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SUPPLEMENTARY DATA

Hydrogen Bonding Reactivities of Atomic Sites in the Nucleobases

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Table S1. Proton affinities (PA), shifts of electrostatic potential at nuclei (ΔV_N), and atomic charges [q_N(NBO) and q_N(Hirsh)] for nitrogen proton accepting sites in the primary nucleobases and in sets of model compounds (Scheme 2) from M06-2X/6-311+G(2d,2p) computations.

Molecule, Substituent	PA [kcal/mol]	ΔV_N [b] [kcal/mol]	q_N(NBO) [e]	q_N(Hirsh) [e]
Pyridine	219.0	2.6	-0.4594	-0.1613
Pyrimidines				
H	208.6	10.5	-0.4837	-0.1640
4-CH_3	214.6	6.1	-0.4932	-0.1714
4-NH_2	224.0	-2.2	-0.5268	-0.1909
4-F	204.2	15.7	-0.4941	-0.1676
4-CHO	203.4	20.2	-0.4657	-0.1528
4-CN	197.1	27.1	-0.4631	-0.1482
4-NO_2	193.9	30.1	-0.4588	-0.1453
Purines (sp^2 N)				
H	210.9	10.3	-0.4885	-0.1971
2-CH_3	214.3	7.7	-0.4877	-0.1987

2-NH_2	219.2	4.2	-0.4828	-0.2000
2-F	206.5	15.4	-0.4806	-0.1930
2-CHO	206.0	17.4	-0.4887	-0.1933
2-CN	201.1	22.7	-0.4832	-0.1889
2-NO_2	199.1	24.8	-0.4823	-0.1876
Purines (NH)				
H	170.2	67.7	-0.5840	0.1018
2- CH_3	174.0	65.0	-0.5834	0.0988
2-NH_2	179.8	60.7	-0.5894	0.0928
2-F	165.2	73.3	-0.5832	0.1076
2-CHO	165.6	74.6	-0.5798	0.1116
2-CN	159.7	81.0	-0.5774	0.1155
2-NO_2	157.5	83.2	-0.5764	0.1194
Anilines				
H	207.3	24.3	-0.8213	0.0720
4-CH_3	210.0	18.9	-0.8156	0.0419
4-NH_2	214.9	15.3	-0.8196	0.0290
4-F	204.6	23.9	-0.8151	0.0460
4-CHO	199.0	34.5	-0.8004	0.0806
4-CN	195.0	37.7	-0.8008	0.0826
4-NO_2	193.0	40.8	-0.7967	0.0917
Pyridin-2(1H)-ones				
H	176.0	57.0	-0.5898	0.1009
5-NH_2	186.8	52.7	-0.5852	0.0922
5-NO_2	158.8	80.0	-0.5734	0.1267
5-CH_3	180.9	53.9	-0.5881	0.0956
5-F	173.3	63.4	-0.5844	0.1039
5-CN	161.4	76.2	-0.5796	0.1208
5-Cl	172.6	64.9	-0.5819	0.1075
Imides				
Imide 1	186.4	49.9	-0.6913	0.0544
Imide 2	174.3	63.7	-0.6923	0.0685
Nucleobases				
Adenine				
N1	222.0	7.4	-0.5720	-0.2066
N3	220.2	1.9	-0.5434	-0.2110
N7	213.6	6.9	-0.5011	-0.2040
N9	177.6	52.5	-0.5772	0.1004
N10	200.0	33.9	-0.7865	0.1173
Guanine				
N3	209.4	9.8	-0.6013	-0.2333
N7	225.0	0.8	-0.4537	-0.1867
N9	179.6	60.9	-0.5702	0.0985

N11	186.5	45.1	-0.8132	0.0929
Thymine				
N1	174.4	64.4	-0.6335	0.0812
N3	174.8	54.4	-0.6648	0.0777
Uracil				
N1	172.4	55.9	-0.6704	0.0783
N3	169.0	68.1	-0.63696	0.0863
Cytosine				
N1	185.3	53.9	-0.6192	0.0840
N3	224.5	-6.7	-0.6165	-0.2182
N7	192.9	29.5	-0.7867	0.1195
Correlation coefficient[a]		**0.986**	**0.167**	**0.817**

[a]Correlation coefficients for the correlations with proton affinities
[b]ΔV_N is defined in Eqns. 2 and 3 in the main text.

Table S2. Proton affinities (PA), shifts of electrostatic potential at nuclei (ΔV_O), and atomic charges [q_O(NBO) and q_O(Hirsh)] for carbonyl oxygen proton accepting sites in the primary nucleobases and in sets of model compounds (Scheme 3) from M06-2X/6-311+G(2d,2p) computations.

Derivative	**PA [kcal/mol]**	**ΔV_O[b] [kcal/mol]**	**q_O(NBO) [e]**	**q_O(Hirsh) [e]**
Cyclohexa-2,4-dienones				
H	209.0	-22.4	-0.5735	-0.2803
4-CH3	211.1	-23.5	-0.5739	-0.2810
4-NH2	211.8	-23.1	-0.5713	-0.2785
4-F	202.5	-15.36	-0.5626	-0.2709
4-Cl	203.3	-14.9	-0.5618	-0.2707
4-Br	203.6	-14.7	-0.5616	-0.2705
4-CHO	202.0	-13.6	-0.5616	-0.2700
4-CN	196.8	-8.36	-0.5544	-0.2645
4-NO	200.2	-11.9	-0.5602	-0.2689
4-NO2	195.6	-6.9	-0.5525	-0.2629
Benzoquinone	188.6	1.3	-0.5110	-0.2370
Pyridin-2(1H)-ones				
H	217.4	-36.9	-0.6543	-0.3450
5-CH_3	220.9	-39.4	-0.6587	-0.3493
5-NH_2	224.7	-42.0	-0.6659	-0.3555
5-F	213.5	-32.8	-0.6519	-0.3430
5-Cl	213.3	-30.4	-0.6453	-0.3376
5-CN	203.9	-18.5	-0.6230	-0.3189
5-NO_2	201.8	-15.0	-0.6156	-0.3127
Nucleobases				
Guanine				

O10	213.2	-29.6	-0.6093	-0.3120
Tymine				
O7	204.9	-20.2	-0.6130	-0.3006
O8	206.1	-20.0	-0.6424	-0.3324
Uracil				
O7	208.5	-19.76	-0.6047	-0.3059
O8	203.2	-16.7	-0.6362	-0.3270
Cytosine				
O8	226.6	-41.9	-0.6445	-0.3438
Correlation coefficient[a]		**0.985**	**0.769**	**0.794**

[a]Correlation coefficients for the correlations with proton affinities and molecular parameters
[b] ΔV_O is defined in eq 4 in the main text.

Figure S1. Plot of theoretically evaluated proton affinities vs. shifts of electrostatic potential at the nuclei for nitrogen atomic sites in model compounds (Scheme 2) and in the nucleobases.

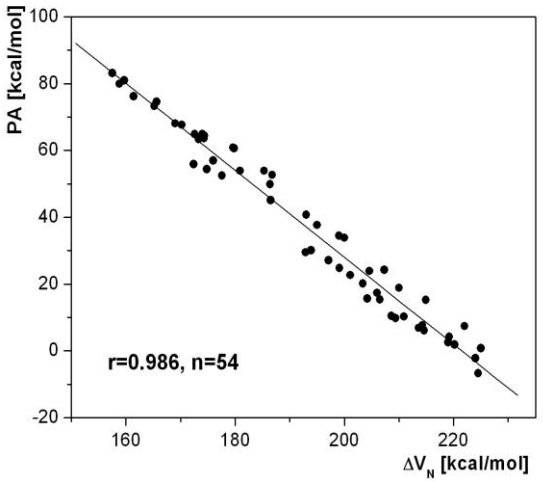

Figure S2. Plot of proton affinities vs. shifts of electrostatic potential at the nuclei for oxygen atomic sites in model compounds (Scheme 2) and in the primary nucleobases.

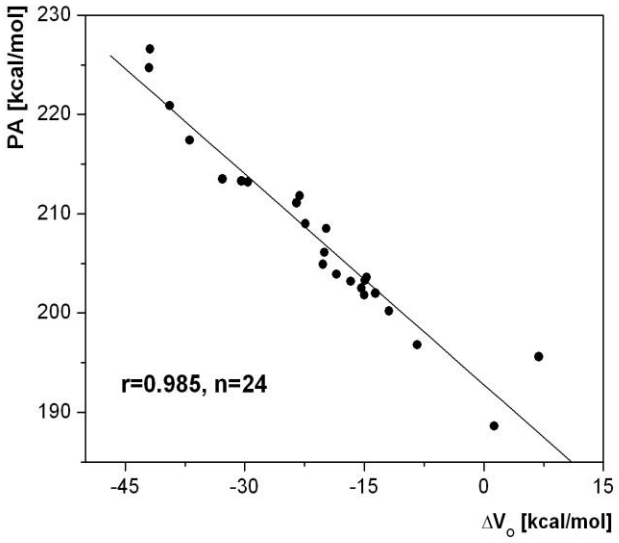

Table S3. Theoretical parameters for N-H proton donating sites in the set of model nitrogen compounds (Scheme 3) and in the nucleobases from M06-2X/6-311+G(2d,2p).

Derivative	Edep [kcal/mol]	ΔV_H [b] [kcal/mol]	q_H(NBO) [e]	q_H(Hirsh) [e]
1,6-dihydropyrimidines				
H	-363.4998	31.89	0.3914	0.1302
4-OCH_3	-361.0473	33.33	0.3930	0.1322
4-NH_2	-363.0383	31.32	0.3911	0.1298
4-F	-354.9421	41.67	0.3920	0.1314
4-Cl	-352.1474	41.99	0.3968	0.1367
4-Br	-350.2850	41.67	0.3970	0.1366
4-CHO	-353.2339	41.24	0.3972	0.1368
4-CN	-347.5278	41.57	0.3989	0.1384
4-NO_2	-345.2926	50.27	0.4008	0.1400
Anilines				
H	-374.3994	17.14	0.3747	0.1142
4-OCH3	-377.2192	13.31	0.3700	0.1108
4-NH2	-377.8860	11.05	0.3697	0.1093

4-F	-372.4906	19.77	0.3742	0.1143
4-Cl	-367.6720	22.91	0.3766	0.1167
4-Br	-366.3538	27.37	0.3771	0.1172
4-CHO	-355.4729	30.57	0.3824	0.1227
4-CN	-354.9064	33.77	0.3834	0.1235
4-NO2	-348.7905	36.91	0.3856	0.1258
Nucleobases				
Adenine				
N9-H	-342.0567	57.56	0.4258	0.1587
N10-H	-361.6756	31.44	0.4043	0.1320
Guanine				
N1-H	-344.4985	50.95	0.4127	0.1424
N9-H	-341.8752	56.85	0.4236	0.1566
N11-H	-350.0580	40.91	0.3860	0.1287
Tymine				
N1-H	-341.5219	56.43	0.4232	0.1533
N3-H	-352.8951	4782	0.4273	0.1526
Uracil				
N1-H	-339.6191	59.86	0.4247	0.1551
N3-H	-352.4227	49.32	0.4284	0.1532
Cytosine				
N1-H	-351.4197	44.93	0.4182	0.1478
N7-H	-360.1006	39.22	0.3914	0.1309
correlation coefficient[a]		**0.956**	**0.781**	**0.854**

[a] Correlation coefficients for the relationships of E_{dep} with ΔV_H, q_H(NBO) and q_H(Hirsh).
[b] ΔV_H is defined in eq 5 in the main text.

