
Hydrogen Bonding and Structure of Uracil-water and Thymine-water Complexes

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TABLES OF SUPPLEMENTARY DATA

Table S1. Observed frequencies (in MHz) and residuals for the rotational transitions of the parent species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{cal.}}$
3	0	3	2	0	2	2	5	2	4	5202.414	0.000
						1	3	1	2	5202.429	0.003
						1	2	1	1	5202.480	0.005
						0	3	0	2	5202.509	0.002
						2	4	2	3	5202.509	-0.001
						1	4	1	3	5202.541	0.002
						2	3	2	2	5202.683	0.002
3	1	2	2	1	1	0	3	0	2	5544.454	0.002
						1	3	1	2	5544.530	0.003
						2	5	2	4	5544.618	0.000
						1	4	1	3	5544.704	-0.001
						2	4	2	3	5544.784	0.000
						2	3	2	2	5544.799	0.002
						1	3	1	2	7452.498	0.002
3	1	3	2	0	2	0	3	0	2	7452.550	-0.001
						2	5	2	4	7452.652	0.001
						1	4	1	3	7453.257	0.000
						1	2	1	1	7453.335	-0.001
						2	4	2	3	7453.462	0.001
						2	3	2	2	7454.055	0.001
						2	6	2	5	6886.688	0.001
4	0	4	3	0	3	1	4	1	3	6886.688	-0.000
						1	5	1	4	6886.830	0.003
						0	4	0	3	6886.722	0.000
						1	3	1	2	6886.800	0.000
						2	5	2	4	6886.814	0.000
						2	4	2	3	6886.974	0.001
						2	6	2	5	6567.055	-0.000
4	1	4	3	1	3	1	4	1	3	6567.098	0.001
						2	5	2	4	6567.126	0.000
						0	4	0	3	6567.146	-0.002
						1	5	1	4	6567.203	0.000
						2	4	2	3	6567.320	0.003
						0	4	0	3	7378.996	-0.001
						1	4	1	3	7379.022	-0.002
4	1	3	3	1	2	2	6	2	5	7379.058	-0.003
						1	5	1	4	7379.127	-0.002
						2	5	2	4	7379.140	-0.002
						2	4	2	3	7379.187	-0.002
						1	4	1	3	8817.166	-0.002
						0	4	0	3	8817.192	0.001
						2	6	2	5	8817.292	0.000
4	1	4	3	0	3	1	5	1	4	8817.920	-0.000
						1	3	1	2	8817.980	0.000
						2	5	2	4	8818.074	-0.002
						2	4	2	3	8818.690	0.000
						1	5	1	4	8532.394	0.001
						0	5	0	4	8532.413	0.002
						2	3	2	2	8532.419	0.001
5	0	5	4	0	4	1	4	1	3	8532.530	-0.004
						2	6	2	5	8532.544	0.000
						1	6	1	5	8532.554	0.001
						2	4	2	3	8532.583	-0.002
						2	5	2	4	8532.711	0.000
						1	5	1	4	8190.623	-0.001
						5	1	5	4	8190.623	-0.001

2	6	2	5	8190.637	-0.005
1	4	1	3	8190.651	0.000
1	6	1	5	8190.704	0.001
2	5	2	4	8190.778	0.001
2	4	2	3	8190.806	-0.002

Table S2. Observed frequencies (in MHz) and residuals for the rotational transitions of C₄N₂O₂H₄-H₂¹⁸O species of uracil-water complex.

J'	K' ₋₁	K' ₊₁	J''	K'' ₋₁	K'' ₊₁	I'	F'	I''	F''	V _{obs.}	V _{obs.} -V _{cal.}
3	0	3	2	0	2	2	5	2	4	4987.018	0.000
						0	3	0	2	4987.111	-0.002
						2	4	2	3	4987.115	0.007
						1	4	1	3	4987.137	0.004
						2	3	2	2	4987.268	0.001
3	1	3	2	0	2	0	3	0	2	7309.703	0.000
						2	5	2	4	7309.807	0.002
						1	4	1	3	7310.412	-0.001
						2	4	2	3	7310.623	0.003
						2	3	2	2	7311.213	0.001
3	1	2	2	1	1	0	3	0	2	5298.444	-0.004
						1	3	1	2	5298.522	0.001
						2	5	2	4	5298.610	-0.001
						1	4	1	3	5298.695	0.004
						2	4	2	3	5298.774	-0.003
4	0	4	3	0	3	2	3	2	2	5298.786	0.002
						2	6	2	5	6607.438	-0.002
						1	4	1	3	6607.438	-0.004
						1	5	1	4	6607.570	0.001
						0	4	0	3	6607.474	-0.002
4	1	4	3	1	3	1	3	1	2	6607.554	0.008
						2	5	2	4	6607.570	0.012
						2	4	2	3	6607.704	-0.001
						2	6	2	5	6306.480	-0.003
						2	5	2	4	6306.546	-0.007
4	1	3	3	1	2	0	4	0	3	6306.572	-0.003
						1	5	1	4	6306.626	0.001
						2	4	2	3	6306.739	0.001
						1	4	1	3	7053.338	-0.003
						2	6	2	5	7053.376	-0.003
4	1	4	3	0	3	1	5	1	4	7053.440	-0.001
						2	4	2	3	7053.497	-0.002
						2	6	2	5	8629.270	0.001
						1	5	1	4	8629.901	-0.003
						1	3	1	2	8629.968	0.002
						2	5	2	4	8630.061	-0.004
						2	4	2	3	8630.681	-0.002

