Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information for

Hydrogen bonding of 3- and 5-methyl-6-aminouracils with natural DNA bases.

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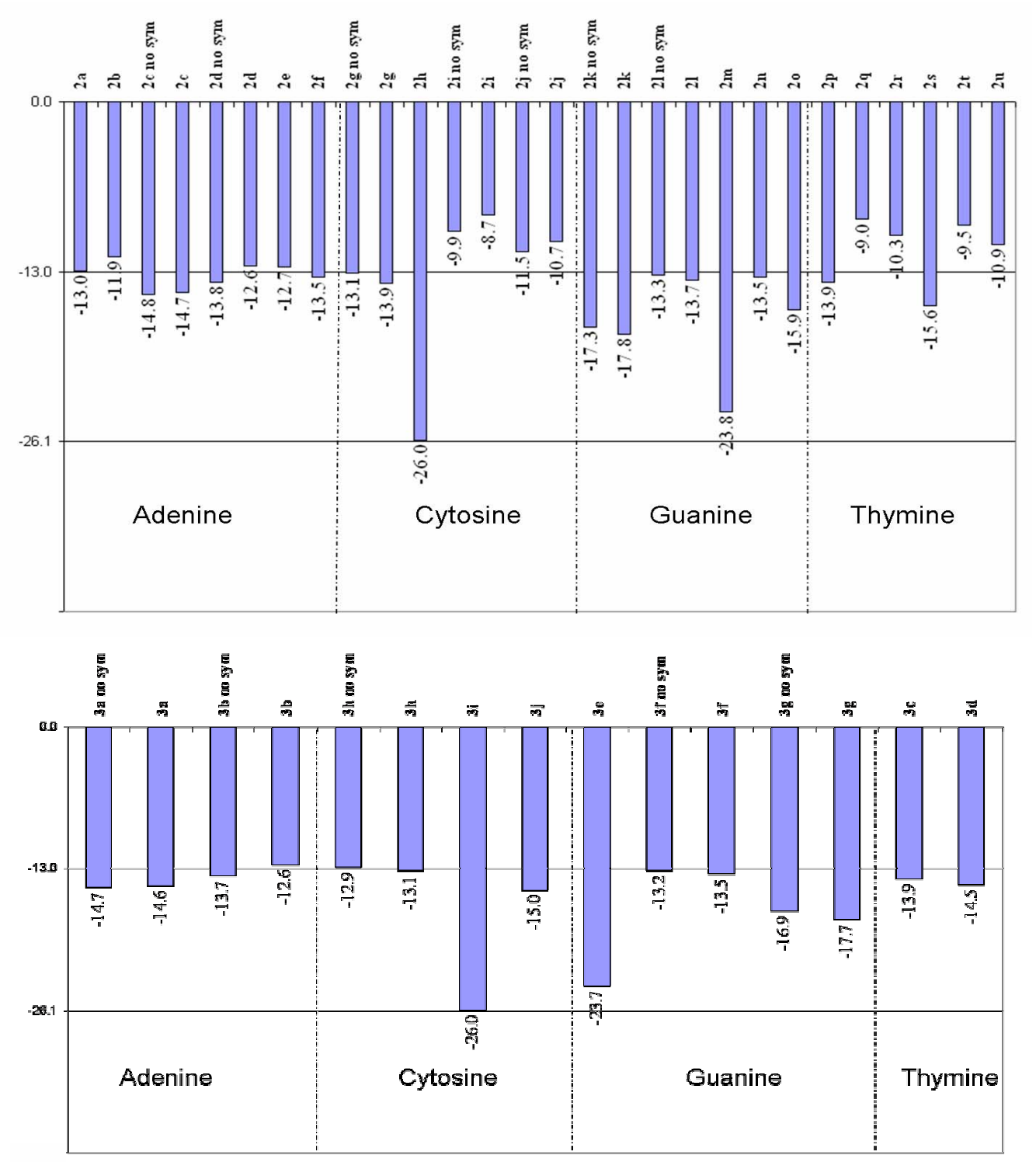

Figure S1 Total bonding energy (in kcal/mol) of 3-methyl-6-aminouracil (top) and 5-methyl-6-aminouracil (bottom) with natural nucleobases. The two horizontal lines show the interaction energy of the natural base-pairs (-13.0 kcal/mol for A-T and -26.1 kcal/mol for G-C)[a]

[a] The A-T and G-C interaction energies are taken from reference 3b

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Table S1. Cartesian coordinates of all calculated duplex systems. The definitions of different bonding arrangements can be found in Figure 2 and Figure 3 in the article.

Adenine — 3-methyl-6-aminouracil

2a: C_s symmetry			
N	2.330677	-0.445582	0.000000
N	0.332637	-1.797396	0.000000
N	-1.687564	-0.419879	0.000000
N	-0.741185	1.636588	0.000000
N	2.337940	1.883779	0.000000
C	1.654589	-1.611460	0.000000
C	-0.321988	-0.623532	0.000000
C	0.238648	0.660631	0.000000
C	1.651554	0.730245	0.000000
C	-1.867245	0.950673	0.000000
C	-2.700266	-1.464227	0.000000
H	2.281325	-2.503909	0.000000
H	-2.861926	1.385157	0.000000
H	3.373140	1.880464	0.000000
H	1.820066	2.751636	0.000000
H	-2.178136	-2.426134	0.000000
H	-3.329989	-1.395228	-0.895675
H	-3.329989	-1.395228	0.895675
N	5.129780	-0.517461	0.000000
N	7.094551	-1.748377	0.000000
N	9.211587	-0.778093	0.000000
C	5.694875	-1.763702	0.000000
C	7.856993	-0.599797	0.000000
C	7.257744	0.640181	0.000000
C	5.816965	0.702683	0.000000
C	8.060510	1.911370	0.000000
O	5.165866	1.767436	0.000000
O	5.074867	-2.822439	0.000000
H	4.065127	-0.486119	0.000000
H	7.520532	-2.669136	0.000000
H	8.702009	2.002217	-0.891764
H	8.702009	2.002217	0.891764
H	7.368967	2.760487	0.000000
H	9.633543	-1.694503	0.000000
H	9.818617	0.027321	0.000000

2b: C_s symmetry			
N	5.169079	0.013384	0.000000
N	7.055155	-1.325781	0.000000
N	9.228459	-0.486264	0.000000
C	5.666455	-1.249557	0.000000
C	7.886741	-0.219810	0.000000
C	7.363937	1.050441	0.000000
C	5.923558	1.210569	0.000000
C	8.240485	2.271923	0.000000
O	5.327340	2.291315	0.000000
O	4.987274	-2.286650	0.000000
H	4.109874	0.102804	0.000000
H	7.425826	-2.269929	0.000000
H	8.886350	2.325184	-0.891675
H	8.886350	2.325184	0.891675
H	7.597804	3.159127	0.000000
H	9.591786	-1.427376	0.000000
H	9.885425	0.278840	0.000000
N	2.367490	0.180659	0.000000
N	0.532437	1.745638	0.000000
N	-1.628058	0.602530	0.000000
N	-0.917275	-1.547345	0.000000
N	2.113604	-2.136638	0.000000
C	1.825834	1.415222	0.000000
C	-0.248349	0.652512	0.000000
C	0.165722	-0.686475	0.000000
C	1.561736	-0.910586	0.000000
C	-1.959418	-0.739335	0.000000
C	-2.517310	1.754072	0.000000
H	2.550262	2.230505	0.000000
H	-2.996555	-1.059652	0.000000
H	3.137092	-2.249074	0.000000
H	1.502914	-2.941702	0.000000
H	-3.150374	1.756185	-0.895768
H	-1.890679	2.651614	0.000000
H	-3.150374	1.756185	0.895768

2c no symmetry:

N	-0.933243	0.164250	-0.099823
N	-2.828069	1.646814	-0.346689
N	-4.950115	0.460047	-0.069828
N	-4.159120	-1.626517	0.313162
N	-1.126066	-2.128595	0.311729
C	-1.528079	1.354704	-0.324101
C	-3.574300	0.553792	-0.108219
C	-3.110134	-0.746047	0.131494
C	-1.707738	-0.934272	0.117779
C	-5.230714	-0.868981	0.187879
C	-5.887224	1.556779	-0.265497
H	-0.846628	2.183949	-0.523611
H	-6.254694	-1.219165	0.269692
H	-0.119124	-2.261183	0.111358
H	-1.730846	-2.935525	0.396139
H	-5.311122	2.433534	-0.577134
H	-6.418086	1.788443	0.666377
H	-6.613311	1.304314	-1.047224
N	3.721669	-1.486201	-0.468579
N	1.899954	-0.134297	-0.035426
N	2.073014	2.157303	0.293906
C	2.365858	-1.405351	-0.281518
C	2.728722	0.966334	0.043323
C	4.087177	0.877344	-0.153249
C	4.659413	-0.418465	-0.442866
C	4.996758	2.071278	-0.060885
O	5.849143	-0.667991	-0.641157
O	1.619256	-2.394684	-0.328276
H	4.101913	-2.411520	-0.650220
H	0.849782	-0.011604	-0.038820
H	4.927382	2.575710	0.917109
H	4.787991	2.818019	-0.842796
H	6.030975	1.733510	-0.187974
H	1.225734	2.087956	0.850105
H	2.674930	2.924594	0.571541

