Electronic Supporting Information for "Nanohydration of uracil: emergence of three-dimensional structures and their influence on proton-induced charge transfer"

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1 Details of quantum chemical calculations

The following methods and basis sets were used to locally reoptimize the most stable configurations obtained for uracil-$(H_2)_n$ clusters:

- DFT with hybrid functional B3LYP [1] and basis set 6-31G*;
- DFT with meta-GGA functional M06-2X [2] and basis set aug-cc-pVTZ;
- Møller-Plesset post-Hartree-Fock method with basis set aug-cc-pVTZ, corrected from basis set superposition error using the counterpoise method [3];
- Coupled-cluster theory with single, double, and perturbative triple excitations and the aug-cc-pVDZ basis set.

2 Configurations and vibrational spectra

Here we provide the equilibrium geometries and static IR absorption spectra with unscaled frequencies, as obtained using the DFT/M06-2X/aug-cc-pVTZ method. The total electronic energy E and the harmonic (unscaled) zero-point vibrational energy correction are also given, as well as associated vertical and adiabatic electron affinities (EA) and ionization potentials (IP). All coordinates are in Å, frequencies in cm^{-1} and intensities in km/mol.

Bare uracil: E =-414.826996138 Hartree; ZPE=55.17026 kcal/mol.
IP: 9.72 eV (vert.) and 9.43 eV (adiab.) / EA: -0.43 eV (vert.) and -0.02 eV (adiab.)

C	0.053289	-1.709260	0.000000
C	1.241517	-1.067980	0.000000
C	1.282118	0.391470	0.000000
C	-1.237459	0.365890	0.000000
N	-1.141025	-1.026459	0.000000
N	0.000000	0.987694	0.000000
H	-2.026071	-1.514266	0.000000
H	-0.020259	2.001463	0.000000
H	-0.031580	-2.790730	0.000000
H	2.180834	-1.603780	0.000000
O	-2.303725	0.951794	0.000000
O	2.284658	1.085450	0.000000

ω	I	ω	I	ω	I
3646.5226	123.233	1395.320	14.651	746.249	12.585
3597.0682	83.728	1238.268	4.601	676.901	77.906
3265.2503	3.768	1213.514	111.132	571.943	42.501
3219.9117	1.346	1098.197	6.428	567.965	3.189
1846.2051	511.292	1006.129	0.125	549.310	8.384
1823.1887	992.839	995.976	8.226	523.500	20.975
1708.6601	96.948	983.252	9.676	404.980	23.653
1519.5766	145.783	842.433	63.837	396.969	24.194
1433.9178	90.239	788.111	37.731	169.530	0.071
1424.2746	38.441	783.305	3.575	155.741	1.667

Table S1: Vibrational frequencies and IR intensities for bare uracil

Uracil-H_2O: E =-491.275288110 Hartree; ZPE=70.98245 kcal/mol.
IP: 9.60 eV (vert.) and 9.07 eV (adiab.) / EA: -0.46 eV (vert.) and 0.10 eV (adiab.)

C	1.775122	-0.883772	0.000000
C	0.607351	-1.565012	-0.000003
N	-0.612330	-0.934325	-0.000005
C	-0.745555	0.444648	-0.000006
N	0.457376	1.119288	-0.000001
C	1.764476	0.573324	0.000002
O	-1.833857	1.016172	-0.000003
O	2.736173	1.310154	0.000005
H	0.561504	-2.648868	-0.000002
H	-1.492184	-1.456310	-0.000006
H	0.395841	2.131373	0.000001
H	2.732155	-1.387356	0.000002
H	-4.304191	-1.467475	-0.000059
O	-3.353196	-1.296452	0.000016
H	-3.230800	-0.325218	0.000009

ω	I	ω	I	ω	I
3951.4284	125.448	1404.492	9.072	602.236	157.479
3684.4305	374.267	1246.358	45.255	580.188	8.488
3607.3204	84.449	1235.065	59.353	556.495	12.996
3475.1797	490.289	1108.178	0.951	527.484	43.472
3248.3939	3.719	1009.926	0.173	417.042	17.710
3228.8161	3.468	1002.418	9.428	413.238	7.002
1826.5038	421.093	990.739	5.203	400.110	150.813
1800.4387	1100.053	835.892	54.631	233.184	130.072
1713.1254	87.429	805.625	122.160	183.461	1.910
1615.8569	243.214	789.488	6.322	175.704	1.507
1542.9499	113.785	777.128	37.180	166.920	4.207
1460.8541	144.732	725.671	13.557	145.042	27.651
1425.3103	10.584	688.808	27.064	51.446	0.621

Table S2: Vibrational frequencies and IR intensities for uracil-H_2O

Uracil-$(H_2O)_2$: E =-567.723491507 Hartree; ZPE=86.79732 kcal/mol.
IP: 9.52 eV (vert.) and 8.87 eV (adiab.) / EA: -0.36 eV (vert.) and 0.14 eV (adiab.)