Table S3. Observed frequencies (in MHz) and residuals for the rotational transitions of $C_4^{15}N_2O_2H_4-H_2O$ species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	2	1	0	1	5956.717	0.001
3	0	3	2	0	2	5185.359	0.002
3	1	3	2	1	2	4916.744	-0.001
3	1	2	2	1	1	5529.610	0.000
3	1	3	2	0	2	7397.912	0.000
4	0	4	3	0	3	6862.892	0.000
4	1	4	3	1	3	6543.377	0.001
4	1	3	3	1	2	7358.716	-0.001
4	1	4	3	0	3	8755.930	-0.001
5	0	5	4	0	4	8501.205	-0.001
5	1	5	4	1	4	8160.586	-0.001
5	0	5	4	1	4	6608.166	-0.000
6	0	6	5	0	5	10098.763	-0.001
6	1	6	5	1	5	9767.308	0.002

Table S4. Observed frequencies (in MHz) and residuals for the rotational transitions of $C_4^{15}N_2O_2H_4-H_2^{18}O$ species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
3	0	3	2	0	2	4971.278	0.002
3	1	2	2	1	1	5284.715	0.001
3	1	3	2	0	2	7256.651	-0.002
4	0	4	3	0	3	6585.558	0.001
4	1	4	3	1	3	6284.528	-0.001
4	1	3	3	1	2	7034.571	-0.001
4	1	4	3	0	3	8569.908	0.003
5	0	5	4	0	4	8166.256	-0.002
5	1	5	4	1	4	7839.898	0.000

Table S5. Observed frequencies (in MHz) and residuals for the rotational transitions of $C_4^{15}N_2O_2H_4-D_0H_wO$ species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
3	0	3	2	0	2	5099.323	0.002
3	1	2	2	1	1	5431.438	-0.004
3	1	3	2	0	2	7336.088	-0.000
4	0	4	3	0	3	6751.377	-0.001
4	1	4	3	1	3	6439.096	-0.000
4	1	3	3	1	2	7228.777	0.004
4	1	4	3	0	3	8675.863	0.001
5	0	5	4	0	4	8366.423	-0.000
5	1	5	4	1	4	8031.370	0.002
6	0	6	5	0	5	9942.550	-0.002

Table S6. Observed frequencies (in MHz) and residuals for the rotational transitions of $C_4^{15}N_2O_2H_4-H_0D_wO$ species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	2	1	0	1	5885.745	-0.001
3	0	3	2	0	2	5019.235	-0.001
3	1	3	2	0	2	7288.716	0.001
4	0	4	3	0	3	6647.904	-0.001
4	1	4	3	1	3	6343.056	-0.002
4	1	3	3	1	2	7106.313	0.001
5	0	5	4	0	4	8241.866	-0.000
5	1	5	4	1	4	7912.493	0.000
6	0	6	5	0	5	9798.879	0.002

Table S7. Observed frequencies (in MHz) and residuals for the rotational transitions of $C_4^{15}N_2O_2H_4-D_2O$ species of uracil-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
3	0	3	2	0	2	4940.174	0.002
3	1	2	2	1	1	5249.250	0.001
3	1	3	2	0	2	7230.325	0.000
4	0	4	3	0	3	6545.117	0.000
4	1	4	3	1	3	6247.037	0.001
4	1	3	3	1	2	6987.584	-0.001
5	0	5	4	0	4	8117.222	-0.002
6	0	6	5	0	5	9654.036	0.000

