Electronic Supplementary Information for…

Diverse Mixtures of 2,4-Dihydroxy Tautomers and O4 Protonated Conformers of Uridine and 2'-Deoxyuridine Coexist in the Gas Phase

R. R. Wu,[†] Bo Yang,[†] C. E. Frieler,[†] G. Berden,[‡] J. Oomens,[‡§] and M. T. Rodgers[†,*]

[†]*Department of Chemistry, Wayne State University, Detroit, Michigan 48202*

[‡]*Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Toernooiveld 7, 6525 ED, Nijmegen, The Netherlands,*

[§]*van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands*

Theoretical Results.

The following discussion focuses primarily on the stable low-energy ring-closed conformations of $[Urd+H]^+$ and $[dUrd+H]^+$ even though calculations suggest that a number of the stable ring-open conformers are more stable than the most stable ring-closed conformers. However, comparison of the measured IRMPD and computed IR spectra for the ring-open forms clearly show that these conformers are not populated in the experiments. Thus, the stable ring-open conformers are only discussed very briefly.

$[Urd+H]^+$. The stable low-energy ring-closed conformers of $[Urd+H]^+$ protonated at either O2 or O4 as well as the 2,4-dihydroxy tautomers and their relative free energies at 298 K are shown in Figure S1. The 2,4-dihydroxy tautomers are the most favorable structures of $[Urd+H]^+$ for both B3LYP and MP2. O4 protonation is found to be the next most favorable based on B3LYP results, whereas MP2 suggests that a couple of O2 protonated conformers are more stable than all of the O4 protonated structures.

The first excited **TA** conformer, which lies only 0.2 kJ/mol (B3LYP) and 0.3 kJ/mol (MP2) above the ground **Ti** conformer, has both hydroxyl substituents pointed towards N3. The sugar remains in the C2'-endo configuration similar to that of **Ti**, but without interaction between the sugar and the anti-oriented 2,4-dihydroxy uracil moiety. The **TB** conformer, which also involves the anti-oriented minor 2,4-dihydroxy uracil moiety with both hydroxyl substituents pointed towards N3, adopts the C3'-endo sugar configuration, and lies 2.5 kJ/mol (B3LYP) and 3.2 kJ/mol (MP2) above the ground-state conformer. The **TC** conformer adopts similar C2'-endo puckering as the ground-state conformer, however the protonated 2,4-dihydroxy uracil residue rotates into the syn orientation and is stabilized by an O2H···O5' hydrogen bond, and lies 2.9 kJ/mol (B3LYP) and 2.2 kJ/mol (MP2) above the ground-state conformer. The primary difference between the **TA** and **Tii** conformers as well as that of the **TB** and **Tiii** conformers is the orientation of the hydroxyl substituents of the sugar moiety. The relative stabilities of these four conformers suggest that when the nucleobase is anti-oriented and has the minor 2,4-dihydroxy tautomeric form with both hydroxyl substituents pointed towards N3, C2'-endo sugar puckering is preferred over C3'-endo sugar puckering, and the C2'-endo sugar prefers the hydroxyl groups to be pointed down and away from the nucleobase, whereas C3'-endo puckering prefers the hydroxyl groups to be pointed up and away from the nucleobase. The **TD** conformer, which has a C2'-endo sugar configuration and the 2,4-dihydroxy uracil moiety with

both hydroxyl substituents pointed towards N3, forms the O5'-H···O2 hydrogen bond to maintain the syn orientation of the nucleobase, and lies > 25 kJ/mol above the ground-state **Ti** conformer.

The most stable O4 protonated conformer, **O4A**, lies 2.9 kJ/mol (B3LYP) and 10.1 kJ/mol (MP2) higher in energy than the ground-state **Ti** conformer, prefers C2'-endo sugar puckering with the 2'- and 3'-hydroxyls pointed down and away from the anti-oriented nucleobase with the 4-hydroxyl hydrogen atom pointed away from N3. The C3'-endo sugar configuration of the **O4i** conformer does not cause a significant difference in free energy vs **O4A**. The **O4B** conformer shares the same nucleobase orientation and sugar configuration with **O4i**, however, the change in the orientation of the 2'- and 3'-hydroxyls leads **O4B** to lie 1.4 kJ/mol (B3LYP) and 1.3 kJ/mol (MP2) higher in free energy than **O4i**. The **O4ii** conformer is one of only two stable conformers found that exhibits C3'-exo sugar puckering that is stabilized by the sugar hydroxyls pointing up and toward the nucleobase to form coupled O3'H···O2'H···O2 hydrogen bonds and lies 3.5 kJ/mol (B3LYP) and 0.9 kJ/mol (MP2) above **O4A**. The primary difference between the **O4A** and **O4iii** conformers is the orientation of the sugar hydroxyls. Both hydroxyls point up and toward the nucleobase in **O4iii**, which destabilizes this conformer by 6.7 kJ/mol (B3LYP) and 5.4 kJ/mol (MP2) relative to **O4A**. **O4C**, **O4iv**, **O4D**, **O4v** and **O4vi** are the 4-hydroxyl rotamers of **O4A**, **O4i**, **O4B**, **O4ii**, and **O4iii**, respectively. Rotation of O4–H^+ toward N3 destabilizes these conformers by > 10 kJ/mol relative to their corresponding rotamers. The **O4E** conformer exhibits a similar nucleobase orientation and sugar puckering to **O4B**, but the 5'-hydroxymethyl in **O4E** rotates away from the nucleobase and forms an O2'H···O3'H···O5'H dual hydrogen-bonding interaction, which destabilizes **O4E** by > 15 kJ/mol vs **O4B**. The **O4F** conformer adopts C2'-endo sugar puckering, O4–H^+ is pointed away from N3, and O2 is interacting with O5'H, where the rotation of the nucleobase into the syn orientation and forcing O5'–H to rotate towards O2, destabilizes this conformer by > 15 kJ/mol vs **O4A**.

The most stable O2 protonated conformer, **O2i**, lies 8.0 kJ/mol (B3LYP) and 8.6 kJ/mol (MP2) above the ground-state **Ti** conformer. The coupled O2H···O2'H···O3'H hydrogen bonds facilitate C2'-endo sugar puckering and the anti nucleobase orientation. The second most stable O2 protonated conformer, **O2B**, which lies only 1.0 kJ/mol (B3LYP) and 0.2 kJ/mol (MP2) above **O2i**, also adopts C2'-endo sugar puckering, but the nucleobase rotates into the syn orientation with the excess proton hydrogen bonded to O5'. The **O2B**, **O2ii**, **O2C** and **O2iii** conformers all have the O2 protonated nucleobase in the anti orientation with the excess proton pointed toward N3. These conformers lie much higher in energy due to the lack of hydrogen-bonding interaction between the nucleobase and the sugar hydroxyls as well as the repulsion between the parallel O2–H^+ and N3–H hydrogen atoms.

[dUrd+H]$^+$. The low-energy ring-closed conformers of [dUrd+H]$^+$ protonated at either O2 or O4 as well as the 2,4-dihydroxy tautomers and their relative free energies at 298 K are shown in Figure S2. The 2,4-dihydroxy tautomers are much preferred by MP2, whereas B3LYP favors O4 protonation with the 2,4-dihydroxy tautomers being only slightly less stable.

As compared to the B3LYP ground-state **O4B** conformer, switching from C3'-endo to C2'-endo sugar puckering together with minor changes in the nucleobase orientation about the glycosidic bond only accounts for 0.4 kJ/mol (B3LYP) change in free energy from the **O4A** conformer. However, according to MP2, **O4A** is 1.2 kJ/mol

more stable than **O4B**. The **O4C** and **O4D** conformers are the 4-hydroxyl rotamers of **O4B** and **O4A**, respectively, and lie > 10 kJ/mol above **O4B** and **O4A**, respectively. The energy difference is caused by the repulsion between the parallel N3–H and O4–H^+. The **O4E** conformer adopts a similar sugar configuration and nucleobase orientation as the B3LYP groud-state **O4B** conformer. However, the 5'-hydroxymethyl substituent of **O4E** staggers away from the base, forming a hydrogen-bonding interaction with the 3'-hydroxyl hydrogen atom and lies 17.3 kJ/mol (B3LYP) and 18.7 kJ/mol (MP2) above **O4B**. The **O4F** conformer, which has C2'-endo sugar puckering and the nucleobase in the syn orientation, facilitating formation of an O5'H···O2 hydrogen-bonding interaction, lies > 30 kJ/mol above **O4B**.

The most stable minor 2,4-dihydroxyl tautomer, **TA**, predicted as the MP2 ground-state conformer, lies 0.7 kJ/mol above the B3LYP ground-state conformer, **O4B**, when computed using B3LYP level of theory. Switching from C2'-endo to C3'-endo sugar puckering accompanied with minor changes in the nucleobase orientation leads **TB** to lie 1.0 kJ/mol (B3LYP) and 3.3 kJ/mol (MP2) above **TA**. The **TC** conformer which has the syn oriented nucleobase stabilized by an O2H···O5' hydrogen bond with C2'-endo puckering of the sugar lies 3.6 kJ/mol(B3LYP) and 2.0 kJ/mol(MP2) above **TA**. The **TD** conformer adopts similar C2'-endo sugar puckering and nucleobase orientation as **TC**, but the O5'H···O2 hydrogen-bonding interaction that stabilizes this conformer is ~30 kJ/mol less favorable than the O2H···O5' hydrogen bond.

The most stable O2 protonated conformer, **O2A**, exhibits C2'-endo sugar puckering with the syn oriented nucleobase and is stabilized by an O2H···O5' hydrogen bond. In contrast, the **O2B**, **O2a, O2C** and **O2b** conformers all have the nucleobase in the anti orientation. The noncanonical C6H···O5' hydrogen-bonding interaction is much less favorable for O2 protonation, destabilizing these conformers by > 35 kJ/mol relative to **O2A**. The **O2B** and **O2a** and the **O2C** and **O2b** conformers are the 2-hydroxyl rotamers of each other. Based on their calculated relative energetics, it can be seen that rotation of the O2–H^+ does not result in a very significant change in free energy, whereas rotation of the O4–H^+ produces much larger (> 10 kJ/mol) differences between the 4-hydroxyl rotamers.

Ring-Open Conformations. The low-energy ring-open conformers of $[Urd+H]^+$ and $[dUrd+H]^+$ protonated at O4 as well as the 2,4-dihydroxy tautomers and their relative free energies at 298 K are shown in Figure S3. O4 protonation is slightly preferred for both B3LTP, whereas MP2 suggests that the 2,4-dihydroxy tautomers are more stable. Ring opening to produce the C4′ carbonyl is favored over C1′ for $[Urd+H]^+$, whereas ring opening to produce the C1′ carbonyl is favored over C4′ for $[dUrd+H]^+$. The structures of these systems enable hydrogen-bonding interactions between the carbonyl and hydroxyl moieties of the nucleobase and ring-open sugar via 6-memebered ring formation help stabilize these structures.

Discussion

Comparison of Experimental IRMPD and Theoretical IR Spectra of $[Urd+H]^+$. The experimental IRMPD and theoretical IR spectra of the **TB**, **O4i**, **Tii**, and **O4iii** ring-closed conformers of $[Urd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S4 and were previously discussed in the main text. The experimental IRMPD and theoretical IR spectra of the **O2i**, **Tiii**, **O2A**, **O4C**, **O4iv**, **O4D** and **O4v** ring-

closed conformers of $[Urd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S5 with the mismatches between the measured and calculated IR bands highlighted. The calculated band at ~1530 cm^{-1} of **O2i** is shifted to a higher frequency relative to the measured band at ~1505 cm^{-1}. The small band predicted at ~965 cm^{-1} for **O2i** is not observed in the measured spectrum. The IR band predicted at ~1060 cm^{-1} of **Tiii** is shifted relative to the measured band at ~1115 cm^{-1} and would tend to broaden this band if **Tiii** was populated. The calculated band at ~1610 cm^{-1} for **O2A** is shifted relative to the measured bands at ~1595 cm^{-1}. In addition, the calculated IR band at ~1155 cm^{-1} of **O2A** would broaden the two consecutive IR bands measured at ~1210 cm^{-1} and ~1115 cm^{-1}, and the calculated IR feature at ~3645 cm^{-1} for **O2A** would also broaden the measured band at ~3665 cm^{-1} if **O2A** was present in the experiments. The calculated bands at ~1620 and ~3600 cm^{-1} of the **O4C**, **O4iv** and **O4D** ring-closed conformers are shifted relative to the measured bands at ~1595 and ~3615 cm^{-1} respectively, and would broaden the measured bands at ~1595, ~1650 and ~ 3615 cm^{-1} if they were present. Likewise, the calculated band at ~1620 cm^{-1} of **O4v** is shifted relative to the measured band at ~1595 cm^{-1} and the calculated band at ~1325 cm^{-1} is not observed in the measured spectrum.

The experimental IRMPD and theoretical IR spectra of the **O4E**, **O4vi**, **O4F**, **O2B**, **O2ii**, **O2C** and **O2iii** ring-closed conformers of $[Urd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S6 with the mismatches between the measured and calculated IR bands highlighted. The calculated IR features at ~1620 cm^{-1} for **O4E** and **O4vi**, and ~1625 cm^{-1} for **O4F** would broaden the measured band at ~1595 cm^{-1} if these conformers were present. The calculated IR feature at ~1050 cm^{-1} for **O4E** is not observed in the measured spectrum. The broad bands calculated at ~3600 cm^{-1} for **O4E** and **O4vi** would tend to broaden the measured bands at ~3615 and ~3565 cm^{-1} if these conformers were present. In addition, above ~3500 cm^{-1}, the calculated bands for **O4F** exhibit large discrepancies with the measured bands. For the O2 protonated conformers, although the calculated IR spectra of these conformers in the hydrogen-stretching region exhibit reasonable agreement with the measured IR spectrum, mismatches observed in the IR fingerprint region allow these O2 protonated conformers to be eliminated. The calculated bands at ~1675 cm^{-1} for these conformers are shifted relative to the measured band at ~1650 cm^{-1}. The calculated band at ~1575 cm^{-1} for **O2iii** is shifted relative to the measured band at ~1595 cm^{-1}. The small bands predicted at ~1330 cm^{-1} for these conformers are not observed in the measured spectrum. Moreover, between ~1000 and ~1100 cm^{-1}, obvious discrepancies are observed between experiment and theory for these four conformers. Therefore, from Figures S5–S6, we conclude that no O2 protonated conformers are populated by ESI, and the 2,4-dihydroxy tautomer, **Tiii**, as well as the higher-energy O4 protonated conformers do not exist in the experiments.

The experimental IRMPD and theoretical IR spectra of the stable low-energy ring-open conformers, **O4A_RO4′**, **TA_RO4′**, **O4A_RO1′**, **TA_RO1′**, and **Ti_RO1′** of $[Urd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S7. In all cases, the IR spectra of the ring-open conformers exhibit obvious differences from the measured IRMPD spectrum that clearly eliminate their presence in the experimental population. Predicted bands that exhibit obvious disagreement with the measured spectrum are highlighted. In particular, the carbonyl stretches associated with the ring-open sugar moieties are significantly shifted to either lower or higher frequencies. In contrast, the C2=O carbonyl stretches are well matched to the measured band,

indicating that the band observed at ~1800 cm^{-1} is indeed contributed by the O4 protonated canonical conformers. Therefore, the ring-open conformations of $[Urd+H]^+$ are not populated by ESI.

Comparison of Experimental IRMPD and Theoretical IR Spectra of $[dUrd+H]^+$. The experimental IRMPD and theoretical IR spectra of the **O2A**, **O4C**, **O4D**, **O4E**, **O4F**, **O2B**, **O2a**, **O2C** and **O2b** ring-closed conformers of $[dUrd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S8 with the mismatches between the measured and calculated IR bands highlighted. For the **O2A** conformer, the calculated bands at ~1665 cm^{-1} and ~1620 cm^{-1} are shifted to higher frequencies relative to the measured bands at ~1640 cm^{-1} and 1590 cm^{-1}. The strong IR bands predicted at ~1620 cm^{-1} for **O4C** and **O4D** are shifted relative to the sharp band measured at ~1590 cm^{-1} and would also broaden this measured band as well as the measured band at ~1640 cm^{-1} if these two conformers were present. The small band predicted at ~3675 cm^{-1} for **O4E** is shifted relative to the measured band at ~3665 cm^{-1}, and the calculated band at ~3610 cm^{-1} is too intense relative to the measured band. The small and broad band predicted at ~1315 cm^{-1} for **O4F** is not observed in the measured IR spectrum in the IR fingerprint region, and the calculated IR feature at ~3645 cm^{-1} for **O4F** is shifted relative to the measured band at ~3665 cm^{-1}. For **O2B**, **O2a**, **O2C** and **O2b** conformers, the calculated bands at ~1670 cm^{-1} for these four conformers are shifted to higher frequencies relative to the measured band at ~1640 cm^{-1}. The calculated bands at ~1540 cm^{-1} for **O2a** and **O2b**, and the calculated bands at ~1330 cm^{-1} for **O2B** and **O2C** are not observed in the measured spectrum. The calculated bands at ~1010 cm^{-1} for **O2C** and **O2b** are too intense compared to those observed in the measured spectrum. Therefore, the presence of these four conformers are eliminated although their calculated IR spectra in the hydrogen-stretching region agree well with the measured spectrum except for the shift of the calculated band at ~3590 cm^{-1} for **O2a** relative to the measured band at ~3575 cm^{-1}. Therefore, similar to $[Urd+H]^+$, no O2 protonated conformers are populated by ESI and the presence of the higher-energy O4 protonated conformers are also eliminated.

The experimental IRMPD and theoretical IR spectra of the stable low-energy ring-open conformers, **O4A_RO1′**, **TA_RO1′**, **Ta_RO1′**, **O4A_RO4′**, and **TA_RO4′** of $[dUrd+H]^+$ in the IR fingerprint and hydrogen-stretching regions are compared in Figure S9. As found for $[Urd+H]^+$, the IR spectra of the ring-open conformers exhibit obvious differences from the measured IRMPD spectrum that clearly eliminate their presence in the experimental population. The carbonyl stretches associated with the ring-open sugar moieties are again significantly shifted relative to the measured spectrum. In contrast, the band positions of the C2=O carbonyl stretches of the O4 protonated species are again well matched with the measured band. Therefore as found for $[Urd+H]^+$, the ring-open conformations of $[dUrd+H]^+$ are not also populated by ESI.

Conformers Populated. Approximate populations of the stable low-energy ring-closed conformers of $[Urd+H]^+$ and $[dUrd+H]^+$ populated in the experiments are estimated by comparing the measured IRMPD spectra to Maxwell-Boltzmann statistically weighted IR spectra for the conformations determined to contribute to the experiments along with least squares fitting of the spectra. Resulta are shown in Figures S10-S11 and discussed in the main text.

Table S1. Relative Enthalpies and Free Energies of Sugar Ring Open Conformers to the Ground-State Conformers Found For $[Urd+H]^+$ and $[dUrd+H]^+$ at 0 and 298 K in kJ/mol[a]

Species	Conformer	B3LYP			MP2(full)		
		ΔH_0	ΔH_{298}	ΔG_{298}	ΔH_0	ΔH_{298}	ΔG_{298}
$[Urd+H]^+$	**Ti**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
	O4A_RO4'	-18.7	-30.5	-26.2	-3.9	0.4	-12.1
	TA_RO4'	-14.1	-11.4	-22.0	-7.2	-2.9	-15.9
	O4A_RO1'	-10.1	-8.9	-15.5	4.5	7.2	-1.6
	TA_RO1'	-8.1	-4.6	-15.4	19.3	24.4	11.3
	Ti_RO1'	-8.3	-5.4	-14.5	11.5	16.0	4.6
$[dUrd+H]^+$	**O4B**	**0.0**	**0.3**	**0.0**	**9.3**	**11.1**	**8.6**
	TA	**0.9**	**0.7**	**0.7**	**0.9**	**2.3**	**0.0**
	O4A_RO1'	-5.2	0.1	-13.9	20.3	25.6	11.6
	TA_RO1'	-5.0	-0.3	-12.8	13.4	18.1	5.6
	Ta_RO1'	1.6	6.2	-7.7	17.2	21.8	7.9
	O4A_RO4'	5.3	10.0	-4.5	13.5	18.2	3.7
	TA_RO4'	11.9	15.5	0.9	26.8	30.4	15.8

[a]Single point energies of the B3LYP/6-311+G(d,p) optimized structures determined at the B3LYP/6-311+G(2d,2p) and MP2(full)/6-311+G(2d,2p) levels of theory including ZPE and thermal corrections.

Table S2. Calculated Cartesian Coordinates of the Stable Low-Energy Ring-Closed Conformers of $[Urd+H]^+$.

