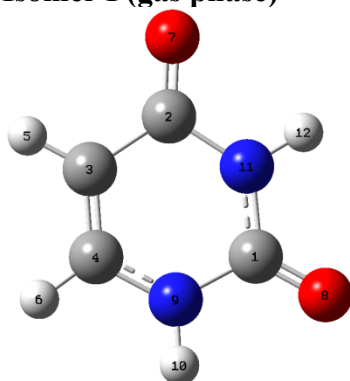


Supplementary Information A.

Geometrical parameters of the uracil isomers in gas and aqueous phases optimized by B3LYP/6-311++g(3df,3pd).

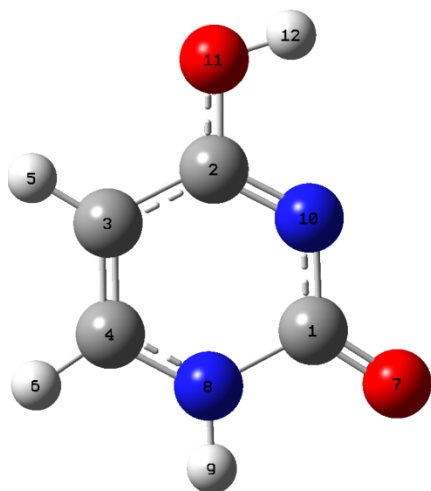
Isomer I (gas phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	2	B6	1	A5	4
O	1	B7	4	A6	3
N	4	B8	3	A7	2
H	9	B9	4	A8	3
N	1	B10	8	A9	9
H	11	B11	1	A10	8
					D9

B1	2.51032707	A5	145.81170506
B2	1.45759291	A6	150.73456364
B3	1.34836854	A7	121.92354109
B4	1.07809591	A8	121.25489933
B5	1.08175699	A9	124.26115124
B6	1.21670891	A10	115.66937409
B7	1.21411190	D1	-0.00000000
B8	1.37345300	D2	180.00000000
B9	1.00756217	D3	-180.00000000
B10	1.38154828	D4	179.99952119
B11	1.01148478	D5	-179.99920380
A1	87.91227156	D6	0.00029007
A2	119.79980014	D7	-179.99965156
A3	118.27192779	D8	-179.99946841
A4	122.79533498	D9	-0.00000000

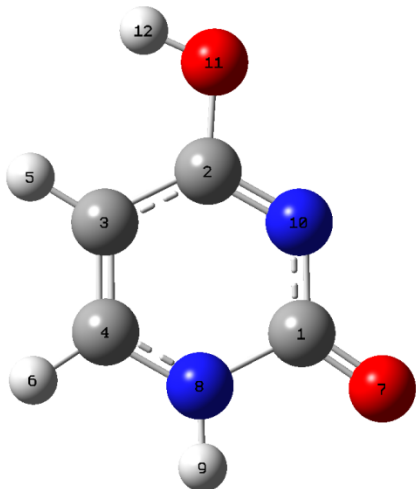
Isomer II (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	4	B7	3	A6	2	D5 0
H	8	B8	4	A7	3	D6 0
N	2	B9	1	A8	7	D7 0
O	2	B10	1	A9	7	D8 0
H	11	B11	2	A10	1	D9 0

B1	2.32039591	A6	120.11322974
B2	1.42454929	A7	121.22255917
B3	1.35491295	A8	30.78742923
B4	1.07623092	A9	148.93808050
B5	1.08066532	A10	106.94921587
B6	1.21079062	D1	0.01207353
B7	1.35060044	D2	-179.99523840
B8	1.00815012	D3	179.99142072
B9	1.30079493	D4	-179.91133757
B10	1.33915326	D5	-0.00686066
B11	0.96839911	D6	179.99404399
A1	94.54012320	D7	0.08058099
A2	115.25412454	D8	0.09815265
A3	121.86175405	D9	-0.01079191
A4	123.06179396		
A5	154.43172283		

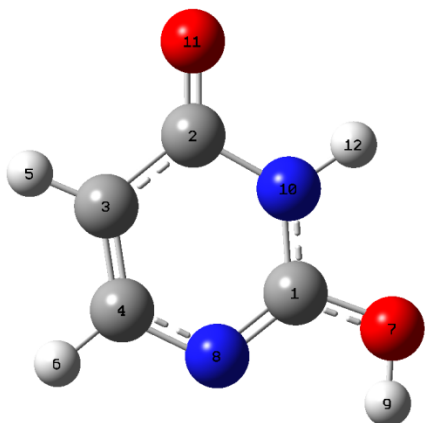
Isomer III (gas phase)



C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
H	3	B4	2	A3	1	D2	0
H	4	B5	3	A4	2	D3	0
O	1	B6	2	A5	3	D4	0
N	4	B7	3	A6	2	D5	0
H	8	B8	4	A7	3	D6	0
N	2	B9	1	A8	7	D7	0
O	2	B10	1	A9	7	D8	0
H	11	B11	2	A10	1	D9	0