Table S4. Hydrogen bonding energies and reactivity descriptors for nitrogen proton accepting centers in model molecules (Scheme 2) from M06-2X/6-311+G(2d,2p) computations.

Molecule	ΔE_{corr} [kcal/mol]	ΔV_N[a] [kcal/mol.]	q_N(NBO) [e]	q_N(Hirsh) [e]	PA [kcal/mol]
sp^2- Hybridized nitrogen atoms					
Pyridine	-9.43	2.64	-0.4594	-0.1613	219.0
Pyrimidines					
H	-8.27	10.47	-0.4837	-0.1640	208.6
4-CH_3	-8.78	6.14	-0.4932	-0.1714	214.6
4-NH2	-9.66	-2.18	-0.5268	-0.1909	224.0
4-F	-7.82	15.71	-0.4941	-0.1676	204.2
4-CHO	-7.33	20.17	-0.4657	-0.1528	203.4
4-CN	-6.91	27.08	-0.4631	-0.1482	197.1

4-NO_2	-6.57	30.09	-0.4588	-0.1453	193.9
Purines					
H	-8.31	10.31	-0.4885	-0.1971	210.9
2-CH_3	-8.57	7.71	-0.4877	-0.1987	214.3
2-NH2	-8.99	4.16	-0.4828	-0.2	219.2
2-F	-7.83	15.44	-0.4806	-0.193	206.5
2-CHO	-7.52	17.42	-0.4887	-0.1933	206.0
2-CN	-7.14	22.69	-0.4832	-0.1889	201.1
2-NO_2	-7.16	24.78	-0.4823	-0.1876	199.1
sp^3- Hybridized nitrogen atoms					
Anilines					
H	-6.83	24.20	-0.8213	0.0720	207.3
4-CH_3	-6.90	18.96	-0.8156	0.0419	210.0
4-OCH3	-7.92	17.61	-0.8181	0.0339	212.0
4-NH2	-7.47	15.30	-0.8196	0.0290	214.9
4-F	-6.77	23.90	-0.8151	0.0460	204.6
4-Cl	-6.19	26.98	-0.8113	0.0559	203.3
4-Br	-6.06	27.72	-0.8106	0.0579	203.1
4-CHO	-4.93	34.54	-0.8004	0.0806	199.0
4-CN	-4.84	37.74	-0.8008	0.0826	195.0
5-Amino-pyrimidines					
H	-5.15	35.71	-0.8105	0.0704	193.1
2-CH_3	-5.36	32.50	-0.8131	0.0621	197.3
2-NH_2	-6.31	26.90	-0.8185	0.0438	204.7
2-F	-4.90	39.23	-0.8117	0.0694	189.9
2-CHO	-3.92	46.42	-0.8002	0.0957	186.8
2-CN	-3.32	51.23	-0.7988	0.1025	
2-NO_2	-3.16	53.60	-0.7974	0.1072	
Correlation coefficients[b]		**0.991**	**0.516**	**0.387**	**0.985**
Correlation coefficients[c]		**0.987**	**0.897**	**0.937**	**0.958**

[a] ΔV_N is defined in Eqns. 2 and 3 in the main text.

[b] Correlation coefficient for the relationship between hydrogen bonding energies and molecular parameters for sp^2-hybridized nitrogen atoms.

[c] Correlation coefficient for the relationship between hydrogen bonding energies and molecular parameters for sp^3-hybridized nitrogen atoms.

Table S5. Hydrogen bonding energies and reactivity descriptors for oxygen proton accepting centers in model molecules (Scheme 3) from M06-2X/6-311+G(2d,2p) computations.

Molecule	ΔE_{corr} [kcal/mol]	ΔV_O[b] [kcal/mol.]	q_O(NBO) [e]	q_O(Hirsh) [e]	PA [kcal/mol]
Cyclohexa-2,4-dienones					
H	-9.72	-22.41	-0.5735	-0.2803	209.0
4-CH_3	-10.11	-23.54	-0.5739	-0.2810	211.1
4-NH_2	-10.00	-23.10	-0.5713	-0.2785	211.8
4-F	-9.14	-15.26	-0.5626	-0.2709	202.5
4-Cl	-8.91	-14.69	-0.5616	-0.2705	203.6
4-Br	-9.21	-14.88	-0.5618	-0.2707	203.3
4-CHO	-8.48	-13.63	-0.5616	-0.2700	202.0
4-CN	-8.56	-8.36	-0.5544	-0.2645	196.8
4-NO	-8.81	-11.87	-0.5602	-0.2689	200.2
4-NO_2	-8.34	-6.91	-0.5525	-0.2629	195.6
Benzoquinone	-6.92	1.31	-0.5110	-0.2370	188.6
Pyridin-2(1H)-ones					
H	-11.38	-36.91	-0.6543	-0.3450	217.4
5-CH3	-11.61	-39.42	-0.6587	-0.3493	220.9
5-NH_2	-12.18	-41.99	-0.6659	-0.3555	224.7
5-F	-10.80	-30.38	-0.6453	-0.3376	213.3
5-Cl	-11.15	-32.83	-0.6519	-0.3430	213.5
5-CN	-9.53	-18.46	-0.6230	-0.3189	203.9
5-NO_2	-9.22	-15.01	-0.6156	-0.3127	201.8
Correlation coefficients[a]		**0.991**	**0.911**	**0.910**	**0.979**

[a] Correlation coefficients for the relationships between ΔE_{cor} and molecular parameters.
[b] ΔV_O is defined in eq 4 in the main text.

Table S6. Hydrogen bonding energies, electrostatic potential at nuclei, NBO and Hirshfeld charges, and deprotonation energies for N-H hydrogen in 1,6-dihydropyrimidine and aniline derivatives from M06-2X/6-311+G(2d,2p).

Derivative	ΔE_{corr} [kcal/mol]	ΔV_H[b] [kcal/mol]	q_H(NBO) [e]	q_H(Hirsh) [e]	E_{dep} [kcal/mol]
1,6-Dihydropyrimidines					
H	-4.57	31.89	0.3914	0.1302	-363.50
4-OCH_3	-4.69	33.33	0.3930	0.1322	-361.05
4-NH_2	-4.72	31.32	0.3911	0.1298	-363.05
4-Br	-5.41	41.67	0.3970	0.1366	-350.29
4-CHO	-5.42	41.24	0.3972	0.1368	-353.23

4-NO_2	-5.85	50.27	0.4008	0.1400	-345.29
Anilines					
H	-3.64	17.14	0.3747	0.1142	-374.40
4-OCH_3	-3.54	13.31	0.3700	0.1108	-377.22
4-Br	-4.04	27.37	0.3771	0.1172	-366.35
4-CHO	-4.49	30.57	0.3824	0.1227	-355.47
4-CN	-4.84	33.77	0.3834	0.1235	-354.91
4-NO_2	-5.18	36.91	0.3856	0.1258	-348.79
Correlation coefficient[a]		**0.988**	**0.930**	**0.942**	**0.964**
Nucleobases					
Adenine					
N9-H		57.56	0.4258	0.1587	
N10-H		31.44	0.4043	0.1320	
Guanine					
N1-H		50.95	0.4127	0.1424	-344.4985
N9-H		56.85	0.4236	0.1566	-341.8752
N11-H		40.91	0.3860	0.1287	-350.0580
Tymine					
N1-H		56.43	0.4232	0.1533	-341.5219
N3-H		47.82	0.4273	0.1526	-352.8951
Uracil					
N1-H		59.86	0.4247	0.1551	-339.6191
N3-H		49.32	0.4284	0.1532	-352.4227
Cytosine					
N1-H		44.93	0.4182	0.1478	-351.4197
N7-H		39.22	0.3914	0.1309	-360.1006

[a] Correlation coefficients for the relationships between ΔE_{corr} and ΔV_H

[b] ΔV_H is defined in eq 5 in the main text.

S7. Cartesian Coordinates, Total Energies (in hartree), and Number of Imaginary Frequencies for the Optimized Structures of Model Sets of Molecules, Used for Calculations the Shifts of EPN from M06-2X/6-311+G(2d,2p) Computations.

NH_3
N,0,-1.6758727194,-0.8117382006,-0.01062624
H,0,-1.2975135118,-1.7508371263,-0.0106263553
H,0,-1.2974965372,-0.3421956769,0.8026533954
H,0,-1.2974965372,-0.3421954771,-0.8239057601
HF=-56.5492627 Nimag=0

CH_2NH
C,0,0.5661033495,0.0364230069,0.
H,0,1.2632890317,-0.7991237473,0.
H,0,0.9979024625,1.0391081601,0.
N,0,-0.6723737983,-0.2042463602,0.
H,0,-1.2097106854,0.6626282305,0.
HF=-94.6151324 Nimag=0

HCHO
C,0,-1.0437002383,0.1479441903,-0.0079707831
H,0,-1.6218085078,1.0870470128,-0.0079608214
H,0,-1.621829146,-0.7911459281,-0.0079831801
O,0,0.152204772,0.1479309884,-0.0079615754
HF=-114.4907506 Nimag=0

H_2
H,0,-0.3691560705,0.,0.
H,0,0.3691560705,0.,0.
HF= -1.1687457 Nimag=0

Table S8. Cartesian Coordinates, Total Energies (in *hartree*), and Number of Imaginary Frequencies for the Optimized Structures of Model Sets of Molecules, Containing Nitrogen Atoms from M06-2X/6-311+G(2d,2p) Computations.