Ti	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.6911694145	-0.704658662	0.0975155152
C	-1.5629775667	-0.5628604396	-1.0221107936
H	-0.7793727527	0.057706569	0.678866614
H	-1.2751053002	0.2904437554	-1.6464205623
H	-2.604210647	-0.4217315688	-0.70621127
C	-1.4773241261	-1.8319529451	-1.8505050275
H	-2.1582973726	-1.7558888856	-2.7006960742
O	-0.1281542638	-1.9674499755	-2.4002363035
C	-1.7388382827	-3.1373569034	-1.0726437329
C	0.4886964322	-3.1154286163	-1.9243641895
H	-2.363643573	-2.9775462324	-0.1919669663
C	-0.3232215083	-3.5919948882	-0.6990343711
O	-2.2543986197	-4.1754447434	-1.9007965872
H	0.5235576862	-3.8958635745	-2.694158317
N	1.9285559366	-2.8121739241	-1.5955176018
H	0.010443981	-3.0751066507	0.1999393942
O	-0.1899992824	-4.9884963573	-0.4956852926
H	-3.216978621	-4.1575712735	-1.9251659979
C	2.4198847909	-1.5403040861	-1.7241122824
C	2.7927631201	-3.831800063	-1.2696647324
H	-0.8902003833	-5.4303795716	-1.0069753507
H	1.6850096689	-0.7897408098	-1.9703479694
C	3.7456240371	-1.2857008265	-1.5635066505
N	4.0890087653	-3.6290092135	-1.1420911594

O	2.35798603	-5.0488100863	-1.0960181884
H	4.1542080868	-0.2909190141	-1.6623870884
C	4.5695817543	-2.4021363532	-1.2910999447
O	5.8677121569	-2.2127528076	-1.1747128836
H	6.3073424779	-3.0591025536	-0.9898388903
H	1.3820133898	-5.1574830985	-0.9053222958

TA	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.7858321452	-1.411024091	-0.0039287596
C	-1.7155786974	-1.6742483921	-1.0622029605
H	-1.4071891677	-1.1680436485	-1.9831488396
H	-2.7217995494	-1.3303977639	-0.7962792651
C	-1.7594000809	-3.1712785665	-1.3103580945
H	-2.4684623722	-3.3729273671	-2.117131755
O	-0.4471001194	-3.6178165713	-1.7674001916
C	0.0545282172	-4.6121091544	-0.9246598992
H	-0.036722364	-5.6078174555	-1.3574574013
N	1.5256985251	-4.3594381644	-0.758347055
C	1.9609862671	-3.0865536173	-0.4963379622
H	1.1818436014	-2.3345512842	-0.432367505
C	3.2867856419	-2.8225402496	-0.3365161268
C	4.1708118005	-3.9175401851	-0.4576508437
O	5.4610216244	-3.708379912	-0.3132089884
N	3.7425702686	-5.152272051	-0.7146861469
C	2.4486760961	-5.3492097442	-0.8571520674
O	1.9865442851	-6.5548424988	-1.114625324
C	-2.0992127703	-4.0474092918	-0.0873378903
H	-2.64670891	-3.4972861701	0.6807031166
C	-0.7179511601	-4.5036881889	0.4143332833
H	-0.2804814958	-3.705177534	1.016560662
O	-0.7073037474	-5.6744850659	1.1714255863
H	-1.4289715545	-6.2376555859	0.8537910748
O	-2.7811526431	-5.2418010581	-0.4594539631
H	-3.7351421694	-5.1170247501	-0.4338135045
H	-0.8753549276	-0.4958005287	0.2817585182
H	5.9524315021	-4.5388905572	-0.4199245717
H	2.7285409827	-7.1773647424	-1.1719889368
H	3.6522391724	-1.8273856099	-0.1298422589

TB	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.5518025278	-1.2074809605	-0.011921974
C	-1.6115207818	-1.8428968975	-0.7364819854
H	-0.7493906779	-0.2703118355	0.08606488
H	-1.6712795221	-1.4542956495	-1.7581745524
H	-2.5777373819	-1.6866443885	-0.2438036357
C	-1.3416668259	-3.330699862	-0.781630273
H	-2.162517809	-3.825087008	-1.3093480724
O	-0.1102747839	-3.5691917465	-1.5161370691
C	-1.1311921241	-4.0220845968	0.5730222626
C	0.6042531761	-4.6295148365	-0.9795592738
H	-0.6464734757	-3.339783711	1.2757434846

C	-0.1917865433	-5.1990961408	0.2105004213
O	-2.3742179667	-4.4840081612	1.0726482061
H	0.7998648724	-5.3992982856	-1.7248115396
N	1.9829117958	-4.1062188419	-0.5618778344
H	0.4588012155	-5.4933821901	1.0426665095
O	-0.9192850148	-6.295935335	-0.2813618336
H	-2.4222030924	-4.3641621008	2.0265998295
C	2.2079772758	-2.7726173717	-0.3609555283
C	3.0292586993	-4.9610892623	-0.4354703818
H	-1.7685862136	-6.3237159162	0.1844480883
H	1.3441045881	-2.1260687845	-0.4723010887
C	3.4539924611	-2.321394513	-0.0359602446
N	4.2520742075	-4.5856563744	-0.1345863484
O	2.7434449658	-6.2327111488	-0.6351676827
H	3.6544212555	-1.2727475705	0.1279771958
C	4.478480524	-3.2854795718	0.0628701135
O	5.6977835014	-2.8909327862	0.3594902218
H	6.3019193343	-3.6501824734	0.3898851004
H	3.5479181684	-6.7676065797	-0.5442909955

TC	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.9234217238	-1.6957685781	-0.4174769663
C	-1.0031322311	-2.1042520291	0.6079254831
H	-1.7796735266	-0.7742863559	-0.6629107317
H	-1.1626546169	-1.5217800349	1.5198843604
H	0.0308464781	-1.9733056963	0.2744972943
C	-1.2830964741	-3.569151687	0.8782911948
H	-0.6607578095	-3.9168289909	1.7062971582
O	-2.6815274131	-3.6681416567	1.2849560094
C	-1.1131013296	-4.5227339474	-0.3310619724
C	-3.3138870426	-4.6746229919	0.5441427252
H	-0.5023234171	-4.0836754418	-1.1218962404
C	-2.5616468992	-4.7786343908	-0.8026310224
O	-0.6090673916	-5.7931401387	0.0685549789
H	-3.2657576575	-5.6409219351	1.0550956552
N	-4.7641717609	-4.3650546409	0.4386761778
H	-2.8728741121	-3.9756413137	-1.4735812573
O	-2.7742132148	-5.9941783441	-1.4533642514
H	0.3475936773	-5.8339203156	-0.0305756267
C	-5.6490936012	-5.3730513231	0.7432288395
C	-5.2731828972	-3.1538354598	0.0199154505
H	-2.1016515241	-6.6179549533	-1.1394775309
H	-5.2039586345	-6.3006483258	1.0738231736
C	-6.9897316947	-5.2082870552	0.6295118372
N	-6.5752564742	-2.9556166986	-0.0948511475
O	-4.5203574212	-2.1468901801	-0.3011212051
H	-7.6889028943	-5.996914333	0.8651603841
C	-7.4190235686	-3.9342428807	0.1873522567
H	-3.5366929293	-2.1810418793	-0.1574298604
O	-8.7106976921	-3.7174416234	0.0591044927
H	-8.8625170035	-2.8077961988	-0.2466496592

O4A	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.7908176058	-0.5817538796	-0.0276615517
C	-1.6811012661	-0.8554031052	-1.1194523421
H	-0.9957674446	0.2838673227	0.3407043667
H	-1.4172711552	-0.2471175262	-1.9910724914
H	-2.7185466038	-0.6361294309	-0.8428131726
C	-1.5696603069	-2.3243958362	-1.4881806984
H	-2.234299529	-2.5236483618	-2.3328146805
O	-0.2090387926	-2.5994598898	-1.9310468197
C	-1.8547965528	-3.3300100787	-0.3541418084
C	0.3707463023	-3.6065599461	-1.1485190901
H	-2.4835391253	-2.9066531277	0.4321780285
C	-0.4493682136	-3.6784668809	0.1648735527
O	-2.3912349885	-4.5525120234	-0.8494785683
H	0.4001660274	-4.5704118247	-1.6576400046
N	1.7989260591	-3.2310084765	-0.9184646082
H	-0.117294241	-2.8837462456	0.836057317
O	-0.3383874776	-4.8876673517	0.8473321583
H	-3.3533169742	-4.531770106	-0.852741819
C	2.1074147871	-1.9743717532	-0.5522923268
C	2.7820332265	-4.2214632593	-1.1289341787
H	-0.9482375614	-5.5189634728	0.4376178968
H	1.2598619528	-1.301716168	-0.4423445295
C	3.4022303722	-1.5569392707	-0.3334446373
N	4.0893136612	-3.748463107	-0.8885916915
O	2.5674128673	-5.3450101564	-1.4768431969
H	3.6183052419	-0.5408211962	-0.0383940883
C	4.414532079	-2.4989533086	-0.513117531
H	4.8275746222	-4.4341652579	-1.0261038986
O	5.706210568	-2.3063300291	-0.3562385119
H	5.9200486813	-1.4017267526	-0.0864536039

O4i	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.2286874664	-1.2315002694	-0.0080080373
C	-1.376202448	-1.8244543563	-0.6327912046
H	-0.4374695766	-0.3256190481	0.2412555505
H	-1.5263021192	-1.4045426375	-1.6326891318
H	-2.2800713225	-1.6560323254	-0.0376891802
C	-1.1596558693	-3.318047818	-0.732134386
H	-2.0160764301	-3.76743641	-1.2437367125
O	0.0338296216	-3.5760068614	-1.5328768977
C	-0.9009041526	-4.0535320342	0.597413547
C	0.7466288147	-4.6556048465	-1.0380632226
H	-0.3103169561	-3.4101157214	1.2537220251
C	-0.0489583948	-5.2571683986	0.1439226829
O	-2.0597620031	-4.3960471841	1.3011469664
H	0.9451069569	-5.3936708487	-1.815832957
N	2.1262969027	-4.1658198661	-0.6020162837
H	0.5934630001	-5.649257456	0.9342889042
O	-0.9497185043	-6.2378399646	-0.3324158015
H	-2.4361019183	-5.1904108759	0.8963252011
C	2.4061612417	-2.8594332503	-0.4671380874

C	3.09329659	-5.1686985309	-0.4194703191
H	-0.5442812166	-7.1114876355	-0.3153278361
H	1.5717800638	-2.1797267126	-0.6237912389
C	3.6672310549	-2.4060766427	-0.1325744465
N	4.3648345148	-4.6641558768	-0.102662291
O	2.8684776796	-6.3439942644	-0.5209965915
H	3.8643630369	-1.3496195386	-0.0246148865
C	4.6670426586	-3.3577206539	0.0437162506
H	5.0943727339	-5.3609460334	0.0260489266
O	5.9272469482	-3.1362198025	0.3488469912
H	6.1290624594	-2.1945997362	0.4476704661

O4B	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.0148987893	-0.6099514544	-0.0057814351
C	-1.0881560411	-1.2093230635	-0.7003378367
H	-0.1719668546	0.3234798268	0.1374991651
H	-1.1728462084	-0.802092062	-1.712884106
H	-2.0304940361	-1.0338361052	-0.1699778208
C	-0.8615554399	-2.702828772	-0.7763519138
H	-1.706059556	-3.1634255879	-1.2971753429
O	0.3486065042	-2.9626741437	-1.5369275939
C	-0.6482338482	-3.4263346894	0.5606125367
C	1.0504445083	-4.0453408978	-1.0200242109
H	-0.1239149049	-2.7757273203	1.265723862
C	0.2392928426	-4.6268071576	0.1518886146
O	-1.8988297166	-3.8463476095	1.0784259396
H	1.2409027791	-4.8056609195	-1.7770481982
N	2.4285920562	-3.552449351	-0.5896868336
H	0.8806059048	-4.9833962041	0.9660117782
O	-0.5383895036	-5.6677659453	-0.3828319017
H	-1.9072258687	-3.7785216111	2.0386174203
C	2.6968049799	-2.246128192	-0.4377937464
C	3.4162433149	-4.5470929535	-0.44783235
H	-1.3718405801	-5.7028525178	0.1090247712
H	1.8543226967	-1.5730467716	-0.5746576609
C	3.9562966646	-1.7793443206	-0.116053974
N	4.6861676871	-4.0255097717	-0.1360893604
O	3.2152958159	-5.7204971481	-0.5770635721
H	4.1405810185	-0.7219483681	0.0037515591
C	4.9726062357	-2.7195499663	0.0274397605
H	5.4276253644	-4.7144963474	-0.0373589288
O	6.2347653012	-2.4829183292	0.3150891351
H	6.4235043948	-1.5396882463	0.422145244

Tii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.157354116	-0.4924516001	-0.1952850205
C	0.7633640539	-0.4533239466	-1.2971370781
H	-0.0536453443	-1.3256262552	0.2762288828
H	0.4494560057	-1.1475224643	-2.0834963528
H	1.773689088	-0.7252291373	-0.9729356855
C	0.7965658286	0.9532467978	-1.8606513842

H	1.4981865998	0.986563394	-2.6963792434
O	-0.5263840633	1.2932246975	-2.3874499108
C	1.1432338127	2.0756237839	-0.8732687499
C	-1.0310839451	2.4246665902	-1.7486932588
H	1.7293864735	1.7103111757	-0.0227317941
C	-0.2449843551	2.5860288743	-0.4362183802
O	1.8365010235	3.0721821411	-1.5965342675
H	-0.9488801296	3.3237986591	-2.3583594534
N	-2.5018516072	2.1928177581	-1.5343242537
H	-0.6501024682	1.9218408416	0.3316981458
O	-0.2687548224	3.940152712	-0.0325880537
H	1.7845608839	3.9050520437	-1.1093325559
C	-2.9213255728	0.9883461093	-1.0318350527
C	-3.4401417387	3.1137313742	-1.8709311678
H	-0.176252913	4.0030542545	0.9240552254
H	-2.1298682812	0.2845406777	-0.7953886369
C	-4.2463306839	0.7277772904	-0.8615676178
N	-4.7346697384	2.9153294076	-1.7315253403
O	-2.9930439134	4.2507318086	-2.359718593
H	-4.5995457146	-0.2139097347	-0.4676410679
C	-5.1472266863	1.749086963	-1.2382767297
O	-6.4372704948	1.5377020725	-1.0976819208
H	-3.7440468324	4.82254312	-2.5844289716
H	-6.9420034491	2.3113974915	-1.3966937131

O4ii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-3.0507516754	1.4507322816	0.0214821818
C	-4.1692596488	1.7465473078	-0.8268561916
H	-3.0089534216	2.1013766455	0.7295347003
H	-3.9360561786	2.5898086549	-1.486880985
H	-5.0560218568	2.0070810943	-0.2390659089
C	-4.4911225882	0.5245117832	-1.6656592153
H	-5.2842474128	0.7723301478	-2.3720497266
O	-3.3273833954	0.142380359	-2.4727380543
C	-4.873341179	-0.7464540166	-0.9060589102
C	-2.748111368	-1.0203284444	-1.9998464024
H	-5.3163228331	-0.5249425641	0.0712194141
C	-3.5341952358	-1.4953198398	-0.7436673966
O	-5.7663060657	-1.4662481826	-1.7260090831
H	-2.7188173313	-1.7945403848	-2.7705463336
N	-1.277420022	-0.7183518805	-1.688108313
H	-3.0284761878	-1.143387309	0.1605348104
O	-3.7929804933	-2.8731316748	-0.7083403063
H	-5.7416514169	-2.3963170411	-1.4629023224
C	-0.7637699935	0.5064651697	-1.8626681666
C	-0.4967296914	-1.7968134448	-1.2575937336
H	-2.9621622343	-3.3575228717	-0.6231956369
H	-1.4732836285	1.2491543458	-2.199189863
C	0.5691029904	0.7973737921	-1.6453604799
N	0.853532569	-1.4745837603	-1.0682296186
O	-0.9235965042	-2.9061693747	-1.06128767
H	0.9523531832	1.7952467955	-1.7992374434
C	1.3906930755	-0.2481634775	-1.239829706

H	1.4497946574	-2.2412473648	-0.7662744904
O	2.6814800384	-0.1960745343	-0.992321398
H	3.0534243483	0.6880968886	-1.1226627507

O2i	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.3604513497	-0.0831535159	0.1093595012
C	0.4702555873	-0.2732553752	-1.03296398
H	-0.2903585621	-0.8432108829	0.6962225736
H	0.1585189226	-1.1477322883	-1.6147010741
H	1.5217604725	-0.4059907413	-0.7482014178
C	0.3597309645	0.9639036293	-1.9053033594
H	1.0301004216	0.8667092522	-2.761649656
O	-0.9994069113	1.0663214062	-2.4404605532
C	0.6162247265	2.2972370031	-1.1725221966
C	-1.6115874092	2.2327844834	-2.0098843064
H	1.2534918029	2.1720216078	-0.2953964402
C	-0.8008198965	2.7411609092	-0.7991821304
O	1.1039636485	3.3198670336	-2.0365242086
H	-1.6314628162	2.9871381623	-2.8067791529
N	-3.0545447075	1.9470978067	-1.6755255564
H	-1.1232468839	2.2425660607	0.1137275608
O	-0.9483388899	4.1458734441	-0.6271197149
H	2.0658245031	3.3069952671	-2.086782339
C	-3.5980352258	0.6717857964	-1.8717037393
C	-3.8641039873	2.9673838769	-1.3272310792
H	-0.2601481174	4.5841357827	-1.1590878782
H	-2.8672165791	-0.0729088601	-2.1445759232
C	-4.9104326808	0.4192500312	-1.7369800906
N	-5.1720835481	2.7422364039	-1.1958068837
O	-3.4528220323	4.1796152169	-1.1235632683
H	-5.3058330822	-0.5742890536	-1.8921730601
C	-5.8435775257	1.4759688242	-1.3837516806
O	-7.0318805425	1.4108448399	-1.232410536
H	-2.4556794828	4.3053963505	-0.960631647
H	-5.754100919	3.5254822288	-0.9102947636

Tiii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.5223077136	-0.7966383158	-0.0142808715
C	-1.6310578759	-1.4321186555	-0.6601093109
H	-0.7453247976	0.1201194546	0.1762057131
H	-1.7593360051	-1.0448679869	-1.6762989019
H	-2.5593122156	-1.2729717417	-0.1005528486
C	-1.3756611283	-2.9218111883	-0.712410283
H	-2.2150880884	-3.4065167389	-1.2201847983
O	-0.1671304896	-3.1782706654	-1.4937359281
C	-1.1113780166	-3.6124514481	0.6395194059
C	0.5549021683	-4.2344854596	-0.9707744192
H	-0.5318416837	-2.9417747277	1.2778072769
C	-0.2416361585	-4.8170008853	0.2211555263
O	-2.2651649902	-3.9523448203	1.3513604257
H	0.7660017691	-4.9842446757	-1.7330889293

N	1.9343489247	-3.7097100434	-0.537539738
H	0.3969410082	-5.1827279913	1.0276462833
O	-1.1271540429	-5.818887949	-0.244665226
H	-2.6486170015	-4.7442850503	0.9490506958
C	2.1646656335	-2.372866155	-0.3605470157
C	2.9741266438	-4.5647966075	-0.3818042421
H	-0.7498006547	-6.69664857	-0.1281919327
H	1.3057777775	-1.7223056043	-0.4907487821
C	3.4102417512	-1.9237653894	-0.029518282
N	4.1950664145	-4.194021495	-0.0753144089
O	2.6850538241	-5.8443711782	-0.5585239582
H	3.6141460446	-0.8732337508	0.1177718607
C	4.4281374459	-2.8902755575	0.0997932533
O	5.6459586249	-2.4979877097	0.4026572394
H	6.2457285548	-3.2592896847	0.4572991142
H	3.4935094771	-6.3715582093	-0.4560169185

O2A	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.6100804668	0.0825240288	-0.0177802822
C	-2.5212510435	-0.241110775	-1.0891935379
H	-1.7732910554	0.9726734543	0.3169300241
H	-2.3313520194	0.4037847446	-1.9512050245
H	-3.5549632452	-0.1088422853	-0.7584801127
C	-2.2629553886	-1.6882095351	-1.4588245337
H	-2.8634473432	-1.9535767725	-2.3323127828
O	-0.8551831199	-1.7857833158	-1.8233345381
C	-2.4962679456	-2.7299766656	-0.336282007
C	-0.2563351278	-2.8430136546	-1.1213023689
H	-3.1413648452	-2.3479096349	0.4572629035
C	-1.0725384783	-3.0353449489	0.1781604722
O	-2.987610542	-3.9589878587	-0.8580228673
H	-0.2765688832	-3.7711088947	-1.6992086839
N	1.1847275447	-2.5418484749	-0.9346947548
H	-0.7854975271	-2.2859721216	0.918931099
O	-0.8993654131	-4.2935020346	0.7531020553
C	2.1112212122	-3.5430643764	-1.269489682
C	1.6430738506	-1.3677464532	-0.446717159
H	1.663576685	-4.4480766145	-1.654116764
C	3.4366081267	-3.4037589104	-1.1233614211
N	2.9627647903	-1.203738266	-0.3074922783
O	0.9215448885	-0.3634989246	-0.0769282004
H	4.1164319287	-4.1998694214	-1.3907830336
C	3.9939960513	-2.1664781227	-0.6041223669
H	3.2776707235	-0.3077498748	0.0548538763
O	5.1433767003	-1.8797516742	-0.4156137448
H	-0.080611892	-0.3411758916	-0.2139111087
H	-1.5515572164	-4.8924344198	0.3585351948
H	-3.9478559893	-4.002045026	-0.8036808027