B1	2.31563087	A5	154.45316854
B2	1.43088603	A6	119.88771546
B3	1.35578292	A7	121.34420604
B4	1.07845207	A8	30.76766379
B5	1.08078024	A9	146.28391492
B6	1.21014475	A10	110.43408473
B7	1.34680984	D1	0.00000000
B8	1.00826100	D2	179.99396585
B9	1.29572117	D3	179.99713430
B10	1.34668341	D4	-179.90630282
B11	0.96252571	D5	0.00352581
A1	94.05759266	D6	179.99074125
A2	115.73257814	D7	0.07539421
A3	122.82429980	D8	0.05135397
A4	123.04564253	D9	-179.97074344

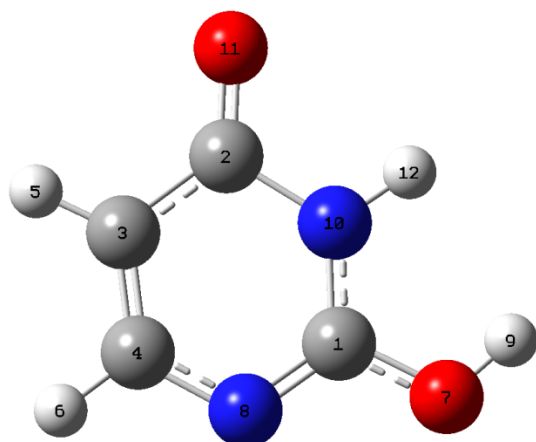
Isomer IV (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	4	A5	3	D4 0
N	1	B7	7	A6	4	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	8	A8	4	D7 0
O	2	B10	1	A9	8	D8 0
H	10	B11	1	A10	8	D9 0

B1	2.43436386	A5	154.38415595
B2	1.44334038	A6	121.14253618
B3	1.35692411	A7	106.99684361
B4	1.07826718	A8	124.64501803
B5	1.08256862	A9	147.32464936
B6	1.33706073	A10	119.98037377
B7	1.29413926	D1	0.00662704
B8	0.96687011	D2	-179.99516121
B9	1.34848485	D3	180.00000000
B10	1.21431171	D4	179.97047329
B11	1.01086720	D5	-0.01837311
A1	84.21536347	D6	0.00875860
A2	120.05031136	D7	0.00865266
A3	117.87192748	D8	-179.99743628
A4	120.47419985	D9	179.99019409

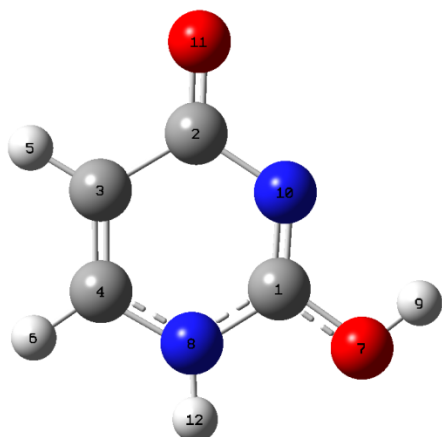
Isomer V (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	4	A5	3	D4 0
N	1	B7	7	A6	4	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	8	A8	4	D7 0
O	2	B10	1	A9	8	D8 0
H	10	B11	1	A10	8	D9 0

B1	2.45205094	A5	150.94327983
B2	1.43880500	A6	117.90158214
B3	1.35823708	A7	112.20330884
B4	1.07832650	A8	123.68941054
B5	1.08287770	A9	146.66239643
B6	1.34205601	A10	122.11269522
B7	1.29025585	D1	-0.00444115
B8	0.96260737	D2	-179.99331659
B9	1.35810370	D3	-179.98390637
B10	1.21480158	D4	179.98027202
B11	1.01110226	D5	-0.00287484
A1	84.27455827	D6	-179.74141956
A2	119.73538216	D7	0.01725867
A3	118.06714523	D8	179.99837574
A4	120.17754321	D9	-179.94607321

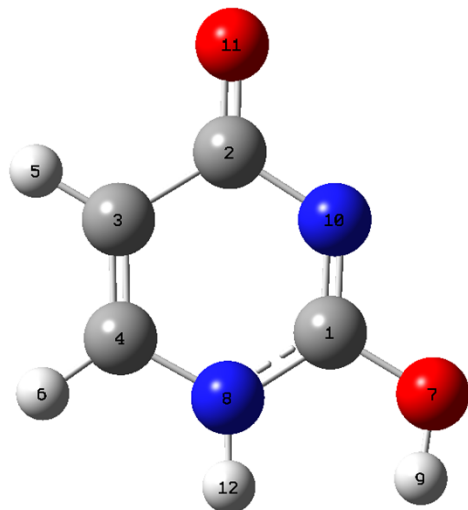
Isomer VI (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	4	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	7	A8	8	D7 0
O	2	B10	1	A9	10	D8 0
H	8	B11	1	A10	10	D9 0

B1	2.32614098	A5	153.53004718
B2	1.47081329	A6	112.60560239
B3	1.34007719	A7	106.51079706
B4	1.07820394	A8	121.75356296
B5	1.07954262	A9	149.84629458
B6	1.34252742	A10	119.50896172
B7	1.36036477	D1	0.00047192
B8	0.96711927	D2	-179.99880157
B9	1.27997172	D3	-180.00000000
B10	1.21328668	D4	-179.98881085
B11	1.00598258	D5	-0.00584780
A1	87.38104817	D6	179.99920650
A2	120.45979161	D7	179.99418320
A3	118.24840744	D8	0.04710354
A4	124.34368987	D9	-179.99905489