2c: C_s symmetry

N	1.865781	0.376536	0.000000
N	-0.068817	1.836209	0.000000
N	-2.165382	0.570202	0.000000
N	-1.323293	-1.531150	0.000000
N	1.704465	-1.960019	0.000000
C	1.235742	1.568839	0.000000
C	-0.792237	0.701689	0.000000
C	-0.296738	-0.606741	0.000000
C	1.111238	-0.759693	0.000000
C	-2.413670	-0.789928	0.000000
C	-3.128616	1.661754	0.000000
H	1.886278	2.447467	0.000000
H	-3.428993	-1.173611	0.000000
H	2.735504	-2.061701	0.000000
H	1.111624	-2.779685	0.000000
H	-2.565413	2.600009	0.000000
H	-3.760187	1.620695	0.895665
H	-3.760187	1.620695	-0.895665
N	6.604095	-1.334145	0.000000
N	4.768958	0.067839	0.000000
N	4.965928	2.376036	0.000000
C	5.239922	-1.225955	0.000000
C	5.603611	1.169337	0.000000
C	6.976710	1.046881	0.000000
C	7.553376	-0.273752	0.000000
C	7.887678	2.242901	0.000000
O	8.752742	-0.555329	0.000000
O	4.487786	-2.212309	0.000000
H	6.985699	-2.276393	0.000000
H	3.725658	0.188548	0.000000
H	7.748819	2.875724	0.891705
H	7.748819	2.875724	-0.891705
H	8.924658	1.889879	0.000000
H	3.958816	2.436453	0.000000
H	5.504331	3.228380	0.000000

2d no symmetry:

N	1.963269	0.139042	-3.981027
N	3.011504	0.082548	-1.801589
N	1.373812	0.038084	0.004084
N	-0.525274	0.020311	-1.206645
N	-0.329279	0.204057	-4.330644
C	3.008348	0.104441	-3.143868
C	1.760040	0.063903	-1.325534
C	0.567208	0.062577	-2.063370
C	0.707374	0.139189	-3.474186
C	0.003175	0.014528	0.006659
C	2.269691	0.060579	1.150145
H	3.989574	0.103591	-3.620923
H	-0.563118	0.002319	0.932239
H	-0.091095	0.341353	-5.306081
H	-1.287423	0.427664	-4.026332
H	2.992371	-0.759382	1.073520
H	2.818153	1.009391	1.185494
H	1.680231	-0.054183	2.065228
N	-5.152649	0.651556	-2.928569
N	-3.324959	-0.105798	-1.737488
N	-3.500920	-1.183864	0.311971
C	-3.788099	0.518762	-2.873541
C	-4.160606	-0.588389	-0.750897
C	-5.526641	-0.448922	-0.813605
C	-6.099461	0.223934	-1.959728
C	-6.446455	-0.985461	0.248365
O	-7.296041	0.428572	-2.165821
O	-3.032875	0.923547	-3.767242
H	-5.532557	1.105775	-3.755157
H	-2.285161	-0.079092	-1.580008
H	-6.314668	-2.068419	0.408105
H	-6.308820	-0.480632	1.217218
H	-7.481414	-0.820323	-0.070408
H	-2.631018	-1.652586	0.071868
H	-4.097992	-1.741051	0.914026

2d: C_s symmetry

N	3.786431	-2.235233	0.000000
N	4.874262	-0.077918	0.000000
N	3.279955	1.757391	0.000000
N	1.343799	0.596119	0.000000
N	1.499377	-2.557426	0.000000
C	4.846651	-1.419803	0.000000
C	3.631121	0.419495	0.000000
C	2.419188	-0.289621	0.000000
C	2.537262	-1.707454	0.000000
C	1.910371	1.791869	0.000000
C	4.206202	2.878997	0.000000
H	5.818777	-1.915436	0.000000
H	3.635317	3.813020	0.000000
H	1.724421	-3.544875	0.000000
H	0.511116	-2.270399	0.000000
H	4.844345	2.840065	0.890360
H	4.844345	2.840065	-0.890360
H	1.388425	2.743847	0.000000
N	-3.402507	-1.319689	0.000000
N	-1.584336	0.104844	0.000000
N	-1.812816	2.410983	0.000000
C	-2.038544	-1.196507	0.000000
C	-2.434725	1.195018	0.000000
C	-3.805389	1.055811	0.000000
C	-4.366180	-0.272850	0.000000
C	-4.729708	2.241892	0.000000
O	-5.561907	-0.568830	0.000000
O	-1.274567	-2.170392	0.000000
H	-3.771849	-2.266873	0.000000
H	-0.549529	0.239321	0.000000
H	-4.598226	2.876307	0.891818
H	-4.598226	2.876307	-0.891818
H	-5.763144	1.878450	0.000000
H	-0.807298	2.478443	0.000000
H	-2.362554	3.256054	0.000000

2e: C_s symmetry

N	-4.608164	-1.863671	0.000000
N	-5.430174	0.413903	0.000000
N	-3.610853	2.048145	0.000000
N	-1.856774	0.643223	0.000000
N	-2.354567	-2.429563	0.000000
C	-5.562733	-0.921343	0.000000
C	-4.137372	0.766272	0.000000
C	-3.029849	-0.091751	0.000000
C	-3.309675	-1.479917	0.000000
C	-2.244684	1.905916	0.000000
C	-4.384823	3.280997	0.000000
H	-6.587338	-1.296297	0.000000
H	-1.561137	2.748857	0.000000
H	-2.660230	-3.394179	0.000000
H	-1.352062	-2.215095	0.000000
H	-4.166262	3.874879	0.895658
H	-5.442932	3.001748	0.000000
H	-4.166262	3.874879	-0.895658
N	0.896316	0.153196	0.000000
N	2.680745	-1.317368	0.000000
N	4.907762	-0.632892	0.000000
C	1.299630	-1.143733	0.000000
C	3.588261	-0.273437	0.000000
C	3.157188	1.031959	0.000000
C	1.732543	1.292896	0.000000
C	4.121932	2.185286	0.000000
O	1.211426	2.414052	0.000000
O	0.546264	-2.125548	0.000000
H	-0.148541	0.320751	0.000000
H	2.984654	-2.285061	0.000000
H	4.770368	2.190116	-0.891412
H	4.770368	2.190116	0.891412
H	3.548164	3.118355	0.000000
H	5.204698	-1.597078	0.000000
H	5.617026	0.084113	0.000000

2f: C_s symmetry

N	2.725645	-2.442302	0.000000
N	3.869104	-0.307381	0.000000
N	2.305948	1.572340	0.000000
N	0.366140	0.436562	0.000000
N	0.413002	-2.675915	0.000000
C	3.806069	-1.648078	0.000000
C	2.640412	0.227489	0.000000
C	1.420421	-0.460773	0.000000
C	1.494528	-1.876130	0.000000
C	0.933373	1.629812	0.000000
C	3.252079	2.678589	0.000000
H	4.765800	-2.167019	0.000000
H	0.383818	2.565481	0.000000
H	0.578282	-3.674303	0.000000
H	-0.552939	-2.320582	0.000000
H	4.257768	2.247017	0.000000
H	3.123820	3.298466	0.895633
H	3.123820	3.298466	-0.895633
N	-2.429365	0.277910	0.000000
N	-4.436223	1.434629	0.000000
N	-6.515665	0.383993	0.000000
C	-3.039190	1.501607	0.000000
C	-5.155205	0.256777	0.000000
C	-4.510248	-0.959988	0.000000
C	-3.067349	-0.969720	0.000000
C	-5.266719	-2.259555	0.000000
O	-2.372241	-2.003283	0.000000
O	-2.455849	2.583012	0.000000
H	-1.370623	0.287051	0.000000
H	-4.897805	2.338090	0.000000
H	-5.904682	-2.373590	-0.891676
H	-5.904682	-2.373590	0.891676
H	-4.545528	-3.083609	0.000000
H	-6.973073	1.283274	0.000000
H	-7.091745	-0.443935	0.000000

Cytosine — 3-methyl-6-aminouracil

2g no symmetry:

C	-3.340588	1.455631	-0.245892
C	-2.270651	-0.590096	0.149631
C	-4.685320	-0.467293	0.138001
C	-4.639231	0.871826	-0.123941
C	-3.586340	-2.641489	0.538576
N	-2.222363	0.752002	-0.095294
N	-3.554254	-1.201569	0.273324
N	-3.207695	2.786559	-0.501231
O	-1.272649	-1.307241	0.268539
H	-5.624343	-1.006389	0.245603
H	-5.552035	1.450805	-0.233493
H	-4.006350	3.326858	-0.802819
H	-2.287196	3.123462	-0.757716
H	-3.061695	-2.859347	1.475450
H	-4.630019	-2.963976	0.607604
H	-3.076838	-3.180441	-0.267914
N	3.711840	-1.117612	-0.415638
N	1.468267	-0.573375	-0.275655
N	0.733410	1.598029	0.122893
C	2.410644	-1.574630	-0.475229
C	1.794261	0.741936	-0.010551
C	3.107219	1.160824	0.071509
C	4.159913	0.197692	-0.134647
C	3.467597	2.595031	0.339874
O	5.375805	0.417927	-0.098502
O	2.105937	-2.745082	-0.681757
H	4.436744	-1.815551	-0.556769
H	0.489236	-0.883165	-0.179783
H	3.122292	2.941551	1.329190
H	4.559016	2.689502	0.320837
H	3.051570	3.277921	-0.418722
H	0.915588	2.473339	0.594464
H	-0.227569	1.244338	0.148890

