The Structure of Uracil: A Laser Ablation Rotational Study

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Supplementary Information

Figure 1. A five MHz section of the $2_{2,0} \leftarrow 1_{1,1}$ rotational transition for the parent species of uracil, illustrating the complicated hyperfine structure (*I*, *F* labels are given). Because of the parallel arrangement of the molecular beam and the axis of the resonator each line appear as a Doppler doublet. The transition frequencies are calculated as the arithmetic mean of the Doppler components.

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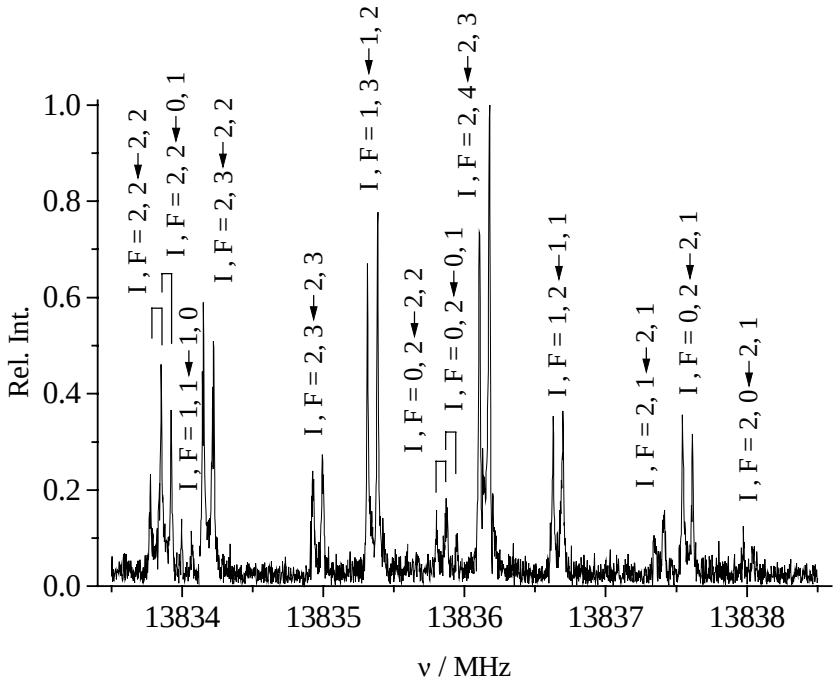


Table S1. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the parent uracil:

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	Obs / MHz	Obs-cal / MHz
2	0	2	1	0	1	2	0	0	1	6547.227	0.002
						0	2	2	2	6547.592	0.005
						0	2	0	1	6547.672	0.002
						2	1	2	2	6547.790	0.001
						2	1	0	1	6547.872	0.000
						1	2	1	2	6548.344	0.001
						1	1	1	0	6548.809	0.001
						2	4	2	3	6548.899	0.003
						1	2	1	1	6548.899	0.005
						1	3	1	2	6549.178	0.003
						0	2	2	1	6549.444	0.004
						2	2	2	2	6549.569	0.006
						2	2	0	1	6549.648	0.003
						2	3	2	3	6550.007	0.002
						1	1	1	1	6550.192	0.004
2	1	2	1	1	1	0	2	2	2	6014.713	0.004
						0	2	0	1	6014.793	0.004
						2	1	0	1	6015.068	-0.002
						1	2	1	2	6015.538	0.004
						2	0	2	1	6015.882	0.003
						1	2	1	1	6016.047	0.003
						2	4	2	3	6016.177	0.003
						0	2	2	1	6016.496	0.001
						1	3	1	2	6016.689	0.004
						2	3	2	2	6016.926	0.004
						2	2	0	1	6017.542	0.005
						2	3	2	3	6017.716	-0.001
3	0	3	2	0	2	0	3	2	3	9470.774	0.001
						2	2	2	2	9471.034	0.000
						1	3	1	3	9471.451	0.001
						2	1	2	1	9471.759	0.002
						1	3	1	2	9472.283	0.000
						2	5	2	4	9472.299	0.002
						1	2	1	1	9472.565	0.001
						1	4	1	3	9472.620	0.003
						2	4	2	3	9472.649	0.002
						2	2	2	1	9472.811	0.004
						2	2	0	2	9473.008	-0.001
						2	3	2	2	9473.026	0.002
						2	3	2	3	9473.412	0.002
						2	4	2	4	9473.755	-0.001
						1	2	1	2	9473.860	0.001
3	1	3	2	1	2	0	3	2	3	8931.718	0.002
						2	2	2	2	8931.970	0.003
						1	3	1	3	8932.646	0.002
						2	1	2	1	8933.160	0.001
						2	5	2	4	8933.768	0.003
						1	3	1	2	8933.797	0.002
						1	2	1	1	8933.917	0.002
						0	3	0	2	8933.931	0.002
						2	4	2	3	8934.002	0.003