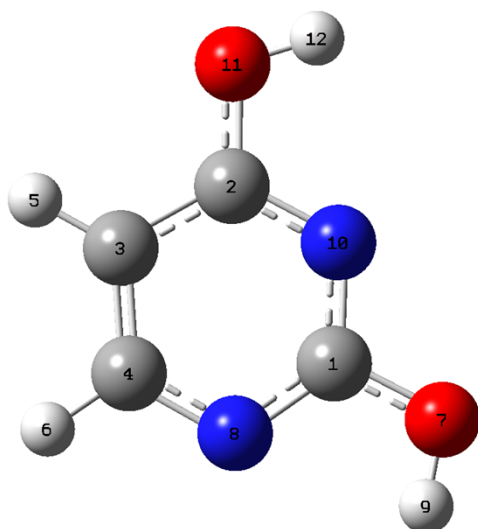
Isomer VII (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	2	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	7	A8	8	D7 0
O	2	B10	1	A9	10	D8 0
H	8	B11	1	A10	10	D9 0

B1	2.32664622	A5	149.93601771
B2	1.47086128	A6	116.85442384
B3	1.33818707	A7	112.59963722
B4	1.07834931	A8	118.45295967
B5	1.07981088	A9	149.51425908
B6	1.34823990	A10	121.67059766
B7	1.37318006	D1	-0.00826581
B8	0.96237624	D2	179.99375053
B9	1.27472871	D3	-179.99682955
B10	1.21331359	D4	-179.98808733
B11	1.00554347	D5	179.99037158
A1	88.03171417	D6	0.00793137
A2	120.17939300	D7	-179.99025459
A3	118.50112842	D8	0.02005695
A4	124.46843855	D9	-179.90509480

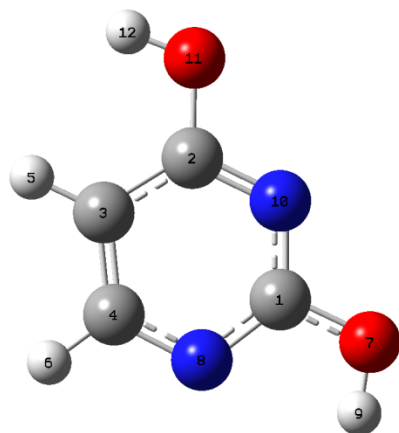
Isomer VIII (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	2	D5 0
H	7	B8	1	A7	8	D6 0
N	2	B9	1	A8	8	D7 0
O	2	B10	1	A9	8	D8 0
H	11	B11	2	A10	1	D9 0

B1	2.24865492	A5	147.33297339
B2	1.39688504	A6	117.48431377
B3	1.37881802	A7	106.79465223
B4	1.07772429	A8	32.10401587
B5	1.08323850	A9	149.73231908
B6	1.33935772	A10	107.30700224
B7	1.32805996	D1	-0.00552071
B8	0.96592515	D2	179.99661663
B9	1.32349023	D3	-179.99834304
B10	1.33973809	D4	179.96714994
B11	0.96735616	D5	179.95559530
A1	90.82311265	D6	-0.01189196
A2	115.33243992	D7	-179.99113657
A3	121.66881351	D8	-180.00000000
A4	120.65913160	D9	0.00654294

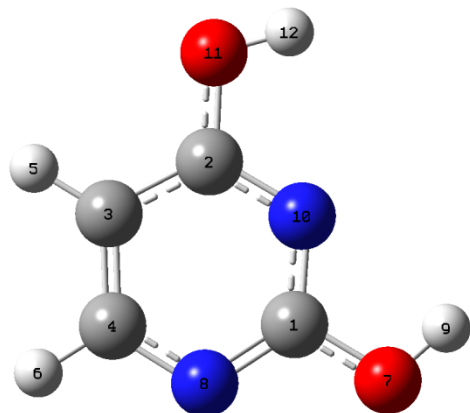
Isomer IX (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	2	D5 0
H	7	B8	1	A7	8	D6 0
N	2	B9	1	A8	8	D7 0
O	2	B10	1	A9	10	D8 0
H	11	B11	2	A10	1	D9 0

B1	2.24332581	A5	147.31234179
B2	1.40060734	A6	117.08285823
B3	1.38041248	A7	106.85160644
B4	1.08004263	A8	32.10636625
B5	1.08350193	A9	146.91289736
B6	1.33885648	A10	110.07699794
B7	1.33208916	D1	-0.00785982
B8	0.96579793	D2	179.99440346
B9	1.31957984	D3	-179.99740791
B10	1.34577440	D4	179.96773208
B11	0.96264125	D5	179.95378978
A1	90.43464990	D6	-0.01180527
A2	115.75607480	D7	-179.99155960
A3	122.50423977	D8	-0.01686038
A4	120.66822537	D9	-179.98295783