2g: C_s symmetry

C	1.403056	0.316986	0.000000
C	-0.328496	-1.258408	0.000000
C	-0.840762	1.105052	0.000000
C	0.488058	1.415587	0.000000
C	-2.687471	-0.533296	0.000000
N	1.002341	-0.952154	0.000000
N	-1.265724	-0.181666	0.000000
N	2.740394	0.549259	0.000000
O	-0.776082	-2.409125	0.000000
H	-1.616125	1.868533	0.000000
H	0.819534	2.450270	0.000000
H	3.114410	1.486023	0.000000
H	3.377096	-0.235967	0.000000
H	-2.923310	-1.132764	0.886276
H	-3.278070	0.388312	0.000000
H	-2.923310	-1.132764	-0.886276
N	0.515541	-7.292132	0.000000
N	0.496184	-4.980906	0.000000
N	2.442952	-3.717461	0.000000
C	-0.255983	-6.147965	0.000000
C	1.875888	-4.957441	0.000000
C	2.619273	-6.122636	0.000000
C	1.930584	-7.387555	0.000000
C	4.122208	-6.105797	0.000000
O	2.450921	-8.509408	0.000000
O	-1.483315	-6.149749	0.000000
H	0.008848	-8.172787	0.000000
H	-0.026611	-4.093008	0.000000
H	4.538835	-5.607073	0.891522
H	4.481110	-7.141094	0.000000
H	4.538835	-5.607073	-0.891522
H	3.449734	-3.660096	0.000000
H	1.899234	-2.851700	0.000000

2h: C_s symmetry

C	-3.009866	1.209792	0.000000
C	-2.989235	-1.150046	0.000000
C	-5.089646	0.044712	0.000000
C	-4.445094	1.242233	0.000000
C	-5.145629	-2.407066	0.000000
N	-2.344496	0.045432	0.000000
N	-4.413891	-1.137836	0.000000
N	-2.289565	2.339848	0.000000
O	-2.398431	-2.242345	0.000000
H	-6.175989	-0.029570	0.000000
H	-5.001024	2.175972	0.000000
H	-2.761800	3.232768	0.000000
H	-1.243422	2.307217	0.000000
H	-4.405696	-3.210182	0.000000
H	-5.773573	-2.484833	-0.896716
H	-5.773573	-2.484833	0.896716
N	2.483975	1.158987	0.000000
N	0.519013	-0.042494	0.000000
N	0.454384	-2.351724	0.000000
C	1.119162	1.188771	0.000000
C	1.222614	-1.236338	0.000000
C	2.607289	-1.248870	0.000000
C	3.317428	-0.001188	0.000000
C	3.383979	-2.535828	0.000000
O	4.540937	0.162223	0.000000
O	0.468325	2.253056	0.000000
H	2.965094	2.054056	0.000000
H	-0.528385	-0.046195	0.000000
H	3.174090	-3.150647	-0.890751
H	3.174090	-3.150647	0.890751
H	4.453724	-2.300139	0.000000
H	0.911253	-3.251138	0.000000
H	-0.576113	-2.310004	0.000000

2i no symmetry:

C	2.554295	1.396190	-0.338759
C	2.768779	-0.769833	0.569184
C	4.725886	0.411096	-0.275111
C	3.961266	1.491139	-0.602939
C	4.988831	-1.849524	0.669855
N	2.001141	0.300282	0.186832
N	4.181373	-0.695654	0.285602
N	1.734139	2.429188	-0.633700
O	2.344653	-1.773345	1.129529
H	5.801957	0.389045	-0.440930
H	4.406612	2.378319	-1.045003
H	2.130476	3.303368	-0.946984
H	0.759870	2.410983	-0.286860
H	6.023365	-1.680630	0.352082
H	4.592679	-2.754913	0.196308
H	4.949596	-1.995466	1.756243
N	-0.909944	-0.016449	0.105154
N	-2.875712	1.150505	0.479891
N	-4.999410	0.182945	0.504335
C	-1.497209	1.192350	0.316983
C	-3.630772	-0.005251	0.367246
C	-3.037202	-1.203943	0.086829
C	-1.590327	-1.249381	-0.092340
C	-3.818169	-2.483215	-0.035244
O	-0.952665	-2.257617	-0.377615
O	-0.903116	2.280988	0.366138
H	0.140206	-0.023200	0.096509
H	-3.325839	2.059518	0.503063
H	-4.475159	-2.492367	-0.919097
H	-4.440596	-2.677997	0.853430
H	-3.109429	-3.312269	-0.138819
H	-5.522502	-0.683148	0.585588
H	-5.279092	0.861941	1.208251

2i: C_s symmetry

C	1.147509	1.289671	0.000000
C	1.357717	-1.058968	0.000000
C	3.342807	0.360676	0.000000
C	2.571024	1.481609	0.000000
C	3.645120	-2.068212	0.000000
N	0.587871	0.077356	0.000000
N	2.794322	-0.879324	0.000000
N	0.329403	2.361254	0.000000
O	0.906034	-2.196902	0.000000
H	4.431591	0.405652	0.000000
H	3.019224	2.471723	0.000000
H	0.719847	3.291704	0.000000
H	-0.696104	2.229854	0.000000
H	4.278734	-2.089168	-0.896764
H	2.978906	-2.935079	0.000000
H	4.278734	-2.089168	0.896764
N	-2.432928	-0.321179	0.000000
N	-4.409952	0.887401	0.000000
N	-6.530767	-0.079437	0.000000
C	-3.021550	0.903908	0.000000
C	-5.174414	-0.266225	0.000000
C	-4.571984	-1.496323	0.000000
C	-3.121060	-1.575431	0.000000
C	-5.366096	-2.772863	0.000000
O	-2.477263	-2.617724	0.000000
O	-2.432487	1.996349	0.000000
H	-1.389043	-0.335327	0.000000
H	-4.835248	1.807794	0.000000
H	-6.006864	-2.868420	-0.891781
H	-6.006864	-2.868420	0.891781
H	-4.664470	-3.614250	0.000000
H	-7.140591	-0.882495	0.000000
H	-6.949335	0.838284	0.000000

2j no symmetry:

C	2.183357	1.467604	-0.317963
C	2.578032	-0.759703	0.356064
C	4.439025	0.691583	-0.251040
C	3.583872	1.723166	-0.499921
C	4.890265	-1.625923	0.454675
N	1.723752	0.269955	0.058169
N	3.986443	-0.518605	0.158606
N	1.276637	2.442459	-0.535634
O	2.234618	-1.859221	0.775089
H	5.517744	0.791186	-0.362095
H	3.955307	2.693108	-0.819311
H	1.595864	3.377319	-0.744569
H	0.288855	2.291479	-0.247498
H	5.915950	-1.318037	0.224347
H	4.617207	-2.501503	-0.145352
H	4.812219	-1.907283	1.511903
N	-1.128867	-0.251843	-0.147314
N	-3.004860	-1.614962	-0.299826
N	-5.189535	-0.865165	0.031448
C	-1.610566	-1.510394	-0.435968
C	-3.839612	-0.566918	0.011879
C	-3.333715	0.691713	0.229076
C	-1.904111	0.879580	0.125472
C	-4.214790	1.861229	0.572672
O	-1.346105	1.986843	0.277412
O	-0.941107	-2.469700	-0.781923
H	-0.082364	-0.136482	-0.109159
H	-3.380535	-2.508690	-0.600149
H	-4.820930	1.675880	1.475030
H	-4.900614	2.126504	-0.247316
H	-3.580739	2.731375	0.772314
H	-5.772769	-0.152578	0.456628
H	-5.440187	-1.805189	0.323449

2j: C_s symmetry

C	1.093669	1.287751	0.000000
C	1.391393	-1.053676	0.000000
C	3.322710	0.438711	0.000000
C	2.509999	1.530081	0.000000
C	3.715156	-1.977132	0.000000
N	0.580416	0.053069	0.000000
N	2.820703	-0.821191	0.000000
N	0.236146	2.325240	0.000000
O	0.982976	-2.208699	0.000000
H	4.409037	0.523626	0.000000
H	2.921081	2.536175	0.000000
H	0.593749	3.269002	0.000000
H	-0.790345	2.157768	0.000000
H	4.349246	-1.974415	-0.896666
H	3.081428	-2.868025	0.000000
H	4.349246	-1.974415	0.896666
N	-2.404645	-0.371664	0.000000
N	-4.373437	-1.611304	0.000000
N	-6.497915	-0.658715	0.000000
C	-2.967868	-1.630708	0.000000
C	-5.144375	-0.473465	0.000000
C	-4.550453	0.768731	0.000000
C	-3.111267	0.839463	0.000000
C	-5.360325	2.035639	0.000000
O	-2.483437	1.919342	0.000000
O	-2.363868	-2.688817	0.000000
H	-1.358546	-0.318506	0.000000
H	-4.789786	-2.536463	0.000000
H	-6.002730	2.122770	0.891691
H	-6.002730	2.122770	-0.891691
H	-4.674534	2.889116	0.000000
H	-7.110111	0.142718	0.000000
H	-6.913752	-1.577931	0.000000

