H	0.986045	-3.014272	-0.001068
H	-2.509930	3.516212	-0.001128

iC:G tWW

35

GiC SCF Done: -1016.58250647 A.U.

C	-2.798802	1.579783	0.000251
O	-2.124833	2.613438	0.000279
N	-2.199933	0.343039	-0.000154
C	-2.901645	-0.768872	-0.000159
N	-2.266829	-1.944014	-0.000559
C	-4.930808	0.449238	0.000610
C	5.695941	0.878118	0.000619
N	0.696466	0.245436	-0.000494
C	1.425826	1.405125	-0.000400
N	0.728624	2.552749	-0.000657
N	2.747376	1.424947	-0.000133
C	3.284764	0.193312	-0.000008
C	2.641126	-1.045435	-0.000104

C	1.218557	-1.054454	-0.000366
O	0.451844	-2.025483	-0.000484
N	3.566085	-2.072967	0.000067
C	4.722612	-1.474576	0.000327
N	4.622888	-0.091970	0.000228
H	-2.766404	-2.811214	-0.000516
H	-6.009178	0.393784	0.000885
H	5.636503	1.513621	-0.882073
H	-0.293463	2.578750	-0.000441
H	1.258301	3.403850	-0.000259
H	5.685119	-1.960288	0.000511
H	5.638158	1.511330	0.885086
H	6.646356	0.349832	-0.000949
H	-1.226494	-1.958657	-0.000763
H	-0.332356	0.311543	-0.000617
C	-5.039912	-2.010056	0.000195
H	-4.819657	-2.601267	-0.889822
H	-4.819203	-2.601574	0.889895
H	-6.099465	-1.773882	0.000507
H	-4.766171	2.556051	0.000955
C	-4.255702	1.606889	0.000643
N	-4.283229	-0.767212	0.000215

A:T tWW

36

AT-trans-gd3bj SCF Done: -1000.53591318 A.U.

C	5.811198	1.516964	0.000649
N	0.881232	0.156885	-0.000925
C	1.467870	1.363917	-0.000872
N	2.766933	1.633954	-0.000522
C	3.503869	0.518150	-0.000202
C	3.032897	-0.792898	-0.000219
C	1.635299	-0.959607	-0.000616
N	1.040095	-2.158567	-0.000769
N	4.079963	-1.692591	0.000190
C	5.150241	-0.939763	0.000369
N	4.874218	0.410444	0.000189
C	-4.562210	-2.408378	0.001181
N	-3.897378	-1.110813	0.000605
C	-2.513810	-1.106569	0.000135
O	-1.876781	-2.157062	0.000196
N	-1.932810	0.126606	-0.000297
C	-2.579707	1.359287	-0.000267
O	-1.940642	2.398675	-0.000680
C	-4.038103	1.285412	0.000245
C	-4.609905	0.067525	0.000665
H	5.232334	2.436551	-0.001616
H	0.782506	2.203046	-0.001127
H	1.614801	-2.981008	-0.000053

H	6.166066	-1.301245	0.000667
H	-4.278234	-2.980743	-0.879765
H	-5.683844	-0.054217	0.001065
H	0.025708	-2.233205	-0.000463
H	-0.886205	0.141309	-0.000627
H	-5.636240	-2.246418	0.000870
H	-4.278621	-2.979841	0.882851
H	6.442345	1.488778	-0.886872
H	6.438933	1.491105	0.890675
C	-4.811335	2.564336	0.000282
H	-4.559927	3.166959	-0.873552
H	-4.559361	3.167253	0.873751
H	-5.884479	2.377089	0.000663