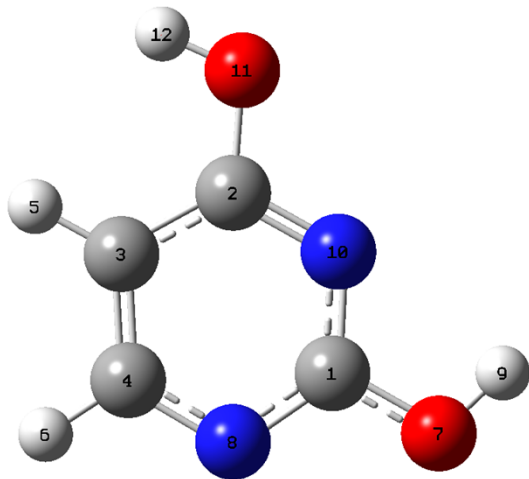
Isomer X (gas phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	4	A5	3
N	1	B7	7	A6	4
H	7	B8	1	A7	8
N	2	B9	1	A8	8
O	2	B10	1	A9	8
H	11	B11	2	A10	1
					D1 0
					D2 0
					D3 0
					D4 0
					D5 0
					D6 0
					D7 0
					D8 0
					D9 0

B1	2.26006106	A5	148.73622050
B2	1.39429711	A6	116.09253112
B3	1.38083399	A7	107.53783580
B4	1.07774714	A8	32.00686918
B5	1.08352778	A9	149.90909516
B6	1.34006804	A10	107.63475500
B7	1.32202470	D1	-0.00416341
B8	0.96500365	D2	179.99761626
B9	1.32485676	D3	-179.99916288
B10	1.34063435	D4	-179.97046820
B11	0.96666861	D5	0.01676908
A1	90.42701463	D6	179.98743690
A2	115.35283941	D7	-179.99209243
A3	121.63653172	D8	-179.99666317
A4	120.34256343	D9	0.00262113

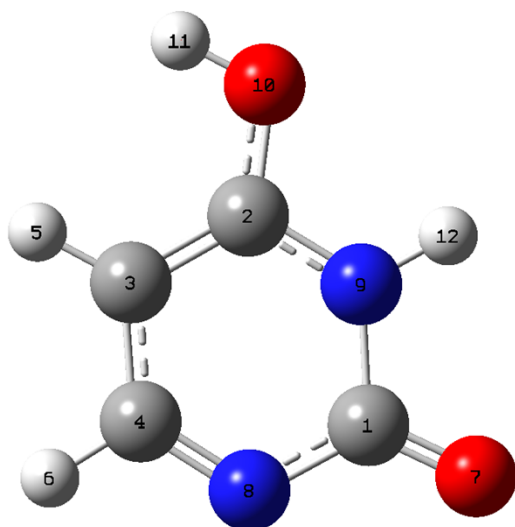
Isomer XI (gas phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	4	A5	3
N	1	B7	7	A6	4
H	7	B8	1	A7	8
N	2	B9	1	A8	8
O	2	B10	1	A9	8
H	11	B11	2	A10	1
					D1
					D2
					D3
					D4
					D5
					D6
					D7
					D8
					D9

B1	2.25487299	A5	148.52923233
B2	1.39784127	A6	115.85871884
B3	1.38266741	A7	107.19123757
B4	1.08006247	A8	31.98558359
B5	1.08380324	A9	146.88766622
B6	1.33893247	A10	110.01946418
B7	1.32594392	D1	-0.00658266
B8	0.96565394	D2	179.99544279
B9	1.32084438	D3	-179.99805666
B10	1.34609002	D4	-179.96914174
B11	0.96271545	D5	0.01718807
A1	90.04837516	D6	179.98659192
A2	115.75086799	D7	-179.99208669
A3	122.47045010	D8	179.99474970
A4	120.33244136	D9	-179.98723072

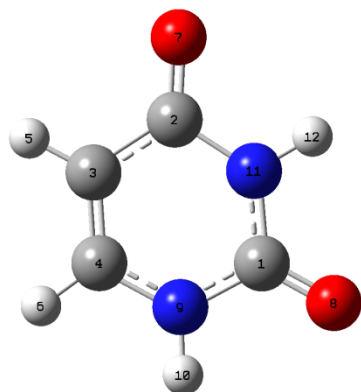
Isomer XII (gas phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	4	A5	3	D4 0
N	4	B7	3	A6	2	D5 0
N	2	B8	1	A7	7	D6 0
O	2	B9	1	A8	7	D7 0
H	10	B10	2	A9	1	D8 0
H	9	B11	2	A10	1	D9 0

B1	2.44897631	A5	155.60681420
B2	1.36944267	A6	126.26120332
B3	1.41211839	A7	28.90526365
B4	1.07820645	A8	142.92953473
B5	1.08668421	A9	110.20914607
B6	1.20892766	A10	119.66725762
B7	1.30624454	D1	-0.00113928
B8	1.34235442	D2	179.99947608
B9	1.34053963	D3	179.99935634
B10	0.96329598	D4	-179.99355209
B11	1.01047161	D5	0.00123471
A1	90.28772831	D6	-0.00414361
A2	115.61306545	D7	-0.00492991
A3	122.15539380	D8	-179.99938952
A4	117.92227940	D9	-180.00000000