Guanine — 3-methyl-6-aminouracil

2k no symmetry:

N	3.453506	-1.866997	0.067429
N	4.399670	0.309440	0.107148
N	2.663285	2.015579	-0.030212
N	0.834686	0.715749	-0.115443
N	5.776797	-1.563677	0.158691
C	4.522007	-1.001052	0.127291
C	3.110045	0.714377	0.010513
C	1.957862	-0.074623	-0.043027
C	2.076711	-1.496567	-0.011348
C	1.284517	1.952210	-0.104462
C	3.494150	3.211331	0.003046
O	1.205842	-2.369207	-0.044253
H	3.613840	-2.871399	0.032397
H	0.651879	2.833239	-0.139376
H	6.512521	-0.895195	0.362705
H	5.886315	-2.462575	0.614666
H	2.843121	4.090256	-0.010529
H	4.102216	3.222721	0.914824
H	4.158598	3.236652	-0.868416
N	-4.003821	1.364455	0.098513
N	-1.975827	0.280790	-0.087091
N	-1.786201	-2.029622	-0.220288
C	-2.637301	1.489736	0.008196
C	-2.605606	-0.947134	-0.085761
C	-3.981743	-1.045881	0.012863
C	-4.761526	0.160446	0.112267
C	-4.685118	-2.374646	0.009926
O	-5.991544	0.240252	0.205758
O	-2.041192	2.571259	0.011044
H	-4.536993	2.226404	0.169800
H	-0.938542	0.354674	-0.129954
H	-4.514284	-2.937218	-0.922503
H	-4.375559	-3.017179	0.851506
H	-5.762557	-2.199907	0.104395
H	-0.769886	-1.966696	-0.126178
H	-2.195588	-2.941796	-0.076888

2k: C_s symmetry

N	-3.422531	-2.136601	0.000000
N	-4.414044	0.021580	0.000000
N	-2.710011	1.763129	0.000000
N	-0.852364	0.501780	0.000000
N	-5.746856	-1.867478	0.000000
C	-4.511802	-1.293021	0.000000
C	-3.131234	0.452739	0.000000
C	-1.961468	-0.312271	0.000000
C	-2.052211	-1.734114	0.000000
C	-1.326350	1.728690	0.000000
C	-3.572768	2.938116	0.000000
O	-1.163508	-2.590166	0.000000
H	-3.552554	-3.145735	0.000000
H	-0.708878	2.620952	0.000000
H	-6.549615	-1.254372	0.000000
H	-5.886997	-2.865849	0.000000
H	-3.394259	3.544909	0.895421
H	-4.609618	2.590066	0.000000
H	-3.394259	3.544909	-0.895421
N	3.989885	1.183697	0.000000
N	1.966425	0.075076	0.000000
N	1.797783	-2.239076	0.000000
C	2.619374	1.292705	0.000000
C	2.608838	-1.146953	0.000000
C	3.990310	-1.228282	0.000000
C	4.759207	-0.012524	0.000000
C	4.710443	-2.548047	0.000000
O	5.991612	0.081502	0.000000
O	2.012634	2.367834	0.000000
H	4.516957	2.052261	0.000000
H	0.927998	0.141617	0.000000
H	4.477587	-3.154809	-0.890998
H	4.477587	-3.154809	0.890998
H	5.789077	-2.355416	0.000000
H	0.776669	-2.190787	0.000000
H	2.224723	-3.153012	0.000000

21 no symmetry:

N	2.796229	1.888995	0.292635
N	4.514160	0.295997	-0.068966
N	3.593038	-1.941153	-0.307466
N	1.396313	-1.513249	-0.032728
N	5.038205	2.550550	0.132857
C	4.114442	1.535638	0.130703
C	3.486310	-0.584915	-0.107587
C	2.118973	-0.341594	0.059469
C	1.677913	1.000530	0.280368
C	2.304569	-2.440665	-0.251699
C	4.826871	-2.680730	-0.531835
O	0.547209	1.456344	0.444534
H	2.534876	2.868741	0.385193
H	2.107773	-3.499298	-0.380203
H	6.000370	2.232546	0.173438
H	4.838469	3.389360	0.664960
H	5.508148	-2.545477	0.316131
H	5.321203	-2.326994	-1.444033
H	4.586544	-3.742826	-0.638036
N	-4.378571	1.249593	-0.378264
N	-2.192225	0.606581	0.016125
N	-1.614980	-1.571654	0.610657
C	-3.058610	1.644651	-0.306190
C	-2.602788	-0.689966	0.258256
C	-3.935231	-1.047878	0.185704
C	-4.913124	-0.042516	-0.146754
C	-4.396412	-2.455418	0.443288
O	-6.133867	-0.208817	-0.250799
O	-2.676613	2.793517	-0.505887
H	-5.049874	1.975228	-0.613362
H	-1.207539	0.874108	0.145783
H	-4.187186	-2.785294	1.474090
H	-3.933023	-3.183530	-0.244161
H	-5.480685	-2.498723	0.291404
H	-0.639445	-1.410933	0.338741
H	-1.891433	-2.545008	0.625657

21: C_s symmetry

N	-0.015436	-2.563719	0.000000
N	1.071309	-0.455521	0.000000
N	-0.544369	1.360580	0.000000
N	-2.473501	0.193004	0.000000
N	2.317892	-2.402117	0.000000
C	1.110693	-1.774314	0.000000
C	-0.190581	0.031203	0.000000
C	-1.399372	-0.673311	0.000000
C	-1.367550	-2.100924	0.000000
C	-1.928172	1.391147	0.000000
C	0.374741	2.491194	0.000000
O	-2.281762	-2.924295	0.000000
H	0.062602	-3.578732	0.000000
H	-2.470847	2.329841	0.000000
H	3.147877	-1.826172	0.000000
H	2.412522	-3.406084	0.000000
H	0.228457	3.106226	-0.896000
H	1.393208	2.092108	0.000000
H	0.228457	3.106226	0.896000
N	-7.019522	-4.510758	0.000000
N	-5.177796	-3.110992	0.000000
N	-5.382543	-0.790270	0.000000
C	-5.643682	-4.421300	0.000000
C	-6.002608	-2.002374	0.000000
C	-7.380288	-2.132168	0.000000
C	-7.960216	-3.449348	0.000000
C	-8.288319	-0.934255	0.000000
O	-9.166015	-3.725264	0.000000
O	-4.894714	-5.393567	0.000000
H	-7.406135	-5.450276	0.000000
H	-4.155300	-3.005014	0.000000
H	-8.149305	-0.299315	-0.891317
H	-8.149305	-0.299315	0.891317
H	-9.326201	-1.285529	0.000000
H	-4.370268	-0.648061	0.000000
H	-5.965400	0.033205	0.000000

2m: C_s symmetry

N	2.127502	-1.331086	0.000000
N	4.385699	-2.075877	0.000000
N	5.919795	-0.197292	0.000000
N	4.464026	1.533530	0.000000
N	2.627284	-3.592802	0.000000
C	3.084314	-2.312532	0.000000
C	4.663774	-0.754377	0.000000
C	3.774994	0.334900	0.000000
C	2.378246	0.053136	0.000000
C	5.727476	1.178388	0.000000
C	7.178010	-0.927963	0.000000
O	1.414605	0.851635	0.000000
H	1.121754	-1.629636	0.000000
H	6.571879	1.859913	0.000000
H	3.302954	-4.342355	0.000000
H	1.636930	-3.796675	0.000000
H	7.764738	-0.688359	-0.895462
H	6.942780	-1.996479	0.000000
H	7.764738	-0.688359	0.895462
N	-2.710271	-1.727266	0.000000
N	-1.123447	-0.061956	0.000000
N	-1.638615	2.182704	0.000000
C	-1.385831	-1.402797	0.000000
C	-2.109648	0.905623	0.000000
C	-3.449880	0.573612	0.000000
C	-3.814876	-0.818820	0.000000
C	-4.533343	1.616140	0.000000
O	-4.953692	-1.288816	0.000000
O	-0.474540	-2.260051	0.000000
H	-2.948519	-2.715234	0.000000
H	-0.109765	0.238850	0.000000
H	-4.490618	2.262950	-0.891277
H	-4.490618	2.262950	0.891277
H	-5.505387	1.111255	0.000000
H	-0.643119	2.369507	0.000000
H	-2.283775	2.957394	0.000000