Pyridine
C,0,-2.301322252,0.4316858104,0.0605264308
N,0,-2.2323087403,-0.8967585033,0.1199275199
C,0,-1.0213102337,-1.4486397625,0.0754759451
C,0,0.1535194666,-0.7159064291,-0.0282057755
C,0,0.0670546565,0.6668505702,-0.0891820855
C,0,-1.1880645358,1.2548962052,-0.0438771878
H,0,-3.295923396,0.8593597388,0.0982607513
H,0,-0.9884511656,-2.5303091446,0.1252103053
H,0,1.1073117317,-1.2211210475,-0.0598445942
H,0,0.9582210771,1.2728459619,-0.1702268755
H,0,-1.3080796358,2.3270935782,-0.0880629
HF=-248.2489657 Nimag=0

Pyrimidines
H
C,0,-2.5792178472,-0.7439168363,0.128727094
N,0,-3.0059499288,0.4906321407,-0.1244530826
C,0,-2.061353049,1.4116590905,-0.2892346328
N,0,-0.7459331259,1.2283713671,-0.2277561018
C,0,-0.3411460734,-0.0133435347,0.0264276682
C,0,-1.232349266,-1.0571136701,0.2165932189
H,0,-3.3419648055,-1.5017666678,0.264592401
H,0,-2.3998578557,2.4197255091,-0.4957795911
H,0,0.7295913385,-0.1726866619,0.0784860631
H,0,-0.8950623868,-2.0615607366,0.4223969631
HF=*-264.2918383* Nimag=0

4-CH_3
C,0,0.862319417,0.013442206,0.0062468555
C,0,0.1394635242,1.1981866775,-0.0737095077
C,0,-1.2414306175,1.1022114706,-0.0628883164
N,0,-1.8759469194,-0.0641723115,0.0194410946
C,0,-1.0929077908,-1.1372448947,0.0912676989
N,0,0.2341255085,-1.1626021918,0.0892296786
C,0,2.3604309135,-0.0175078312,0.0082275399
H,0,0.6354943308,2.1551660363,-0.142102052
H,0,-1.8622561537,1.9886460256,-0.122650238
H,0,-1.593166723,-2.0963133515,0.1581719501
H,0,2.713323007,-0.672129263,-0.7873428741
H,0,2.7160042075,-0.4321267255,0.9511544741
H,0,2.7832275059,0.975137153,-0.1265640335
HF=-303.6057028 Nimag=0

4-NH_2
C,0,0.166583532,1.2066660991,0.0150187755
C,0,0.8909707529,0.0059667985,0.0380274884
N,0,0.2694736938,-1.1737811168,0.0358732267
C,0,-1.0589907252,-1.1454555972,0.0055819927
N,0,-1.8449964581,-0.0783955557,-0.0167148738
C,0,-1.2034274931,1.0964805739,-0.0101152109
N,0,2.2573291671,-0.0154166784,0.022110771
H,0,0.6607218085,2.1669664559,0.0115842926
H,0,-1.5521484509,-2.1107979192,0.0022269552
H,0,-1.8247561796,1.9841233933,-0.0272537786
H,0,2.6778259068,-0.8999897693,0.2534014009
H,0,2.7498197358,0.8060229957,0.3243050803
HF=-319.6641017 Nimag=0

4-F
C,0,-1.1300337659,0.1889627746,0.0328119507
C,0,-1.0720117106,-1.194765247,0.0198861204

N,0,0.0318581198,-1.8900651326,-0.0132851111
C,0,1.1571714673,-1.1719781768,-0.0349418588
N,0,1.2534915339,0.1487573409,-0.0256134604
C,0,0.0989456026,0.8188339234,0.0083564436
F,0,-2.2065143027,-1.8830133714,0.0409865547
H,0,-2.068551018,0.7182930293,0.0601037149
H,0,2.0827760615,-1.7328507499,-0.061900115
H,0,0.1655500122,1.8995896096,0.015962761
HF=-363.544721 Nimag=0

4-CHO

C,0,-0.53647031,0.7184528072,0.024215086
C,0,-0.5068928348,-0.6662510763,0.0115431227
N,0,0.627074717,-1.362117013,-0.015676758
C,0,1.7481399907,-0.6481834872,-0.0298976146
N,0,1.8419619768,0.6782456493,-0.020547651
C,0,0.694748011,1.3534324793,0.0069939804
C,0,-1.7710606562,-1.4725204985,0.0276836273
O,0,-2.8594700306,-0.9712757671,0.0522728599
H,0,-1.4754817081,1.2508274585,0.0461080273
H,0,2.6783179406,-1.2018070433,-0.0532054934
H,0,0.7696740134,2.4341582734,0.014489211
H,0,-1.6147661098,-2.5634927823,0.0148706025
HF=-377.6096452 Nimag=0

4-CN

C,0,-0.6179969206,0.4348955074,0.0271556338
C,0,-0.5757179001,-0.9510338515,0.0136051076
N,0,0.5625383272,-1.6407833231,-0.0137848468
C,0,1.6741711836,-0.9150503936,-0.0271341303
N,0,1.7600881206,0.4135367565,-0.0163697546
C,0,0.6105403186,1.0782622765,0.0109265802
C,0,-1.8102940068,-1.7098463462,0.02849992
N,0,-2.8105489245,-2.2683866562,0.0412534632
H,0,-1.5533873123,0.972064953,0.0490529359
H,0,2.6070927122,-1.4638299036,-0.049753348
H,0,0.6719384019,2.1595699808,0.019649439
HF=-356.5252833 Nimag=0

4-NO_2

C,0,-0.5482154176,0.7958446572,-0.1045325824
C,0,-0.4744244598,-0.5802923995,-0.121190931
N,0,0.6297266119,-1.2765568796,-0.1810336031
C,0,1.7498404196,-0.5581350317,-0.2281731485
N,0,1.8325396137,0.7678942216,-0.2196007003
C,0,0.6834161253,1.4344547498,-0.157892003
N,0,-1.750143999,-1.3738046311,-0.0672796597
O,0,-1.6642617684,-2.5718432367,-0.0834309874
O,0,-2.7734099396,-0.7236358521,-0.0112113153
H,0,-1.4882258008,1.3190726161,-0.0542060497
H,0,2.6787336952,-1.1109862548,-0.2782135754
H,0,0.7470059194,2.5152670409,-0.1507494443
HF=-468.7815566 Nimag=0

Purines

H

N,0,1.0184670902,-1.9347938115,0.0760436206
C,0,2.148941418,-1.2670769244,0.2864762016
N,0,2.3051118353,0.0553948798,0.4324531693
C,0,1.2268868766,0.8291520975,0.3657500356
C,0,-0.0193544667,0.2594051089,0.1495145511
C,0,-0.0339829209,-1.1353573603,0.015128153
N,0,-1.2995577063,0.7728376486,0.0317955669
C,0,-2.0450363679,-0.2721875226,-0.1644634551
N,0,-1.3499822423,-1.4587792353,-0.186824872
H,0,3.0510212436,-1.8618656928,0.3473130187
H,0,1.3606945601,1.8975475709,0.4846319394
H,0,-3.1142000474,-0.250350114,-0.3014385238
H,0,-1.7216642722,-2.3828436447,-0.3226724055
HF= -411.9126643 Nimag=0

2-CH_3

C,0,0.862319417,0.013442206,0.0062468555
C,0,0.1394635242,1.1981866775,-0.0737095077
C,0,-1.2414306175,1.1022114706,-0.0628883164
N,0,-1.8759469194,-0.0641723115,0.0194410946
C,0,-1.0929077908,-1.1372448947,0.0912676989
N,0,0.2341255085,-1.1626021918,0.0892296786
C,0,2.3604309135,-0.0175078312,0.0082275399
H,0,0.6354943308,2.1551660363,-0.142102052
H,0,-1.8622561537,1.9886460256,-0.122650238
H,0,-1.593166723,-2.0963133515,0.1581719501
H,0,2.713323007,-0.672129263,-0.7873428741
H,0,2.7160042075,-0.4321267255,0.9511544741
H,0,2.7832275059,0.975137153,-0.1265640335
HF=-303.6057028 Nimag=0

2-NH_2

N,0,1.0918093965,-1.0694490839,0.9059088981
C,0,2.0363492265,-0.6470492626,0.0626423496
N,0,1.952396687,0.3793606977,-0.8104716967
C,0,0.8159757999,1.0549258478,-0.8741857724
C,0,-0.2537183582,0.7091326804,-0.060511869
C,0,-0.024955518,-0.3677872949,0.803953313
N,0,-1.5369118648,1.2077819638,0.1078275658
C,0,-2.0522775936,0.4592475097,1.031253366
N,0,-1.1922044569,-0.514627856,1.5017330995
H,0,0.7618555813,1.8785282062,-1.5763371929
H,0,-3.051759789,0.5559299412,1.4233835501
H,0,-1.3783782443,-1.2036614526,2.2090043179
N,0,3.2138412571,-1.3458469601,0.0484341001
H,0,3.9941317555,-0.8705872848,-0.3696349139
H,0,3.4020947409,-1.9095104819,0.8585828048
HF=-467.2849791 Nimag=0

2-F

N,0,0.8933772444,-1.4143395019,0.0000721809
C,0,1.978244702,-0.6734511367,0.0001452192
N,0,2.1113859565,0.6432066539,0.0000244023
C,0,0.9956560572,1.3672759328,-0.000012956
C,0,-0.2382308093,0.7352787522,0.0000093862
C,0,-0.2003745488,-0.6659913448,0.0000329724
N,0,-1.5481155359,1.1841025835,-0.0000047932
C,0,-2.2575891431,0.0984814538,0.0000152633
N,0,-1.5078718205,-1.0593214754,-0.0000153301
H,0,1.0969377649,2.4451210496,-0.0000605141
H,0,-3.33511308,0.0633696908,0.0000046744
H,0,-1.8447505093,-2.0066884246,0.0001188128
F,0,3.1170525619,-1.3488528431,-0.0001347231
HF=-511.1658356 Nimag=0

2-CHO

N,0,-0.6879677885,-0.8760530915,-0.0248107546
C,0,-1.4612291759,0.2060158926,-0.0072463101
N,0,-1.0753418121,1.4890024133,0.0274888522
C,0,0.2245649048,1.7628889968,0.0479718973
C,0,1.1408913478,0.7219395483,0.0330128198
C,0,0.5939550303,-0.573185618,-0.0037830759
N,0,2.5205570879,0.6653325637,0.0463108426
C,0,2.7877168678,-0.6069278392,0.018285543
N,0,1.6764424921,-1.4129007135,-0.0129507883
C,0,-2.9505552112,0.0053958831,-0.0281615453
O,0,-3.4774072472,-1.0680912133,-0.0593434696
H,0,0.5269792346,2.8024003105,0.0761638115
H,0,3.7809303368,-1.0268954349,0.0188977828
H,0,1.6483840703,-2.4179478144,-0.0366933258

H,0,-3.5192911375,0.9496137264,-0.0120189897
HF=-525.2276826 Nimag=0

2-CN

N,0,0.8959853236,-1.4223142203,0.0000454086
C,0,2.0046199824,-0.6882744919,0.0000619604
N,0,2.1191742752,0.6446191857,0.0000118003
C,0,1.0042111326,1.366305532,-0.0000097233
C,0,-0.2283365078,0.7295721862,0.0000011415
C,0,-0.1925483278,-0.6738420948,0.0000228123
N,0,-1.533052458,1.179580256,-0.0000095884
C,0,-2.2457380212,0.0925827374,0.00001243
N,0,-1.503005081,-1.0642705815,-0.0000070678
H,0,1.1018785937,2.4445011814,-0.0000385741
H,0,-3.3235020655,0.0622186503,0.0000062792
H,0,-1.8430050938,-2.0109703391,0.0001402607
C,0,3.2545881111,-1.4293295726,0.0000102804
N,0,4.2374048964,-2.0177343785,-0.0000280597
HF=-504.1458213 Nimag=0

2-NO_2

N,0,0.2442463872,-0.9489564368,0.
C,0,1.0446901812,0.0917873777,0.
N,0,0.7715446782,1.3815244013,0.
C,0,-0.5107415032,1.7339431644,0.
C,0,-1.4902516938,0.7506692799,0.
C,0,-1.0231945532,-0.5748295742,0.
N,0,-2.8692324614,0.7754831258,0.
C,0,-3.2113291774,-0.4787140912,0.
N,0,-2.1487262112,-1.3502282111,0.
H,0,-0.74388674,2.7908703129,0.
H,0,-4.2271632218,-0.8400952976,0.
H,0,-2.1808124633,-2.3558974617,0.
N,0,2.5152687845,-0.2492992009,0.
O,0,2.7981884452,-1.4234558329,0.
O,0,3.289588789,0.6748577745,0.
HF=-616.3999032 Nimag=0