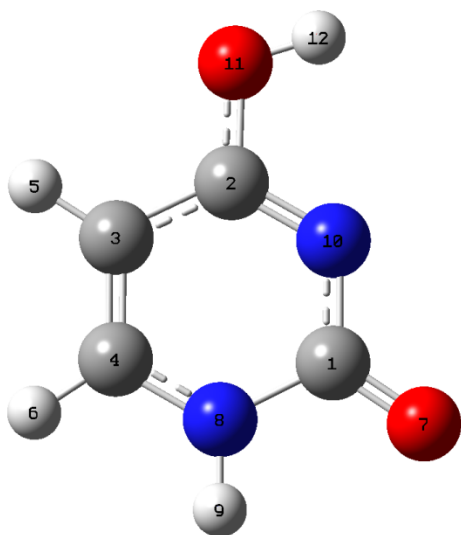
Isomer I (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	2	B6	1	A5	4	D4 0
O	1	B7	4	A6	3	D5 0
N	4	B8	3	A7	2	D6 0
H	9	B9	4	A8	3	D7 0
N	1	B10	8	A9	9	D8 0
H	11	B11	1	A10	8	D9 0

B1	2.49081142	A5	145.82927420
B2	1.44517103	A6	151.23679814
B3	1.34704610	A7	121.88108734
B4	1.07671851	A8	120.42282758
B5	1.07930877	A9	123.36372269
B6	1.22361933	A10	115.83193473
B7	1.21836491	D1	0.00305386
B8	1.36666874	D2	-179.99821857
B9	1.00832496	D3	179.99804304
B10	1.37721266	D4	-179.99045590
B11	1.01097855	D5	179.99700993
A1	88.04852730	D6	-0.00255860
A2	119.61798981	D7	180.00000000
A3	118.88986961	D8	179.99578779
A4	122.78237702	D9	0.00307007

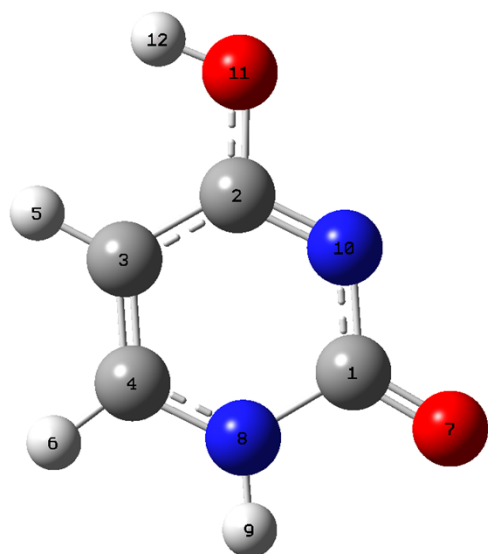
Isomer II (Aqueous phase)



C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
H	3	B4	2	A3	1	D2	0
H	4	B5	3	A4	2	D3	0
O	1	B6	2	A5	3	D4	0
N	4	B7	3	A6	2	D5	0
H	8	B8	4	A7	3	D6	0
N	2	B9	1	A8	7	D7	0
O	2	B10	1	A9	7	D8	0
H	11	B11	2	A10	1	D9	0

B1	2.31673726	A5	153.38841849
B2	1.41769251	A6	120.04466293
B3	1.35651942	A7	120.22192515
B4	1.07619547	A8	30.80553892
B5	1.07934897	A9	149.05886530
B6	1.22569978	A10	108.30036460
B7	1.35051991	D1	-0.00648077
B8	1.00929559	D2	179.99768392
B9	1.30903636	D3	-179.99520947
B10	1.33633310	D4	179.95295658
B11	0.96873874	D5	0.00364116
A1	94.05780443	D6	-179.99604415
A2	115.47465553	D7	-0.04316754
A3	121.97725019	D8	-0.05203956
A4	123.35086937	D9	0.00548569

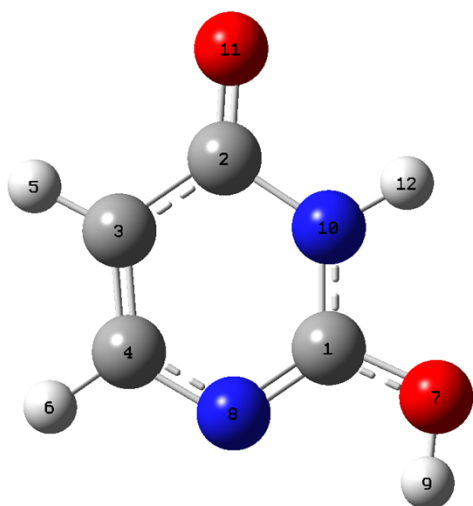
Isomer III (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	4	B7	3	A6	2	D5 0
H	8	B8	4	A7	3	D6 0
N	2	B9	1	A8	7	D7 0
O	2	B10	1	A9	7	D8 0
H	11	B11	2	A10	1	D9 0