						1	4	1	3	8934.063	0.003
						2	3	2	2	8934.393	0.003
						2	2	2	1	8934.435	0.001
						2	2	0	2	8934.715	-0.001
						2	3	2	3	8934.929	0.002
						2	4	2	4	8935.548	0.004
						1	2	1	2	8935.714	0.000
4	0	4	3	0	3	0	4	2	4	12158.347	-0.001
						2	3	2	3	12158.589	-0.002
						1	4	1	4	12159.018	-0.003
						2	2	2	2	12159.197	-0.004
						1	4	1	3	12160.187	0.000
						2	6	2	5	12160.187	0.000
						1	3	1	2	12160.455	-0.001
						1	5	1	4	12160.483	-0.001
						2	5	2	4	12160.491	0.000
						2	3	2	2	12160.580	-0.001
						2	4	2	3	12160.816	-0.001
						2	3	0	3	12161.227	-0.001
						2	4	2	4	12161.581	0.001
						2	5	2	5	12161.947	-0.004
						1	3	1	3	12162.031	-0.001
4	1	4	3	1	3	1	4	1	4	11770.174	-0.003
						2	2	2	2	11770.452	-0.002
						2	6	2	5	11771.558	0.000
						1	4	1	3	11771.593	0.000
						0	4	0	3	11771.646	-0.001
						1	3	1	2	11771.689	-0.001
						2	5	2	4	11771.708	0.002
						1	5	1	4	11771.773	0.000
						2	3	2	2	11771.958	0.001
						2	4	2	3	11771.967	0.000
						2	3	0	3	11772.744	-0.002
						2	4	2	4	11772.893	0.000
						2	5	2	5	11773.482	-0.002
						1	3	1	3	11773.609	0.000
5	1	5	4	1	4	1	4	1	3	14539.594	-0.005
						1	6	1	5	14539.648	-0.003
						2	4	2	3	14539.758	-0.004
						2	5	2	4	14539.789	-0.004
1	1	1	0	0	0	2	1	2	2	5213.635	0.003
						2	1	0	0	5213.635	0.003
						1	1	1	1	5214.369	0.001
						2	3	2	2	5214.625	0.004
						1	2	1	1	5214.883	0.004
						0	1	2	2	5215.340	0.004
						0	1	0	0	5215.340	0.003
						2	2	2	2	5215.416	0.000
						1	0	1	1	5215.677	0.003
2	1	2	1	0	1	2	0	0	1	7874.293	0.003
						0	2	2	2	7874.824	0.002
						2	1	1	0	7874.832	0.004
						0	2	0	1	7874.907	0.002
						2	1	2	2	7875.104	0.000
						1	2	2	2	7875.112	0.004

						2	1	0	1	7875.187	0.000
						1	2	1	2	7875.665	0.003
						2	0	2	1	7876.064	0.003
						1	2	1	1	7876.216	0.003
						2	4	2	3	7876.326	0.006
						1	1	1	0	7876.636	0.005
						0	2	2	1	7876.679	0.003
						1	3	1	2	7876.817	0.004
						2	1	2	1	7876.956	-0.001
						2	3	2	2	7877.038	0.003
						2	2	0	1	7877.657	0.003
						2	3	2	3	7877.865	0.001
						1	1	1	1	7878.015	0.004
						2	2	2	3	7878.403	0.002
2	2	0	1	1	1	2	2	0	1	13833.906	-0.002
						1	1	1	0	13834.049	-0.002
						2	3	2	2	13834.217	0.002
						2	3	2	3	13835.010	0.000
						1	3	1	2	13835.310	0.001
						2	4	2	3	13836.121	0.001
						1	2	1	1	13836.652	0.002
						0	2	2	1	13837.590	0.001
2	2	1	1	1	0	1	2	2	1	12980.633	-0.002
						2	1	2	1	12980.641	0.003
						0	2	2	1	12980.784	0.002
						2	0	2	1	12981.095	-0.002
						1	1	1	1	12981.175	-0.002
						2	2	2	3	12981.374	0.000
						2	3	2	3	12981.648	0.000
						1	2	1	1	12982.098	0.000
						2	4	2	3	12982.441	0.003
						1	3	1	2	12982.585	0.001
						2	2	0	1	12982.833	0.001
						2	2	2	2	12982.989	-0.004
						1	2	1	2	12983.175	0.002
						2	3	2	2	12983.264	-0.004
						1	1	1	0	12983.872	0.000
						1	2	0	1	12984.091	-0.003
						2	1	0	1	12984.100	0.004
						0	2	0	1	12984.242	0.002
						2	1	2	2	12984.263	0.006
						0	2	2	2	12984.400	-0.002
						2	0	0	1	12984.554	-0.001
3	1	3	2	0	2	2	1	2	2	10258.700	-0.001
						0	3	2	3	10259.580	0.004
						2	2	2	2	10259.975	0.000
						1	3	1	3	10260.286	0.003
						2	1	2	1	10260.475	0.002
						1	3	1	2	10261.119	0.004
						1	4	2	3	10261.141	-0.002
						2	5	2	4	10261.193	0.003
						1	4	1	3	10261.701	0.003
						1	2	1	1	10261.738	0.000
						2	4	2	3	10261.863	0.003
						2	3	2	2	10262.402	0.003