O4iii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	2.8184580328	-1.0296121344	0.6009294955

C	2.6117058645	-0.9776660207	2.0236927911
H	3.7516498457	-1.186359531	0.4231695459
H	3.0037405021	-0.0397927861	2.43033175
H	3.1154270401	-1.8130064219	2.521337374
C	1.1255647316	-1.0621712046	2.3110792057
H	0.9686307525	-1.0061843911	3.3902088685
O	0.4556853248	0.0882319463	1.7088496631
C	0.3932378843	-2.2955052635	1.7660896546
C	-0.5137387163	-0.327986236	0.7919020012
H	1.0700336767	-3.1451765325	1.6194919188
C	-0.1856701764	-1.7878155371	0.4300736728
O	-0.6432405235	-2.6075847848	2.6732321409
H	-1.5302796034	-0.2440147402	1.1777332307
N	-0.4490385718	0.6093270923	-0.375801439
H	0.5920600939	-1.8212784583	-0.338004186
O	-1.3625835542	-2.4529589412	0.0203332095
H	-1.3297391383	-3.1002952424	2.2036549415
C	0.747309698	0.9502671285	-0.8881070514
C	-1.6577602117	1.1757990527	-0.8344944335
H	-1.1459134348	-3.176012762	-0.5777969078
H	1.6047313819	0.4636656893	-0.427666165
C	0.888825238	1.853076289	-1.9190153988
N	-1.4614898626	2.093432937	-1.8896672687
O	-2.7443553227	0.9325790292	-0.4003860486
H	1.8635188497	2.104250943	-2.3104810901
C	-0.2748736361	2.4370530618	-2.4196983897
H	-2.3094131621	2.5278660179	-2.2454933784
O	-0.3568799861	3.323344313	-3.3877730412
H	0.5077175334	3.5636112777	-3.7507003555

O4C	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.4327757173	0.5731335382	-0.0117097368
C	-1.3218595743	0.2667314409	-1.0950179009
H	-1.0686687407	0.8604070046	-1.979786143
H	-2.3616032277	0.4774096558	-0.8198991137
C	-1.1917305619	-1.207854559	-1.4340546008
H	-1.8602226766	-1.434603859	-2.2686116701
O	0.1690059311	-1.47357425	-1.8827858327
C	0.7704228117	-2.4528410218	-1.0821758026
H	0.8113979318	-3.4272727033	-1.5700157305
N	2.1941506303	-2.049484325	-0.8701289055
C	2.4850724569	-0.7781109061	-0.5232701336
H	1.6257418957	-0.1202928019	-0.4184597308
C	3.7700683335	-0.3361572383	-0.3191108401
C	4.8031687937	-1.2570670315	-0.4866824717
O	6.0486035959	-0.8819137808	-0.2978575042
N	4.4976528289	-2.5213864226	-0.8434592299
C	3.1874857304	-3.0194592801	-1.071855112
O	3.0045749175	-4.1542017264	-1.4036107176
C	-1.4530736915	-2.1927486486	-0.2762844478
H	-2.0815867274	-1.7614465143	0.5058365581
C	-0.0387504069	-2.5099357375	0.2384011137
H	0.2862810352	-1.6979046711	0.8919046819

O	0.0955760474	-3.7052418939	0.9420305064
H	-0.5139999378	-4.349794779	0.5530525993
O	-1.9759907009	-3.4335068515	-0.7405155901
H	-2.9382678335	-3.4257150811	-0.7368115723
H	-0.6369945266	1.4496449388	0.3305360973
H	6.7103279123	-1.5762683951	-0.4310161795
H	3.9897485258	0.6824663737	-0.0397767997
H	5.2151890849	-3.2265149641	-0.9856564807

O4iv	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.1253699502	-0.6857472134	-0.0090914821
C	-1.2702702878	-1.2775102878	-0.6379453807
H	-0.3282443284	0.2248330795	0.2277629117
H	-1.4161865132	-0.859208102	-1.6391983918
H	-2.1768208593	-1.1081715496	-0.0470264375
C	-1.0538144902	-2.7713628936	-0.7346107658
H	-1.9096074527	-3.2216672475	-1.2464551854
O	0.140550463	-3.0314333194	-1.5338939172
C	-0.796196342	-3.50450667	0.5965276861
C	0.85293355	-4.1092491222	-1.0362455947
H	-0.2061821938	-2.859844697	1.2520667753
C	0.0560294289	-4.7089005208	0.1455803096
O	-1.9553895515	-3.8462089483	1.3001889366
H	1.0526747868	-4.8485916999	-1.8125702661
N	2.2332371538	-3.6181941616	-0.5994278271
H	0.6972525345	-5.100213099	0.9374601608
O	-0.8446564347	-5.6900785008	-0.330641745
H	-2.3337980891	-4.638693276	0.89374152
C	2.512449542	-2.307567618	-0.4581874845
C	3.1980629821	-4.6134462828	-0.4243116928
H	-0.4401568339	-6.5640155726	-0.3114077963
H	1.6756379498	-1.6301360563	-0.6099544482
C	3.7700343253	-1.854072611	-0.126081115
N	4.478973586	-4.107997645	-0.1071302181
O	2.988633811	-5.7921745498	-0.5271106699
H	3.9840789819	-0.8028869013	-0.0099422223
C	4.7785493586	-2.7970785464	0.0446196191
H	5.1790888516	-4.8353279474	0.0079350314
O	5.996914144	-2.4082748204	0.3482392907
H	6.6447720775	-3.1213225115	0.4448443991

O4D	Coordinates (Angstrom)		
Atom	X	Y	Z
O	1.2375789955	1.1805363455	-0.0077707138
C	0.1423924928	0.5787463265	-0.7112141162
H	1.0577038328	2.1179768108	0.1173667681
H	0.0675120465	0.9814060327	-1.7263815656
H	-0.8056406433	0.7554035334	-0.1912991311
C	0.371531885	-0.9148953344	-0.7789522399
H	-0.4699897904	-1.3796806534	-1.3009094437
O	1.5853380491	-1.1767835434	-1.5329345948
C	0.5806068296	-1.6304776943	0.5631211226

C	2.2862148718	-2.2560304445	-1.008629854
H	1.0991686118	-0.9740902339	1.2669728367
C	1.4739145439	-2.8307420395	0.1660196858
O	-0.6706880476	-2.0529315793	1.0775749463
H	2.4775002966	-3.0209938054	-1.7607502422
N	3.6644691568	-1.7604888088	-0.5799578965
H	2.1149181536	-3.1773499294	0.984930895
O	0.7016391175	-3.8800770451	-0.3601789683
H	-0.6875040112	-1.9699956167	2.0364318835
C	3.9274745558	-0.4503577131	-0.4111580908
C	4.653261424	-2.7448217128	-0.4548870089
H	-0.1352606358	-3.9092544356	0.1263658089
H	3.0801240379	0.2185524585	-0.5369280767
C	5.1822135275	0.0186813728	-0.0903859596
N	5.9317481996	-2.2196940312	-0.1430188963
O	4.4717489386	-3.9210508019	-0.593000511
H	5.3798907458	1.0705711082	0.0455543865
C	6.2108764819	-0.9098897581	0.0369099401
H	6.646804183	-2.9373104293	-0.0647749929
O	7.4279419458	-0.5055798255	0.3276200932
H	8.090463505	-1.2090811527	0.3872759354

O4v	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.4538548923	-2.6491549735	0.0230717357
C	0.6605916148	-2.953466363	-0.8268838126
H	-0.5152540704	-3.3143158749	0.7161519441
H	0.4214175124	-3.7958844753	-1.485853067
H	1.5472005022	-3.2182539052	-0.2405264812
C	0.9875148329	-1.734185693	-1.6675556212
H	1.7816595375	-1.9853726918	-2.371540271
O	-0.1729387335	-1.3501701511	-2.478625251
C	1.3704658272	-0.4626330059	-0.9092810852
C	-0.7525924267	-0.1880084496	-2.0068644354
H	1.8119663061	-0.6833603017	0.0687890399
C	0.0316101402	0.287177153	-0.749820872
O	2.2650026951	0.2553828325	-1.7292631413
H	-0.7811374363	0.5858135252	-2.7780291363
N	-2.2248611138	-0.4896848973	-1.6962556692
H	-0.4754319338	-0.064035764	0.153855055
O	0.2906672111	1.6654591706	-0.7147867673
H	2.2438414042	1.1851590046	-1.4651047064
C	-2.7416117212	-1.717978312	-1.8721489381
C	-3.0016337755	0.5826078788	-1.2683962601
H	-0.5398365534	2.1499260638	-0.6291515786
H	-2.0317442432	-2.4594674186	-2.2095711406
C	-4.0709703573	-2.0075348843	-1.6559182642
N	-4.3614111583	0.2628331405	-1.077857403
O	-2.586329022	1.696378819	-1.0676478988
H	-4.4729295821	-2.9975328702	-1.8058259042
C	-4.8994627728	-0.9678218155	-1.2501243033
H	-4.9203187049	1.05548294	-0.7747156313
O	-6.1786409032	-1.1867298896	-1.0421651479
H	-6.6922471829	-0.4101618917	-0.7764259874

O4E	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.968510763	-1.9903432942	0.0089160876
C	-2.1312925587	-2.1526615174	-0.8018824663
H	-0.4011094728	-2.7648216076	-0.0520696476
H	-2.858363165	-2.8159935945	-0.3137933316
H	-1.8854822209	-2.5625947438	-1.7860945046
C	-2.7067027268	-0.752625623	-0.9328059501
H	-2.0518488834	-0.1325948571	-1.5513105913
O	-4.0199536078	-0.8173446503	-1.5466980495
C	-2.9714445401	-0.0412959544	0.4009270998
C	-4.7733269817	0.294785209	-1.1511807243
H	-3.4216849543	-0.7500831842	1.1120340938
C	-4.0129069227	1.0168854974	-0.0128555499
O	-1.8598795357	0.6061649425	0.962426667
H	-4.9570357427	0.9843715118	-1.9764547878
N	-6.1397885907	-0.2116076037	-0.7292123307
H	-4.6713416849	1.3047269512	0.8137375439
O	-3.3999639036	2.1378704927	-0.5965423442
H	-1.1349857826	-0.0314832299	1.0247105324
C	-6.4089456259	-1.5187961371	-0.6035595494
C	-7.1338305202	0.7774225729	-0.5678859152
H	-2.5960583918	2.3315330512	-0.0923653379
H	-5.5716681137	-2.1750797303	-0.8032264907
C	-7.6557236375	-2.000322033	-0.262357238
N	-8.3890039078	0.2446259604	-0.2130016013
O	-6.9469343018	1.9493768259	-0.7120452534
H	-7.8362844859	-3.0610009752	-0.169417961
C	-8.668966732	-1.0636488656	-0.0641881881
H	-9.1294121858	0.9298951807	-0.0820205748
O	-9.9189712748	-1.3092081925	0.2591929921
H	-10.1040418855	-2.2540278019	0.3608373712

O4vi	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.8724522667	-0.316290972	-0.0105257823
C	-2.7453119943	-0.601687549	-1.1171783114
H	-2.0779344983	0.5577483174	0.3372710925
H	-2.4633965399	-0.00201004	-1.9887130945
H	-3.7863443458	-0.3788445058	-0.8601929207
C	-2.6337335908	-2.0723121718	-1.4681925047
H	-3.2901603971	-2.2863773793	-2.3140669174
O	-1.2651117513	-2.3629478162	-1.8897744278
C	-2.9353924309	-3.0676634575	-0.3401383012
C	-0.6909681584	-3.3363643371	-1.0675574798
H	-3.591039172	-2.6370279428	0.4253206696
C	-1.5340105284	-3.3854993568	0.2190907576
O	-3.5094981796	-4.2152917126	-0.9307088954
H	-0.6465923781	-4.3192294835	-1.5379854908
N	0.7345699313	-2.9361851986	-0.8362924129
H	-1.2279122698	-2.589450891	0.9033537887
O	-1.4231658118	-4.6634527643	0.8118742324

H	-3.3686593781	-4.9704990209	-0.3440190697
C	1.0236605482	-1.6572572625	-0.5138734107
C	1.7314353879	-3.8978976224	-1.0595935546
H	-1.5712775697	-4.6033888435	1.7615977726
H	0.1612412595	-1.0042148916	-0.3997377678
C	2.3089031803	-1.2022327644	-0.3459373006
N	3.0439413424	-3.3839202308	-0.8743498765
O	1.5523166661	-5.0373520908	-1.3749731536
H	2.5264512094	-0.1781020781	-0.0855095003
C	3.3468768144	-2.1132548697	-0.5406900627
O	4.5930104221	-1.7214292534	-0.3980045482
H	5.2591837789	-2.4059814536	-0.5577909589
H	3.7642296506	-4.0812932472	-1.0396395811

O4F	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.8045032832	-1.4595088065	-0.0855195931
C	-1.3458581152	-1.8856698784	-1.32275081
H	0.1462067038	-1.3318440131	-0.1838138097
H	-1.0105428199	-1.2577047543	-2.1561087046
H	-2.4313950672	-1.7790387523	-1.2438800587
C	-1.0279945628	-3.3407649173	-1.638317211
H	-1.6125657894	-3.6718643421	-2.5009998806
O	0.3893869031	-3.456686143	-2.0168129585
C	-1.2333702839	-4.3180306418	-0.4599272087
C	0.9836793808	-4.4542000916	-1.2596620521
H	-1.8747645743	-3.8940674345	0.3135723045
C	0.1959679652	-4.563850697	0.0641866884
O	-1.7055436201	-5.5964163516	-0.8892209096
H	0.9669773464	-5.4279954624	-1.7642442675
N	2.4442427214	-4.1544893962	-1.0960506691
H	0.4744008524	-3.7538716448	0.7373116249
O	0.400463628	-5.7864454801	0.7122969582
H	-2.6668773335	-5.6307622266	-0.8592006214
C	3.3460122727	-5.0795336672	-1.4768705757
C	2.8500011602	-2.9330345334	-0.5182292835
H	-0.2775912598	-6.400382748	0.3900423668
H	2.9339532048	-5.9817480726	-1.9112735709
C	4.7064270728	-4.9272385333	-1.3393932196
N	4.2494990423	-2.8049698464	-0.4190048062
O	2.1219004992	-2.0652238195	-0.1287987873
H	5.3884539732	-5.7016023741	-1.6578172495
C	5.1555819585	-3.7287966014	-0.785546538
H	4.5703819251	-1.9321604436	-0.0060038693
O	6.4008828029	-3.3733803415	-0.5722565871
H	7.0400922964	-4.0512460857	-0.8364457011

TD	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.0939526366	0.8788441751	-0.0685995003
C	-0.4362424364	0.2655616868	-1.2339831742
H	1.0082383445	1.1180793913	-0.2487505256
H	-0.2108540111	0.8466250178	-2.1349153103

H	-1.5224775734	0.2445352741	-1.1154634719
C	0.0664676738	-1.1575294716	-1.411272074
H	-0.4155085211	-1.6223773263	-2.2765669004
O	1.5089201853	-1.1030874923	-1.68143005
C	-0.1093566531	-2.0807108779	-0.178415247
C	2.1173369249	-2.1275770295	-0.9639661588
H	-0.7533359748	-1.6309643138	0.5780007286
C	1.3287308512	-2.275390881	0.3540642277
O	-0.5700466839	-3.3804457125	-0.5463769153
H	2.0910699008	-3.0835141133	-1.5002252715
N	3.5811433807	-1.8379526903	-0.8203075651
H	1.5721322151	-1.4562087429	1.0294003892
O	1.5705365048	-3.4879862967	1.0033151653
C	4.4766415971	-2.7440873652	-1.3290807111
C	4.0911234849	-0.7397105363	-0.1980618166
H	4.0432551935	-3.6009404615	-1.8251265765
C	5.820195567	-2.5708678079	-1.2105822377
N	5.378759302	-0.5148026739	-0.0562951846
O	3.2272857491	0.1285191257	0.2883681678
H	6.527391098	-3.2845013981	-1.6074051903
C	6.245561051	-1.4027112778	-0.5413068839
O	7.5318210204	-1.1870945749	-0.3971113991
H	7.6898367556	-0.3543653902	0.077060158
H	3.7220778169	0.8283291648	0.7462353626
H	-1.5233759401	-3.4495890664	-0.4341542355
H	0.9057202606	-4.1218520454	0.6912812507

O2B	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.5076646563	-1.9997843666	-0.0105803555
C	-1.3635417934	-2.306718719	-1.1170451194
H	-1.084657641	-1.7202201721	-1.9989136576
H	-2.4114556167	-2.0947130041	-0.874823905
C	-1.226852466	-3.7833870218	-1.4404354432
H	-1.8938400519	-4.025439771	-2.2714333797
O	0.1368333657	-4.0521068265	-1.8911688626
C	0.7327302601	-5.0235736582	-1.086466899
H	0.7518423544	-6.0018085992	-1.5660659961
N	2.1648074347	-4.6210094887	-0.8808865321
C	2.442770258	-3.303094825	-0.4961377033
H	1.5609511862	-2.6809760307	-0.3937609532
C	3.693271505	-2.8586967839	-0.2846243357
C	4.8345963196	-3.7368045706	-0.4468706844
O	6.0017510668	-3.513725505	-0.2984543805
N	4.4259349885	-5.0792083621	-0.8525853386
C	3.1703056364	-5.4796852859	-1.0537718267
O	2.8698457289	-6.704822657	-1.4245561036
C	-1.4807388675	-4.7532357375	-0.2674073256
H	-2.100480117	-4.3084832559	0.5136017426
C	-0.0632183082	-5.0713108894	0.2396915923
H	0.2680765133	-4.2620507372	0.8925975209
O	0.0766529515	-6.2763256052	0.930362479
H	-0.5881828099	-6.8911648108	0.5850990989

O	-2.0126254767	-5.9993989324	-0.7094898196
H	-2.9750495737	-5.9865120243	-0.700839932
H	-0.6973762821	-1.110600176	0.3068693786
H	3.6396191938	-7.2764343036	-1.5561560534
H	3.8814116357	-1.8364643666	0.0112778476
H	5.198997992	-5.7279833133	-0.9700617435

O2ii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.3223261989	-0.3514662819	-0.7069818283
C	1.1011792175	-0.2466721254	-1.9081295597
H	0.4568815044	-1.2203367121	-0.3141125893
H	0.6864315793	-0.8875887628	-2.6929896772
H	2.140823488	-0.5413160332	-1.7279302474
C	1.0818594804	1.1926884441	-2.3817537973
H	1.6930020977	1.2815694893	-3.2818660852
O	-0.2876431888	1.5651317604	-2.7470082265
C	1.5332382373	2.2497032593	-1.3639111953
C	-0.7119999247	2.6524839434	-1.9869827961
H	2.2063739338	1.8325177373	-0.6072688968
C	0.1985462267	2.7208136115	-0.7508449463
O	2.1454251024	3.2957119641	-2.0915813898
H	-0.6680440751	3.5911340321	-2.5382852206
N	-2.1565440979	2.4199392632	-1.6475316829
H	-0.1263386851	2.001540881	0.0050066858
O	0.2121330552	4.0438761163	-0.25285266
H	2.1803321831	4.0857957297	-1.5367931516
C	-2.5270671786	1.177628399	-1.1160764426
C	-3.0959431634	3.33345522	-1.897737398
H	0.407428476	4.0412772339	0.6904253235
H	-1.6963491632	0.4936938507	-0.9806433424
C	-3.8003437049	0.8677075111	-0.8184946604
N	-4.3713779426	3.0662608226	-1.6150192038
O	-2.7117423967	4.4776099412	-2.4174345157
H	-4.0606753562	-0.0978876396	-0.4088400236
C	-4.8714073293	1.817903154	-1.0438230943
H	-5.0931746776	3.7611164862	-1.7841804237
O	-6.0454202366	1.7146802428	-0.832400123
H	-3.43963868	5.0792152715	-2.6297428218

O2C	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.1470954578	-1.776262418	-0.016362895
C	-0.8793045704	-2.4252716279	-0.7742549374
H	-0.0368741071	-0.8323678901	0.0309828135
H	-0.8966088567	-2.0568855584	-1.8049415134
H	-1.8661075364	-2.2621646601	-0.3262115075
C	-0.6055590891	-3.9133073223	-0.7787119303
H	-1.4122070626	-4.4228046798	-1.3139896467
O	0.6441962241	-4.1659997514	-1.4765519414
C	-0.4279650875	-4.568057035	0.5996381252
C	1.3394557837	-5.2208144231	-0.9077994925
H	0.0261260924	-3.8612673401	1.298038765
C	0.5367432069	-5.7434185213	0.3010249411

O	-1.6785291895	-5.0359326687	1.073915772
H	1.5150255265,	-6.0180283639	-1.6281950543
N	2.7302824812	-4.7039465881	-0.5158166435
H	1.1834949401	-5.9829911805	1.1541901628
O	-0.1629384475	-6.8791107093	-0.1407939237
H	-1.7706531534	-4.8648210934	2.0167774853
C	2.936923048	-3.3488423005	-0.2389239928
C	3.764823331	-5.5434170951	-0.4776736921
H	-1.0271342923	-6.8858390201	0.2985410379
H	2.0441926105	-2.7367595939	-0.30340587
C	4.1485557611	-2.8533549205	0.0739969193
N	4.9835282757	-5.0950261221	-0.180679842
O	3.5095845167	-6.8084019731	-0.7369651204
H	4.280908598	-1.801783878	0.2852974707
C	5.3185175428	-3.7050111756	0.1301544795
O	6.4567220917	-3.4348338072	0.3860448196
H	4.2897777762	-7.3814456035	-0.739180679
H	5.7749866473	-5.7313453691	-0.1434711797

O2iii	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.0052113052	0.3182112428	-0.0040248115
C	-1.0752446339	-0.3262177267	-0.6847565726
H	-0.2139598001	1.2435877469	0.1449910019
H	-1.1655342606	0.0467944608	-1.7103649354
H	-2.025264065	-0.1632927132	-0.1637825994
C	-0.8158146536	-1.8157761819	-0.7082651055
H	-1.6435515488	-2.3099805477	-1.2261700928
O	0.40938277	-2.0852361846	-1.4611520822
C	-0.5772940934	-2.4843548153	0.6593752276
C	1.1108582118	-3.1423842503	-0.9173724127
H	-0.0072618617	-1.8044479827	1.296218354
C	0.2956034233	-3.6984899398	0.2748972851
O	-1.7432051531	-2.8101358365	1.3570240222
H	1.3138751127	-3.9066505627	-1.6668892903
N	2.5002409666	-2.6238299947	-0.4854086604
H	0.9213495713	-4.0506537505	1.0975023215
O	-0.5804131507	-4.7101115669	-0.1921511119
H	-2.1344824981	-3.5942614309	0.9472161878
C	2.7154763464	-1.2602374752	-0.2534945172
C	3.527036201	-3.4665597276	-0.4025943097
H	-0.2541891076	-5.5859001266	0.0363525621
H	1.8291259161	-0.6419369952	-0.3449646311
C	3.9277746474	-0.7650362443	0.0577768705
N	4.7453818587	-3.0216844279	-0.1042812895
O	3.2650378998	-4.7432248067	-0.6193451301
H	4.0649160187	0.292303387	0.2350272646
C	5.0902298584	-1.6216484852	0.1594639646
O	6.2276547578	-1.3543949267	0.4193792672
H	4.0510391652	-5.3083608285	-0.6307302602
H	5.5288308462	-3.6640005592	-0.0239495364

Table S3. Calculated Cartesian Coordinates of the Stable Low-Energy ring-Closed Conformers of $[dUrd+H]^+$.