B1	2.31506628	A5	153.32506942
B2	1.42071478	A6	119.94577650
B3	1.35721748	A7	120.30566520
B4	1.07746564	A8	30.75139740
B5	1.07934633	A9	145.61007640
B6	1.22613620	A10	110.94522766
B7	1.34833614	D1	0.00388198
B8	1.00937497	D2	-179.99318416
B9	1.30769761	D3	179.99949059
B10	1.34088286	D4	179.94930651
B11	0.96496623	D5	-0.00613594
A1	93.72462448	D6	-179.99370762
A2	115.76561194	D7	-0.03364311
A3	122.66628185	D8	-0.00161062
A4	123.30051549	D9	179.95700800

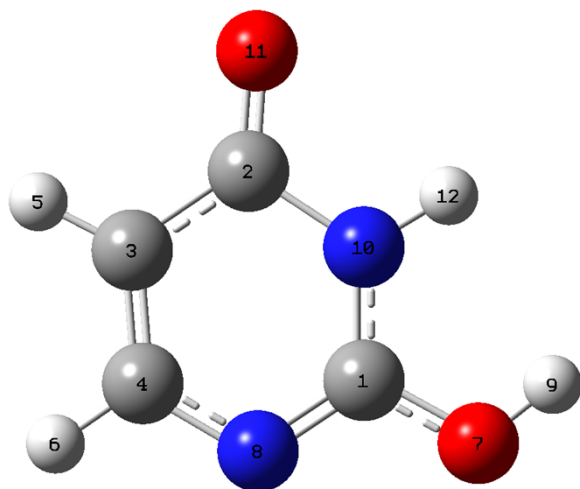
Isomer IV (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	4	A5	3	D4 0
N	1	B7	7	A6	4	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	8	A8	4	D7 0
O	2	B10	1	A9	8	D8 0
H	10	B11	1	A10	8	D9 0

B1	2.42389843	A5	154.74642263
B2	1.43638354	A6	121.68304281
B3	1.35965143	A7	108.35331972
B4	1.07827304	A8	124.22582868
B5	1.08234437	A9	147.50220849
B6	1.33001265	A10	119.36853154
B7	1.29860640	D1	0.02703658
B8	0.96797517	D2	-179.97982159
B9	1.35019203	D3	179.98596733
B10	1.22631178	D4	-179.97799939
B11	1.01191443	D5	0.01689060
A1	84.77425455	D6	-0.00219734
A2	119.72036481	D7	0.01200958
A3	118.51899362	D8	-179.89455529
A4	120.26587683	D9	-179.99138300

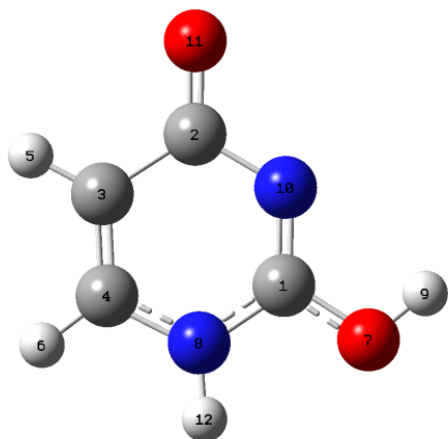
Isomer V (Aqueous phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	4	A5	3
N	1	B7	7	A6	4
H	7	B8	1	A7	8
N	1	B9	8	A8	4
O	2	B10	1	A9	8
H	10	B11	1	A10	8
					D1 0
					D2 0
					D3 0
					D4 0
					D5 0
					D6 0
					D7 0
					D8 0
					D9 0

B1	2.43506017	A5	150.44303887
B2	1.43322203	A6	117.57500003
B3	1.36015972	A7	112.96543840
B4	1.07828743	A8	123.50692909
B5	1.08253822	A9	147.02555006
B6	1.33295968	A10	121.00541056
B7	1.29839148	D1	-0.02284892
B8	0.96532865	D2	179.98324462
B9	1.35469984	D3	-179.98484689
B10	1.22603326	D4	179.96833197
B11	1.01198988	D5	-0.01977159
A1	84.90945229	D6	-179.94058811
A2	119.47727200	D7	-0.00312938
A3	118.63439929	D8	179.89626523
A4	120.05400355	D9	179.99052528

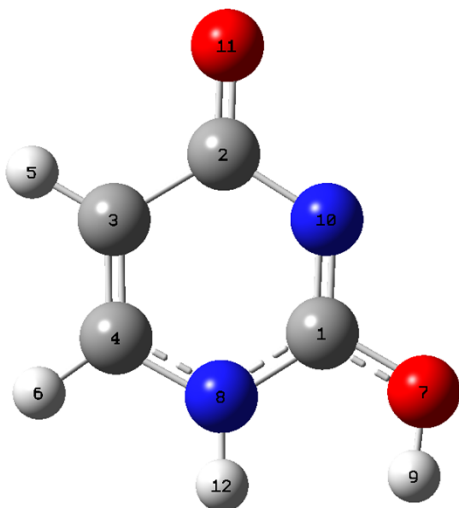
Isomer VI (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	4	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	7	A8	8	D7 0
O	2	B10	1	A9	10	D8 0
H	8	B11	1	A10	10	D9 0