Anilines

H

C,0,-1.1567914664,-1.1965922871,0.0013822866
C,0,-1.8619530566,0.0000005434,-0.0127316443
C,0,-1.1567914049,1.1965927428,0.0014339125
C,0,0.2290066438,1.2013843813,0.029316356
C,0,0.9389518045,-0.0000007722,0.0453068969
C,0,0.229006593,-1.2013851808,0.0292645594
N,0,2.3371220112,-0.0000000882,0.0139251015
H,0,-1.6890861248,-2.1379199481,-0.0091627676
H,0,-2.9417589644,0.0000010515,-0.0343988133
H,0,-1.6890860373,2.1379208716,-0.0090705737
H,0,0.7707474648,2.1386563764,0.034366209
H,0,0.7707473576,-2.1386574295,0.0342739595
H,0,2.7606530194,-0.8315936625,0.3936840748
H,0,2.7606530702,0.8315767034,0.3937207525
HF=-287.5667192 Nimag=0

4-CH_3

C,0,0.6687283684,1.18803449,-0.0013626827
C,0,1.3917807714,-0.0021167096,-0.0105609845
C,0,0.668927894,-1.1910250854,-0.0224096536
C,0,-0.717788593,-1.1986386896,-0.0197193421
C,0,-1.4315657113,-0.0017390717,-0.0046562346
C,0,-0.7168299143,1.1959424599,0.0013787447
N,0,-2.8313568552,-0.0000160731,-0.0663265225
C,0,2.8975251911,0.0008472517,0.0163731566
H,0,1.2005957013,2.1315931555,0.0011356562
H,0,1.2002151467,-2.1346288892,-0.0366357962
H,0,-1.2546309258,-2.1386890235,-0.0383645843
H,0,-1.2537638093,2.1361446414,-0.0008663192
H,0,-3.2574484913,0.8261507413,0.3232169343
H,0,-3.25862705,-0.8337659235,0.3053543105
H,0,3.2983176334,-0.926232354,-0.3909393212
H,0,3.2741486085,0.1043837053,1.0355116186
H,0,3.2995096153,0.8280925846,-0.5675942499
HF=-326.8743802 Nimag=0

4-OCH_3

C,0,2.030017081,-0.2003252115,-0.0048787843
C,0,1.4894372518,1.0883645499,-0.0006923855
C,0,0.123054444,1.2841395996,0.0151710663
C,0,-0.7489493855,0.1974275445,0.0234636166
C,0,-0.2253518098,-1.0882174673,0.0160312583
C,0,1.154347566,-1.2773015997,0.00147505
N,0,3.4209013381,-0.393210333,-0.0840234871
O,0,-2.0804927758,0.4973104039,0.0393634947
C,0,-2.9825238267,-0.5845335011,0.0385605068
H,0,2.1522263527,1.944299957,-0.0144363184
H,0,-0.2948070822,2.2809393506,0.0206802977
H,0,-0.8697755744,-1.9539060967,0.0216375515
H,0,1.5487119521,-2.2853727126,-0.0100289237
H,0,3.7254303156,-1.2744072255,0.3003944468
H,0,3.9527721464,0.3629778929,0.3188161906
H,0,-2.8642680887,-1.198472353,-0.8579137288
H,0,-2.8511667795,-1.2113372954,0.9242816096
H,0,-3.9780991249,-0.1511775025,0.049270539
HF=-402.0805518 Nimag=0

4-NH_2

C,0,-1.3750324781,0.7065962653,0.0070831847
C,0,-1.4022345173,-0.6840603735,0.0739922032
C,0,-0.1864087732,-1.3588681849,0.1494850984
C,0,1.0148038896,-0.667351195,0.1530828343
C,0,1.042101343,0.7230776001,0.0810918386
C,0,-0.1737836114,1.3981053278,0.0104254606
N,0,2.2593966216,1.4284066447,0.1492947676
N,0,-2.6235673466,-1.3826534091,0.1349900123
H,0,-2.3067846242,1.2557299509,-0.0434825634
H,0,-0.1801620171,-2.4397964216,0.2113600076
H,0,1.9461437596,-1.2157377641,0.217588792
H,0,-0.1805405218,2.4797443977,-0.037342412
H,0,2.222114211,2.3293833333,-0.3026044149
H,0,3.0442743753,0.900491434,-0.2008809841
H,0,-2.559838771,-2.3251957169,-0.2183180868
H,0,-3.3821665394,-0.8963928887,-0.318180738
HF=-342.9198605 Nimag=0

4-F

C,0,0.7166176337,1.2043819458,0.0018923988
C,0,1.3899273959,0.0000020648,-0.000197192
C,0,0.7165677682,-1.204354573,0.0020737052
C,0,-0.6700901963,-1.1999837218,0.006395309
C,0,-1.3811163313,0.0000579354,0.0105113716
C,0,-0.6700454392,1.2000666366,0.006234578
N,0,-2.7822005532,0.0000574506,-0.0479258571
F,0,2.7379169816,-0.0000275216,-0.0031916635
H,0,1.2764026377,2.1283092349,0.0002048078
H,0,1.2763178948,-2.1283033694,0.0005229299
H,0,-1.2082760034,-2.1387796664,0.0018796626
H,0,-1.2081865165,2.1388882947,0.0016222684
H,0,-3.2065849421,0.8301530418,0.3344912521
H,0,-3.2066133901,-0.8297681025,0.3350477793
HF=-386.8087841 Nimag=0

4-Cl

C,0,0.869684175,-1.2017191427,-0.130492779
C,0,1.5385632693,-0.0000437945,0.0291796386
C,0,0.8699597605,1.2020359052,-0.1285809355

C,0,-0.4778711454,1.2004534424,-0.4483633399
C,0,-1.170916285,0.0007791893,-0.6155559606
C,0,-0.478146295,-1.1993193492,-0.4502658094
N,0,-2.5422445171,0.0011393832,-0.8789798865
H,0,1.4011283275,-2.1336918795,-0.0053356708
H,0,1.4016168803,2.1336869755,-0.0019424974
H,0,-1.0011049537,2.1403864659,-0.5657383306
H,0,-1.0016006277,-2.138943077,-0.5691233831
H,0,-2.8801939485,0.8335531955,-1.3348635394
H,0,-2.8803596096,-0.8304234614,-1.3362914218
Cl,0,3.2384579695,-0.0005588527,0.4314319153
HF=-386.8087841 Nimag=0

4-Br

C,0,-0.1856154945,1.2020821601,-0.2279248447
C,0,-0.8602915623,0.0000155904,-0.0976002313
C,0,-0.1855922425,-1.2020106136,-0.2281769642
C,0,1.1746141005,-1.1998231571,-0.4913287093
C,0,1.8739239819,0.0000977166,-0.6285178063
C,0,1.1745908676,1.1999762272,-0.4910773859
N,0,3.2539920427,0.0001324195,-0.8347923472
H,0,-0.7175360669,2.1363949846,-0.12517294
H,0,-0.7174946947,-2.1363552796,-0.1256209628
H,0,1.7021402434,-2.1397933934,-0.5875739684
H,0,1.7020985776,2.1399769176,-0.5871261045
H,0,3.6126869022,-0.8322955696,-1.2743405841
H,0,3.6126716924,0.8326616468,-1.2741612253
Br,0,-2.7262873473,-0.0000400964,0.2614210742
HF=-2861.1361665 Nimag=0

4-CHO

C,0,-1.1583567231,0.7353298225,0.0125449065
C,0,-1.1735086672,-0.6610216206,-0.0045369995
C,0,0.0352112365,-1.3516356832,0.0152337009
C,0,1.2390424094,-0.6738730576,0.0501141558
C,0,1.2538777985,0.7243390654,0.0651366686
C,0,0.0352922703,1.4208883488,0.0482773009
N,0,2.4498201528,1.4149036524,0.1532251108
C,0,-2.44404638,-1.4005352817,-0.0448626237
O,0,-3.5356278841,-0.8891132501,-0.0691663784
H,0,-2.1026058447,1.262780998,-0.0034537218
H,0,0.0297042153,-2.4349846078,0.001944006
H,0,2.1746796873,-1.2170731015,0.0693779572
H,0,0.0447800673,2.5029553721,0.0667005162
H,0,2.4303005013,2.3724472475,-0.1561653695
H,0,3.2702006449,0.9189949042,-0.1530326173
H,0,-2.3409204846,-2.5025508086,-0.0523256127
HF=-400.8907636 Nimag=0

4-CN

C,0,-1.2205255403,0.7157681054,0.0079519867
C,0,-1.23093141,-0.6795080428,-0.0104343433
C,0,-0.0202068027,-1.3731068584,0.0103123951
C,0,1.1759730094,-0.6861117512,0.0480497149
C,0,1.1922453203,0.7129788735,0.0643865001
C,0,-0.0246937211,1.403419801,0.0457567561
N,0,2.3895749733,1.4011756344,0.1565911307
C,0,-2.4735212721,-1.39334937,-0.0521986311
N,0,-3.4690939664,-1.965098135,-0.0863495433
H,0,-2.1566487124,1.2552840534,-0.0082808877
H,0,-0.0255457698,-2.4535815734,-0.0041214363
H,0,2.1109948294,-1.2297999786,0.0685993569
H,0,-0.0236298237,2.4850376494,0.0647584019
H,0,2.3733504991,2.3582067789,-0.1542006765
H,0,3.2089933869,0.9034898134,-0.1494167243
HF=-379.8113149 Nimag=0

4-NO_2

C,0,-1.1616260646,0.7564646523,-0.0918987577
C,0,-1.1446948065,-0.6296573276,-0.113059042
C,0,0.0465810137,-1.3388709669,-0.1213294998
C,0,1.2406588961,-0.648440607,-0.1082895897
C,0,1.2529990161,0.7525267371,-0.0889491837
C,0,0.0343113104,1.4437567816,-0.0789665848
N,0,2.4477426277,1.4403961679,-0.0243742801
N,0,-2.4101257414,-1.3590751016,-0.1292334567
O,0,-2.3631701606,-2.5735516909,-0.1493970457
O,0,-3.4377364632,-0.7098265921,-0.1218404057
H,0,-2.1074669518,1.2757361745,-0.0864460103
H,0,0.0220603232,-2.4174811184,-0.1383312936
H,0,2.1773687422,-1.189137944,-0.1098945836
H,0,0.0356619748,2.5251187167,-0.0580396248
H,0,2.4272785125,2.4040853664,-0.3122525655
H,0,3.2675387715,0.946732752,-0.334442076
HF=-492.0682745 Nimag=0