2n: C_s symmetry

N	3.098578	0.825689	0.000000
N	5.389373	1.450462	0.000000
N	6.824500	-0.505536	0.000000
N	5.284220	-2.159492	0.000000
N	3.719368	3.061667	0.000000
C	4.103310	1.753329	0.000000
C	5.596580	0.112817	0.000000
C	4.655040	-0.929181	0.000000
C	3.266160	-0.580619	0.000000
C	6.564237	-1.869758	0.000000
C	8.116108	0.161810	0.000000
O	2.263940	-1.311667	0.000000
H	2.108892	1.150456	0.000000
H	7.373093	-2.593121	0.000000
H	4.437950	3.769923	0.000000
H	2.744213	3.323381	0.000000
H	8.691314	-0.105671	0.895339
H	7.933841	1.240750	0.000000
H	8.691314	-0.105671	-0.895339
N	-0.377276	-0.378877	0.000000
N	-1.768501	1.469598	0.000000
N	-4.096622	1.343644	0.000000
C	-0.475553	0.971962	0.000000
C	-2.903547	0.674059	0.000000
C	-2.794280	-0.692170	0.000000
C	-1.473431	-1.294107	0.000000
C	-4.001507	-1.588084	0.000000
O	-1.246448	-2.499633	0.000000
O	0.484231	1.768521	0.000000
H	0.592587	-0.784821	0.000000
H	-1.830712	2.481584	0.000000
H	-4.632126	-1.441238	-0.891830
H	-4.632126	-1.441238	0.891830
H	-3.658761	-2.628509	0.000000
H	-4.152482	2.350809	0.000000
H	-4.957680	0.818511	0.000000

2o: C_s symmetry

N	-0.749605	-1.325131	0.000000
N	-1.502592	-3.576700	0.000000
N	-3.925235	-3.680680	0.000000
N	-4.444368	-1.480968	0.000000
N	0.766472	-3.074174	0.000000
C	-0.536354	-2.674098	0.000000
C	-2.728437	-3.004023	0.000000
C	-3.071459	-1.641721	0.000000
C	-2.006753	-0.685283	0.000000
C	-4.914808	-2.706315	0.000000
C	-4.083960	-5.125592	0.000000
O	-2.054366	0.557257	0.000000
H	0.082902	-0.686010	0.000000
H	-5.965716	-2.977080	0.000000
H	0.965211	-4.063108	0.000000
H	1.517916	-2.398441	0.000000
H	-4.624337	-5.457517	0.895461
H	-3.083583	-5.569288	0.000000
H	-4.624337	-5.457517	-0.895461
N	0.232014	2.117596	0.000000
N	1.246347	4.210180	0.000000
N	3.554179	4.515930	0.000000
C	0.045098	3.481920	0.000000
C	2.500596	3.649017	0.000000
C	2.651376	2.277672	0.000000
C	1.466576	1.465125	0.000000
C	4.009390	1.631718	0.000000
O	1.497126	0.209071	0.000000
O	-1.032486	4.053602	0.000000
H	-0.645460	1.527453	0.000000
H	1.113729	5.216328	0.000000
H	4.600201	1.897756	0.891678
H	4.600201	1.897756	-0.891678
H	3.882714	0.544499	0.000000
H	3.426356	5.516954	0.000000
H	4.496360	4.155705	0.000000

Thymine — 3-methyl-6-aminouracil

2p: C_s symmetry

C	-2.674668	-1.364966	0.000000
C	-1.441440	0.798168	0.000000
C	-3.857439	0.746629	0.000000
C	-3.929409	-0.605647	0.000000
C	-5.218509	-1.370697	0.000000
C	-2.697583	2.916452	0.000000
N	-1.507715	-0.567909	0.000000
N	-2.665854	1.453851	0.000000
O	-2.597104	-2.586862	0.000000
O	-0.365916	1.430323	0.000000
H	-0.589977	-1.073840	0.000000
H	-4.749998	1.371662	0.000000
H	-6.083849	-0.697263	0.000000
H	-5.278080	-2.026808	0.878878
H	-5.278080	-2.026808	-0.878878
H	-1.666622	3.274617	0.000000
H	-3.212835	3.284981	0.896060
H	-3.212835	3.284981	-0.896060
N	3.312869	-1.777181	0.000000
N	2.112694	0.191106	0.000000
N	3.104497	2.279622	0.000000
C	2.080211	-1.183740	0.000000
C	3.281060	0.926101	0.000000
C	4.517796	0.317087	0.000000
C	4.579593	-1.124089	0.000000
C	5.798500	1.104815	0.000000
O	5.598955	-1.815941	0.000000
O	1.015062	-1.819282	0.000000
H	3.332424	-2.793655	0.000000
H	1.182600	0.659034	0.000000
H	5.896472	1.745409	-0.891613
H	6.639351	0.402694	0.000000
H	5.896472	1.745409	0.891613
H	2.179350	2.685528	0.000000
H	3.906458	2.890530	0.000000

2q: C_s symmetry

C	3.078444	-0.106805	0.000000
C	0.933741	-1.383804	0.000000
C	3.063780	-2.528920	0.000000
C	3.794188	-1.386292	0.000000
C	5.293541	-1.358557	0.000000
C	0.978461	-3.843985	0.000000
N	1.674849	-0.227332	0.000000
N	1.681578	-2.560428	0.000000
O	3.616124	0.996814	0.000000
O	-0.304598	-1.398552	0.000000
H	1.114700	0.649387	0.000000
H	3.535537	-3.511391	0.000000
H	5.712259	-2.372401	0.000000
H	5.671266	-0.819040	0.879308
H	5.671266	-0.819040	-0.879308
H	-0.093619	-3.635290	0.000000
H	1.239599	-4.420925	0.896501
H	1.239599	-4.420925	-0.896501
N	-2.033025	0.853044	0.000000
N	-2.019759	3.165522	0.000000
N	-3.955164	4.463303	0.000000
C	-1.282557	1.988189	0.000000
C	-3.403139	3.211853	0.000000
C	-4.143085	2.054866	0.000000
C	-3.453674	0.779206	0.000000
C	-5.646422	2.074628	0.000000
O	-3.996138	-0.325269	0.000000
O	-0.045185	2.031741	0.000000
H	-1.498482	-0.036239	0.000000
H	-1.458427	4.010384	0.000000
H	-6.059180	2.574299	0.891681
H	-6.006793	1.040133	0.000000
H	-6.059180	2.574299	-0.891681
H	-3.393506	5.301321	0.000000
H	-4.958939	4.561242	0.000000

2r: C_s symmetry

C	-2.534127	-1.673537	0.000000
C	-1.550338	0.613301	0.000000
C	-3.946297	0.294970	0.000000
C	-3.865395	-1.058100	0.000000
C	-5.061473	-1.962067	0.000000
C	-3.027061	2.581760	0.000000
N	-1.467185	-0.755146	0.000000
N	-2.844445	1.130239	0.000000
O	-2.326275	-2.883010	0.000000
O	-0.556265	1.354837	0.000000
H	-0.491413	-1.135264	0.000000
H	-4.904617	0.814112	0.000000
H	-5.996144	-1.388345	0.000000
H	-5.048862	-2.620877	0.879031
H	-5.048862	-2.620877	-0.879031
H	-2.036181	3.041103	0.000000
H	-3.576868	2.896521	0.896331
H	-3.576868	2.896521	-0.896331
N	2.114442	0.485412	0.000000
N	4.412663	0.779624	0.000000
N	5.929510	-0.987797	0.000000
C	3.150062	1.387085	0.000000
C	4.625219	-0.582500	0.000000
C	3.562201	-1.458320	0.000000
C	2.229200	-0.912717	0.000000
C	3.756771	-2.949243	0.000000
O	1.193413	-1.605894	0.000000
O	3.034707	2.604619	0.000000
H	1.146092	0.867423	0.000000
H	5.185203	1.437194	0.000000
H	4.300982	-3.300458	-0.891804
H	2.773028	-3.430158	0.000000
H	4.300982	-3.300458	0.891804
H	6.696959	-0.332813	0.000000
H	6.142825	-1.973657	0.000000

2s: C_s symmetry

C	-1.875951	-1.184818	0.000000
C	-3.421763	0.759216	0.000000
C	-4.258181	-1.519024	0.000000
C	-3.019177	-2.081700	0.000000
C	-2.784385	-3.563869	0.000000
C	-5.851722	0.357806	0.000000
N	-2.163291	0.169868	0.000000
N	-4.483969	-0.165630	0.000000
O	-0.692068	-1.589690	0.000000
O	-3.597591	1.967176	0.000000
H	-1.353278	0.839620	0.000000
H	-5.159605	-2.131948	0.000000
H	-2.203968	-3.869865	0.880986
H	-2.203968	-3.869865	-0.880986
H	-3.733750	-4.112921	0.000000
H	-6.387906	0.023560	-0.896972
H	-5.783186	1.448329	0.000000
H	-6.387906	0.023560	0.896972
N	2.335501	2.214911	0.000000
N	1.473767	0.078306	0.000000
N	2.785826	-1.820346	0.000000
C	1.217560	1.426654	0.000000
C	2.745112	-0.456610	0.000000
C	3.867056	0.345284	0.000000
C	3.692754	1.776736	0.000000
C	5.258035	-0.225299	0.000000
O	4.584752	2.627039	0.000000
O	0.060530	1.879200	0.000000
H	2.189664	3.220985	0.000000
H	0.632383	-0.544157	0.000000
H	5.457360	-0.842267	0.891510
H	5.975341	0.602603	0.000000
H	5.457360	-0.842267	-0.891510
H	1.934612	-2.365856	0.000000
H	3.673760	-2.297441	0.000000