O4A	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.197310167	-0.1865292447	-0.0173276279
C	-2.1598703559	-0.5516193039	-1.0190351459
H	-1.9808827002	0.0107245248	-1.9416602472
C	-2.0328375299	-2.0353004463	-1.3087637656
H	-2.736509857	-2.3028443044	-2.0996901588
O	-0.6924862296	-2.3135258596	-1.8012443237
C	0.0452751921	-3.2520480532	-0.9906616834
H	0.0389292011	-4.2196961744	-1.4853251269
N	1.3793411111	-2.7811057824	-0.8205016325
C	1.6588930923	-1.4699491097	-0.7429069341
H	0.7948374425	-0.8116391084	-0.7613726323
C	2.9475104933	-0.9889260186	-0.6347910666
C	3.9795857509	-1.9244155486	-0.6229293895
O	5.2695679119	-1.6770954673	-0.5462098503
N	3.6784965618	-3.2348018436	-0.6935254829
H	4.4301011513	-3.9195502298	-0.6758070496
C	2.3779295718	-3.7709122159	-0.7656667748
O	2.1714605024	-4.9509296111	-0.7775607823
C	-2.2478527883	-2.9862597755	-0.1161405983
H	-2.819102337	-2.506121182	0.6834278966
C	-0.8176567703	-3.3207122564	0.3315973954
H	-0.4590038574	-2.5506597557	1.0179576301
O	-2.9337500694	-4.1205530521	-0.6295929677
H	-3.1800076857	-0.3444206423	-0.6785497844
H	-1.4175955369	0.6835944729	0.3306547906
H	-3.2154341034	-4.6909779303	0.0938839944
H	-0.7398528626	-4.2969148973	0.8102846488
H	3.141885605	0.0716799573	-0.5743199292
H	5.4676098872	-0.7306927914	-0.5020904022

O4B	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.8298691603	-0.9638143199	-0.0080551156
C	-2.8955972788	-1.6473500299	-0.6826953321
H	-3.0389273757	-1.2368870956	-1.6874205031
C	-2.55261153	-3.1171819796	-0.7810160054
H	-3.3680141625	-3.6299973646	-1.3015089983
O	-1.335158509	-3.2792739645	-1.5624257983
C	-0.538699429	-4.2958464506	-1.0518455148
H	-0.2517525757	-4.9989790462	-1.8329852818
N	0.7967998241	-3.6736972574	-0.6158656553
C	0.9456673795	-2.3504840214	-0.4584912182
H	0.0465336745	-1.7544469653	-0.5936966372
C	2.1577577769	-1.7745569472	-0.1274185509
C	3.2515569612	-2.6211606475	0.0200394272
O	4.4867700295	-2.2763140981	0.316839249
N	3.0826019572	-3.9478012203	-0.1490884965
H	3.8812340749	-4.568749621	-0.045988484
C	1.8651713542	-4.575666461	-0.4681725083

O	1.766694848	-5.7639209143	-0.5990725101
C	-2.2871716563	-3.8497669646	0.5410756755
H	-1.8338469375	-3.1617105727	1.2623498
C	-1.2916228719	-4.9438574498	0.113132038
H	-0.6354641633	-5.2974640334	0.9077726069
O	-3.5242980179	-4.3379339488	1.0200628994
H	-3.8351086968	-1.558783955	-0.1268716597
H	-2.104628555	-0.0609624046	0.1814662679
H	-3.4640927856	-4.5401990619	1.9591907005
H	-1.8532942758	-5.8005775499	-0.2668917129
H	2.2463208949	-0.7055097338	-0.0019069319
H	4.5912994862	-1.3206159713	0.4284482499

TA	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.5922587766	-0.8050463014	-0.0344258671
C	-1.4882991405	-1.2441020803	-1.0659354149
H	-1.2624268091	-0.7391807727	-2.011102451
C	-1.3296371633	-2.7410496535	-1.2523926222
H	-2.0129928252	-3.0757017477	-2.0353339913
O	0.0252908718	-3.0313034322	-1.7009451285
C	0.6644601691	-3.9066494241	-0.8186721158
H	0.7461814307	-4.9057393879	-1.2438080793
N	2.087619392	-3.4119718665	-0.6696703098
C	2.321497659	-2.0697526191	-0.5296368091
H	1.4343250316	-1.4456197311	-0.4990157332
C	3.5936010489	-1.5914288313	-0.4374760295
C	4.636675634	-2.5406485152	-0.5061202647
O	5.8813637589	-2.1211048348	-0.4415037832
N	4.4019324878	-3.8467179776	-0.6315468319
C	3.1516259315	-4.250151896	-0.7044458031
O	2.8737461772	-5.535760098	-0.8085224518
C	-1.5492942494	-3.6082281375	0.0022335171
H	-2.1445806408	-3.0833826551	0.7538337686
C	-0.1202775563	-3.8779200009	0.4971140947
H	0.2145760373	-3.047388775	1.1217729154
O	-2.1977688065	-4.7959351627	-0.4350613485
H	-2.529286332	-1.0325009358	-0.7981240831
H	-0.8168125804	0.0959161651	0.2203626659
H	-2.5387764868	-5.283332326	0.322549659
H	-0.0362040542	-4.809575848	1.0569626427
H	3.8020024049	-0.5373238494	-0.3272994445
H	6.4953891288	-2.8706702981	-0.5018289778
H	3.7015995578	-6.0400169573	-0.8530467233

TB	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.4199966478	-1.3153365605	-0.0152926763
C	-0.6019762798	-2.039434486	-0.7100523332
H	-0.7198591896	-1.6597384763	-1.730170704
C	-0.2188533777	-3.5017749001	-0.75828295
H	-1.011829349	-4.0525218625	-1.2745534668
O	1.0147674758	-3.6567807875	-1.5182304539

C	1.8204513354	-4.6452067615	-0.977366409
H	2.1163629997	-5.3625449634	-1.7414991276
N	3.1545631733	-3.9882214277	-0.5549353643
C	3.2558743329	-2.6394348242	-0.3626448944
H	2.3369238836	-2.0739799863	-0.4762581887
C	4.455096035	-2.0735263403	-0.0379131563
C	5.56322727	-2.9379792137	0.0688626864
O	6.7413413849	-2.4318173291	0.364068395
N	5.4566003126	-4.2553502091	-0.1195866328
C	4.2731375562	-4.7406439356	-0.4193520687
O	4.1075179294	-6.0382332069	-0.6087364545
C	0.0480090404	-4.1855818961	0.5896963356
H	0.4740636138	-3.4639335245	1.2935638506
C	1.0764366225	-5.267960169	0.2075796367
H	1.7342764682	-5.5716388821	1.02170428
O	-1.1779766322	-4.6982947676	1.070475348
H	-1.5638163507	-1.9627840722	-0.1913615786
H	0.1351610474	-0.40457881	0.1117774093
H	-1.1493634139	-4.7965611339	2.0273952403
H	0.5367649021	-6.151674094	-0.1415397836
H	4.5573944651	-1.0099279075	0.1203178824
H	7.4119302084	-3.132547153	0.4012211158
H	4.9615787282	-6.4892817097	-0.5155329375

TC	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.7320111287	-0.7614630149	-0.0474447006
C	-1.6177170849	-1.3409623112	-1.0235260394
H	-1.4520744257	-0.8858877456	-2.0040158279
C	-1.2965883528	-2.8196392018	-1.0823225902
H	-1.9037679935	-3.2995902488	-1.8525108508
O	0.1060799502	-2.9437446681	-1.4484532523
C	0.7523233134	-3.8124129382	-0.5534390586
H	0.7518657673	-4.8345395977	-0.9415482046
N	2.1932326409	-3.4290328602	-0.4951622022
C	3.1228604744	-4.4052357554	-0.7649747444
H	2.7202396262	-5.3737644176	-1.0275162961
C	4.4552934614	-4.1644500591	-0.7015033297
C	4.8260463235	-2.8435964856	-0.3501600147
O	6.1071800099	-2.5564358702	-0.2590788899
N	3.9385323452	-1.8909809481	-0.1211458563
C	2.6449848272	-2.1600573226	-0.199686815
O	1.8471661813	-1.168238372	0.0412713727
C	-1.4655019582	-3.6027400308	0.2414831644
H	-2.1044217592	-3.066161221	0.9468411689
C	-0.0239904315	-3.7413970917	0.7646767165
H	0.2561444938	-2.8648280144	1.3513345238
O	-2.0236856504	-4.8628791745	-0.1074727111
H	-2.6610515675	-1.1951166521	-0.7295116685
H	-0.9002045789	0.1829588924	0.0504391335
H	-2.3804141188	-5.2959004616	0.6756710023
H	0.1112157068	-4.6338859695	1.3757586527
H	5.1901629074	-4.9277328387	-0.9107578213
H	0.8660660568	-1.2328581334	-0.1394063785

H	6.2183239746	-1.6205600074	-0.022761483

O2A	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.5081409396	-0.1015145805	-0.0515144049
C	-2.4195095687	-0.6652465667	-1.0228812268
H	-2.2584714102	-0.1992221765	-1.9982493289
C	-2.1212307963	-2.1477657347	-1.1005998495
H	-2.7367065838	-2.6042334283	-1.878569103
O	-0.7225641376	-2.2849252716	-1.4680634192
C	-0.0769307226	-3.1577620523	-0.5725483833
H	-0.0645221907	-4.1748851407	-0.9713741338
N	1.357180501	-2.7654873783	-0.499255694
C	2.322660515	-3.754579182	-0.7423697802
H	1.910957084	-4.7252992856	-0.9807787613
C	3.643533463	-3.5311043537	-0.6853777995
C	4.1516912586	-2.2048036315	-0.375598964
O	5.290699923	-1.8402367725	-0.2818873845
N	3.0823024774	-1.2590337499	-0.1816006811
H	3.3613993394	-0.3012164068	0.0131781537
C	1.7675937297	-1.5045763212	-0.2339389249
O	1.007280305	-0.4916761619	0.0017643159
C	-2.30367948	-2.9502932251	0.2097044237
H	-2.9467451441	-2.423182798	0.9189586663
C	-0.8666761825	-3.102211134	0.7389305998
H	-0.5862231415	-2.2356130496	1.3406667537
O	-2.8634969941	-4.2005989808	-0.1664757338
H	-3.4523206553	-0.5003116195	-0.7060501785
H	-1.6900006208	0.8359312481	0.0865245449
H	-3.2178107894	-4.6532299155	0.6067894747
H	-0.7382145435	-4.0024767725	1.3399048672
H	4.3553088745	-4.3211211265	-0.8772572766
H	-0.0020226201	-0.511507172	-0.138848772

O4C	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.4888913621	0.7058005122	-0.0089211154
C	-1.5483128896	0.0212847801	-0.6909181533
H	-1.6824963381	0.4276768718	-1.6985928404
C	-1.2040947122	-1.44889623	-0.780789362
H	-2.0169738345	-1.965116845	-1.3018465866
O	0.0165574441	-1.6142697174	-1.5567393325
C	0.8114877812	-2.6276516837	-1.0386969462
H	1.0994759145	-3.3354819168	-1.8152439606
N	2.1474582145	-2.0033105728	-0.6044257965
C	2.2927611587	-0.6763915104	-0.4357606935
H	1.390048886	-0.0842734867	-0.5626410556
C	3.5006527396	-0.0991848378	-0.1075344173
C	4.6045093375	-0.9341479972	0.0277805539
O	5.7808492517	-0.4263341822	0.3254707209
N	4.4411815312	-2.2645586853	-0.1516219849
H	5.2151675807	-2.9171454967	-0.0661807236
C	3.2147530458	-2.8960912335	-0.4689449295

O	3.1339573566	-4.0859477484	-0.6035752011
C	-0.9430251848	-2.1740485573	0.5464238268
H	-0.4945581079	-1.4810658588	1.2657919311
C	0.0564583644	-3.2687593098	0.1287136748
H	0.7109912777	-3.6150131226	0.9280581905
O	-2.1806564546	-2.6636687248	1.0229617483
H	-2.4930800309	0.1117326218	-0.1442077633
H	-0.7571559249	1.6142514103	0.1624636352
H	-2.128890543	-2.8439821068	1.9669822034
H	-0.5028107308	-4.1292502072	-0.2463102421
H	3.6046294868	0.9659370364	0.0294934118
H	6.5004416622	-1.0704183514	0.3928052076

O4D	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.8063871869	-1.0923203582	-0.0205810516
C	-1.7532185266	-1.460251603	-1.035760321
H	-1.5551109997	-0.9077760791	-1.9603913389
C	-1.6303286599	-2.9473826392	-1.3093819803
H	-2.3302640095	-3.2204784686	-2.1017026891
O	-0.2882827057	-3.2376011149	-1.7903208541
C	0.3491717328	-4.1701046999	-0.9647047927
H	0.4287855363	-5.144460699	-1.4467029393
N	1.775565505	-3.7051622481	-0.7951140075
C	2.0539984805	-2.3909682307	-0.6831112449
H	1.1869779644	-1.7360589291	-0.67597438
C	3.3381819989	-1.9095371256	-0.5761468944
C	4.3795257679	-2.8343077144	-0.6015061071
O	5.6246796388	-2.4205127703	-0.5211644651
N	4.0822925665	-4.1473183761	-0.7074651427
H	4.8048645498	-4.8614777671	-0.7201778588
C	2.7727259584	-4.6863923082	-0.7833816102
O	2.5857041985	-5.8693385087	-0.8297774733
C	-1.8568273622	-3.8831820202	-0.1068921486
H	-2.4316032912	-3.3912444583	0.6827517113
C	-0.4306005537	-4.2166610563	0.3539997019
H	-0.0734924418	-3.4383305275	1.0316902099
O	-2.542788835	-5.022161452	-0.6104556644
H	-2.7778651333	-1.2442957957	-0.7144326584
H	-1.0158366767	-0.2103640837	0.3037153484
H	-2.8390839006	-5.5773958094	0.1189279121
H	-0.3599157661	-5.1863450994	0.8470269083
H	3.5493710444	-0.8551941648	-0.4880159988
H	6.2925981265	-3.1208168324	-0.5520318406

O4E	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.0618903668	-0.0928691403	0.0317499837
C	1.2150984003	-0.2918370605	0.8445484241
H	1.93529448	-0.956027443	0.3464176993
C	1.8204556523	1.0919758252	1.014073077
H	1.171330306	1.7104772809	1.6423634792
O	3.1219075992	0.9723881199	1.6496698901

C	3.9340983295	2.0429945161	1.2629644634
H	4.1877432293	2.6759186886	2.1145098801
N	5.27671684	1.4559735772	0.8284872495
C	5.471345579	0.1379533322	0.6946599955
H	4.6007429362	-0.4716989189	0.9006354555
C	6.6867523151	-0.4093832354	0.3360011125
C	7.7458994215	0.4720251217	0.1293667338
O	8.9771446138	0.1626140221	-0.2116632297
N	7.5390652781	1.7936113606	0.2886518848
H	8.3138728931	2.4382781636	0.1510493956
C	6.3188592965	2.3884173488	0.661007692
O	6.195537426	3.5696431958	0.8145146608
C	2.1067303849	1.8397164973	-0.2972392581
H	2.4750521878	1.1224495866	-1.0468393849
C	3.2223427545	2.7999933038	0.1318222435
H	3.8866526203	3.0966241749	-0.6779396665
O	1.0164643832	2.5691898828	-0.7954708483
H	0.9573230092	-0.7210083968	1.8178568934
H	-0.5126356078	-0.8636405863	0.066719316
H	0.2958931772	1.9488644096	-0.9699183435
H	2.7657617415	3.7063158608	0.5349031117
H	6.8084169302	-1.4777095285	0.2350882747
H	9.1104047161	-0.7899708688	-0.3213691852

O4F	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.1226425677	0.3670612593	-0.0516204287
C	-0.6139090485	-0.095709603	-1.2981771576
H	0.8357303666	0.4559281327	-0.1025249541
H	-0.2322909042	0.5013782254	-2.1345454614
H	-1.6996453033	0.027614405	-1.2712661589
C	-0.3093738593	-1.5641231217	-1.5562306411
H	-0.8655208658	-1.9145850955	-2.4286677943
O	1.1177764955	-1.7244361842	-1.8611533928
C	-0.5863785245	-2.5071037937	-0.3675717548
C	1.6582246047	-2.7042954204	-1.0330717641
H	-1.2633863947	-2.0458914862	0.3532737145
C	0.8111701854	-2.7400161417	0.2388890537
O	-1.1282830444	-3.7138559551	-0.9001002623
H	1.653912322	-3.6864906441	-1.52021057
N	3.1264140513	-2.3989685265	-0.8670493914
H	1.0655815187	-1.9211024081	0.9101532904
H	-1.6112656949	-4.1853304983	-0.2134294675
C	4.0300833997	-3.2627434	-1.3671091156
C	3.5292919747	-1.1753573486	-0.2912733364
H	3.6190404833	-4.1556176896	-1.822535044
C	5.3907894163	-3.0651109193	-1.3233624151
N	4.929802408	-1.0083870217	-0.2670881137
O	2.8017455705	-0.3351811709	0.1537328037
H	6.0734934945	-3.7936949484	-1.734921898
C	5.8379891537	-1.8761933816	-0.7458586956
H	5.2481553491	-0.1354000767	0.1477251219
O	7.0822861525	-1.4819602854	-0.6105790962
H	7.7231394078	-2.1168513484	-0.9630225412

H	0.879713263	-3.6925765031	0.7652201608

TD	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.0786108421	-0.6013601325	-0.0669208873
C	-0.6295201992	-1.3922766077	-1.1109835602
H	-0.4026834934	-0.9704474128	-2.0963449874
C	-0.1531931773	-2.83374404	-1.0570726542
H	-0.6488027475	-3.4236348369	-1.8325956344
O	1.2874914582	-2.8576306766	-1.3231191347
C	1.8800915105	-3.738567429	-0.4173900418
H	1.8576765816	-4.7682870244	-0.7909420766
N	3.353046367	-3.4217741161	-0.3579238191
C	4.2372488743	-4.3667026265	-0.81233981
H	3.7952224253	-5.2896367949	-1.161408684
C	5.5799549557	-4.1517643416	-0.8206689662
C	6.0159498402	-2.8933315001	-0.3501899107
O	7.3018458514	-2.6329920746	-0.3362249263
N	5.1591026697	-1.9657873109	0.0733563237
C	3.8709634808	-2.233335434	0.057174759
O	3.018035646	-1.3188021475	0.470056302
C	-0.3468594448	-3.5496621105	0.3014719557
H	-1.0068123404	-2.9803867475	0.9584749704
C	1.0804035936	-3.6371580398	0.8799988097
H	1.3179269042	-2.7237632789	1.4230979289
O	-0.8795202841	-4.8399948561	0.019204587
H	-1.7142411986	-1.3761757318	-0.9831357348
H	0.8454566019	-0.4383975865	-0.2787081419
H	-1.3162990462	-5.19381701	0.8012022962
H	1.2099560938	-4.5035166156	1.5290495186
H	6.2781005438	-4.895906165	-1.175418671
H	7.468125605	-1.7370635541	-0.0000175616
H	3.5202391504	-0.5457984981	0.7774175908

