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Uracil
E(NN)=358.335960, E(HF/6-31(+)G*)=-412.480723, E(CCSD/6-31(+)G*)=-413.683919

C	1.282409	0.344117	0.000000
O	2.305402	1.000355	0.000000
N	0.034953	0.973561	0.000000
C	-1.214176	0.400371	0.000000
N	-1.169168	-0.978725	0.000000
C	-0.007293	-1.695619	0.000000
C	1.195482	-1.099235	0.000000
H	2.102515	-1.668441	0.000000
H	-0.122433	-2.764793	0.000000
H	-2.063639	-1.435070	0.000000
O	-2.250828	1.027713	0.000000
H	0.047936	1.982097	0.000000

Stacked uracil dimer, the geometry of the neutral
E(NN)=1161.470703, E(HF/6-31(+)G*)=-824.960277, E(CCSD/6-31(+)G*)=-827.387312

N	-2.072256	1.105980	-0.071103
C	-2.059504	0.589911	-1.337439
H	-2.367357	1.268570	-2.118682
C	-1.681094	-0.681127	-1.585525
H	-1.672908	-1.080128	-2.585041
C	-1.230666	-1.524219	-0.493625
O	-0.782296	-2.655801	-0.599081
N	-1.330922	-0.910847	0.761600
H	-0.977606	-1.439511	1.550335
C	-1.669186	0.398162	1.045691
O	-1.609958	0.888541	2.156770
H	-2.242063	2.086718	0.083778
N	2.072256	-1.105980	-0.071103
C	2.059504	-0.589911	-1.337439
H	2.367357	-1.268570	-2.118682
C	1.681094	0.681127	-1.585525
H	1.672908	1.080128	-2.585041
C	1.230666	1.524219	-0.493625
O	0.782296	2.655801	-0.599081
N	1.330922	0.910847	0.761600
H	0.977606	1.439511	1.550335
C	1.669186	-0.398162	1.045691
O	1.609958	-0.888541	2.156770
H	2.242063	-2.086718	0.083778

Stacked uracil dimer, the cation geometry
E(NN)=1152.637409, E(HF/6-31(+)G*)=-824.933002, E(CCSD/6-31(+)G*)=-827.352475

N	1.444053	1.105646	-0.823447
H	1.262853	1.632814	-1.662002
C	2.363500	0.097169	-0.944097
O	2.921317	-0.206549	-1.941200
C	0.757351	1.484087	0.317679
O	-0.070474	2.348460	0.296920
N	2.604736	-0.589913	0.263726
H	3.259739	-1.350492	0.186024
C	2.040503	-0.287749	1.419215
H	2.346338	-0.866403	2.273578
C	1.097947	0.710321	1.509375
H	0.768243	1.074880	2.461650
C	-1.097947	-0.710321	1.509376
H	-0.768243	-1.074879	2.461650
C	-2.040503	0.287749	1.419215
H	-2.346338	0.866404	2.273578
N	-2.604736	0.589913	0.263726

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H    -3.259739     1.350492     0.186024
C    -2.363500    -0.097169    -0.944097
O    -2.921317     0.206549    -1.941200
N    -1.444053    -1.105646    -0.823447
H    -1.262853    -1.632814    -1.662001
C    -0.757351    -1.484087     0.317679
O     0.070474    -2.348460     0.296920

H-bonded uracil dimer, the geometry of the neutral
E(NN)=1032.281916, E(HF/6-31(+)G*)=-824.983139, E(CCSD/6-31(+)G*)=-827.399595
O    -0.999831    -1.474772     0.000000
C    -1.908930    -0.644185     0.000000
N    -1.694255     0.706319     0.000000
C    -2.718913     1.613974     0.000000
C    -4.016749     1.243246     0.000000
C    -4.360922    -0.165195     0.000000
N    -3.231326    -1.004870     0.000000
O    -5.481203    -0.643233     0.000000
H    -4.810563     1.970059     0.000000
H    -0.714742     1.017291     0.000000
H    -3.415735    -1.998756     0.000000
H    -2.410651     2.648930     0.000000
O     0.999831     1.474772     0.000000
C     1.908930     0.644185     0.000000
N     1.694255    -0.706319     0.000000
C     2.718913    -1.613974     0.000000
C     4.016749    -1.243246     0.000000
C     4.360922     0.165195     0.000000
N     3.231326     1.004870     0.000000
O     5.481203     0.643233     0.000000
H     4.810563    -1.970059     0.000000
H     0.714742    -1.017291     0.000000
H     3.415735     1.998756     0.000000
H     2.410651    -2.648930     0.000000
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