2t: C_s symmetry

C	0.959653	-1.419772	0.000000
C	2.992987	0.017764	0.000000
C	3.158837	-2.404920	0.000000
C	1.814079	-2.601214	0.000000
C	1.171072	-3.956208	0.000000
C	5.213117	-1.047152	0.000000
N	1.625713	-0.199344	0.000000
N	3.755191	-1.164062	0.000000
O	-0.281400	-1.466656	0.000000
O	3.495921	1.133399	0.000000
H	1.026336	0.654350	0.000000
H	3.855921	-3.243040	0.000000
H	0.525083	-4.081227	-0.879577
H	0.525083	-4.081227	0.879577
H	1.925344	-4.752499	0.000000
H	5.635468	-1.519178	0.896398
H	5.454464	0.018613	0.000000
H	5.635468	-1.519178	-0.896398
N	-2.055848	0.739494	0.000000
N	-2.130180	3.052527	0.000000
N	-4.110752	4.279778	0.000000
C	-1.352573	1.902615	0.000000
C	-3.514089	3.048779	0.000000
C	-4.209344	1.865374	0.000000
C	-3.472971	0.615608	0.000000
C	-5.711990	1.825682	0.000000
O	-3.977170	-0.505857	0.000000
O	-0.116910	1.996250	0.000000
H	-1.486102	-0.132661	0.000000
H	-1.598821	3.916552	0.000000
H	-6.144476	2.308013	0.891773
H	-6.028721	0.777048	0.000000
H	-6.144476	2.308013	-0.891773
H	-3.579424	5.137346	0.000000
H	-5.117275	4.341888	0.000000

2u: C_s symmetry

C	-0.371751	1.648427	0.000000
C	2.063036	2.148033	0.000000
C	0.406851	3.926746	0.000000
C	-0.654338	3.077907	0.000000
C	-2.084119	3.531859	0.000000
C	2.801000	4.497333	0.000000
N	0.971497	1.295870	0.000000
N	1.719004	3.513507	0.000000
O	-1.259372	0.777023	0.000000
O	3.223913	1.760878	0.000000
H	1.180625	0.266830	0.000000
H	0.270617	5.008404	0.000000
H	-2.616743	3.145206	0.879503
H	-2.616743	3.145206	-0.879503
H	-2.151839	4.626738	0.000000
H	2.745663	5.128149	-0.896578
H	3.743276	3.943914	0.000000
H	2.745663	5.128149	0.896578
N	-0.830214	-1.981465	0.000000
N	-1.521790	-4.194237	0.000000
N	-0.047967	-5.997147	0.000000
C	-1.899089	-2.843946	0.000000
C	-0.218889	-4.642053	0.000000
C	0.829388	-3.748487	0.000000
C	0.524373	-2.341083	0.000000
C	2.263073	-4.201363	0.000000
O	1.392520	-1.444455	0.000000
O	-3.078166	-2.520010	0.000000
H	-1.039479	-0.956854	0.000000
H	-2.304958	-4.839101	0.000000
H	2.513412	-4.798811	0.891727
H	2.908943	-3.317115	0.000000
H	2.513412	-4.798811	-0.891727
H	-0.827603	-6.637559	0.000000
H	0.885170	-6.380052	0.000000

Adenine — 5-methyl-6-aminouracil

3a: no symmetry

N	0.951400	-0.352400	0.039400
N	2.992200	-1.608100	0.362400
N	4.975100	-0.202500	0.083200
N	3.967500	1.772700	-0.374100
N	0.894300	1.934400	-0.432900
C	1.668400	-1.463000	0.308900
C	3.617400	-0.446000	0.103800
C	3.018000	0.787800	-0.181800
C	1.603300	0.819300	-0.196400
C	5.113200	1.141400	-0.209900
C	6.021800	-1.183900	0.329300
H	1.077800	-2.356600	0.520000
H	6.094000	1.599500	-0.287500
H	-0.126800	1.953000	-0.259900
H	1.404100	2.802500	-0.533800
H	6.612200	-1.360900	-0.578200
H	5.535800	-2.117600	0.629000
H	6.682900	-0.845400	1.136000
N	-3.895200	0.788700	0.177800
N	-1.889200	-0.380800	-0.147300
N	-1.754700	-2.677000	-0.465200
C	-2.524300	0.829000	0.056200
C	-2.562200	-1.570100	-0.269100
C	-3.924600	-1.612000	-0.153300
C	-4.681200	-0.416900	0.100500
C	-4.583600	2.062500	0.393500
O	-5.903500	-0.359400	0.228000
O	-1.880900	1.889300	0.123600
H	-0.834100	-0.369100	-0.087800
H	-4.476900	-2.540500	-0.261700
H	-0.906600	-2.508900	-0.999000
H	-2.246600	-3.513300	-0.758200
H	-4.221700	2.536500	1.313000
H	-5.649300	1.834800	0.471000
H	-4.394200	2.741000	-0.446200

3a: C_s symmetry

N	0.297493	-0.964275	0.000000
N	0.842463	-3.325434	0.000000
N	3.261886	-3.702372	0.000000
N	3.967006	-1.551161	0.000000
N	1.920232	0.723433	0.000000
C	0.014509	-2.282413	0.000000
C	2.125564	-2.920512	0.000000
C	2.586461	-1.599511	0.000000
C	1.605467	-0.577816	0.000000
C	4.326252	-2.819766	0.000000
C	3.295994	-5.157746	0.000000
H	-1.048270	-2.538949	0.000000
H	5.350966	-3.177310	0.000000
H	1.193358	1.462736	0.000000
H	2.900895	0.971563	0.000000
H	3.805502	-5.533220	-0.895672
H	2.260680	-5.512105	0.000000
H	3.805502	-5.533220	0.895672
N	-2.224001	3.433842	0.000000
N	-1.723923	1.143822	0.000000
N	-3.330743	-0.522511	0.000000
C	-1.267090	2.448283	0.000000
C	-3.058020	0.814962	0.000000
C	-4.012791	1.799477	0.000000
C	-3.646175	3.184718	0.000000
C	-1.754553	4.820243	0.000000
O	-4.428187	4.134637	0.000000
O	-0.051126	2.702762	0.000000
H	-0.991546	0.392508	0.000000
H	-5.071795	1.560675	0.000000
H	-2.588721	-1.205609	0.000000
H	-4.285883	-0.843746	0.000000
H	-1.144454	5.012967	0.889845
H	-2.645817	5.452072	0.000000
H	-1.144454	5.012967	-0.889845

3b: no symmetry

N	3.426637	-2.320009	-0.424707
N	4.668631	-0.293063	0.022967
N	3.203458	1.622792	0.388452
N	1.204719	0.628135	0.091124
N	1.109869	-2.454975	-0.448351
C	4.543698	-1.598335	-0.263996
C	3.467454	0.290872	0.113283
C	2.213817	-0.313163	-0.058983
C	2.222669	-1.710243	-0.310551
C	1.838860	1.757890	0.362839
C	4.203176	2.640763	0.680729
H	5.477613	-2.151637	-0.373252
H	1.354642	2.709200	0.557627
H	1.251777	-3.453660	-0.544635
H	0.176705	-2.117337	-0.171827
H	5.181666	2.221941	0.426471
H	4.192234	2.904483	1.745752
H	4.021822	3.538219	0.078281
N	-3.605344	-0.778100	0.260643
N	-1.630574	0.404051	-0.188381
N	-1.556188	2.649903	-0.779402
C	-2.231555	-0.793321	0.152984
C	-2.336454	1.549721	-0.455932
C	-3.699756	1.564348	-0.356656
C	-4.424602	0.384442	0.032199
C	-4.260639	-2.037869	0.617895
O	-5.646196	0.307106	0.153276
O	-1.556921	-1.815110	0.347956
H	-0.583421	0.438169	-0.106564
H	-4.278530	2.454544	-0.583783
H	-0.709437	2.432491	-1.299052
H	-2.074824	3.420759	-1.186143
H	-4.030670	-2.807272	-0.128055
H	-5.334182	-1.837356	0.645501
H	-3.907600	-2.383849	1.596054

3b: C_s symmetry

N	-4.193533	-2.970791	0.000000
N	-5.562315	-0.980337	0.000000
N	-4.232082	1.055751	0.000000
N	-2.157954	0.164702	0.000000
N	-1.883212	-2.977753	0.000000
C	-5.354183	-2.305939	0.000000
C	-4.399392	-0.317987	0.000000
C	-3.103374	-0.857352	0.000000
C	-3.027636	-2.278021	0.000000
C	-2.879326	1.274318	0.000000
C	-5.305702	2.039281	0.000000
H	-6.250697	-2.927831	0.000000
H	-2.487067	2.286806	0.000000
H	-1.971201	-3.986643	0.000000
H	-0.942885	-2.558135	0.000000
H	-6.250274	1.486601	0.000000
H	-5.254974	2.668811	-0.896631
H	-5.254974	2.668811	0.896631
N	2.830768	-1.133174	0.000000
N	0.813558	0.062086	0.000000
N	0.692831	2.374893	0.000000
C	1.456241	-1.163535	0.000000
C	1.484691	1.261920	0.000000
C	2.854865	1.288977	0.000000
C	3.618955	0.075857	0.000000
C	3.525739	-2.421812	0.000000
O	4.847121	0.002547	0.000000
O	0.813017	-2.223274	0.000000
H	-0.228460	0.038917	0.000000
H	3.402241	2.226565	0.000000
H	1.108764	3.292770	0.000000
H	-0.311201	2.291919	0.000000
H	3.251343	-2.999551	0.890004
H	4.595597	-2.200447	0.000000
H	3.251343	-2.999551	-0.890004