O2B	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.1125756536	-1.2614645257	1.7390294914
C	-1.0862187938	-1.1579315078	0.6907232832
H	-0.8542113965	-0.3157812541	0.0303479398
C	-1.0777383456	-2.4402879543	-0.1189705224
H	-1.8478396546	-2.3788197306	-0.8902343079
O	0.2052752705	-2.5831363535	-0.7954469916
C	0.8289292502	-3.7780656593	-0.4248027345
H	0.7705496557	-4.5154688981	-1.2235760045
N	2.2982129113	-3.461480401	-0.2593046626
C	2.658208613	-2.3513377148	0.5157491316
H	1.8158113864	-1.8404886749	0.9698766235
C	3.9340143686	-1.9547796422	0.6634809427
C	5.0173563978	-2.6632267897	0.0121712312
O	6.1961133794	-2.4540038162	0.0354395408
N	4.524327012	-3.7953888915	-0.7699970246
H	5.2561892947	-4.3324067551	-1.2265027661
C	3.2457820517	-4.1541168952	-0.888775661
O	2.8676936729	-5.1952156288	-1.6016703608

C	-1.2737083012	-3.7432304899	0.6804907404
H	-1.7650617626	-3.5566723196	1.6384192303
C	0.16240487	-4.2572700639	0.867987735
H	0.6145226017	-3.7775955142	1.7381570379
O	-2.0456936609	-4.6127172663	-0.138973834
H	-2.0909101547	-1.0122484898	1.1027257004
H	-0.2227363656	-0.5263322117	2.3511297205
H	-2.3955429922	-5.3385331137	0.3887486954
H	0.2086772529	-5.3400678076	0.9869521764
H	4.1858188656	-1.094949558	1.2678635208
H	3.5843788168	-5.6079840925	-2.1045812713

O2a	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.5223881048	0.2313517205	0.5428055206
C	-1.4857453119	0.3146552253	-0.5151046519
H	-1.246152893	1.1394641192	-1.1943410487
C	-1.4765072728	-0.9864830972	-1.2940794546
H	-2.2453308316	-0.9465209569	-2.0675221276
O	-0.1899530977	-1.1426925567	-1.9681465278
C	0.4421857831	-2.3122203009	-1.5499657723
H	0.3250000971	-3.0943574302	-2.3102155451
N	1.9051753628	-2.0103253606	-1.4340337925
C	2.2820206664	-0.9292694893	-0.6152468197
H	1.4465514375	-0.4192054265	-0.1489509852
C	3.5618023994	-0.5611198133	-0.4513084208
C	4.6372140003	-1.2622973556	-1.1327076039
O	5.8179698339	-1.0676196689	-1.0828103009
N	4.1288758008	-2.3241178048	-1.9792317868
H	4.8195517716	-2.8441299347	-2.5151528063
C	2.8507015558	-2.6611712114	-2.1224609489
O	2.6269678853	-3.6559929483	-2.9503035412
C	-1.6608171064	-2.2715109918	-0.4636807271
H	-2.1771773061	-2.0722534875	0.4776843739
C	-0.2176913061	-2.7491978166	-0.237781199
H	0.2224118559	-2.2224703079	0.6098096796
O	-2.3867087408	-3.1871124871	-1.2769017526
H	-2.4938930409	0.473068179	-0.1159388975
H	-0.6192028062	0.9929007322	1.1243099477
H	-2.7914440585	-3.868006157	-0.7289634371
H	-0.1528248248	-3.8245894485	-0.0704966655
H	3.8256663823	0.2722952722	0.1842346029
H	1.6888057192	-3.8343911066	-3.1095531017

O2C	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.520077129	-1.9245222857	0.1041861344
C	-1.5121612199	-2.6487689385	-0.6303221457
H	-1.6149365451	-2.2489936562	-1.6443946679
C	-1.1013045813	-4.1024073419	-0.7026703653
H	-1.8816263457	-4.6594755215	-1.2311407236
O	0.1378983703	-4.2222792993	-1.4621316597
C	0.9512251367	-5.2153241124	-0.9465901133

H	1.2368597523	-5.9193300737	-1.7263850562
N	2.2931388282	-4.555174226	-0.5341941534
C	2.3558335668	-3.1929741979	-0.2277880923
H	1.4031629487	-2.6766044704	-0.2703602197
C	3.5100165441	-2.577474983	0.0916063623
C	4.764673272	-3.2990980655	0.1248317991
O	5.8695591707	-2.915042577	0.3820459908
N	4.5772781503	-4.7102236347	-0.2143062333
H	5.431269657	-5.2603455644	-0.1892527
C	3.4101470167	-5.2771980805	-0.516721756
O	3.2921358629	-6.5607365534	-0.8000960887
C	-0.8254412368	-4.8036717054	0.6350198255
H	-0.4168953876	-4.0862949928	1.3529149684
C	0.2254672696	-5.8599552914	0.2379688987
H	0.8930990723	-6.1542158283	1.0480517439
O	-2.0402999752	-5.3530593561	1.1028301234
H	-2.4868232262	-2.6018240173	-0.1321085916
H	-0.8072311407	-1.0126633799	0.2179422769
H	-2.0292363069	-5.4266564789	2.0622430724
H	-0.2988777102	-6.7522180132	-0.1131357136
H	3.5296122823	-1.52272017	0.3263648928
H	4.1348087836	-7.0355169149	-0.8368234386

O2b	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.6354831432	-0.07326505	0.1142994877
C	-1.6248227368	-0.7920018419	-0.6264933809
H	-1.7238889125	-0.3903451373	-1.6401995346
C	-1.2126955012	-2.2453948139	-0.7003334892
H	-1.9881085048	-2.8048404365	-1.2330373592
O	0.0319556167	-2.3566799733	-1.4556792929
C	0.8467814906	-3.3475356308	-0.9430186265
H	1.0991293805	-4.0462101534	-1.7491926847
N	2.1891270674	-2.7104226736	-0.5487486558
C	2.2569752195	-1.3438095821	-0.2346967037
H	1.3073465083	-0.8236244688	-0.2802392208
C	3.4119879285	-0.7405235595	0.0952354417
C	4.664934193	-1.4733192108	0.1337124761
O	5.7653749324	-1.0839581192	0.4032362756
N	4.4728315334	-2.8702208314	-0.2127839636
H	5.3034224655	-3.457419245	-0.206001926
C	3.3111443558	-3.4342072469	-0.5251348943
O	3.3649271919	-4.7239298911	-0.7885616933
C	-0.935571765	-2.9451851708	0.6380557315
H	-0.5280654765	-2.2272678906	1.3551046556
C	0.1212014063	-3.9997315028	0.2418712482
H	0.7865022672	-4.284749555	1.058474976
O	-2.1422123114	-3.507508936	1.1056810325
H	-2.602301784	-0.7476002072	-0.1332612994
H	-0.917947824	0.8403346816	0.226987806
H	-2.156103798	-3.5288153143	2.0677081829
H	-0.4073743444	-4.8921748531	-0.1037728468
H	3.4368709931	0.3130644716	0.3349212018
H	2.5177108117	-5.1211100878	-1.0309203039

Table S4. Calculated Cartesian Coordinates of the Stable Low-Energy Ring-Open Conformers of $[Urd+H]^+$.

O4A_RO4'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.036731259	0.1304310109	-0.5106546562
C	-0.5447324561	-1.0841837176	-0.8842387063
H	-0.2402132582	-1.9065952373	-0.2168040334
C	-2.0485449518	-1.0450392315	-0.8630291932
O	-2.6416795494	-0.0516028459	-0.4727920983
C	-4.3818897749	-2.1521316721	0.8515703675
N	-5.5992511125	-1.5783575991	0.219833345
C	-5.6646059409	-0.2766899852	-0.121439946
H	-4.7421609058	0.2798085019	0.0031825174
C	-6.8034983756	0.309938715	-0.6298330732
C	-7.9291868464	-0.4991663285	-0.7776740932
O	-9.1084938412	-0.1371145386	-1.2288832542
N	-7.8494906865	-1.799332592	-0.4366128249
C	-6.7073914412	-2.4424294173	0.0769847685
O	-6.6986199212	-3.6047287226	0.3619348741
C	-2.8538679078	-2.2753654959	-1.2919360023
H	-3.6427234395	-1.9222198298	-1.968132263
C	-3.5090898383	-3.000922567	-0.0841017276
H	-4.1133809615	-3.8108980734	-0.5083845899
O	-2.0538754737	-3.2742375771	-1.906224449
H	-0.2031085072	-1.3707230606	-1.8868431036
H	-6.8164644755	1.3575239731	-0.8925548139
H	-4.7134142783	-2.8029662819	1.6592429393
H	-3.8133807742	-1.3279810177	1.2752024307
H	-1.9936926791	-3.1384519537	-2.85702367
H	-0.6558396814	0.705551133	-0.1571690996
H	-9.1524332007	0.8017582115	-1.4619686808
H	-8.6707996346	-2.3909034098	-0.5385877148
O	-2.5138862412	-3.5149420041	0.7758691983
H	-2.0135645542	-4.1921605367	0.3034039726

TA_RO4'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	0.0616398484	0.7251877211	-0.4516815082
C	-0.5499725662	-0.4276294733	-0.9494754054
H	-0.283443906	-1.315594513	-0.3548771471
C	-2.0519861813	-0.3363838148	-0.9562778666
O	-2.6197175369	0.6483948901	-0.5131511047
C	-4.4712991628	-1.4680507291	0.6176686488
N	-5.6895018412	-0.8681703755	0.0028001713
C	-5.7137092459	0.4561504843	-0.3570310765
H	-4.7739391836	0.9813110044	-0.2362529598
C	-6.8455919953	1.0268245636	-0.8548071665
C	-7.9795623933	0.1927893343	-0.9735287389
O	-9.0952378851	0.7042478996	-1.4401293227
N	-7.9520582345	-1.0951366094	-0.6276713291
C	-6.8303926438	-1.5900597212	-0.1539911607
O	-6.7546314206	-2.8547939371	0.2079834432
C	-2.8910362961	-1.5028156338	-1.4906941712

H	-3.646374594	-1.0737073429	-2.161286626
C	-3.6062667476	-2.2841319417	-0.3542305469
H	-4.2303789345	-3.0356864047	-0.854022889
O	-2.1159857142	-2.4926346612	-2.1498175838
H	-0.1982414701	-0.6336886575	-1.969464811
H	-6.8815470245	2.0684876598	-1.139173284
H	-9.7961651199	0.0325319626	-1.4661841893
H	-7.6180282911	-3.2811410047	0.0855327438
H	-4.7944301015	-2.1399742366	1.41006826
H	-3.9047335356	-0.6541500366	1.0627130976
H	-1.9846056903	-2.2749146177	-3.0781665708
H	-0.6264492383	1.3187144081	-0.1197179605
O	-2.6598037061	-2.9033934174	0.4894411607
H	-2.1313428082	-3.5189247498	-0.0348932769

O4A_RO1'		Coordinates (Angstrom)	
Atom	X	Y	Z
O	-0.7421729611	-0.2839074893	0.0446664217
C	-0.6162129753	1.0675381941	0.532816548
H	0.2156274581	1.5697372552	0.0287783145
C	-1.9099828798	1.8040340221	0.1937607917
H	-1.841865006	2.8230216009	0.5877840123
O	-4.6234591226	-0.6372535955	3.1750921892
C	-4.6568759742	0.3451367796	2.5073434955
N	-5.9489056323	0.5916556878	1.7577174768
C	-6.6117065206	-0.5129115699	1.3423590185
H	-6.1208484983	-1.4508811138	1.5697831249
C	-7.8108361955	-0.4611371562	0.6801283217
C	-8.3614542318	0.8051963654	0.4561014304
O	-9.493405582	1.0709714816	-0.1484764572
N	-7.6998337706	1.8929015885	0.8879991116
C	-6.4609020185	1.8902927459	1.5637271509
O	-5.940208119	2.904037195	1.9270948023
C	-3.2300106101	1.1741641852	0.6697632185
H	-4.0312626726	1.7682630727	0.2143023101
C	-3.4707108374	1.250596648	2.2126876021
O	-3.420835197	-0.1667640962	0.2276256371
H	-0.4330243976	1.0647292628	1.6079804851
H	0.0733345025	-0.772361132	0.1943193976
H	-3.710578152	2.2819812894	2.4800205535
H	-8.3035441084	-1.3624137243	0.3456988176
H	-1.9833682083	1.8887381205	-0.8949438355
H	-2.5442265954	-0.5665053807	0.0807463322
H	-8.1065089669	2.8137135218	0.738299307
H	-9.958528025	0.2769548458	-0.4515145904
O	-2.389432356	0.8518778355	3.0097368741
H	-2.4149386662	-0.1035704201	3.1502601281

TA_RO1'		Coordinates (Angstrom)	
Atom	X	Y	Z
O	-0.5244078407	0.4602975685	0.3337517604
C	-0.5037127717	1.7835558045	0.9064532763
H	-1.3101236808	1.8857805756	1.6392501719

C	0.8337117867	1.9511792601	1.624152022
H	0.8731967222	2.9573465794	2.0533050927
O	3.4828173089	2.0837499041	-2.2873868168
C	3.5486494608	2.2824145196	-1.1226344639
N	4.8118418155	1.7836705272	-0.4192656833
C	5.1264939117	0.4535392331	-0.5472317544
H	4.3814450406	-0.1527729202	-1.0429832988
C	6.2923145728	-0.0300146745	-0.0398808588
C	7.1456149556	0.9024911122	0.5942554696
O	8.2795621865	0.4771014402	1.097514154
N	6.8400430291	2.1992470487	0.6960278481
C	5.6993701329	2.607401981	0.1914685708
O	5.3497610267	3.8775296734	0.2399827776
C	2.1107366204	1.7085432076	0.8022561996
H	2.9430818869	1.7060916077	1.5184743006
C	2.4486788269	2.8313581723	-0.2301194407
O	2.1423399685	0.446960223	0.1418179933
H	-0.6330481244	2.5354418803	0.1267884868
H	-1.3735855895	0.2859957951	-0.0844301314
H	2.8200244828	3.7045196286	0.3157737661
H	6.5593727534	-1.0742244126	-0.1132176302
H	8.7750477425	1.210495379	1.4976963976
H	6.0523822185	4.396858349	0.6632554733
H	0.8645020328	1.2472608761	2.4614327446
H	1.2244334313	0.1396332887	0.0174438958
O	1.3812518718	3.263611372	-1.026243663
H	1.3248280315	2.7273666202	-1.8281790898

Ti_RO1'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.8611592147	0.0926743892	-0.2195750211
C	-0.790790322	-0.8808887417	-1.2779483246
H	0.0666688443	-1.5433866113	-1.1243140546
C	-2.0677260393	-1.7186473064	-1.2219922265
H	-2.0642230115	-2.4117511585	-2.069757923
O	-4.9511507952	1.8176415922	-2.1741333759
C	-5.0207089433	0.6160251809	-2.2295506764
N	-6.285646532	-0.0262483533	-1.8773998976
C	-6.5419974317	-1.3446852868	-2.2169375526
H	-5.7977311828	-1.8342222687	-2.8245536715
C	-7.6771952005	-1.9656363364	-1.8290900928
C	-8.5797095884	-1.1977456021	-1.0406601903
O	-9.6675245757	-1.7812460379	-0.6059895999
N	-8.3683685339	0.0745196716	-0.7458125127
C	-7.271229656	0.6678165152	-1.1647327727
O	-7.1245102692	1.9220416382	-0.8922246509
C	-3.412058798	-0.9693422185	-1.1868952173
H	-4.1827686636	-1.7352692392	-1.0264089188
C	-3.788253845	-0.2435124074	-2.5263471145
O	-3.5365636005	-0.0500275509	-0.1187239629
H	-0.6835368734	-0.3812525067	-2.2420928108
H	-0.02255419	0.5546582261	-0.122912464
H	-3.9983860985	-0.9943308192	-3.2946982948
H	-7.8933817824	-2.9893828949	-2.0983791604

H	-10.2032197438	-1.1553250793	-0.0880580021
H	-6.29382245	2.2725387966	-1.3040172735
H	-2.0418907452	-2.3288349708	-0.3140180356
H	-2.6458436504	0.2503642691	0.1374098395
O	-2.7923862463	0.5766459891	-3.0569743172
H	-2.741346471	1.4001835221	-2.5524840346

Table S5. Calculated Cartesian Coordinates of the Stable Low-Energy Ring-Open Conformers of $[dUrd+H]^+$.

O4A_RO1'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-1.6967560968	-0.2323951219	0.1737337448
C	-1.7679198639	1.0515097575	0.8147993632
H	-2.6596206672	1.1151614701	1.4461528853
C	-0.5258725929	1.2055878253	1.6869306227
H	-0.5551753006	2.1908664522	2.1638914125
O	2.0779728889	1.463271073	-2.2329841994
C	2.145571405	1.6270291898	-1.0607410707
N	3.4687137748	1.1800010887	-0.418656613
C	4.0392545212	0.0778351906	-0.948123746
H	3.4920851978	-0.3706526443	-1.76792297
C	5.2227563982	-0.4485611685	-0.493078352
C	5.8513661271	0.2201269164	0.5603573743
O	6.9807713945	-0.1134519345	1.1389874257
N	5.2809634679	1.327673164	1.0662391689
C	4.0698465029	1.9040259914	0.6257189502
O	3.6428302784	2.9130581873	1.1094791357
C	0.8243346527	1.0344371133	0.9745353672
H	1.6020833507	1.1479925571	1.7350246249
C	1.074755024	2.1003145239	-0.1269252815
H	0.1996818541	2.2487419338	-0.7604629684
O	1.0089910888	-0.2705324271	0.4230508133
H	-1.8347568207	1.8449299882	0.0608172068
H	-2.4981147915	-0.4054114983	-0.3305137863
H	1.3560998976	3.0568776607	0.3190566015
H	5.6413594444	-1.3433663572	-0.9298473095
H	-0.5644650404	0.4617684254	2.4880509624
H	0.139395376	-0.6007127179	0.1384828323
H	5.7480361942	1.827249551	1.8194202066
H	7.3771968846	-0.91281849	0.7621901685

TA_RO1'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-3.0313809942	-0.0262267283	-2.7075378571
C	-2.8830803112	-0.8929641404	-1.5720748193
H	-1.86839271	-0.8254757319	-1.1679101625
C	-3.876395425	-0.4355681101	-0.5076387896
H	-3.7915171901	-1.1016185771	0.3575019478
O	-7.4622658944	-1.9096704092	-3.2376194074
C	-7.1893993024	-1.5342596714	-2.1523365801
N	-8.2463506846	-0.5987678299	-1.4932775377
C	-8.6021197568	0.532438655	-2.1783969371
H	-8.0375894583	0.7277665429	-3.0785594674
C	-9.5905595905	1.3436163976	-1.711371368

C	-10.2218614256	0.9470529049	-0.5113417126
O	-11.1790162617	1.7013581312	-0.0222279035
N	-9.8827162129	-0.1680856596	0.1407886199
C	-8.9187533508	-0.9066455482	-0.3605898393
O	-8.5558224238	-2.0312602466	0.2297612228
C	-5.3466479347	-0.365474943	-0.9471444928
H	-5.921288966	0.009158552	-0.0935843497
C	-5.9383620424	-1.7406798331	-1.3538644733
H	-5.2693711009	-2.3035902277	-2.0060225693
O	-5.5744547731	0.5668940477	-2.0040824697
H	-3.0566916274	-1.934570135	-1.8680607838
H	-2.3669141778	-0.2207055207	-3.3763124414
H	-6.1546570716	-2.349202459	-0.4714188072
H	-9.881411484	2.2479128481	-2.2256483052
H	-11.5320584503	1.3172655381	0.7967571248
H	-9.1108676808	-2.179810979	1.0119261122
H	-3.5930626774	0.5651075377	-0.1689945471
H	-4.7774127513	0.588298675	-2.5629893466

Ta_RO1'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	1.1060854351	2.39351594	-5.3356269114
C	0.2545960366	1.2430671024	-5.230888501
H	-0.1502527571	0.9736252406	-6.2110957586
C	1.1036752054	0.0873510405	-4.7091061833
H	0.4718807515	-0.8035645205	-4.6270815513
O	0.995482932	2.4835575526	-0.8751734243
C	1.42232521	1.382978842	-1.1230350518
N	2.619891861	0.9321873086	-0.400420852
C	3.0352019748	-0.3855865213	-0.4534813647
H	2.3844174324	-1.0677927531	-0.9753329957
C	4.1816810807	-0.7921824672	0.1347246823
C	4.9448854937	0.2132785271	0.7895100508
O	6.0821568563	-0.1344347189	1.338783911
N	4.5484180744	1.4723010717	0.8722636721
C	3.4139028288	1.8361803256	0.3122736433
O	3.0493588917	3.0691590981	0.4416253454
C	1.8163141148	0.3246251699	-3.369125609
H	2.4415004511	-0.5542756972	-3.1816114733
C	0.8231060254	0.4834930094	-2.16890952
H	-0.0884148486	0.9988066726	-2.4710138799
O	2.7035958576	1.4355759349	-3.3813613425
H	-0.5926000953	1.4603106661	-4.5684391732
H	0.6433637353	3.1270243415	-5.7535055196
H	0.5270620177	-0.4875458621	-1.7605193683
H	4.5090104858	-1.8213139868	0.106961835
H	6.5050566978	0.6376605954	1.7528876281
H	2.1642978569	3.2088218788	0.011647732
H	1.8771312378	-0.1383872702	-5.4489299913
H	2.3826382263	2.0789308494	-4.0384119788