						2	3	2	3	10262.788	0.003
						2	4	2	4	10262.969	0.001
						1	2	1	2	10263.035	0.002
3	2	2	2	1	1	2	1	2	0	15643.509	-0.003
						0	3	0	2	15643.796	-0.006
						2	1	2	1	15643.932	-0.008
						2	2	2	1	15643.932	-0.008
						1	3	1	2	15643.953	-0.007
						1	2	1	2	15643.963	0.002
						1	4	1	3	15644.499	-0.004
						1	3	1	3	15644.499	-0.004
						1	2	1	1	15644.832	-0.006
						2	3	2	3	15644.897	-0.005
						2	4	2	3	15644.897	-0.005
						0	3	2	2	15644.897	-0.005
						2	3	2	2	15645.149	-0.006
						2	2	2	2	15645.149	-0.007
3	0	3	2	1	2	0	3	2	3	8142.915	0.001
						2	2	2	2	8143.023	-0.003
						2	2	2	3	8143.560	-0.002
						1	3	1	3	8143.812	0.000
						2	1	2	1	8144.442	0.000
						1	2	1	1	8144.742	0.001
						2	4	2	3	8144.788	0.001
						2	5	2	4	8144.873	0.001
						1	4	1	3	8144.979	0.001
						0	3	0	2	8145.129	0.002
						2	1	2	0	8145.335	-0.003
						2	2	2	1	8145.492	-0.001
						2	3	2	3	8145.553	0.002
						2	2	0	2	8145.772	-0.002
						2	4	2	4	8146.333	0.001
						1	2	1	2	8146.538	-0.002
4	1	4	3	0	3	0	4	2	4	12558.574	-0.002
						2	3	2	3	12558.912	0.000
						1	4	1	4	12559.257	-0.002
						2	2	2	2	12559.392	-0.003
						1	4	1	3	12560.426	0.000
						0	4	0	3	12560.450	0.001
						1	5	1	4	12560.853	-0.001
						1	3	1	2	12560.865	0.001
						2	3	2	2	12560.898	-0.003
						2	5	2	4	12560.918	0.000
						2	4	2	3	12561.344	0.001
						2	4	2	4	12562.106	0.000
						2	5	2	5	12562.376	-0.002
						1	3	1	3	12562.442	0.001
4	0	4	3	1	3	0	4	2	4	11369.132	-0.004
						2	3	2	3	11369.211	-0.005
						1	4	1	4	11369.937	-0.002
						2	2	2	2	11370.255	-0.003
						2	5	2	4	11371.275	-0.003
						2	6	2	5	11371.293	-0.001
						1	5	1	4	11371.401	-0.002
						0	4	0	3	11371.417	-0.002

2	4	2	3	11371.438	-0.003
2	2	2	1	11371.531	-0.003
2	3	2	2	11371.637	-0.002
2	4	2	4	11372.365	-0.003
2	3	0	3	11372.424	-0.001
2	5	2	5	11373.055	-0.001
1	3	1	3	11373.198	-0.002

Table S2. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the $^{15}N(1)$ and $^{15}N(3)$ isotopically substituted uracil:

								$^{15}N_1$-$^{14}N_3$		$^{14}N_1$-$^{15}N_3$	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	Obs / MHz	Obs-cal / MHz	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	2	1	5176.563	0.002	5184.802	0.001
						1	1	5177.013	-0.001	5185.398	0.002
						0	1	5175.875	-0.004	5183.910	0.001
2	1	2	1	0	1	3	2	7821.700	0.003	7840.335	0.000
						2	1	7822.222	-0.003	7841.012	0.002
2	2	0	1	1	1	3	2	13735.298	0.000	13758.853	0.001
						2	1	13734.005	0.001	13757.429	0.000
						1	0	13736.446	0.001	13760.204	0.000
2	2	1	1	1	0	3	2	12884.660	0.003	12899.020	-0.002
						2	1	12885.065	-0.005	12899.578	-0.001
3	1	3	2	0	2	4	3	10191.430	0.000	10218.903	0.000
						3	2	10191.963	0.003	10219.544	0.000
4	0	4	3	1	3	5	4	11306.228	-0.001	11363.676	-0.002
						4	3	11306.287	-0.001	11363.720	0.000
						3	2	11306.342	0.000	11363.804	0.001