C	1.775122	-0.883772	0.000000
C	2.340951	-0.733796	0.089553
C	1.167129	-1.405559	0.086291
N	-0.051914	-0.772412	0.078123
C	-0.170469	0.600041	0.058102
N	1.032683	1.271672	0.068323
C	2.339141	0.722037	0.083403
O	-1.251231	1.194645	0.037285
O	3.312118	1.457293	0.088049
H	1.111422	-2.489095	0.088531
H	-0.927236	-1.334331	0.092616
H	0.974261	2.283771	0.049608
H	3.294500	-1.244153	0.094754
H	-2.670712	-2.499238	0.996840

O	-2.387598	-2.287815	0.094422
H	-3.012405	-1.572709	-0.201785
H	-2.846901	0.511846	-0.435282
O	-3.670269	-0.011399	-0.580598
H	-4.306667	0.356554	0.050251

ω	I	ω	I	ω	I
3940.4673	114.515	1408.056	8.148	560.873	21.388
3931.8791	93.624	1254.666	112.892	530.687	58.294
3603.2910	83.034	1236.964	41.386	449.223	96.024
3578.0264	1018.573	1112.894	0.899	422.638	7.519
3488.1709	647.337	1016.508	0.504	413.659	17.802
3262.2151	1.935	1005.277	11.476	399.307	40.938
3241.5192	1110.268	992.879	2.281	320.557	94.683
3218.1429	15.111	909.486	79.455	254.595	37.637
1824.4837	526.559	862.553	178.827	213.258	94.823
1789.7842	1110.207	844.218	81.064	189.396	1.208
1714.5459	141.868	800.605	22.637	175.867	4.169
1656.9806	92.451	793.137	11.189	171.780	15.382
1635.5414	64.988	743.917	0.084	164.583	11.891
1566.7169	28.361	695.858	38.487	63.967	1.760
1470.8551	169.593	681.773	183.887	60.125	2.238
1429.1182	8.393	579.851	2.562	34.716	0.315

Table S3: Vibrational frequencies and IR intensities for uracil-$(H_2O)_2$

Uracil-$(H_2O)_3$: E =-644.168053636 Hartree; ZPE=102.36098 kcal/mol.
IP: 9.44 eV (vert.) and 8.58 eV (adiab.) / EA: -0.48 eV (vert.) and 0.28 eV (adiab.)

C	0.788549	-2.613558	0.522460
C	-0.350477	-1.884446	0.490969
N	-0.357033	-0.522546	0.313838
C	0.797902	0.205776	0.150461
N	1.951556	-0.547292	0.190830
C	2.074012	-1.948566	0.368892
O	0.820465	1.428388	-0.014021
O	3.177041	-2.469307	0.378598
H	-1.336706	-2.322738	0.601234
H	-1.270931	-0.025151	0.343153
H	2.818355	-0.035905	0.067927
H	0.780490	-3.686378	0.659578
H	-3.170490	1.148262	-0.099426
O	-2.944220	0.368798	0.482630
H	-3.169013	0.671534	1.375176
H	-0.520905	4.058316	-0.946059
O	-0.785833	3.224698	-1.362219
H	-0.242855	2.541096	-0.904195
H	-3.725963	2.416379	-1.846761
O	-3.374852	2.586921	-0.960044
H	-2.439272	2.889886	-1.115394

ω	I	ω	I	ω	I
3942.8849	95.109	1407.526	11.385	485.097	40.539
3942.1003	116.472	1248.116	114.909	429.854	19.720
3940.6952	83.539	1237.676	77.412	422.422	10.590
3609.4786	90.895	1113.504	1.919	413.002	2.004
3583.1885	975.713	1020.451	1.499	398.379	72.031
3475.8484	1182.207	1007.216	12.386	308.159	115.608
3383.7826	779.147	993.242	2.108	280.227	8.526
3272.3219	1.937	951.628	69.883	260.195	138.797
3233.5202	1264.727	909.029	112.029	235.449	64.306
3214.7329	21.967	850.836	76.688	228.919	39.682
1825.0901	551.835	801.537	33.257	188.186	4.589
1788.9820	1189.963	794.703	11.283	173.899	16.123
1709.9252	165.112	783.039	163.579	161.928	11.771
1670.8525	76.328	749.447	0.367	153.504	11.698
1655.4186	44.741	699.038	46.591	69.620	0.872
1635.8188	61.029	662.207	102.744	53.618	1.613
1553.2406	53.859	580.874	7.638	46.522	1.634
1467.4529	136.760	560.600	18.375	38.692	0.879
1428.6855	4.038	532.644	51.853	27.544	0.382