B1	2.32090709	A5	153.29053928
B2	1.45687088	A6	113.39011933
B3	1.34479151	A7	108.19584802
B4	1.07812037	A8	121.76205510
B5	1.07858926	A9	149.28630195
B6	1.33288645	A10	119.72230394
B7	1.35320959	D1	0.00105182
B8	0.96770493	D2	-179.99942964
B9	1.29189592	D3	179.99929998
B10	1.23174738	D4	-179.99752392
B11	1.00878633	D5	-0.00077132
A1	87.97494058	D6	-179.99922172
A2	119.88045445	D7	179.99814874
A3	119.24591684	D8	0.00400770
A4	124.30524482	D9	-179.99930388

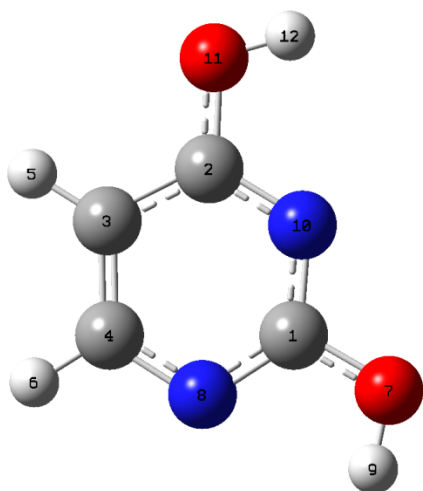
Isomer VII (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	2	D5 0
H	7	B8	1	A7	8	D6 0
N	1	B9	7	A8	8	D7 0
O	2	B10	1	A9	10	D8 0
H	8	B11	1	A10	10	D9 0

B1	2.32340506	A5	148.84149169
B2	1.45582768	A6	118.29281187
B3	1.34346312	A7	113.11149576
B4	1.07814965	A8	117.54988529
B5	1.07859044	A9	148.98579373
B6	1.33605037	A10	121.38898354
B7	1.35890584	D1	0.00750566
B8	0.96530109	D2	-179.99555471
B9	1.29074958	D3	179.99602140
B10	1.23212278	D4	179.99970351
B11	1.00872614	D5	-179.99398527
A1	88.36381723	D6	0.01696231
A2	119.65489913	D7	180.00000000
A3	119.45031068	D8	0.02004192
A4	124.37015319	D9	-179.96919836

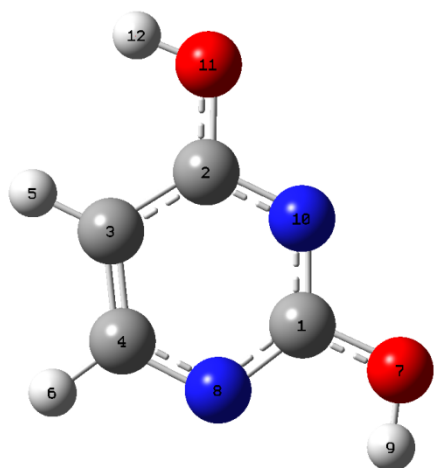
Isomer VIII (Aqueous phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	2	A5	3
N	1	B7	7	A6	2
H	7	B8	1	A7	8
N	2	B9	1	A8	8
O	2	B10	1	A9	8
H	11	B11	2	A10	1
					D9

B1	2.25188408	A5	146.82051181
B2	1.39731671	A6	117.90356916
B3	1.37751848	A7	107.89815467
B4	1.07777443	A8	32.07036578
B5	1.08258637	A9	150.09269173
B6	1.34130647	A10	108.54025051
B7	1.32617262	D1	-0.01186276
B8	0.96678152	D2	179.99252761
B9	1.32555179	D3	-179.99554189
B10	1.33751668	D4	179.93527292
B11	0.96803361	D5	179.91070455
A1	90.64527546	D6	-0.02282109
A2	115.54679945	D7	-179.98300823
A3	121.79729655	D8	179.99490195
A4	120.56457115	D9	0.01807429

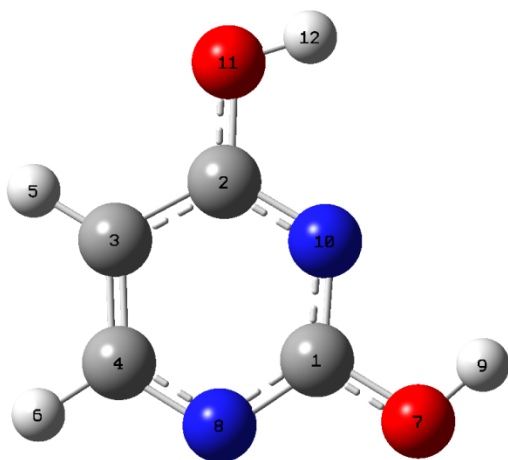
Isomer IX (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	2	A5	3	D4 0
N	1	B7	7	A6	2	D5 0
H	7	B8	1	A7	8	D6 0
N	2	B9	1	A8	8	D7 0
O	2	B10	1	A9	8	D8 0
H	11	B11	2	A10	1	D9 0

B1	2.25015345	A5	146.81745760
B2	1.39910989	A6	117.63626503
B3	1.37852331	A7	107.87791249
B4	1.07896002	A8	32.03310144
B5	1.08266452	A9	146.56765140
B6	1.34194510	A10	110.71394201
B7	1.32789691	D1	-0.01362902
B8	0.96670635	D2	179.99109756
B9	1.32506267	D3	-179.99502297
B10	1.34147889	D4	179.92917785
B11	0.96495711	D5	179.90188065
A1	90.36332535	D6	-0.02487469
A2	115.82008318	D7	-179.98163592
A3	122.37918424	D8	179.99404826
A4	120.51670288	D9	-179.97663668