O4A_RO4'	Coordinates (Angstrom)		
Atom	X	Y	Z

O	0.6955796885	1.6335044766	-0.0175165987
C	-0.0943437175	2.2593261249	0.952559823
H	0.2636114408	3.2810520915	1.124437522
C	-1.552740204	2.2976261327	0.5804975779
O	-1.9639894432	1.6966951193	-0.4001585273
C	-3.8063666829	4.0614838737	-0.6551015853
N	-5.0082445285	3.1754457123	-0.5817744985
C	-4.955195089	1.8909115851	-0.9816124326
H	-3.9722057549	1.5387380774	-1.2748031965
C	-6.0553187236	1.0595957633	-0.9847567958
C	-7.2667161041	1.6004300287	-0.5578043987
O	-8.427167492	0.9878833946	-0.493406544
N	-7.3039230255	2.8857185887	-0.1561843656
C	-6.2057669058	3.7653791819	-0.1280982776
O	-6.3008105502	4.900126362	0.2438460469
C	-2.5359674143	3.0863688234	1.4427204574
H	-3.3470293747	2.3876966026	1.6943726418
C	-3.112798538	4.3089512576	0.6876489641
H	-3.801674701	4.8259165465	1.3619607318
O	-1.854043686	3.501553131	2.6104196056
H	-0.0277262128	1.7573904595	1.9314276723
H	-2.2931688389	5.0073214125	0.4916571737
H	-5.973061334	0.0333307365	-1.3113386041
H	-4.1542797386	5.0133789816	-1.0555961756
H	-3.1364057049	3.6037103809	-1.3788104228
H	-2.4601312224	3.9261967241	3.2268207039
H	0.1194300099	1.1130661212	-0.5934410046
H	-8.3854569717	0.0668843657	-0.7896267831
H	-8.1878576203	3.2843105539	0.1512908106

TA_RO4'	Coordinates (Angstrom)		
Atom	X	Y	Z
O	-0.8522854709	-0.6872956642	-2.200657819
C	-1.6640857518	-0.1376940555	-1.2048297056
H	-1.4090572847	0.9180318481	-1.0583137091
C	-3.1350872115	-0.2623026919	-1.5157654422
O	-3.5197117952	-0.9389100568	-2.4553209828
C	-5.4136198756	1.4309517235	-2.7605005068
N	-6.6539907882	0.5920816235	-2.6781475153
C	-6.6085372731	-0.7507258514	-2.9530037614
H	-5.621807237	-1.1434324016	-3.1679328076
C	-7.7375805599	-1.5124051787	-2.9181087668
C	-8.9413394662	-0.8500019719	-2.5907802376
O	-10.0558190969	-1.5441461719	-2.5531676377
N	-8.9814451222	0.4551054422	-2.3189692631
C	-7.8582029295	1.1365427709	-2.3677294632
O	-7.8470139722	2.4300576236	-2.112620582
C	-4.1596390578	0.4805092555	-0.6516757269
H	-4.9605150732	-0.2353927897	-0.4235878048
C	-4.7449215919	1.6927185361	-1.4105384203
H	-5.4372395731	2.1924234946	-0.7292996464
O	-3.6028025434	1.0175831199	0.5341844244
H	-1.4969984777	-0.6202308821	-0.2263237275

H	-3.9335235905	2.4047651375	-1.5922563798
H	-7.7191088118	-2.5707264508	-3.1344094166
H	-10.8070981905	-0.9737987117	-2.3222643204
H	-8.7499792449	2.7314389422	-1.9231686713
H	-5.7056736403	2.3778616165	-3.2111357306
H	-4.7531651394	0.9137459936	-3.4529433714
H	-3.5736005199	0.3520680953	1.2295412384
H	-1.3794002107	-1.3116808149	-2.7178368966

Table S6. Important Geometric Parameters of Stable Low-Energy Ring-Closed Conformers of $[Urd+H]^+$.[a]

Conformer	χ (degrees)	*P* (degrees)	τ (degrees)	Nucleobase Orientation	Sugar Puckering
Ti	-171.6	172.0	-64.8	anti	C2'-endo
TA	-134.0	165.5	-63.4	anti	C2'-endo
TB	-157.6	16.7	-63.2	anti	C3'-endo
TC	51.1	151.2	-58.6	syn	C2'-endo
O4A	-132.4	166.0	-62.2	anti	C2'-endo
O4i	-163.4	12.3	-60.0	anti	C3'-endo
O4B	-160.4	14.0	-62.2	anti	C3'-endo
Tii	-131.0	168.1	-63.1	anti	C2'-endo
O4ii	-176.9	196.7	-58.8	anti	C3'-exo
O2i	-175.2	169.9	-66.2	anti	C2'-endo
Tiii	-159.6	13.2	-61.4	anti	C3'-endo
O2A	50.0	153.2	-57.4	syn	C2'-endo
O4iii	-130.6	175.8	-61.9	anti	C2'-endo
O4C	-132.0	166.2	-62.6	anti	C2'-endo
O4iv	-163.0	4.5	-60.2	anti	C3'-endo
O4D	-159.3	14.4	-62.5	anti	C3'-endo
O4v	-176.9	196.7	-59.1	anti	C3'-exo
O4E	-167.0	33.8	-170.3	anti	C3'-endo
O4vi	-129.5	168.9	-62.4	anti	C2'-endo
O4F	57.3	153.8	-73.4	syn	C2'-endo
TD	60.4	139.3	-66.6	syn	C2'-endo
O2B	-131.6	165.2	-64.5	anti	C2'-endo
O2ii	-127.2	167.7	-64.3	anti	C2'-endo
O2C	-152.0	20.6	-64.4	anti	C3'-endo
O2iii	-155.0	14.7	-62.5	anti	C3'-endo

[a]Dihedral angles are based on the designations of Hauser and Keese provided in reference 20 and defined as χ = ∠O4'C1'N1C2, $P = \arctan[\ (\nu_4 + \nu_1) - (\nu_3 + \nu_0)/2\nu_2(\sin 36° + \sin 72°)\ ]$ where ν_0=∠C4'O4'C1'C2', ν_1=∠O4'C1'C2'C3', ν_2=∠C1'C2'C3'C4', ν_3=∠C2'C3'C4'O4', and ν_4=∠C3'C4'O4'C1', and τ = ∠O5'C5'C4'O4'.

Table S7. Important Geometric Parameters of Stable Low-Energy Ring-Closed Conformers of $[dUrd+H]^+$.[a]

Conformer	χ (degrees)	*P* (degrees)	τ (degrees)	Nucleobase Orientation	Sugar Puckering
O4A	-144.1	168.1	-60.5	anti	C2'-endo
O4B	-161.0	11.9	-61.6	anti	C3'-endo
TA	-135.4	167.0	-62.9	anti	C2'-endo
TB	-157.8	14.0	-63.0	anti	C3'-endo
TC	52.5	154.4	-57.9	syn	C2'-endo
O2A	52.5	154.3	-57.9	syn	C2'-endo
O4C	-160.1	12.2	-61.9	anti	C3'-endo
O4D	-141.3	168.1	-61.2	anti	C2'-endo
O4E	-167.6	33.7	-170.9	anti	C3'-endo
O4F	60.5	155.6	-73.2	syn	C2'-endo
TD	62.1	142.8	-65.8	syn	C2'-endo
O2B	-126.7	167.3	-65.1	anti	C2'-endo
O2a	-121.0	168.5	-65.7	anti	C2'-endo
O2C	-153.2	16.1	-64.2	anti	C3'-endo
O2b	-153.6	16.6	-64.2	anti	C3'-endo

[a]Dihedral angles are based on the designations of Hauser and Keese provided in reference 20 and defined as χ = ∠O4'C1'N1C2, P = arctan[$(\nu_4 + \nu_1) - (\nu_3 + \nu_0)/2\nu_2(\sin 36° + \sin 72°)$] where ν_0=∠C4'O4'C1'C2', ν_1=∠O4'C1'C2'C3', ν_2=∠C1'C2'C3'C4', ν_3=∠C2'C3'C4'O4', and ν_4=∠C3'C4'O4'C1', and τ = ∠O5'C5'C4'O4'.

Figure Captions

Figure S1. B3LYP/6-311+G(d,p) stable low-energy ring-closed conformers of $[Urd+H]^+$ and their relative Gibbs free energies at 298 K calculated at the B3LYP/6-311+G(2d,2p) (shown in black) and MP2(full)/6-311+G(2d,2p) (shown in red) levels of theory. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer.

Figure S2. B3LYP/6-311+G(d,p) stable low-energy ring-closed conformers of $[dUrd+H]^+$ and their relative Gibbs free energies at 298 K calculated at the B3LYP/6-311+G(2d,2p) (shown in black) and MP2(full)/6-311+G(2d,2p) (shown in red) levels of theory. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer.

Figure S3. B3LYP/6-311+G(d,p) stable low-energy sugar ring-open conformers of $[Urd+H]^+$ and $[dUrd+H]^+$ and their relative Gibbs free energies at 298 K calculated at the B3LYP/6-311+G(2d,2p) (shown in black) and MP2(full)/6-311+G(2d,2p) (shown in red) levels of theory.

Figure S4. Comparison of the measured IRMPD action spectrum of $[Urd+H]^+$ with the theoretical linear IR spectra for the **TB**, **O4i**, **Tii** and **O4iii** conformers of $[Urd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer. To facilitate comparisons, the measured IRMPD

spectrum is overlaid with each theoretical spectrum and scaled to match the intensity of the most intense computed band in both IR fingerprint and hydrogen-stretching regions.

Figure S5. Comparison of the measured IRMPD action spectrum of $[Urd+H]^+$ with the theoretical linear IR spectra for the **O2i**, **Tiii**, **O2A**, **O4C**, **O4iv**, **O4D** and **O4v** conformers of $[Urd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer. To facilitate comparisons, the measured IRMPD spectrum is overlaid with each theoretical spectrum and scaled to match the intensity of the most intense computed band in both IR fingerprint and hydrogen-stretching regions.

Figure S6. Comparison of the measured IRMPD action spectrum of $[Urd+H]^+$ with the theoretical linear IR spectra for the **O4E**, **O4vi**, **O4F**, **O2B**, **O2ii**, **O2C**, and **O2iii** conformers of $[Urd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer. To facilitate comparisons, the measured IRMPD spectrum is overlaid with each theoretical spectrum and scaled to match the intensity of the most intense computed band in both IR fingerprint and hydrogen-stretching regions.

Figure S7. Comparison of the measured IRMPD action spectrum of $[Urd+H]^+$ with the theoretical linear IR spectra for the stable low-energy ring-open conformers of $[Urd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K.

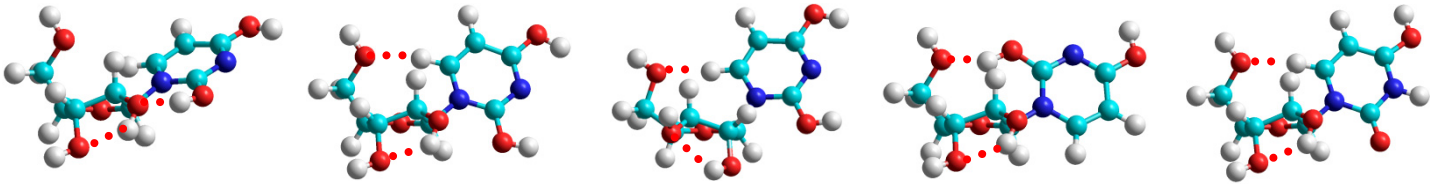
Figure S8. Comparison of the measured IRMPD action spectrum of $[dUrd+H]^+$ with the theoretical linear IR spectra for the **O2A**, **O4C**, **O4D**, **O4E**, **O4F** and **O2B**, **O2a**, **O2C and O2b** conformers of $[dUrd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K. The site of protonation, nucleobase orientation, and sugar puckering are also indicated for each conformer. To facilitate comparisons, the measured IRMPD spectrum is overlaid with each theoretical spectrum and scaled to match the intensity of the most intense computed band in both IR fingerprint and hydrogen-stretching regions.

Figure S9. Comparison of the measured IRMPD action spectrum of $[dUrd+H]^+$ with the theoretical linear IR spectra for the stable low-energy ring-open conformers of $[dUrd+H]^+$ and the corresponding optimized structures calculated at B3LYP/6-311+G(d,p) level of theory. Also shown in black are the B3LYP/6-311+G(2d,2p) and in red the MP2(full)/6-311+G(2d,2p) relative Gibbs free energies at 298 K.

Figure S10. Comparison of the measured IRMPD action spectrum of $[Urd+H]^+$ (in grey) with the linear IR spectra based on a statistically weighted averages of the calculated IR spectra of the **Ti**, **TA**, **TB**, **TC**, **O4A**, **O4i**, **O4B**, **Tii, O4ii**, **O4iii**, and **TD** conformers of $[Urd+H]^+$ using their relative Maxwell-Boltzmann populations at room temperature calculated at the B3LYP/6-311+G(2d,2p) (in black) and MP2(full)/6-311+G(2d,2p) (in red) levels of theory as well as least squares fitting (in blue).

Figure S11. Comparison of the measured IRMPD action spectrum of $[dUrd+H]^+$ (in grey) with the linear IR spectra based on a statistically weighted averages of the calculated IR spectra of the **O4A**, **O4B**, **TA**, **TB**, **TC**, and **TD** conformers of $[dUrd+H]^+$ using their relative Maxwell-Boltzmann populations at room temperature calculated at the B3LYP/6-311+G(2d,2p) (in black) and MP2(full)/6-311+G(2d,2p) (in red) levels of theory as well as least squares fitting (in blue).

Figure S1.



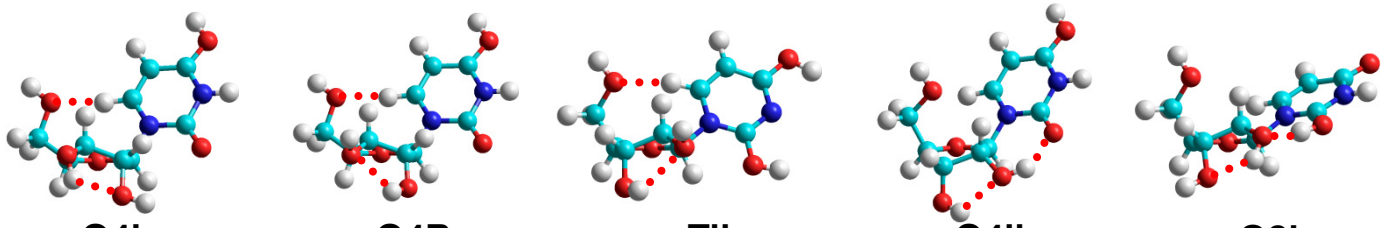
Ti
anti, C2'-endo
0.0, 0.0 kJ/mol

TA
anti, C2'-endo
0.2, 0.3 kJ/mol

TB
anti, C3'-endo
2.5, 3.2 kJ/mol

TC
syn, C2'-endo
2.9, 2.2 kJ/mol

O4A
anti, C2'-endo
2.9, 10.1 kJ/mol



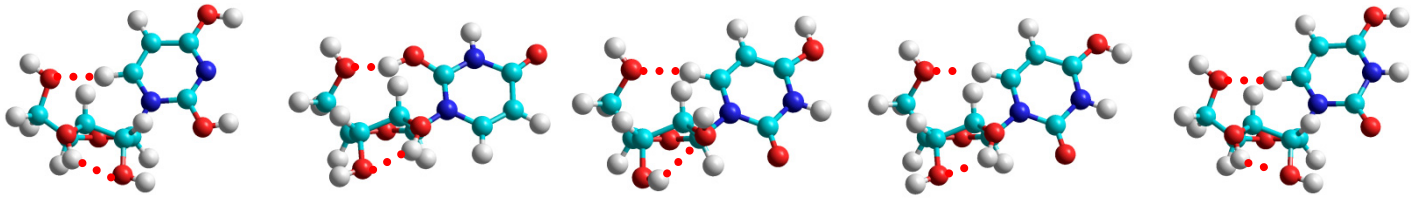
O4i
anti, C3'-endo
3.0, 10.1 kJ/mol

O4B
anti, C3'-endo
4.4, 11.4 kJ/mol

Tii
anti, C2'-endo
5.5, 4.2 kJ/mol

O4ii
anti, C3'-exo
6.4, 11.0 kJ/mol

O2i
anti, C2'-endo
8.0, 8.6 kJ/mol



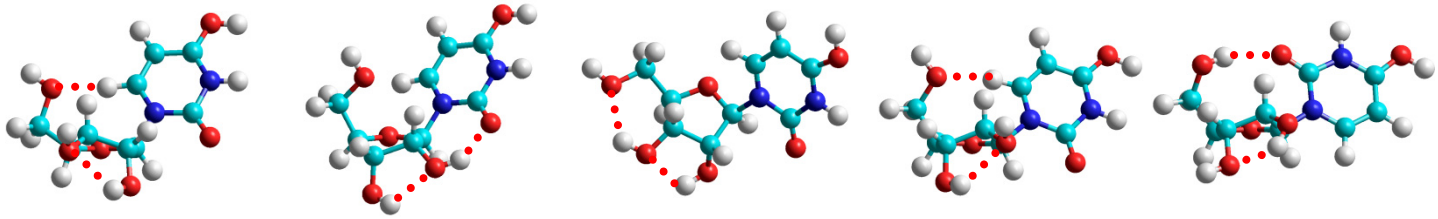
Tiii
anti, C3'-endo
8.1, 8.1 kJ/mol

O2A
syn, C2'-endo
9.0, 8.8 kJ/mol

O4iii
anti, C2'-endo
9.6, 15.5 kJ/mol

O4C
anti, C2'-endo
13.8, 21.1 kJ/mol

O4iv
anti, C3'-endo
15.1, 22.6 kJ/mol



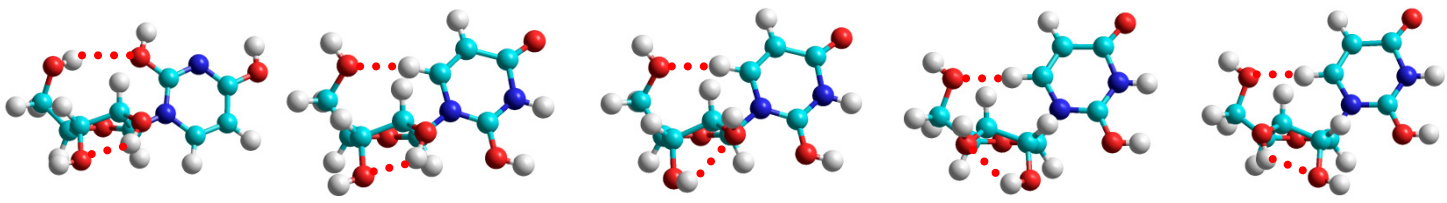
O4D
anti, C3'-endo
15.8, 23.3 kJ/mol

O4v
anti, C3'-exo
18.5, 23.4 kJ/mol

O4E
anti, C3'-endo
20.3, 28.3 kJ/mol

O4vi
anti, C2'-endo
20.4, 26.3 kJ/mol

O4F
syn, C2'-endo
21.9, 30.2 kJ/mol



TD
syn, C2'-endo
26.8, 29.5 kJ/mol

O2B
anti, C2'-endo
42.0, 41.6 kJ/mol

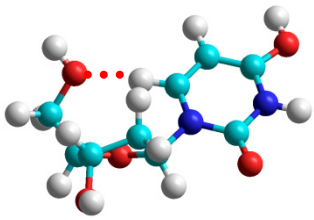
O2ii
anti, C2'-endo
47.2, 45.1 kJ/mol

O2C
anti, C3'-endo
47.2, 49.3 kJ/mol

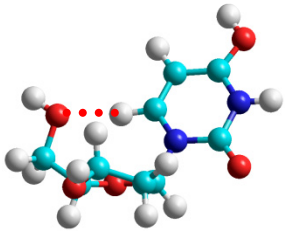
O2iii
anti, C3'-endo
56.6, 57.6 kJ/mol

$[Urd+H]^+$

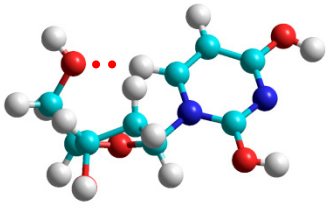
Figure S2.