Thymine — 5-methyl-6-aminouracil

3c: C_s symmetry

N	0.034573	0.024476	0.000000
N	-1.341640	1.905912	0.000000
C	-0.052075	1.389789	0.000000
C	-2.446845	1.070157	0.000000
C	-2.367639	-0.281907	0.000000
C	-1.036271	-0.897811	0.000000
C	-3.563620	-1.185675	0.000000
C	-1.535563	3.356235	0.000000
O	-0.824923	-2.104330	0.000000
O	0.946607	2.137879	0.000000
H	1.004699	-0.375431	0.000000
H	-3.403380	1.591930	0.000000
H	-4.498887	-0.612934	0.000000
H	-3.549642	-1.844115	0.879150
H	-3.549642	-1.844115	-0.879150
H	-0.550927	3.827016	0.000000
H	-2.088646	3.665491	0.896155
H	-2.088646	3.665491	-0.896155
N	4.957799	-0.693474	0.000000
N	3.539039	1.166283	0.000000
N	4.263136	3.360594	0.000000
C	3.673895	-0.207477	0.000000
C	4.599967	2.037671	0.000000
C	5.882804	1.551906	0.000000
C	6.138737	0.140363	0.000000
C	5.123063	-2.148310	0.000000
O	7.251630	-0.385233	0.000000
O	2.672696	-0.944047	0.000000
H	2.558481	1.515213	0.000000
H	6.741497	2.216176	0.000000
H	3.295494	3.650238	0.000000
H	4.983195	4.065612	0.000000
H	4.651929	-2.581978	0.889430
H	6.198316	-2.341505	0.000000
H	4.651929	-2.581978	-0.889430

3d: C_s symmetry

N	-0.609094	-1.430770	0.000000
N	-0.871787	-3.758476	0.000000
C	-1.498043	-2.496241	0.000000
C	0.494046	-3.879714	0.000000
C	1.355769	-2.824821	0.000000
C	0.775028	-1.491645	0.000000
C	2.853974	-2.985039	0.000000
C	-1.723726	-4.949638	0.000000
O	1.454595	-0.440508	0.000000
O	-2.711675	-2.360795	0.000000
H	-1.053203	-0.476094	0.000000
H	0.856893	-4.908066	0.000000
H	3.206069	-3.527945	-0.887710
H	3.206069	-3.527945	0.887710
H	3.320726	-1.995087	0.000000
H	-2.761265	-4.607149	0.000000
H	-1.536171	-5.553285	0.896908
H	-1.536171	-5.553285	-0.896908
N	-1.573623	3.408112	0.000000
N	0.346471	2.072613	0.000000
N	2.505081	2.888670	0.000000
C	-1.029240	2.148851	0.000000
C	1.170149	3.170506	0.000000
C	0.628704	4.431629	0.000000
C	-0.792345	4.624925	0.000000
C	-3.034242	3.509154	0.000000
O	-1.368431	5.712472	0.000000
O	-1.722564	1.115521	0.000000
H	0.742833	1.104929	0.000000
H	1.254421	5.318738	0.000000
H	2.832553	1.932605	0.000000
H	3.180368	3.636494	0.000000
H	-3.447576	3.019707	-0.889214
H	-3.274249	4.574992	0.000000
H	-3.447576	3.019707	0.889214

Guanine — 5-methyl-6-aminouracil

3e: C_s symmetry

N	-1.749485	0.068170	0.000000
N	-4.127099	0.059085	0.000000
N	-4.986708	-2.208736	0.000000
N	-3.057631	-3.389278	0.000000
N	-2.937618	2.054757	0.000000
C	-2.967481	0.695579	0.000000
C	-3.971691	-1.282468	0.000000
C	-2.783348	-2.034121	0.000000
C	-1.547781	-1.323550	0.000000
C	-4.368543	-3.452754	0.000000
C	-6.411327	-1.913192	0.000000
O	-0.379553	-1.772841	0.000000
H	-0.890675	0.672792	0.000000
H	-4.953296	-4.366967	0.000000
H	-3.814849	2.553527	0.000000
H	-2.060948	2.558908	0.000000
H	-6.525458	-0.825044	0.000000
H	-6.892577	-2.325673	0.895610
H	-6.892577	-2.325673	-0.895610
N	2.685624	2.052037	0.000000
N	1.721227	-0.073266	0.000000
N	2.902734	-2.047253	0.000000
C	1.550766	1.287744	0.000000
C	2.950703	-0.687301	0.000000
C	4.095766	0.072158	0.000000
C	4.029988	1.501853	0.000000
C	2.527152	3.506244	0.000000
O	4.989724	2.271251	0.000000
O	0.402013	1.788452	0.000000
H	0.853387	-0.674846	0.000000
H	5.080824	-0.384054	0.000000
H	2.013588	-2.532671	0.000000
H	3.755047	-2.585024	0.000000
H	1.976077	3.828426	-0.891198
H	3.534885	3.928932	0.000000
H	1.976077	3.828426	0.891198

3f: no symmetry

N	-2.641068	1.911306	-0.389812
N	-4.438756	0.527996	0.298093
N	-3.745146	-1.797965	0.439440
N	-1.574985	-1.616175	-0.144237
N	-4.770370	2.808904	0.000599
C	-3.945718	1.711068	-0.007674
C	-3.523202	-0.463976	0.189904
C	-2.174323	-0.373666	-0.169219
C	-1.631607	0.907076	-0.501346
C	-2.537782	-2.436038	0.221637
C	-5.009322	-2.396771	0.842957
O	-0.497560	1.229887	-0.851977
H	-2.319689	2.840830	-0.653159
H	-2.438190	-3.507722	0.353663
H	-5.666271	2.644185	0.446949
H	-4.362285	3.718337	0.183802
H	-5.760157	-2.271122	0.053935
H	-5.374969	-1.920869	1.759897
H	-4.850936	-3.463732	1.026602
N	4.360513	0.636474	0.331674
N	2.132291	0.163212	-0.241206
N	1.390106	-1.941971	-0.913322
C	3.069327	1.112601	0.164478
C	2.427628	-1.159055	-0.469987
C	3.713743	-1.608013	-0.294395
C	4.767101	-0.723185	0.110198
C	5.363468	1.610942	0.757669
O	5.945832	-1.047804	0.283108
O	2.752568	2.284558	0.355076
H	1.194604	0.532835	-0.446304
H	3.970730	-2.650502	-0.456408
H	0.428507	-1.719821	-0.631511
H	1.589035	-2.934453	-0.928978
H	5.444015	2.419723	0.021473
H	6.310313	1.072373	0.843483
H	5.078993	2.050790	1.721053

3f: C_s symmetry

N	2.364812	2.602848	0.000000
N	4.080185	0.964721	0.000000
N	3.145870	-1.278610	0.000000
N	0.941407	-0.805568	0.000000
N	4.622585	3.211910	0.000000
C	3.686726	2.224150	0.000000
C	3.045741	0.093196	0.000000
C	1.673596	0.364119	0.000000
C	1.237734	1.723895	0.000000
C	1.848166	-1.760018	0.000000
C	4.386520	-2.042272	0.000000
O	0.105287	2.203159	0.000000
H	2.107126	3.587700	0.000000
H	1.640929	-2.824390	0.000000
H	5.594911	2.938407	0.000000
H	4.384383	4.191805	0.000000
H	4.452107	-2.670594	0.896156
H	5.214923	-1.328008	0.000000
H	4.452107	-2.670594	-0.896156
N	-4.916961	2.180377	0.000000
N	-2.694936	1.417681	0.000000
N	-2.118340	-0.839987	0.000000
C	-3.570805	2.503602	0.000000
C	-3.099792	0.104200	0.000000
C	-4.444116	-0.190612	0.000000
C	-5.436871	0.840511	0.000000
C	-5.855578	3.300906	0.000000
O	-6.658514	0.659031	0.000000
O	-3.154357	3.659468	0.000000
H	-1.697866	1.666130	0.000000
H	-4.791046	-1.219459	0.000000
H	-1.115256	-0.643700	0.000000
H	-2.398687	-1.808718	0.000000
H	-5.701554	3.925182	0.888350
H	-6.860031	2.870658	0.000000
H	-5.701554	3.925182	-0.888350