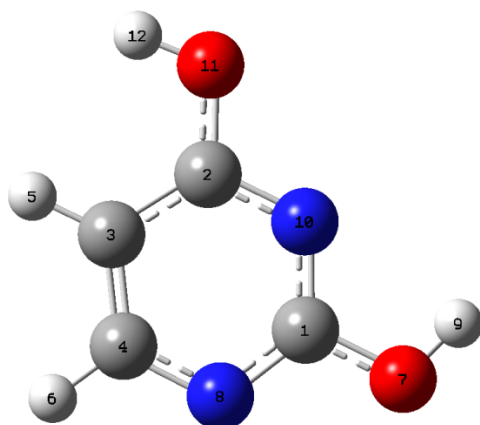
Isomer X (Aqueous phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	4	A5	3
N	1	B7	7	A6	4
H	7	B8	1	A7	8
N	2	B9	1	A8	8
O	2	B10	1	A9	8
H	11	B11	2	A10	1
				D1	0
				D2	0
				D3	0
				D4	0
				D5	0
				D6	0
				D7	0
				D8	0
				D9	0

B1	2.25848387	A5	148.36684905
B2	1.39631022	A6	115.68641394
B3	1.37837053	A7	108.38338025
B4	1.07779760	A8	31.93716373
B5	1.08276034	A9	150.12277233
B6	1.34159598	A10	108.67960996
B7	1.32391507	D1	-0.01193983
B8	0.96641597	D2	179.99241976
B9	1.32594054	D3	-179.99600605
B10	1.33729987	D4	-179.93087816
B11	0.96796477	D5	0.03849351
A1	90.41297907	D6	179.96933805
A2	115.55288442	D7	-179.98210701
A3	121.77484705	D8	179.99577119
A4	120.33804920	D9	0.01744315

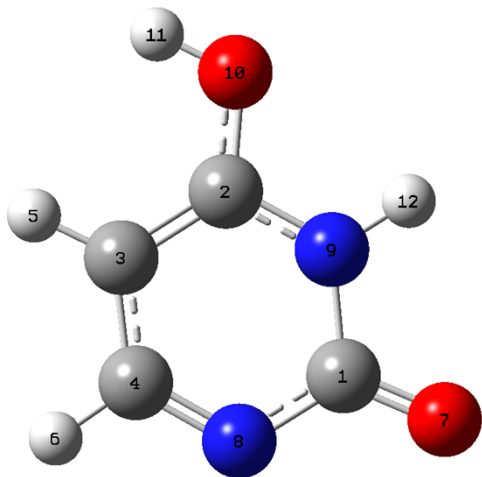
Isomer XI (Aqueous phase)



C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1
H	3	B4	2	A3	1
H	4	B5	3	A4	2
O	1	B6	4	A5	3
N	1	B7	7	A6	4
H	7	B8	1	A7	8
N	2	B9	1	A8	8
O	2	B10	1	A9	8
H	11	B11	2	A10	1
					D1 0
					D2 0
					D3 0
					D4 0
					D5 0
					D6 0
					D7 0
					D8 0
					D9 0

B1	2.25686447	A5	148.19724469
B2	1.39807749	A6	115.47954818
B3	1.37936831	A7	108.23570017
B4	1.07903989	A8	31.89644994
B5	1.08281349	A9	146.54008905
B6	1.34204289	A10	110.70937991
B7	1.32555306	D1	-0.01566682
B8	0.96646943	D2	179.98982715
B9	1.32547501	D3	-179.99496289
B10	1.34098339	D4	-179.91562623
B11	0.96504559	D5	0.04696110
A1	90.12967659	D6	179.96245420
A2	115.82208651	D7	-179.97837977
A3	122.36094568	D8	179.99351141
A4	120.28665084	D9	-179.97381580

Isomer XII (Aqueous phase)



C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
H	3	B4	2	A3	1	D2 0
H	4	B5	3	A4	2	D3 0
O	1	B6	4	A5	3	D4 0
N	4	B7	3	A6	2	D5 0
N	2	B8	1	A7	7	D6 0
O	2	B9	1	A8	7	D7 0
H	10	B10	2	A9	1	D8 0
H	9	B11	2	A10	1	D9 0

B1	2.43191532	A5	154.75074645
B2	1.37536571	A6	125.93326509
B3	1.39898614	A7	28.71710270
B4	1.07733213	A8	142.78509449
B5	1.08494849	A9	111.03775349
B6	1.22562032	A10	119.01641633
B7	1.31915374	D1	-0.00035979
B8	1.34597252	D2	180.00000000
B9	1.32766049	D3	179.99938142
B10	0.96593561	D4	-179.99928633
B11	1.01165933	D5	0.00060954
A1	90.16342740	D6	-0.00038891
A2	115.80147768	D7	-0.00067838
A3	121.87813696	D8	-179.99965771
A4	118.19663025	D9	-180.00000000