Table S8. Observed frequencies (in MHz) and residuals for the nuclear quadrupole coupling hyperfine components of the A-state of the parent species of thymine-water complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	2	1	0	1	2	4	2	3	4436.231	0.002
2	1	2	1	0	1	0	2	2	1	4436.523	0.002
2	1	2	1	0	1	1	3	1	2	4436.720	0.004
2	2	1	1	1	0	2	4	2	3	8404.682	-0.001
2	2	1	1	1	0	1	3	1	2	8404.854	-0.004
2	2	0	1	1	1	2	3	2	2	8601.728	0.003
2	2	0	1	1	1	1	3	1	2	8602.687	0.002
2	2	0	1	1	1	2	4	2	3	8603.328	-0.003
3	1	3	2	0	2	2	5	2	4	5575.425	0.001
3	1	3	2	0	2	1	4	1	3	5576.001	0.002
3	1	3	2	0	2	2	4	2	3	5576.223	0.002
3	1	3	2	0	2	2	3	2	2	5576.793	0.002
4	0	4	3	0	3	2	6	2	5	5512.435	-0.003
4	0	4	3	0	3	2	4	2	3	5512.801	0.004
4	1	4	3	1	3	2	6	2	5	5248.752	0.000
4	1	4	3	1	3	1	5	1	4	5248.912	0.001
4	1	4	3	1	3	2	4	2	3	5249.036	0.000
4	1	4	3	1	3	2	3	2	2	5249.092	-0.003
4	1	4	3	0	3	1	4	1	3	6645.176	-0.003
4	1	4	3	0	3	0	4	0	3	6645.188	0.001
4	1	4	3	0	3	2	6	2	5	6645.281	-0.000
4	1	4	3	0	3	1	5	1	4	6645.858	-0.002
4	1	4	3	0	3	2	5	2	4	6646.029	-0.001
4	1	4	3	0	3	2	4	2	3	6646.599	-0.002
5	0	5	4	0	4	2	6	2	5	6803.754	-0.002
5	0	5	4	0	4	2	5	2	4	6803.953	0.000
5	1	5	4	0	4	2	4	2	3	7672.918	0.002
5	1	5	4	0	4	1	6	1	5	7672.988	-0.005
5	1	5	4	0	4	2	6	2	5	7673.107	-0.004
5	1	5	4	0	4	2	5	2	4	7673.637	0.003
6	1	6	5	0	5	2	6	2	5	8689.026	0.004

Table S9. Observed frequencies (in MHz) and residuals for the nuclear quadrupole coupling hyperfine components of the A-state of the thymine-H₂¹⁸O.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	2	1	0	1	2	4	2	3	4355.438	0.001
2	1	2	1	0	1	1	3	1	2	4355.925	0.001
2	2	1	1	1	0	2	4	2	3	8330.129	0.000
2	2	1	1	1	0	1	3	1	2	8330.307	0.001
2	2	0	1	1	1	2	3	2	2	8512.720	-0.000
2	2	0	1	1	1	1	3	1	2	8513.678	-0.001
3	1	3	2	0	2	2	5	2	4	5458.246	0.001
3	1	3	2	0	2	1	4	1	3	5458.822	0.001
3	1	3	2	0	2	2	4	2	3	5459.048	0.000
4	0	4	3	0	3	2	6	2	5	5311.450	0.000
4	1	4	3	1	3	2	6	2	5	5059.012	0.001
4	1	4	3	1	3	1	5	1	4	5059.169	0.001
4	1	4	3	1	3	2	4	2	3	5059.290	0.003
4	1	4	3	1	3	2	3	2	2	5059.348	-0.004
4	1	4	3	0	3	2	6	2	5	6494.868	-0.003
4	1	4	3	0	3	1	5	1	4	6495.453	-0.002
4	1	4	3	0	3	2	5	2	4	6495.631	-0.002
4	1	4	3	0	3	2	4	2	3	6496.205	-0.002
5	0	5	4	0	4	2	6	2	5	6562.842	-0.002
5	0	5	4	0	4	2	5	2	4	6563.032	-0.001
5	1	5	4	0	4	2	6	2	5	7489.213	0.002
5	1	5	4	0	4	2	5	2	4	7489.746	0.002

Table S3. Average splittings values (in MHz), residuals and average standard deviations for the observed A-E internal rotation components of the parent species of thymine-water complex

Transition $J_{K'_{-1},K'_{+1}} \leftarrow J_{K''_{-1},K''_{+1}}$	$v_A - v_E$		σ^a
	obs.	obs.-cal.	
$2_{12} \leftarrow 1_{01}$	0.040	-0.001	0.002
$2_{20} \leftarrow 1_{11}$	-0.506	0.000	0.004
$2_{21} \leftarrow 1_{10}$	0.725	0.000	0.004
$3_{13} \leftarrow 2_{02}$	0.041	0.005	0.002
$4_{14} \leftarrow 3_{03}$	0.033	-0.001	0.002
$5_{15} \leftarrow 4_{04}$	0.031	-0.001	0.008

^aStandard deviation