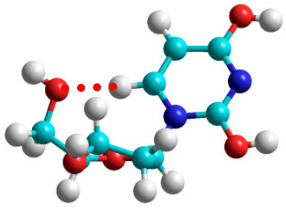
O4A
anti, C2'-endo
0.4, 7.4 kJ/mol



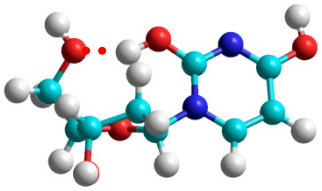
O4B
anti, C3'-endo
0.0, 8.6 kJ/mol



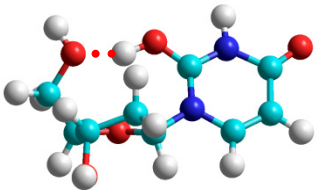
TA
anti, C2'-endo
0.7, 0.0 kJ/mol



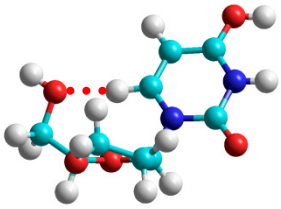
TB
anti, C3'-endo
1.7, 3.3 kJ/mol



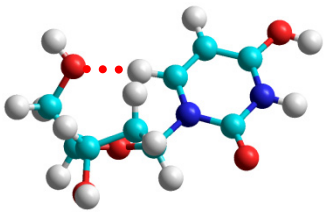
TC
syn, C2'-endo
4.3, 2.0 kJ/mol



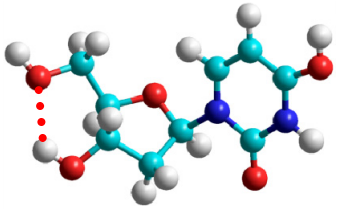
O2A
syn, C2'-endo
8.8, 7.2 kJ/mol



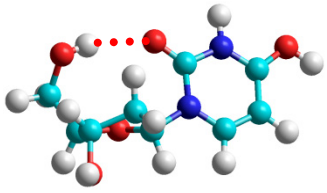
O4C
anti, C3'-endo
11.9, 21.0 kJ/mol



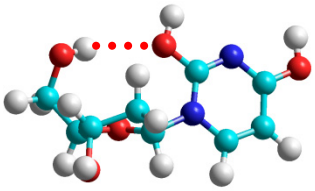
O4D
anti, C2'-endo
12.3, 19.5 kJ/mol



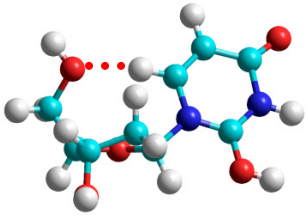
O4E
anti, C3'-endo
17.3, 27.3 kJ/mol



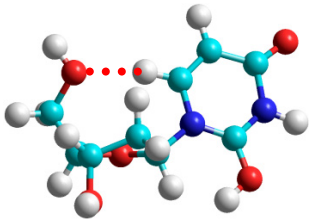
O4F
syn, C2'-endo
30.0, 36.9 kJ/mol



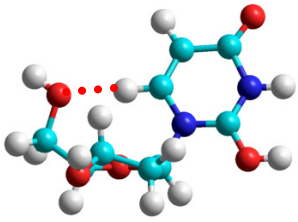
TD
syn, C2'-endo
33.7, 34.6 kJ/mol



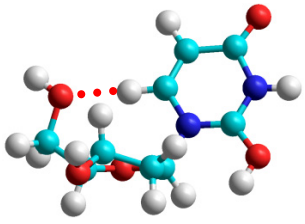
O2B
anti, C2'-endo
45.4, 44.1 kJ/mol



O2a
anti, C2'-endo
46.4, 44.8 kJ/mol



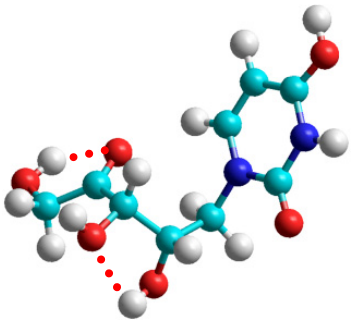
O2C
anti, C3'-endo
48.2, 51.0 kJ/mol



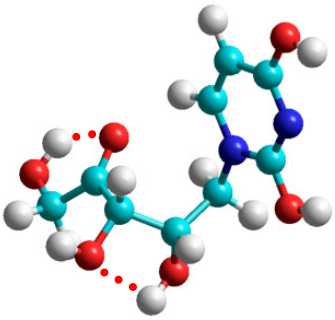
O2b
anti, C3'-endo
53.6, 56.5 kJ/mol

$[dUrd+H]^+$

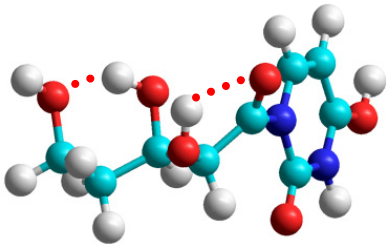
Figure S3.



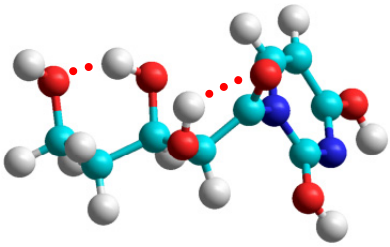
O4A_RO4'
-13.9, 11.6 kJ/mol



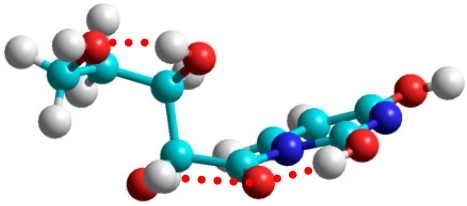
TA_RO4'
-12.8, 5.6 kJ/mol



O4A_RO1'
-7.7, 7.9 kJ/mol

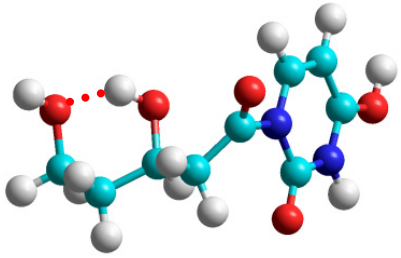


TA_RO1'
-4.5, 3.7 kJ/mol

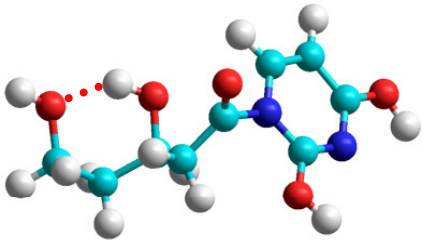


Ti_RO1'
0.9, 15.8 kJ/mol

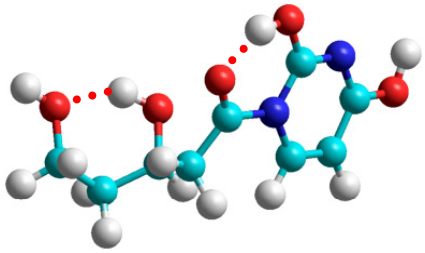
$[Urd+H]^+$



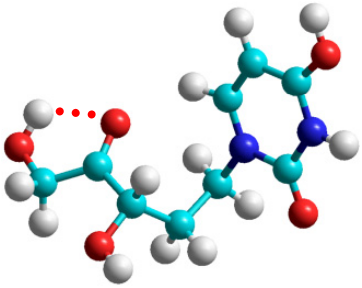
O4A_RO1'
-26.2, -12.1 kJ/mol



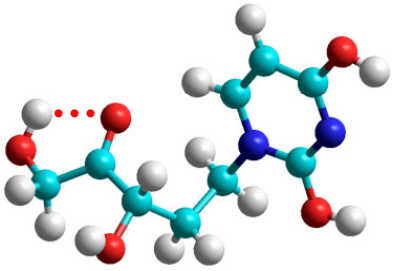
TA_RO1'
-22.0, -15.9 kJ/mol



Ta_RO1'
-15.5, -1.6 kJ/mol



O4A_RO4'
-15.4, -11.3 kJ/mol



TA_RO4'
-14.5, 4.6 kJ/mol

$[dUrd+H]^+$

Figure S4.

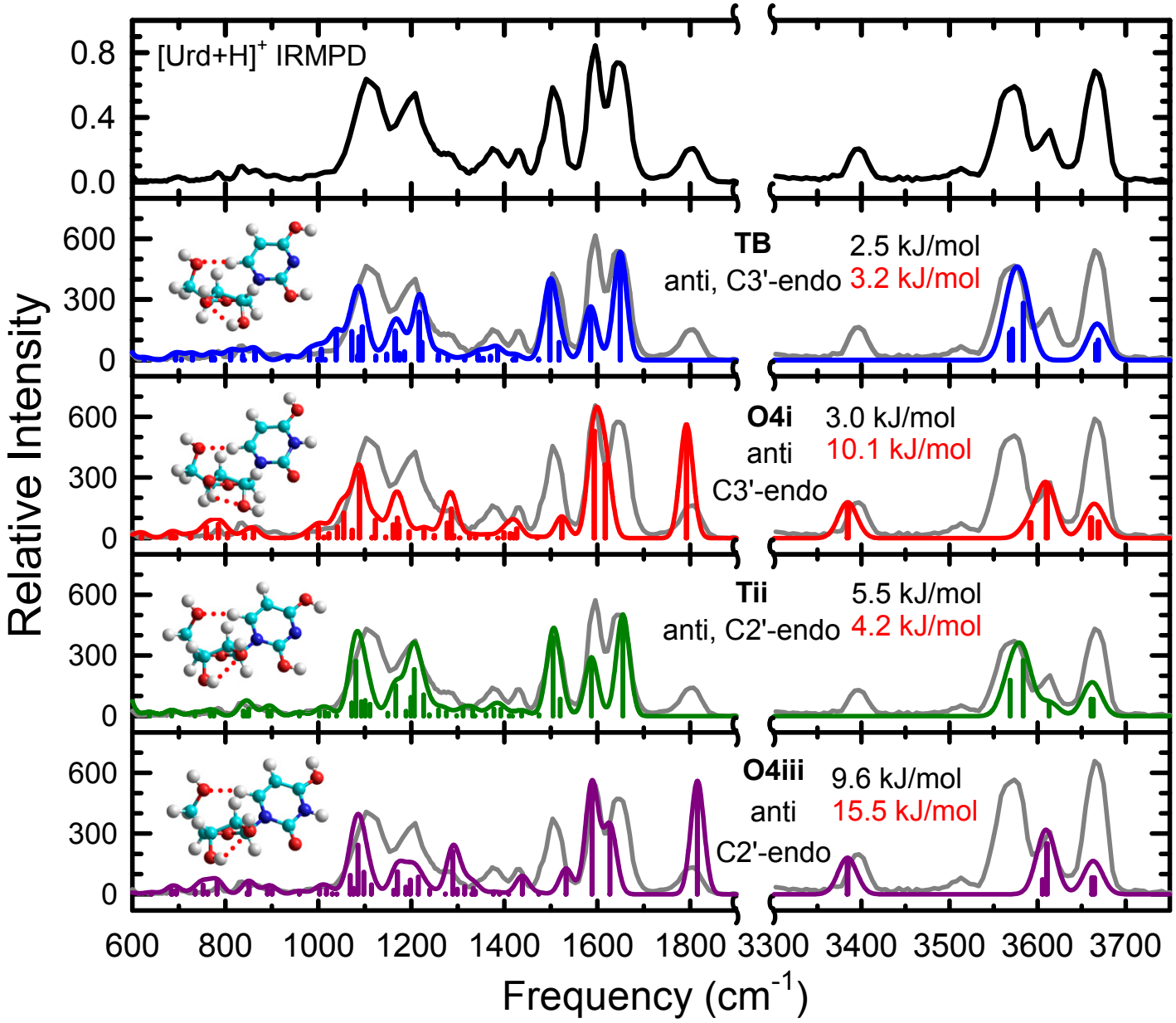

[Urd+H]+ IRMPD
0.8
0.4
0.0
TB
anti, C3'-endo
2.5 kJ/mol
3.2 kJ/mol
O4i
anti
C3'-endo
3.0 kJ/mol
10.1 kJ/mol
Tii
anti, C2'-endo
5.5 kJ/mol
4.2 kJ/mol
O4iii
anti
C2'-endo
9.6 kJ/mol
15.5 kJ/mol
600
300
0
Relative Intensity
600 800 1000 1200 1400 1600 1800 3300 3400 3500 3600 3700
Frequency (cm-1)

Figure S5.

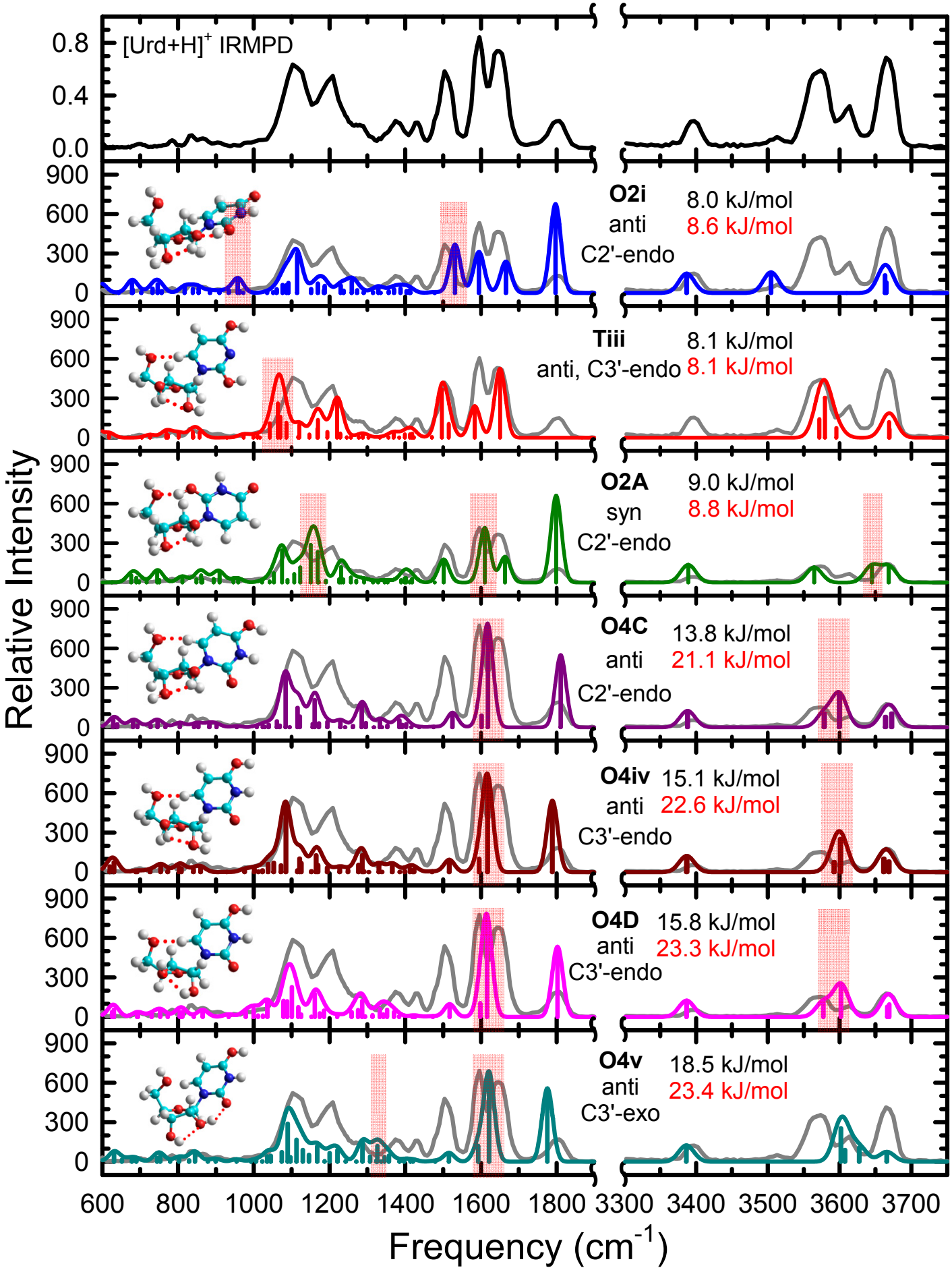

[Urd+H]+ IRMPD
O2i
anti
C2'-endo
8.0 kJ/mol
8.6 kJ/mol
Tiii
anti, C3'-endo
8.1 kJ/mol
8.1 kJ/mol
O2A
syn
C2'-endo
9.0 kJ/mol
8.8 kJ/mol
O4C
anti
C2'-endo
13.8 kJ/mol
21.1 kJ/mol
O4iv
anti
C3'-endo
15.1 kJ/mol
22.6 kJ/mol
O4D
anti
C3'-endo
15.8 kJ/mol
23.3 kJ/mol
O4v
anti
C3'-exo
18.5 kJ/mol
23.4 kJ/mol
Relative Intensity
Frequency (cm-1)

Figure S6.

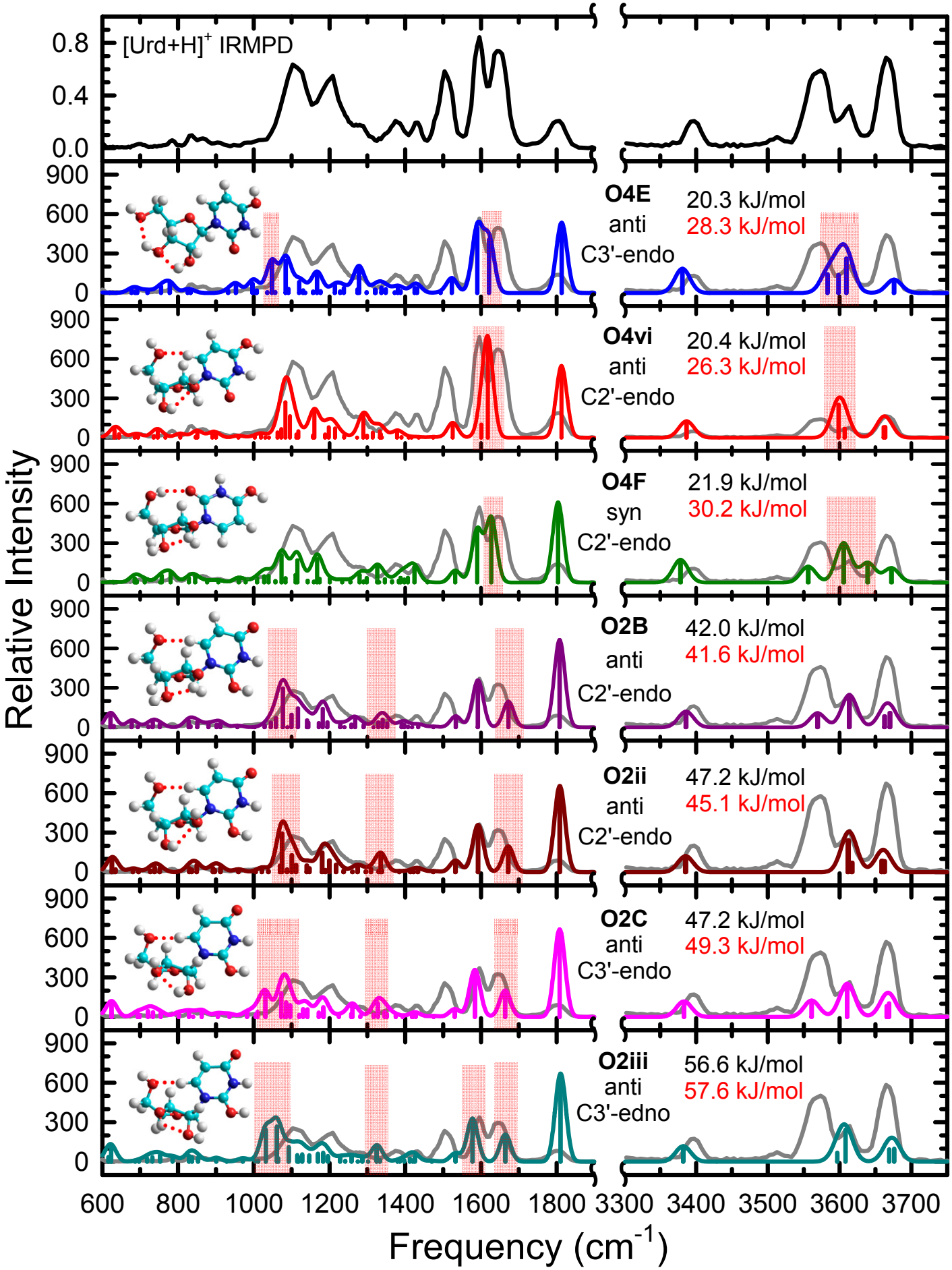

[Urd+H]+ IRMPD
O4E
anti
C3'-endo
20.3 kJ/mol
28.3 kJ/mol
O4vi
anti
C2'-endo
20.4 kJ/mol
26.3 kJ/mol
O4F
syn
C2'-endo
21.9 kJ/mol
30.2 kJ/mol
O2B
anti
C2'-endo
42.0 kJ/mol
41.6 kJ/mol
O2ii
anti
C2'-endo
47.2 kJ/mol
45.1 kJ/mol
O2C
anti
C3'-endo
47.2 kJ/mol
49.3 kJ/mol
O2iii
anti
C3'-edno
56.6 kJ/mol
57.6 kJ/mol
Relative Intensity
Frequency (cm-1)

Figure S7.