Pyridin-2(1H)-ones

H

C,0,-0.307691048,1.2424742154,0.0001725966
C,0,-1.0431962609,-0.0074918693,0.0001376039
C,0,1.1435128813,-1.1133406513,-0.0002663195
C,0,1.8126430159,0.0619876648,-0.0002326163
C,0,1.046772539,1.2644265896,-0.0000061325
O,0,-2.2529704283,-0.1378831326,0.0002783002
H,0,-0.9010648807,2.1438482758,0.0003435442
H,0,1.6339991845,-2.0753953406,-0.0004334022
H,0,2.8895998266,0.0766271912,-0.00037172
H,0,1.563401478,2.2153521238,0.0000236811
N,0,-0.2159040238,-1.1358378894,-0.000100747
H,0,-0.7104425836,-2.0154307574,-0.0001421186
HF=-323.487398 Nimag=0

5-CH_3

C,0,0.7640407962,-1.2456283183,0.0012074195
C,0,1.5351375613,-0.0161441873,0.0009025747
C,0,-0.6264031457,1.1388175904,-0.0010585739
C,0,-1.3408116241,-0.0098410504,-0.0007442771
C,0,-0.5888828528,-1.2279497043,0.0005159014
O,0,2.7496595181,0.0766273926,0.0013630892
C,0,-2.8421548358,-0.0259516969,-0.0018947889
H,0,1.3303772913,-2.1643897154,0.0020976891
H,0,-1.0893043032,2.1155208336,-0.0019444852
H,0,-1.1328600162,-2.165663578,0.0008151961
H,0,-3.244248116,0.9855290295,-0.0005772739
H,0,-3.229838957,-0.5431439444,0.8765750713
H,0,-3.2285977002,-0.5403734674,-0.8825399048
N,0,0.7381339472,1.1270553006,-0.0000305507
H,0,1.2512993169,1.9955099358,-0.0004550698
HF=-362.7955676 Nimag=0

5-NH_2

C,0,-0.3115178476,1.236734734,0.0042281169
C,0,-1.0478372216,-0.0160863701,0.0146844704
C,0,1.1499227121,-1.1070607111,-0.0526204035
C,0,1.8212267345,0.067281459,-0.0519830994
C,0,1.0393718008,1.2650947777,-0.0154902208
O,0,-2.2616194481,-0.135693262,0.0401710339
H,0,-0.9034205751,2.1388834616,0.0265574636
H,0,1.6421283586,-2.06810267,-0.0789996557
H,0,1.5616737524,2.2143628281,0.001414646
N,0,-0.2209837851,-1.1292696957,-0.0028983295
H,0,-0.7062979499,-2.0130597945,0.0059709135
N,0,3.2298084817,0.1654916002,-0.0038126787
H,0,3.6871528804,-0.7229435987,-0.1495054415
H,0,3.5898513867,0.8323719715,-0.6725581852
HF=-378.8363014 Nimag=0

5-F

C,0,-0.3051598037,1.2418365746,0.0001898004

C,0,-1.0424988803,-0.011769876,-0.0000838113
C,0,1.1454412287,-1.1246785685,-0.0005491841
C,0,1.7830355993,0.0601097808,-0.0003315565
C,0,1.0476668975,1.2716043827,0.0000909484
O,0,-2.2532057132,-0.1309105875,-0.0001303119
H,0,-0.8981514383,2.1431001828,0.0004042521
H,0,1.6644563626,-2.0701418994,-0.0007802074
H,0,1.5930858952,2.2059197304,0.0002485303
N,0,-0.2199708022,-1.1387611012,-0.0001536401
H,0,-0.7127578937,-2.0189291146,0.0008305177
F,0,3.1252610981,0.1099735058,-0.0004501978
HF=-422.7220493 Nimag=0

5-Cl

C,0,-0.3066832937,1.2420896004,0.0001798922
C,0,-1.0427352222,-0.0102304268,0.0002659532
C,0,1.1459516299,-1.1171102206,-0.0002234734
C,0,1.7984080523,0.0644630308,-0.0002646059
C,0,1.0455844094,1.2725214916,-0.0000738739
O,0,-2.2512899874,-0.1368483204,0.0004641886
H,0,-0.8985760701,2.1442662919,0.0003471538
H,0,1.653547912,-2.0693168969,-0.000391156
H,0,1.5770072219,2.2144386894,-0.0001176409
N,0,-0.2145267293,-1.136472667,-0.0000561252
H,0,-0.7044849588,-2.0186980977,-0.0004458583
Cl,0,3.534079926,0.1156958053,-0.0005783645
HF=-783.0845354 Nimag=0

5-CN

C,0,-0.2996111469,1.2508671635,0.0001948042
C,0,-1.0258069838,-0.0068228108,0.000429069
C,0,1.1615847963,-1.1082714273,-0.0002256846
C,0,1.8229880821,0.0813407263,-0.0003671943
C,0,1.0499501233,1.2883330283,-0.0001568935
O,0,-2.2280594824,-0.1508015017,0.0006116525
H,0,-0.8993812475,2.1477034423,0.000364249
H,0,1.6741750157,-2.0588923196,-0.0004264661
H,0,1.5729254559,2.234851918,-0.0002855174
N,0,-0.1860146246,-1.1369177931,0.0000227586
H,0,-0.6747130896,-2.0207518655,-0.0007038189
C,0,3.2511584643,0.1094798814,-0.0007509708
N,0,4.3988847073,0.1431112882,-0.0010548976
HF=-415.7273753 Nimag=0

5-NO2

C,0,-0.3097127882,1.2539798434,0.00018116
C,0,-1.0319879936,-0.0069963122,0.0002202875
C,0,1.1543701052,-1.1100480452,-0.0004123414
C,0,1.7880169492,0.089196193,-0.000449431
C,0,1.0401635622,1.2986595021,-0.0001754201
O,0,-2.2322176915,-0.1566804318,0.0005623931
H,0,-0.9139545216,2.147604636,0.0004474875
H,0,1.6928497081,-2.045433113,-0.0006176258
H,0,1.5773703535,2.235754195,-0.0001998337
N,0,-0.1891290828,-1.1408905531,-0.0001881195
H,0,-0.6768021986,-2.0255737943,-0.0001335772
N,0,3.2372754911,0.1133171172,-0.0007583507
O,0,3.7727946161,1.2028170142,-0.000771536
O,0,3.8240774509,-0.9523269813,-0.0009972428
HF=-378.8363014 Nimag=0

Imides

Imide1

C,0,-1.2929599168,-0.208297881,0.0977681575
O,0,-2.2121785431,-0.9836601297,0.193173517
N,0,-0.0005272443,-0.7298440311,0.0464776984
H,0,0.001279098,-1.7419757857,0.0844798431
C,0,1.290251112,-0.2090080805,-0.0425325935
O,0,2.2121683727,-0.9861216403,-0.0789186914
C,0,1.5139758031,1.279808914,-0.0764373
H,0,1.1955869977,1.7385603478,0.857889458
H,0,2.5797733268,1.43412128,-0.2053723224
H,0,0.9745291069,1.7523853177,-0.8930742476
C,0,-1.5219705184,1.2781126267,0.0199792763
H,0,-0.984411518,1.8125966431,0.7988370603
H,0,-1.2048583666,1.6664956287,-0.9461683389
H,0,-2.5883813801,1.4377300602,0.1367188731
HF=-361.8329325 Nimag=0

Imide2

C,0,-3.2338851332,2.0721172912,0.1387987155
O,0,-3.6317815665,0.9721818721,0.3941045236
N,0,-1.8542685014,2.2990082905,0.0603901567
H,0,-1.3266080539,1.4340719085,0.06341537
C,0,-1.0605357784,3.4113372463,-0.167006266
O,0,0.0773776511,3.2816692691,-0.5381507478
C,0,-1.6095789647,4.7984933745,0.1195459502
H,0,-2.2794985425,5.1366288773,-0.6721995142
H,0,-0.7555194999,5.4660913668,0.1874018826
C,0,-4.183794867,3.2100832063,-0.2004658671
H,0,-4.1464173791,3.9872424724,0.5597119852
H,0,-3.9185688081,3.627090171,-1.1746470006
F,0,-2.2924349669,4.8160830256,1.3178427119
F,0,-5.4511466494,2.7157586085,-0.2687296701
HF=-560.292206 Nimag=0

1,6-dihydropyrimidines

H

C,0,-1.4299783115,0.0081361828,0.0803950663
C,0,-0.5854826893,1.2457733968,-0.0489548727
C,0,0.7440130162,1.1750380788,-0.0145003607
N,0,1.4821059003,-0.0159870441,0.1067421775
C,0,0.7816424151,-1.0843589704,0.0206254852
N,0,-0.5660942774,-1.148730184,-0.1407349217
H,0,-2.2301005115,0.0039648909,-0.6624197991
H,0,-1.9079465458,-0.0426724339,1.067530835
H,0,-1.0858861803,2.1983673426,-0.1439080265
H,0,1.3450583273,2.0710577471,-0.0900353803
H,0,1.2823360329,-2.0479602375,0.0402080342
H,0,-0.9869191761,-2.0603637691,-0.1412162372
HF=-265.4725004 Nimag=0

4-OCH_3

C,0,-1.2321362658,-0.7427215303,0.1765758188
C,0,-1.0698053263,-2.2290267096,0.3686260829
C,0,0.1243998338,-2.8208678409,0.1901795432
N,0,1.3009852026,-2.1505043733,-0.1440595305
C,0,1.2088756735,-0.8706042801,-0.1993843707
N,0,0.0918537197,-0.1351266065,0.0181816981
H,0,-1.7332210147,-0.2893061399,1.0381119261
H,0,-1.8553920167,-0.5154663679,-0.7001972647
H,0,-1.9550142565,-2.7863314333,0.6274133409
H,0,2.1001461413,-0.2911034344,-0.4200073467
H,0,0.1521925702,0.8600222803,-0.1037558024
O,0,0.3733489533,-4.1483132704,0.3170401754
C,0,-0.713901057,-4.9904491838,0.6602726825
H,0,-1.1335890958,-4.7189017291,1.6321473331
H,0,-1.5014154281,-4.9491295489,-0.0964649835
H,0,-0.3099548555,-5.9973832779,0.7084563583
HF=-380.1569468 Nimag=0

4-NH_2

C,0,1.2793532987,1.159234563,0.0668161567
C,0,-0.2193959435,1.197405624,-0.0272879774
C,0,-0.9492907981,0.0741639302,0.0269960992
N,0,-0.4015559797,-1.2198445928,0.0927485511
C,0,0.8748899524,-1.2732267876,0.0021963684
N,0,1.7174844057,-0.2230585601,-0.1128998375
H,0,1.6381143961,1.5417261786,1.0313365411
H,0,1.7373916913,1.7776958933,-0.7091473015
H,0,-0.6984477996,2.1637965435,-0.0860723501
H,0,1.356815719,-2.246365626,-0.0117319341
H,0,2.7024820851,-0.416898715,-0.1180834907
N,0,-2.3390269514,0.0449830109,0.0584693696

H,0,-2.7110777228,-0.8211153817,-0.2994621848
H,0,-2.7921603531,0.8581689198,-0.3250170101
HF=-320.8365101 Nimag=0