Table S3. Observed frequencies and residuals (in MHz) for the rotational transitions of the $^{15}N_1$-$^{15}N_3$, $^{15}N_1$-$^{15}N_3$- $^{13}C_2$ and $^{15}N_1$-$^{15}N_3$- $^{13}C_4$ isotopically substituted uracil:

						$^{15}N_1$-$^{15}N_3$		$^{15}N_1$-$^{15}N_3$- $^{13}C_2$		$^{15}N_1$-$^{15}N_3$- $^{13}C_4$	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	Obs / MHz	Obs-cal / MHz	Obs / MHz	Obs-cal / MHz	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	5146.656	0.001	5137.289	0.001	5138.198	0.000
2	1	2	1	0	1	7785.579	0.001	7765.468	0.000	7765.132	-0.001
2	2	0	1	1	1	13657.869	0.001	13631.419	0.001	13633.390	0.001
2	2	1	1	1	0	12801.035	-0.002	12783.679	-0.002	12787.654	-0.001
3	1	3	2	0	2	10148.977	0.001	10119.708	0.001	10118.396	0.001
4	0	4	3	1	3	11298.342	-0.001	11239.934	-0.001	11231.021	0.000

Table S4. Observed frequencies and residuals (in MHz) for the rotational transitions of the $^{15}N_1$-$^{15}N_3$- $^{13}C_5$ and $^{15}N_1$-$^{15}N_3$- $^{13}C_6$ isotopically substituted uracil:

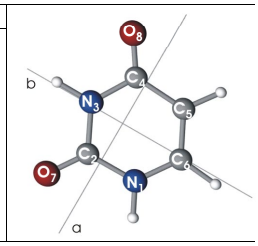
						$^{15}N_1$-$^{15}N_3$- $^{13}C_5$		$^{15}N_1$-$^{15}N_3$- $^{13}C_6$	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	Obs / MHz	Obs-cal / MHz	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	5099.704	0.000	5051.099	-0.001
2	1	2	1	0	1	7719.790	0.000	7669.464	0.000
2	2	0	1	1	1	13534.754	0.000	13413.108	0.000
2	2	1	1	1	0	12679.020	-0.001	12534.931	0.000
3	1	3	2	0	2	10065.915	0.000	10012.363	0.001
4	0	4	3	1	3	11228.562	0.000	11268.368	0.000

Table S5. Observed frequencies and residuals (in MHz) for the rotational transitions of the $^{15}N_1$-$^{15}N_3$- $^{18}O_7$ and $^{15}N_1$-$^{15}N_3$- $^{18}O_8$ isotopically substituted uracil:

						$^{15}N_1$-$^{15}N_3$- $^{18}O_7$		$^{15}N_1$-$^{15}N_3$- $^{18}O_8$	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	Obs / MHz	Obs-cal / MHz	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	5053.130	0.002	5059.229	0.002
2	1	2	1	0	1	7612.797	0.003	7615.268	0.002
2	2	0	1	1	1	13402.177	0.002	13417.007	0.001
2	2	1	1	1	0	12599.715	-0.004	12621.640	-0.002
3	1	3	2	0	2	9907.756	0.000	9907.561	0.000
4	0	4	3	1	3	10892.528	-0.001	10862.284	-0.001

Table S6. Atom coordinates in the principal inertial axis system of uracil.

	a	b	c[b]
N_1	1.1884(10)[a]	-1.0115(12)	0
C_2	1.1975(10)	0.375(3)	0
N_3	-0.091(13)	0.9640(12)	0
C_4	-1.2925(9)	0.295(4)	0
C_5	-1.1992(10)	-1.1535(10)	0
C_6	0.05(2)	-1.7396(7)	0
O_7	2.2323(5)	1.0189(12)	0
O_8	-2.3273(5)	0.9432(13)	0



[a] Derived errors in parentheses in units of the last digit, calculated according to Costain's formula (*J.Chem.Phys.* **1958,** *28*, 864): $\delta z_i = 0.0012/|z_i|$. [b] Assumed value for all atoms.

Complete reference [20]:

Gaussian 03, Revision B.04,

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