3g: no symmetry

N	-3.246528	2.426815	-0.062559
N	-4.382291	0.367221	-0.380977
N	-2.806485	-1.491474	-0.464069
N	-0.875950	-0.390891	-0.141539
N	-5.576198	2.362258	-0.318445
C	-4.386646	1.675838	-0.239063
C	-3.134897	-0.160807	-0.338566
C	-1.921182	0.503198	-0.140650
C	-1.912511	1.922787	0.007410
C	-1.432047	-1.567358	-0.336019
C	-3.736964	-2.589283	-0.688574
O	-0.969023	2.701094	0.166366
H	-3.307365	3.441938	-0.022288
H	-0.882366	-2.501432	-0.391352
H	-6.391606	1.759024	-0.286790
H	-5.667885	3.221191	0.212444
H	-4.281579	-2.438117	-1.627753
H	-4.457684	-2.649367	0.135139
H	-3.169498	-3.522768	-0.743899
N	3.900022	-1.549298	0.144901
N	1.951575	-0.250751	0.207418
N	1.928704	2.038497	0.601125
C	2.522639	-1.504571	0.052302
C	2.664258	0.901097	0.432420
C	4.036662	0.842926	0.510289
C	4.738330	-0.397414	0.372522
C	4.533117	-2.857313	-0.009257
O	5.963044	-0.540177	0.433667
O	1.821187	-2.501643	-0.154678
H	0.916334	-0.234756	0.108179
H	4.628301	1.734892	0.692795
H	0.934188	2.088497	0.369288
H	2.428038	2.916160	0.610141
H	4.167093	-3.549555	0.758488
H	5.609313	-2.699255	0.096404
H	4.300535	-3.279425	-0.994410

3g: C_s symmetry

N	-3.701876	2.445859	0.000000
N	-4.872078	0.379991	0.000000
N	-3.321902	-1.498863	0.000000
N	-1.363469	-0.399853	0.000000
N	-6.040173	2.375354	0.000000
C	-4.858536	1.698028	0.000000
C	-3.630189	-0.157753	0.000000
C	-2.399507	0.505298	0.000000
C	-2.370653	1.929612	0.000000
C	-1.940021	-1.582095	0.000000
C	-4.282151	-2.595303	0.000000
O	-1.414173	2.709264	0.000000
H	-3.745492	3.462406	0.000000
H	-1.400131	-2.523236	0.000000
H	-6.892243	1.832955	0.000000
H	-6.094586	3.382078	0.000000
H	-4.156277	-3.214672	-0.895771
H	-5.285248	-2.159235	0.000000
H	-4.156277	-3.214672	0.895771
N	3.419347	-1.536756	0.000000
N	1.485454	-0.214846	0.000000
N	1.502019	2.104977	0.000000
C	2.039550	-1.485520	0.000000
C	2.216913	0.947419	0.000000
C	3.592197	0.880484	0.000000
C	4.275930	-0.376275	0.000000
C	4.034652	-2.862086	0.000000
O	5.501092	-0.527850	0.000000
O	1.320383	-2.490934	0.000000
H	0.445390	-0.204000	0.000000
H	4.199637	1.780445	0.000000
H	0.480823	2.143450	0.000000
H	2.003410	2.979874	0.000000
H	3.726336	-3.425025	0.889256
H	5.116275	-2.705666	0.000000
H	3.726336	-3.425025	-0.889256

Cytosine — 5-methyl-6-aminouracil

3h: no symmetry

N	-2.313659	0.392286	0.091450
N	-3.304648	-1.779220	-0.101872
N	-3.621427	2.281507	0.045317
C	-2.144250	-0.962242	0.053405
C	-4.534639	-1.220722	-0.207557
C	-4.707974	0.132537	-0.163531
C	-3.529295	0.924008	-0.000074
C	-3.100038	-3.228782	-0.142806
O	-1.051322	-1.528146	0.148202
H	-5.367948	-1.910259	-0.326241
H	-5.697965	0.571747	-0.249692
H	-2.798244	2.801393	0.322668
H	-4.520813	2.727511	0.156241
H	-2.635590	-3.566853	0.790235
H	-2.426723	-3.486152	-0.967826
H	-4.069699	-3.717677	-0.280191
N	3.956995	-0.801997	-0.023154
N	1.637100	-0.519271	0.199465
N	0.586874	1.559009	0.221779
C	2.715062	-1.399317	0.131028
C	1.753195	0.844348	0.099199
C	2.990892	1.415109	-0.067781
C	4.177429	0.612699	-0.138107
C	5.106734	-1.702103	-0.092439
O	5.324245	1.046302	-0.284545
O	2.555029	-2.615431	0.202819
H	0.703614	-0.952045	0.250676
H	3.109593	2.492485	-0.132726
H	-0.316861	1.089307	0.115153
H	0.624538	2.511227	-0.116428
H	5.164543	-2.311542	0.817045
H	5.994508	-1.073487	-0.195155
H	5.010318	-2.376685	-0.951869

3h: C_s symmetry

N	-1.987583	-0.829658	0.000000
N	-3.170974	1.252911	0.000000
N	-3.130171	-2.821385	0.000000
C	-1.932959	0.536430	0.000000
C	-4.352690	0.586767	0.000000
C	-4.409010	-0.775369	0.000000
C	-3.155886	-1.464614	0.000000
C	-3.144736	2.720517	0.000000
O	-0.877570	1.175747	0.000000
H	-5.249444	1.204146	0.000000
H	-5.362442	-1.296573	0.000000
H	-2.238513	-3.297851	0.000000
H	-3.979133	-3.366132	0.000000
H	-3.643778	3.106879	-0.897305
H	-2.097146	3.029061	0.000000
H	-3.643778	3.106879	0.897305
N	4.191333	0.861534	0.000000
N	1.888272	0.411574	0.000000
N	0.995953	-1.730386	0.000000
C	2.901100	1.367619	0.000000
C	2.109941	-0.943074	0.000000
C	3.397853	-1.424244	0.000000
C	4.523135	-0.537233	0.000000
C	5.274913	1.842619	0.000000
O	5.707857	-0.886330	0.000000
O	2.645917	2.569911	0.000000
H	0.924138	0.771916	0.000000
H	3.600176	-2.491084	0.000000
H	0.045317	-1.355173	0.000000
H	1.122729	-2.730378	0.000000
H	5.207768	2.481926	-0.888451
H	6.211049	1.279074	0.000000
H	5.207768	2.481926	0.888451

3i: C_s symmetry

N	-0.302763	-1.404587	0.000000
N	-1.937126	-3.141915	0.000000
N	1.940494	-1.886184	0.000000
C	-1.615458	-1.753059	0.000000
C	-0.945062	-4.074914	0.000000
C	0.369929	-3.727210	0.000000
C	0.673902	-2.323906	0.000000
C	-3.342421	-3.555568	0.000000
O	-2.540151	-0.924059	0.000000
H	-1.270802	-5.113775	0.000000
H	1.148183	-4.485802	0.000000
H	2.149635	-0.860029	0.000000
H	2.699770	-2.552372	0.000000
H	-3.949359	-2.647672	0.000000
H	-3.565547	-4.147698	0.896727
H	-3.565547	-4.147698	-0.896727
N	1.968248	3.043812	0.000000
N	0.292448	1.413634	0.000000
N	-1.970168	1.877568	0.000000
C	1.634452	1.714845	0.000000
C	-0.706363	2.364068	0.000000
C	-0.366375	3.699245	0.000000
C	0.997740	4.121220	0.000000
C	3.390645	3.382995	0.000000
O	1.398745	5.286557	0.000000
O	2.497834	0.812185	0.000000
H	0.053032	0.395357	0.000000
H	-1.129262	4.471725	0.000000
H	-2.169787	0.866062	0.000000
H	-2.739368	2.529996	0.000000
H	3.880196	2.970506	0.890001
H	3.449700	4.474229	0.000000
H	3.880196	2.970506	-0.890001

3j: C_s symmetry

N	1.350562	0.000000	0.000000
N	-0.649332	1.276424	0.000000
N	3.424637	0.966545	0.000000
C	0.000000	0.000000	0.000000
C	0.094433	2.418212	0.000000
C	1.457635	2.402679	0.000000
C	2.082583	1.109149	0.000000
C	-2.111172	1.342258	0.000000
O	-0.686515	-1.035659	0.000000
H	-0.470404	3.349229	0.000000
H	2.024283	3.330494	0.000000
H	3.870133	0.030615	0.000000
H	4.019742	1.782195	0.000000
H	-2.479174	0.313296	0.000000
H	-2.472315	1.862589	-0.896600
H	-2.472315	1.862589	0.896600
N	4.783331	-3.967498	0.000000
N	2.684190	-5.034229	0.000000
N	0.658299	-3.827933	0.000000
C	4.077523	-5.160191	0.000000
C	2.015743	-3.828147	0.000000
C	2.751598	-2.673663	0.000000
C	4.164717	-2.678543	0.000000
C	6.242745	-4.070965	0.000000
O	4.874067	-1.648314	0.000000
O	4.605663	-6.268225	0.000000
H	2.196260	-5.923753	0.000000
H	2.236388	-1.716132	0.000000
H	0.120883	-4.681466	0.000000
H	0.167811	-2.926056	0.000000
H	6.583700	-4.614046	0.889154
H	6.632327	-3.050360	0.000000
H	6.583700	-4.614046	-0.889154