4-F

C,0,-1.435840627,-0.0000265346,0.0703114182
C,0,-0.5997104498,1.247839602,0.0089336309
C,0,0.7235103672,1.1604942524,-0.0596589379
N,0,1.4915092266,0.0154787735,-0.0843342657
C,0,0.8044218304,-1.0681222054,-0.0331419419
N,0,-0.5403875375,-1.1577697804,0.0389656619
H,0,-2.1313517855,-0.0506058845,-0.7732944195
H,0,-2.0385577973,-0.0263764057,0.9835539689
H,0,-1.0834021543,2.2113821293,0.021135338
H,0,1.3246729427,-2.0202651433,-0.047419804
H,0,-0.9449727956,-2.0760154299,0.0731298037
F,0,1.4640926131,2.2716064867,-0.1140859366
HF=-364.7230132 Nimag=0

4-Cl

C,0,-1.4295136257,-0.0039913746,0.0908287816
C,0,-0.5978706491,1.2443687475,-0.0260506045
C,0,0.7293191895,1.1685767012,-0.0441071747
N,0,1.4913750001,0.0086841872,0.0081326425
C,0,0.7994292491,-1.0723113428,-0.0096604703
N,0,-0.5482220385,-1.1608032074,-0.0498736378
H,0,-2.1928895776,-0.0313319482,-0.6905397408
H,0,-1.952987536,-0.038104396,1.0532783509
H,0,-1.10189056,2.1963477788,-0.0755619509
H,0,1.3205319786,-2.0241416137,-0.0115679871
H,0,-0.9561435054,-2.0781313659,-0.0369487162
Cl,0,1.6855818171,2.6237589147,-0.1558122875
HF= -725.0769425 Nimag=0

4-Br

C,0,-1.4258175327,-0.0036777549,0.0992652964
C,0,-0.5978251453,1.2467242206,-0.0362677469
C,0,0.7288258575,1.1687465337,-0.0357017187
N,0,1.4884196858,0.0101215821,0.0455087233
C,0,0.7978857504,-1.0716432359,-0.0000469874
N,0,-0.5482932721,-1.1574415306,-0.080976577
H,0,-2.2113051511,-0.0250099667,-0.6589911677
H,0,-1.9196709934,-0.0445178279,1.0773941951
H,0,-1.1065994383,2.1944184733,-0.1108170003
H,0,1.3199013785,-2.0229261107,0.0014823699
H,0,-0.957772813,-2.0742930661,-0.0836140863
Br,0,1.7717024527,2.7542177322,-0.1790569233
HF=-2839.0429253 Nimag=0

4-CHO

C,0,-1.4125026279,0.0105483899,0.101102612
C,0,-0.5621888153,1.2401238809,-0.0183775821
C,0,0.7731719392,1.167898871,-0.0508892287
N,0,1.5132295231,-0.0200783949,0.0004903786
C,0,0.8035844585,-1.0850486132,-0.0224187698
N,0,-0.5516977612,-1.1547187278,-0.0719315979
H,0,-2.1939050096,0.0083701135,-0.6626955444
H,0,-1.9175947032,-0.0142069952,1.0742932514
H,0,-1.0571189845,2.201329933,-0.0602882723
H,0,1.3026321433,-2.0493286798,-0.0271555824
H,0,-0.9724469519,-2.0660344677,-0.0489961535
C,0,1.5354101407,2.4402955141,-0.1572166873
O,0,2.7299074116,2.52169707,-0.1974293539
H,0,0.896431157,3.3436197572,-0.1978101235
HF=-378.7908503 Nimag=0

4-CN

C,0,-1.5274974187,1.2046814426,0.0449547173
C,0,-0.028641497,1.1650353952,-0.0126521449
C,0,0.6276174595,0.0022490545,0.0313381455
N,0,0.0344580623,-1.2681175417,0.1053674614
C,0,-1.2444671112,-1.2524895023,0.0148118778
N,0,-2.0294931058,-0.1572529467,-0.1120811948
H,0,-1.9220668872,1.8356704608,-0.7543398526
H,0,-1.8652421925,1.6381821578,0.9935179191
H,0,0.5105439032,2.0985986865,-0.0716235955
H,0,-1.7775887441,-2.1975595019,0.0146205341
H,0,-3.0229417522,-0.2975143272,-0.1530275902
C,0,2.0721385142,0.0062599379,-0.0102402328
N,0,3.2179907695,0.0360066844,-0.0441980444
HF=-357.7128127 Nimag=0

4-NO_2

C,0,1.86391544,1.2066500912,0.0000363546
C,0,0.3635916534,1.1660047011,-0.0000199507
C,0,-0.2667304695,-0.0024402852,0.000020087
N,0,0.2902674034,-1.2641778875,0.000099754
C,0,1.5733941747,-1.2581324576,0.0000062575
N,0,2.369261882,-0.1649594677,-0.0001266852
H,0,2.2284523402,1.745441121,0.8797558716
H,0,2.2285083159,1.7456437589,-0.8795305486
H,0,-0.1919179878,2.0897648109,-0.0000642626
H,0,2.101080138,-2.2059109642,0.0000041761
H,0,3.3629967448,-0.308893501,-0.0001786098
N,0,-1.7585464219,0.0070405788,0.0000091464
O,0,-2.3061626103,1.0931139272,-0.0001041545
O,0,-2.319998603,-1.0587284259,0.0000935643
HF=-469.9690384 Nimag=0

5-aminopyrimidines

H

C,0,-0.6163688345,1.1784847194,-0.030849548
N,0,0.7085481517,1.1837251617,0.0069673051
C,0,1.3119760064,-0.0001071207,0.0249898378
N,0,0.707845499,-1.1835798824,0.0053813014
C,0,-0.6170495283,-1.1774991072,-0.0324048913
C,0,-1.3612651587,0.0007349719,-0.0532704423
H,0,-1.1150242231,2.1430311136,-0.0429516509
H,0,2.3933697085,-0.0004536656,0.0568305378
H,0,-1.116298111,-2.1417226662,-0.0457599026
N,0,-2.7519904738,0.001082213,-0.0299191571
H,0,-3.1804836979,0.8347286574,-0.4001264211
H,0,-3.1809291284,-0.8316475351,-0.4016653686
HF=-319.6481355 Nimag=0

2-CH_3

C,0,0.6340439215,1.1648023054,0.0924282113
N,0,-0.689947186,1.1714554044,0.0930882898
C,0,-1.313326109,-0.0043980485,-0.0072587995
N,0,-0.6924093865,-1.1799792977,-0.1060654288
C,0,0.6333031876,-1.1750703043,-0.1050431442
C,0,1.3812843972,-0.0063459518,-0.0051342447
H,0,1.131484977,2.1273671938,0.1693267315
H,0,1.1285782586,-2.137931094,-0.1903443697
N,0,2.7742897389,0.0000370864,-0.0722299022
H,0,3.2078886957,0.7938585799,0.3730022885
H,0,3.2079847657,-0.8614322362,0.2213052258
C,0,-2.8125572318,0.0002681734,0.0172872391
H,0,-3.1978279679,-0.9111805428,-0.4307833817
H,0,-3.1670887741,0.0541142979,1.0477393939
H,0,-3.1936680369,0.8712232141,-0.5102003791
HF=-358.9607667 Nimag=0

2-NH_2

C,0,-0.616937073,1.1777483181,-0.0487445367
N,0,0.7077542572,1.1978059092,-0.0636210526

C,0,1.3233386979,0.014576389,-0.0724365706
N,0,0.7184344959,-1.174139401,-0.090432243
C,0,-0.6063211813,-1.1663960737,-0.074950995
C,0,-1.3597816955,0.0021739995,-0.0483855561
H,0,-1.1170481884,2.1417955417,-0.0395501107
H,0,-1.097762858,-2.1348511128,-0.087314088
N,0,-2.7615779152,-0.0054133297,0.0411814784
H,0,-3.1896348489,0.824006311,-0.342255764
H,0,-3.1823156094,-0.8271295507,-0.3662046898
N,0,2.6998811277,0.0201132552,-0.0203433972
H,0,3.1371918338,-0.8263138582,-0.3425279811
H,0,3.1296806971,0.8775197125,-0.3229957436
HF=-358.9607667 Nimag=0

2-F

C,0,-0.6105982212,1.1765061847,-0.0300683402
N,0,0.7166504715,1.1813384623,0.0049673144
C,0,1.2872401587,-0.0000688584,0.0206729695
N,0,0.7160000326,-1.1811757191,0.0034905447
C,0,-0.6112188177,-1.1755730844,-0.0314240291
C,0,-1.3568868695,0.0006963523,-0.0517794196
H,0,-1.1018801872,2.1437542006,-0.0400157971
H,0,-1.1030653242,-2.1425208476,-0.0424301637
N,0,-2.7507888183,0.0009307585,-0.0223710249
H,0,-3.1749191882,0.8322638514,-0.4034471256
H,0,-3.1753050014,-0.8289061203,-0.4062696059
F,0,2.6138459749,-0.0004690599,0.0558960275
HF=-418.9005455 Nimag=0

2-CHO

C,0,-0.593237304,1.1734340696,-0.0461511465
N,0,0.7297356871,1.1566758053,-0.0166308466
C,0,1.3221155179,-0.0352980165,-0.0017688297
N,0,0.7020347571,-1.2131663303,-0.0159482025
C,0,-0.6159955426,-1.1906355986,-0.044562294
C,0,-1.3497169356,0.0017904241,-0.0624696648
H,0,-1.0793224563,2.1437038506,-0.05638546
H,0,-1.1291356177,-2.1475716913,-0.0536921948
N,0,-2.7292916138,0.0126628756,-0.0350708369
H,0,-3.1725755566,0.8549710633,-0.3635249343
H,0,-3.1851551561,-0.823422102,-0.3624971223
C,0,2.8180583587,-0.0036039232,0.0306734253
O,0,3.5129729337,-0.9784144073,0.0423495251
H,0,3.2311503083,1.0192307409,0.042858862
HF=-432.9641073 Nimag=0

2-CN

C,0,-0.5990300439,1.1822112696,-0.0433227971
N,0,0.7225427334,1.186721307,-0.011307222
C,0,1.3199365308,0.0000774957,0.0033989233
N,0,0.7219717968,-1.1862661364,-0.0129316555
C,0,-0.5995925042,-1.1810744565,-0.0449464496
C,0,-1.345210844,0.0007618657,-0.0631142198
H,0,-1.0943060338,2.1475343366,-0.0534269787
H,0,-1.0953386985,-2.1461425414,-0.0563816172
N,0,-2.7231138156,0.001071915,-0.0393809196
H,0,-3.1749969548,0.8413042978,-0.3609090655
H,0,-3.1753858109,-0.8385382922,-0.3619890518
C,0,2.7703815219,-0.0002998174,0.0376037383
N,0,3.9157973327,-0.0005971534,0.0639303752
HF=-411.883154 Nimag=0

2-NO_2

C,0,-1.2660712378,-1.1805181313,-0.0710100309
N,0,0.0571510514,-1.1804243833,-0.0620760319
C,0,0.6254167229,0.0000631174,-0.0011264627
N,0,0.057355147,1.1806679301,0.0593198816
C,0,-1.2659235804,1.1812736505,0.0629132644
C,0,-2.012286428,0.0004591607,-0.0045408745
H,0,-1.7586862527,-2.1448572398,-0.1328558467
H,0,-1.758402578,2.1459766927,0.1201679243
N,0,-3.3875009074,0.0035958706,-0.0631440158
H,0,-3.8505218989,-0.8526049175,0.1930908864
H,0,-3.850874243,0.8264865383,0.2850835235
N,0,2.1257702085,-0.000202545,0.0026692862
O,0,2.6714689369,1.0585295147,-0.1971828229
O,0,2.6701650594,-1.0590912579,0.2054843191
HF==-524.1374885 Nimag=0

Table S9 Cartesian Coordinates, Total Energies (in *hartree*), and Number of Imaginary Frequencies for the Optimized Structures for Nucleobases from M06-2X/6-311+G(2d,2p) Computations.