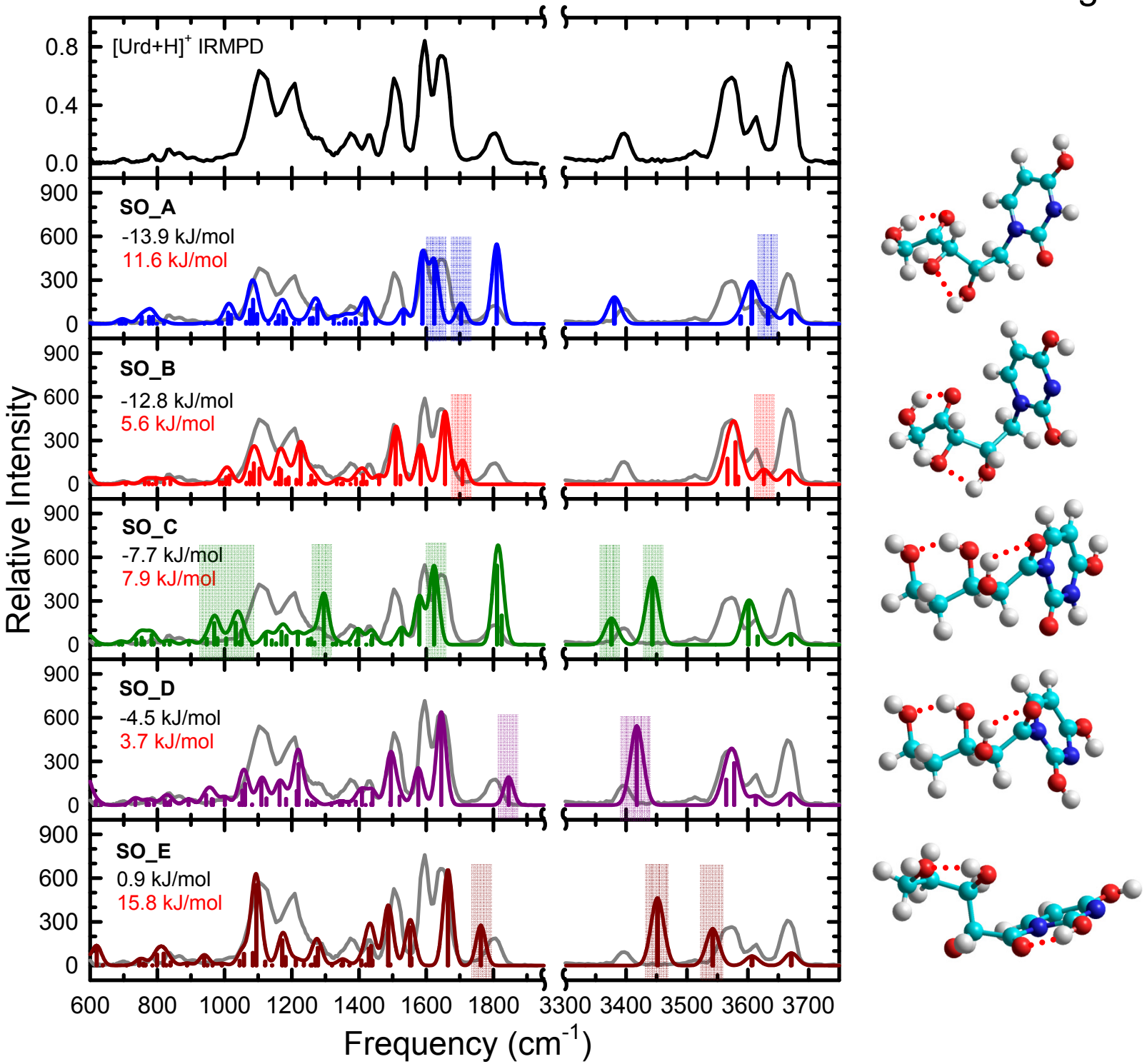

[Urd+H]+ IRMPD
SO_A
-13.9 kJ/mol
11.6 kJ/mol
SO_B
-12.8 kJ/mol
5.6 kJ/mol
SO_C
-7.7 kJ/mol
7.9 kJ/mol
SO_D
-4.5 kJ/mol
3.7 kJ/mol
SO_E
0.9 kJ/mol
15.8 kJ/mol
Relative Intensity
Frequency (cm-1)

Figure S8.

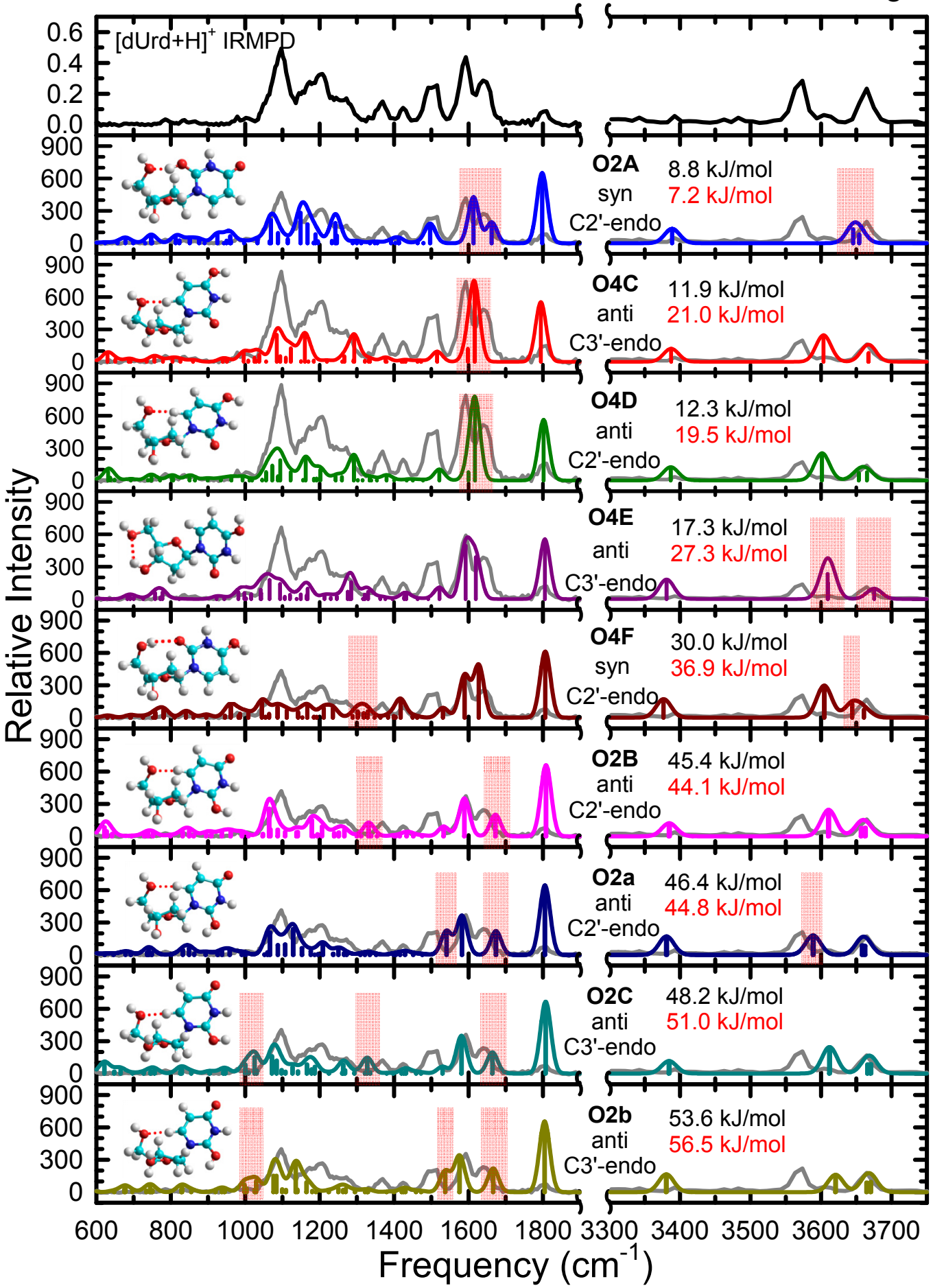
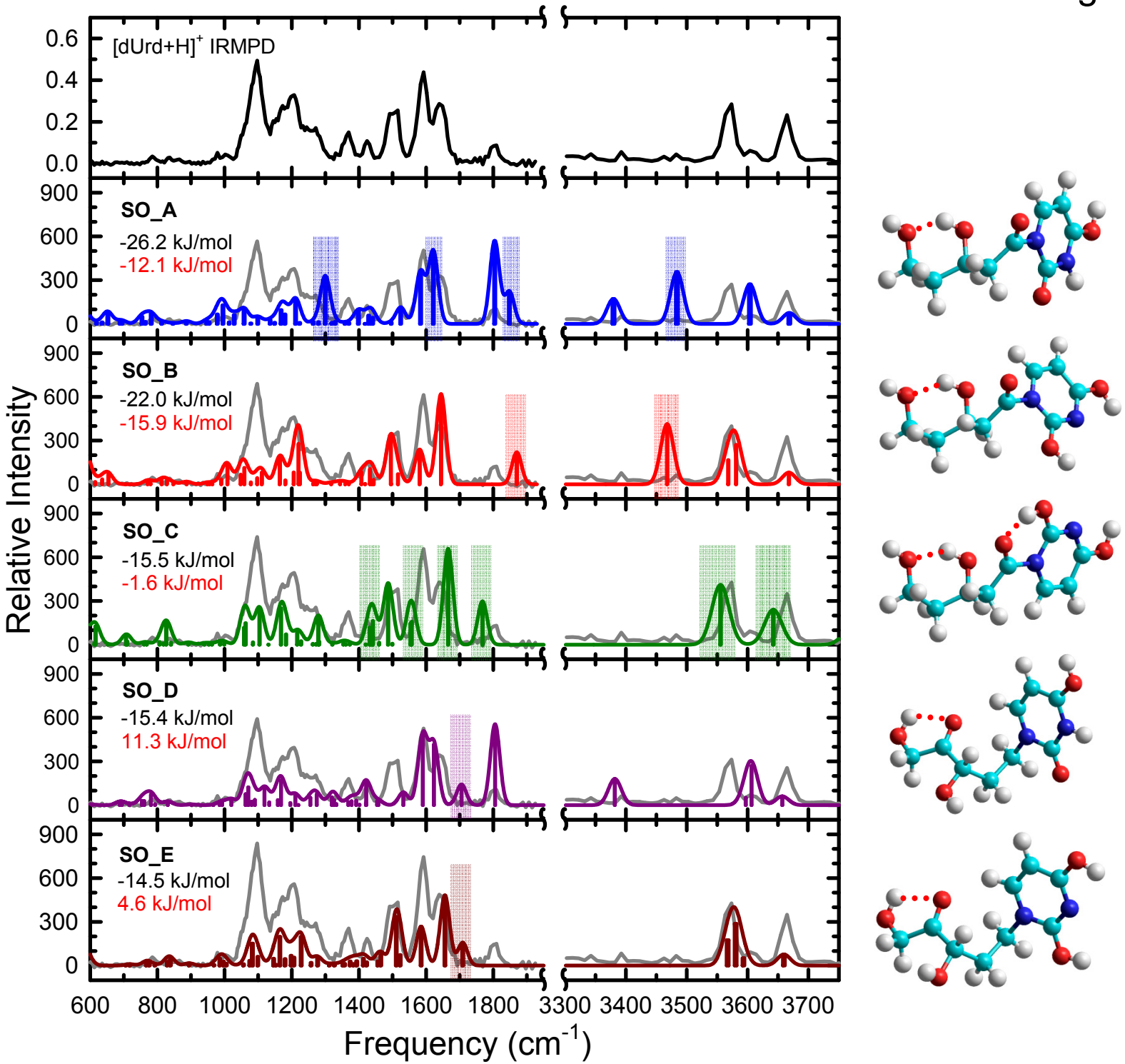
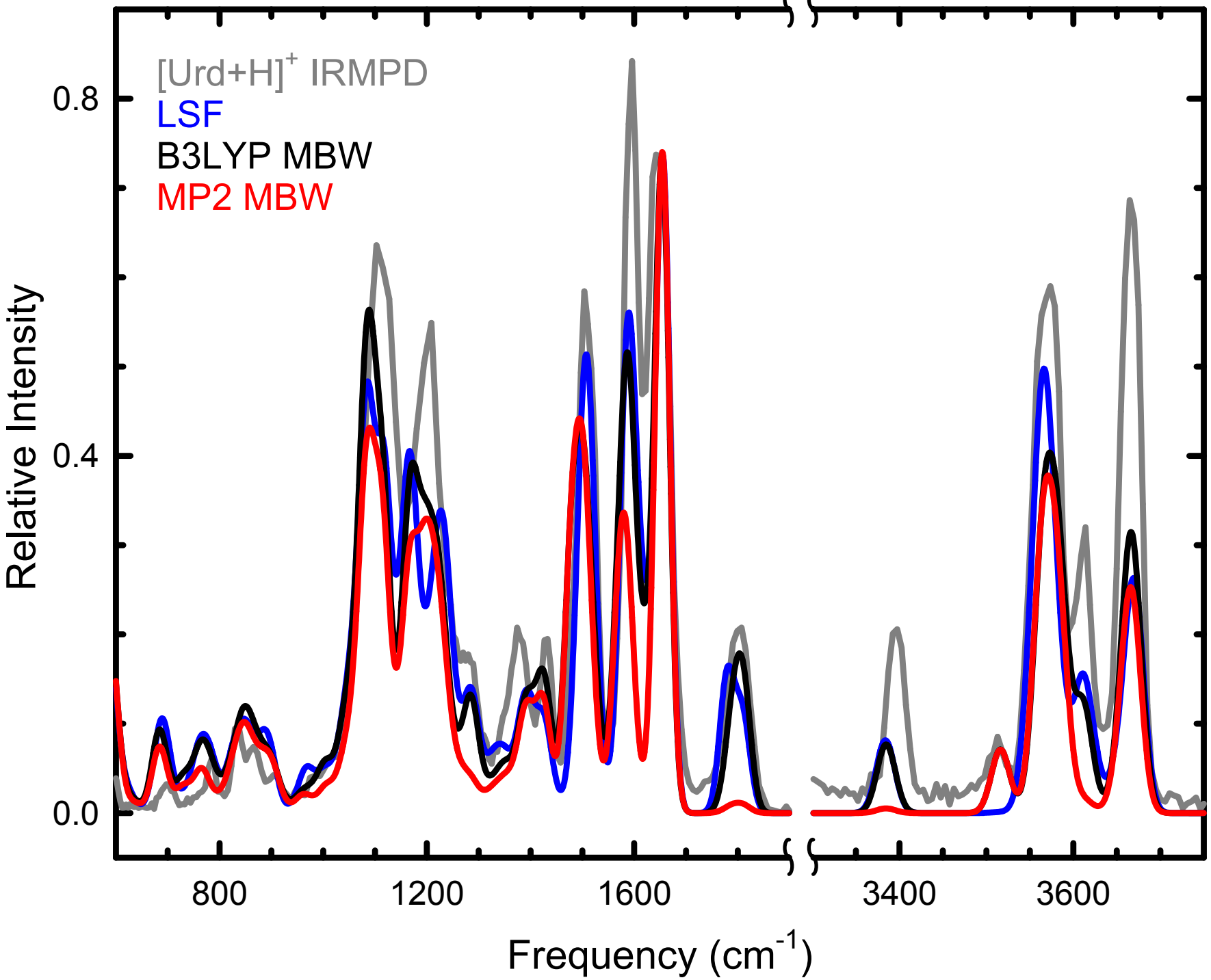
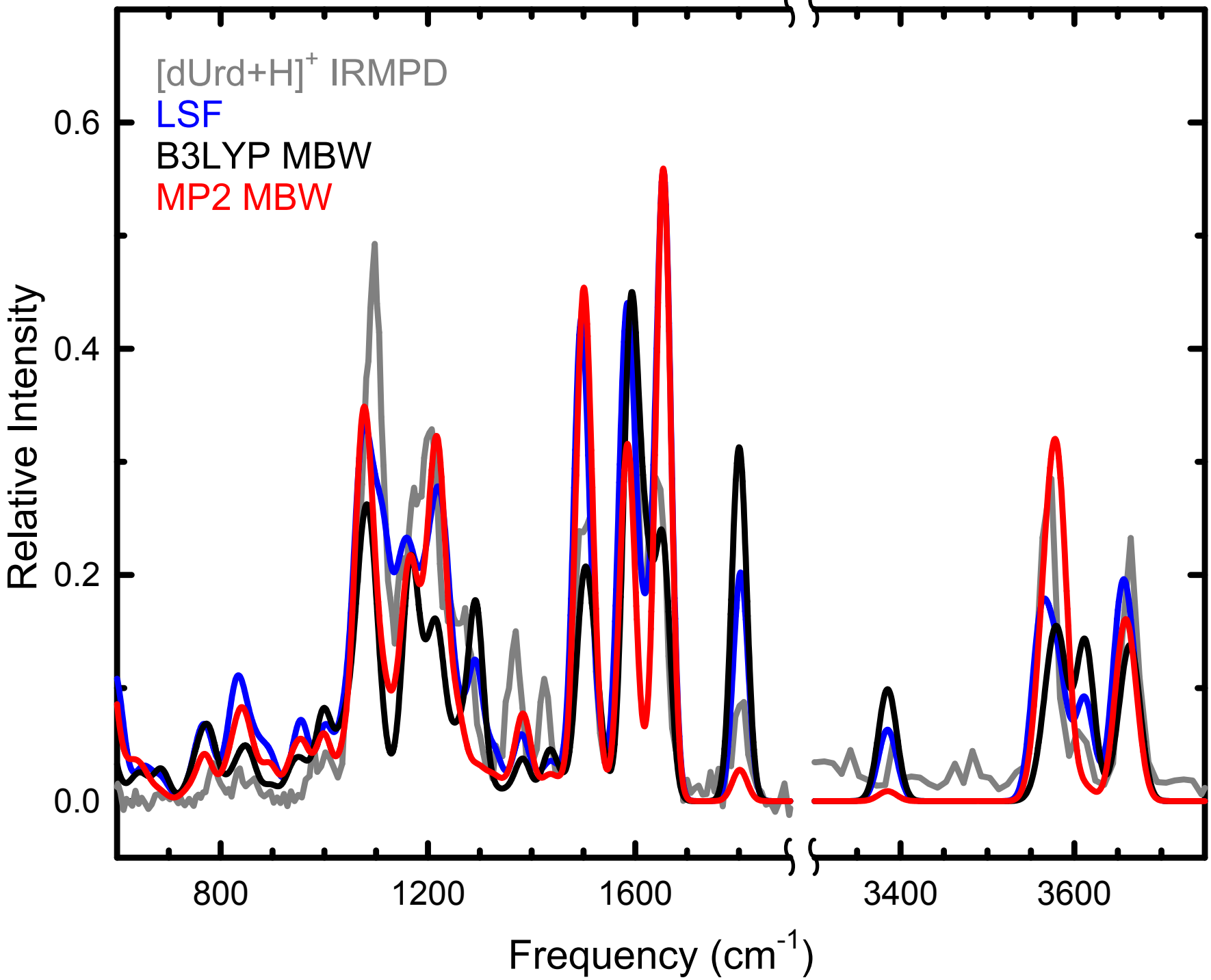

[dUrd+H]+ IRMPD
O2A
syn
C2'-endo
8.8 kJ/mol
7.2 kJ/mol
O4C
anti
C3'-endo
11.9 kJ/mol
21.0 kJ/mol
O4D
anti
C2'-endo
12.3 kJ/mol
19.5 kJ/mol
O4E
anti
C3'-endo
17.3 kJ/mol
27.3 kJ/mol
O4F
syn
C2'-endo
30.0 kJ/mol
36.9 kJ/mol
O2B
anti
C2'-endo
45.4 kJ/mol
44.1 kJ/mol
O2a
anti
C2'-endo
46.4 kJ/mol
44.8 kJ/mol
O2C
anti
C3'-endo
48.2 kJ/mol
51.0 kJ/mol
O2b
anti
C3'-endo
53.6 kJ/mol
56.5 kJ/mol
Relative Intensity
Frequency (cm-1)

Figure S9.


[dUrd+H]+ IRMPD
SO_A
-26.2 kJ/mol
-12.1 kJ/mol
SO_B
-22.0 kJ/mol
-15.9 kJ/mol
SO_C
-15.5 kJ/mol
-1.6 kJ/mol
SO_D
-15.4 kJ/mol
11.3 kJ/mol
SO_E
-14.5 kJ/mol
4.6 kJ/mol
Relative Intensity
Frequency (cm-1)


[Urd+H]+ IRMPD
LSF
B3LYP MBW
MP2 MBW
Relative Intensity
0.8
0.4
0.0
800
1200
1600
3400
3600
Frequency (cm-1)


[dUrd+H]+ IRMPD
LSF
B3LYP MBW
MP2 MBW
Relative Intensity
0.0
0.2
0.4
0.6
800
1200
1600
3400
3600
Frequency (cm-1)