Adenine

N,0,1.9364904463,0.5208035012,0.1223733951
C,0,1.2845825305,1.6907168186,0.1296718053
N,0,-0.0218558488,1.910077563,0.0801973468
C,0,-0.7055645787,0.7666313343,0.0140921554
C,0,-0.1754951825,-0.515384302,-0.0001492954
C,0,1.2238698441,-0.6042940812,0.0625713074
N,0,-2.0626579173,0.5803945916,-0.0591934504
C,0,-2.2707231511,-0.7762838696,-0.1149248338
N,0,-1.1702669595,-1.4700402477,-0.0828904572
N,0,1.8622167759,-1.7957422347,0.0900747091
H,0,1.9134758201,2.570756635,0.1814166782
H,0,-2.7583141026,1.3056410269,-0.0709648856
H,0,-3.2636013418,-1.1900704759,-0.1792207441
H,0,2.8588559596,-1.794770794,-0.0352520284
H,0,1.3409065158,-2.6263447054,-0.1271753824
HF=-467.2886498 Nimag=0

Guanine

N,0,-2.1337892713,0.7657195159,0.0594120844
C,0,-1.2632369381,-0.2845301433,0.0342428885
N,0,0.0208151011,-0.1560178719,-0.1186212705
C,0,0.401579745,1.1428057305,-0.2321658675
C,0,-0.3777249637,2.284875756,-0.2304490694
C,0,-1.8000156505,2.1465806761,-0.0675370681
N,0,1.6798889754,1.5864305959,-0.3904159366
C,0,1.6139065119,2.9603276105,-0.4741957912
N,0,0.3993400293,3.4105462943,-0.3819398743
O,0,-2.6747501152,2.9748902457,-0.0203943513
N,0,-1.8068254277,-1.5318812829,0.2350627781
H,0,-3.1109249063,0.5982032103,0.2490356845
H,0,2.5000572491,1.0068448014,-0.4322651285
H,0,2.4981786243,3.5617253621,-0.6025856803
H,0,-1.1556010216,-2.2727658638,0.0285951577
H,0,-2.7276393686,-1.6873955324,-0.1421827895
HF=-542.5266766 Nimag=0

Thymine

C,0,-1.2147395192,0.338126211,-0.1869869888
N,0,-1.2908210034,-0.8343636741,0.5307163819
C,0,-0.1859855189,-1.5227757249,0.9884642363
N,0,1.0052168334,-0.914888164,0.6528953867

C,0,1.1867071407,0.2684233155,-0.0679913636
C,0,-0.0505501718,0.919881307,-0.5073755189
C,0,0.0753916625,2.1907788844,-1.2839248445
O,0,-0.2615943132,-2.5504598894,1.6171163241
O,0,2.2995097962,0.6869480568,-0.2898767747
H,0,-2.1663451337,0.7614514298,-0.4771527796
H,0,-2.1780642603,-1.2502032359,0.7578437114
H,0,1.8419495825,-1.3847938975,0.9679660834
H,0,0.6076633518,2.9418330916,-0.7010018287
H,0,-0.9042750095,2.5799192381,-1.5541264426
H,0,0.6551425864,2.0262875904,-2.1916823327
HF=-454.1067815 Nimag=0

Uracil

N,0,1.3559135485,0.4277898937,0.0196811375
C,0,1.3390137123,-0.9493723975,0.0275338287
N,0,0.0628723445,-1.4804891821,0.1203235759
C,0,-1.0707681507,-0.7126656027,0.1973553915
C,0,-1.0267288917,0.6259358784,0.1879923018
C,0,0.2618809542,1.3021694449,0.0931562279
O,0,0.4345608123,2.4969025937,0.0756052089
O,0,2.3281915686,-1.6358755042,-0.0391426032
H,0,2.2692938755,0.8540105955,-0.0469220484
H,0,0.0183665777,-2.4855287985,0.1287186566
H,0,-1.9974179607,-1.2633557132,0.2657740445
H,0,-1.9154093904,1.2296907921,0.2483662785
HF=-414.7954267 Nimag=0

Cytosine

C,0,-1.267909672,-0.4834344911,-0.3571190007
C,0,-0.593431126,0.6676347915,-0.1587916627
C,0,0.8407961985,0.5662274333,-0.173121372
N,0,1.4969988791,-0.5489721881,-0.3666865625
C,0,0.8180547385,-1.7215188967,-0.5642052297
N,0,-0.5950176018,-1.6366204411,-0.5515551531
N,0,1.572420783,1.6861668462,0.054624205
O,0,1.3278510909,-2.8025637594,-0.7466681362
H,0,-2.3469381641,-0.540571546,-0.3684213887
H,0,-1.1010422286,1.6028824418,0.0078533696
H,0,-1.0755392893,-2.508853323,-0.7010169713
H,0,2.5648060691,1.6170041111,-0.0931741058
H,0,1.1427933225,2.5903520215,-0.0032469919
HF=-394.9067298 Nimag=0

Table S10. Cartesian Coordinates, Total Energies (in *hartree*), and Number of Imaginary Frequencies for the Optimized Structures for Carbonyl Oxygen Proton Accepting Sites from M06-2X/6-311+G(2d,2p) Computations.

Cyclohexa-2,4-dienones

H

C,0,-1.4187588306,-0.0069684398,0.02738463
C,0,-0.7334109777,0.6873011961,-1.0741550219
C,0,0.7866355962,0.672065931,-1.0738623686
C,0,1.4436798723,-0.0514464786,0.055504032
C,0,0.7369315816,-0.6531429979,1.012585761
C,0,-0.722817619,-0.6262531752,0.9913613419
O,0,-1.3441363417,1.253367676,-1.9537213454
H,0,-2.4995824537,0.0126366653,0.0124564582
H,0,1.1206158594,1.7136291842,-1.1029755685
H,0,1.1058863708,0.2500737144,-2.0316321207
H,0,2.5259208738,-0.0739489669,0.075251153
H,0,1.2314149967,-1.1718364713,1.821712987
H,0,-1.2499929279,-1.1302998374,1.7918820619
HF=-307.4026795 Nimag=0

4-CH_3

C,0,-1.4291466411,0.0549339035,-0.0391148358
C,0,-0.7601284487,0.7698076729,-1.136851257
C,0,0.7579937892,0.75901949,-1.1479004178
C,0,1.4278588733,0.0276244737,-0.0301867217
C,0,0.7484993163,-0.5964129175,0.9346408238
C,0,-0.7178103842,-0.5694897934,0.9082575005
O,0,-1.3841390453,1.3455972327,-2.0008348141
C,0,1.4061902954,-1.3359047196,2.0634046208
H,0,-2.5100771202,0.0649561495,-0.0415898959
H,0,1.0860772157,1.8023774045,-1.1732102524
H,0,1.0672287059,0.3458063459,-2.1128429295
H,0,2.5114583367,0.0151854372,-0.0227138654
H,0,-1.2354413429,-1.0885063269,1.708000372
H,0,2.4901801783,-1.295811605,1.9826497291
H,0,1.099177937,-2.3833073609,2.0693975942
H,0,1.1160033346,-0.9094093865,3.0253163492
HF=-346.7128085 Nimag=0

4-NH_2

C,0,-1.4379195658,0.0081837095,-0.2652670812
C,0,-0.7579684171,0.6119473181,-1.4247973158
C,0,0.756293474,0.6861434108,-1.3795683113
C,0,1.4238595299,-0.0480384008,-0.2602998088
C,0,0.7269882962,-0.614115185,0.730996741
C,0,-0.73742921,-0.554702841,0.7244621117
O,0,-1.3800742953,1.0462833,-2.3686770276
N,0,1.2980572893,-1.2168854656,1.8627902
H,0,-2.5185592001,0.0281186297,-0.2703891606
H,0,1.0013848189,1.75372746,-1.3346739661
H,0,1.1250113853,0.3520511152,-2.3516271094
H,0,2.5061218729,-0.0878476111,-0.2552208883
H,0,-1.2529958541,-0.9970260776,1.5698447875
H,0,2.2819392817,-1.4145302638,1.7589625129
H,0,0.8055055942,-2.0409960984,2.174440316
HF=-362.7589985 Nimag=0

4-F

C,0,-1.4291503995,0.0003755898,0.0159848313
C,0,-0.7381346314,0.695559589,-1.0870274403
C,0,0.7840899457,0.6840410512,-1.0926984247
C,0,1.4517218563,-0.0376051619,0.0336008159
C,0,0.7185349448,-0.6245117209,0.9678170615
C,0,-0.7346226918,-0.6174590286,0.9777000711
O,0,-1.3530758835,1.2590986748,-1.9627076908
F,0,1.2845665661,-1.2821518761,1.9946092162
H,0,-2.5093290171,0.0194781115,0.0018322656
H,0,1.1079657649,1.7279777256,-1.1229274811
H,0,1.093194943,0.2622175684,-2.05301181
H,0,2.5305534174,-0.079680167,0.0841822738
H,0,-1.2239288148,-1.1321623559,1.7944383113
HF=-406.6451159 Nimag=0

4-Cl

C,0,-1.4253773365,-0.1326172111,-0.1148865835
C,0,-0.7368413199,0.5717852867,-1.2107489914
C,0,0.7828973587,0.5641390083,-1.205678806
C,0,1.4451031314,-0.1637421688,-0.0807002965
C,0,0.7228441531,-0.7665194567,0.8573629963

C,0,-0.7365929362,-0.7557868954,0.8480089508
O,0,-1.3488358471,1.1381904106,-2.0866587179
H,0,-2.5057909358,-0.1184110476,-0.1316493808
H,0,1.1104861631,1.6075918544,-1.223581569
H,0,1.1063943397,0.1494810624,-2.1647430009
H,0,2.5251500893,-0.1908809608,-0.044021066
H,0,-1.244892693,-1.2721469814,1.6511593468
Cl,0,1.4790688333,-1.6198769008,2.176506118
HF=-767.0041856 Nimag=0

4-Br

C,0,-1.4259697729,-0.090875961,-0.1800605669
C,0,-0.7369915986,0.6130764462,-1.275342234
C,0,0.7822948062,0.6043496974,-1.2685414119
C,0,1.4436896216,-0.1241700438,-0.1423456993
C,0,0.7205076935,-0.7264135819,0.7949934922
C,0,-0.739128674,-0.7148222706,0.784248279
O,0,-1.3477623074,1.1798063808,-2.1518920148
H,0,-2.5064263949,-0.0763754564,-0.1973423776
H,0,1.1120424475,1.6471745273,-1.2855047438
H,0,1.1079665552,0.1889001862,-2.2265680473
H,0,2.5238522609,-0.1483511079,-0.1101638284
H,0,-1.2532836562,-1.2293111179,1.5846005191
Br,0,1.5472600191,-1.6546466985,2.2302206336
HF=-2880.9708155 Nimag=0

4-CHO

C,0,-1.4378501911,0.0438224593,-0.0217689961
C,0,-0.7487542994,0.7536666131,-1.113703679
C,0,0.773937571,0.7394570025,-1.1159065872
C,0,1.4239128805,0.0065587225,0.0042843313
C,0,0.7108155335,-0.6085397242,0.9546206615
C,0,-0.7516997281,-0.5877146735,0.9372469195
O,0,-1.3540950514,1.3326957501,-1.9854655976
C,0,1.4086627076,-1.3230748549,2.043613795
O,0,0.8431103732,-1.8991611768,2.9347139971
H,0,-2.5182929551,0.0654307592,-0.0425821234
H,0,1.1126230036,1.7795440261,-1.1362844956
H,0,1.0956803479,0.3241491366,-2.0758152535
H,0,2.5078208714,-0.0224033035,0.0388327234
H,0,-1.2542643003,-1.1099322834,1.7411863358
H,0,2.5124582367,-1.296013453,1.9889519689
HF=-420.7243725 Nimag=0

4-CN

C,0,-1.4160287016,0.0257723868,0.0046350772
C,0,-0.7341653741,0.7395880052,-1.0896579078
C,0,0.7862932676,0.7269792506,-1.097522733
C,0,1.4515605156,-0.0035479445,0.0162187245
C,0,0.7424561305,-0.6207592555,0.9689714107
C,0,-0.7247834046,-0.6046858116,0.959540102
O,0,-1.3482543161,1.3169024385,-1.9552353118
C,0,1.4042909139,-1.3216220234,2.0357762928
N,0,1.9106525486,-1.8866543154,2.8965203133
H,0,-2.4964652267,0.0420456088,-0.0071807892
H,0,1.1250650704,1.767174575,-1.1169570431
H,0,1.1066999007,0.3119485237,-2.0581141714
H,0,2.5328741849,-0.0285732962,0.0431170184
H,0,-1.2339475091,-1.1251441423,1.7598610176
HF=-399.6417814 Nimag=0

4-NO

C,0,-1.4565198191,-0.2380562905,0.0564965441
C,0,-0.7699868785,0.4670155104,-1.0405620364
C,0,0.7538875787,0.4624684654,-1.0403167872
C,0,1.4165603592,-0.2606997819,0.0771489652
C,0,0.6949554048,-0.8684456368,1.0222146966
C,0,-0.7605027327,-0.8589186125,1.0160921121
O,0,-1.3771499372,1.0346375423,-1.9181791587
N,0,1.2905034898,-1.5888778274,2.1393863554
O,0,2.4869820257,-1.6080866664,2.1478093594
H,0,-2.5368182943,-0.2236086233,0.0399643116
H,0,1.0865834553,1.5049629723,-1.0613022295
H,0,1.082285571,0.0505202531,-1.9996856752
H,0,2.4978634357,-0.2960682534,0.1274445124
H,0,-1.2556926584,-1.3794640514,1.8268130302
HF=-436.6873319 Nimag=0

4-NO_2

C,0,-1.467833649,0.0426178461,-0.3750603098
C,0,-0.7671222936,0.7450053621,-1.4658408811
C,0,0.7546654671,0.7071585112,-1.4663582016
C,0,1.4017245457,-0.0455557423,-0.3579817718
C,0,0.6589934301,-0.640856763,0.5704670196
C,0,-0.7962019726,-0.6085232218,0.5811372733
O,0,-1.3644802949,1.3338136834,-2.3348386242
N,0,1.3324056878,-1.3789425684,1.656190217
O,0,0.6192485289,-1.9079781804,2.4828160823
O,0,2.5432292484,-1.4117135135,1.6565649214
H,0,-2.5474194117,0.0821751283,-0.3912704338
H,0,1.1122742444,1.7411892761,-1.46923296
H,0,1.0766492126,0.2989027736,-2.4289371313
H,0,2.4795549707,-0.1089609981,-0.3063736133
H,0,-1.303300714,-1.1252535934,1.3821844132
HF=-511.8978812 Nimag=0

Benzoquinone

C,0,-2.4470396116,-0.1166481848,1.1079214352
C,0,-2.4129653381,-0.7899517296,-0.0395242182
C,0,-1.1370975347,-1.329221696,-0.5767371032
C,0,0.099446326,-1.0904890207,0.2114341417
C,0,0.0653721449,-0.4171856029,1.3588801317
C,0,-1.2105350401,0.12186243,1.8962220591
O,0,-1.1061054097,-1.9409938571,-1.6196404458
O,0,-1.2414731516,0.7339390001,2.9389483715
H,0,-3.3582854029,0.2889054125,1.52671144
H,0,-3.2940198652,-0.9809746846,-0.6374211307
H,0,1.0107152037,-1.4959116605,-0.207432306
H,0,0.9464498191,-0.2260315647,1.9567011351
HF=-381.4171527 Nimag=0

Table S11. Cartesian Coordinates, Total Energies (in hartree), and Number of Imaginary Frequencies for the Optimized Structures for Base Pairs from M06-2X/6-311+G(2d,2p) Computations.

Adenine-Thymine

N,0,-5.2767795357,-0.1565657614,0.3501328297
C,0,-5.4332996668,-1.4900720558,0.3169498285
N,0,-6.5493062872,-2.1726827237,0.1289895295
C,0,-7.5971016568,-1.3588368492,-0.0391890888
C,0,-7.587537213,0.0272262294,-0.0298933572
C,0,-6.3403347437,0.6436114646,0.1789055502
N,0,-8.9082962886,-1.6935127557,-0.2570154591
C,0,-9.603662574,-0.5136594192,-0.3652994171
N,0,-8.8519522765,0.5406192868,-0.2356320097
N,0,-6.185132487,1.9711567886,0.2111916369
H,0,-4.5224028663,-2.0585565807,0.4640459229
H,0,-9.2746454773,-2.6271307397,-0.3230316641
H,0,-10.6666896661,-0.5007829658,-0.5404817147
H,0,-5.2673616983,2.3783782118,0.3660203918
H,0,-6.9916354936,2.5550352147,0.0828390425
N,0,-2.6610393182,0.8064432008,0.7889018694
C,0,-1.6929114833,-0.1542534034,0.942337435
N,0,-0.4267046213,0.3602779893,1.1533456143
C,0,-0.1586698516,1.7064817658,1.2050186707
C,0,-1.1124064473,2.6382550207,1.0534189049
C,0,-2.4801902162,2.1733444996,0.82580643
O,0,-3.4279043996,2.9311535816,0.6738133395
O,0,-1.9135482669,-1.3437824188,0.8990818017
C,0,-0.8694267003,4.1123045548,1.1015537069
H,0,-3.6321377741,0.453623837,0.6263357324
H,0,0.3022024979,-0.3231253532,1.2693076602
H,0,0.8767983026,1.9657169968,1.3767107122
H,0,-1.1764638881,4.580629535,0.1667140961
H,0,0.18309733,4.3268665001,1.2759267601
H,0,-1.4606122327,4.5710973492,1.8937252453
HF=-921.4178597 Nimag=0

Adenine-Uracil

N,0,-1.6876457474,-0.4223400492,0.0175485635
C,0,-1.9987552313,-1.7291081334,0.0079678507
N,0,-3.1991402952,-2.2793459254,0.0518976552
C,0,-4.1598194113,-1.3504474458,0.1118714165
C,0,-3.990908696,0.0252225081,0.1292170691
C,0,-2.6652006207,0.4948433695,0.0779981459
N,0,-5.5165982613,-1.5323917985,0.1692623662
C,0,-6.0807802241,-0.2802151351,0.217171181
N,0,-5.2034141351,0.680575865,0.1952915129
N,0,-2.3571513892,1.7956187773,0.0877203417
H,0,-1.1473026123,-2.3985718731,-0.0424387937
H,0,-5.992401006,-2.4178686619,0.1744362097
H,0,-7.1487606414,-0.1455932365,0.267476506
H,0,-1.3873227226,2.0949360657,0.0461706488
H,0,-3.1014889796,2.4677026253,0.1309784359
N,0,1.0520589628,0.2195368798,-0.1054841976
C,0,1.911778381,-0.8467458032,-0.1681507871
N,0,3.2516491427,-0.4893612195,-0.2335200361
C,0,3.6791457966,0.8102362451,-0.2358246495
C,0,2.8193609098,1.8370463966,-0.174107522
C,0,1.3924266701,1.5605631869,-0.1029065499
O,0,0.5269381018,2.4196665887,-0.0440813252
O,0,1.5544247241,-2.002138461,-0.1676969846
H,0,0.0338238428,-0.0185385522,-0.0567078401
H,0,3.8996038847,-1.2576152823,-0.2802217663
H,0,4.7490566542,0.948200155,-0.2904452347
H,0,3.1465089029,2.8620499142,-0.1755662162
HF=-882.1066865 Nimag=0

Guanine-Cytosine

N,0,-5.0634347309,0.3996896946,0.1926126616
C,0,-5.4623190746,-0.8925157366,0.1102605561
N,0,-6.8967833709,-1.1588610686,0.1195666006
C,0,-7.6030040327,-0.0449660442,0.1636546056
C,0,-7.2843015187,1.1241423528,0.3251748256
C,0,-5.8858043957,1.4502848055,0.2317784188
N,0,-5.3937605268,2.6717970584,0.2110182095
O,0,-4.7305115926,-1.8576436302,0.0065699033
H,0,-7.1922289437,-2.0815398624,-0.1594308946
H,0,-4.3727304194,2.8151349946,0.1345310015
H,0,-6.0233879672,3.451750332,0.2609593463
N,0,-2.1256945976,0.761515865,0.0409267178
C,0,-1.2537929951,-0.2926916477,0.0077112555
N,0,0.0422355901,-0.1543920673,-0.1382380191
C,0,0.4131969559,1.1379667925,-0.2394428736
C,0,-0.374002282,2.2796725311,-0.2137695673
C,0,-1.7820948297,2.1132313208,-0.063558752
N,0,1.6875466123,1.5963487833,-0.3969225962
C,0,1.6111201019,2.9733849604,-0.4576601104
N,0,0.3967132216,3.4155630467,-0.3520447598
O,0,-2.6583165778,2.9723063512,-0.0213184976
N,0,-1.7945568449,-1.5196460901,0.1680495284
H,0,-3.1287214267,0.5747832362,0.1378883616
H,0,2.5113612423,1.0234621006,-0.4520039642
H,0,2.4914231515,3.5818723301,-0.5800122844
H,0,-1.1781887691,-2.2934098707,-0.0032742887
H,0,-2.7949699795,-1.6636085377,0.0772656158
HF=-936.1296521 Nimag=0