Table S4: Vibrational frequencies and IR intensities for uracil-$(H_2O)_3$

Uracil-$(H_2O)_4$ / isomer 4a: E =-720.616433382 Hartree; ZPE=117.93107 kcal/mol.
IP: 9.40 eV (vert.) and 8.71 eV (adiab.) / EA: -0.36 eV (vert.) and 0.42 eV (adiab.)

```
C          -0.484719        -2.327927         0.142929
C          -1.630164        -1.607131         0.113769
N          -1.631473        -0.239600         0.064075
C          -0.463796         0.499124         0.032415
N           0.697719        -0.242331         0.077083
C           0.789735        -1.635437         0.119282
O          -0.449533         1.730401        -0.035575
O           1.885553        -2.206637         0.132548
H          -2.614378        -2.063986         0.123496
H          -2.535710         0.274557         0.040607
H           1.583871         0.311699         0.101516
H          -0.482542        -3.408746         0.176918
H          -4.474551         1.197065         0.833515
O          -4.071499         1.098690        -0.042714
H          -3.707283         2.004096        -0.241295
H           3.190643         1.735896        -0.592666
O           3.113918         1.159658         0.182392
H           3.745905         0.412463         0.013613
H          -2.565202         3.689316        -1.261411
O          -2.656782         3.360095        -0.354728
H          -1.813503         2.876100        -0.182360
H           3.543454        -1.617528        -0.191885
O           4.416200        -1.162745        -0.270432
H           4.901739        -1.447437         0.518638
```

ω	I	ω	I	ω	I
3942.0751	74.096	1422.006	17.736	434.296	21.337
3940.4985	125.677	1272.066	99.032	422.082	86.503
3938.8959	119.229	1255.916	56.309	401.757	40.221
3932.6284	93.286	1119.534	0.179	369.925	68.424
3597.3202	952.727	1032.649	5.378	283.597	72.253
3564.7426	1242.105	1012.594	0.803	269.381	91.534
3522.9001	446.214	1000.057	18.830	254.356	82.274
3464.8944	689.392	961.162	120.460	250.888	43.450
3262.9436	1.240	909.418	43.395	231.787	70.793
3242.5216	952.526	863.201	167.413	196.353	29.061
3208.6095	6.142	842.952	53.847	188.686	17.629
3182.1290	1182.905	828.963	106.332	185.513	22.906
1794.6195	647.267	804.237	4.686	182.714	38.263
1773.3092	1089.976	797.546	6.658	176.415	6.465
1706.0496	65.778	743.653	3.471	164.978	1.751
1657.0453	69.738	681.071	172.782	154.423	42.498
1647.1390	100.203	679.808	178.055	77.057	1.251
1635.6429	64.628	585.451	1.393	69.095	3.874
1625.1403	105.269	574.506	25.186	51.081	0.791
1571.4066	40.689	543.067	96.453	46.343	0.841
1511.6281	32.997	460.334	96.326	28.609	0.342
1478.7845	161.960	438.350	14.748	25.188	1.068

Table S5: Vibrational frequencies and IR intensities for uracil-$(H_2O)_4$, planar isomer 4a

Uracil-$(H_2O)_4$ / isomer 4b: E =-720.617227404 Hartree; ZPE=119.24792 kcal/mol.
IP: 9.67 eV (vert.) and 9.00 eV (adiab.) / EA: -0.26 eV (vert.) and 0.54 eV (adiab.)

```
C          -1.883099         -1.586683          1.252381
C          -0.936661         -1.951416          2.143575
N           0.395387         -1.704705          1.913042
C           0.871220         -1.069777          0.770759
N          -0.108100         -0.759104         -0.146081
C          -1.493462         -0.903619          0.026539
O           2.065564         -0.834084          0.623351
O          -2.280525         -0.479019         -0.816198
H          -1.164178         -2.446373          3.081441
H           1.101085         -1.932576          2.600062
H           0.218488         -0.308433         -1.020582
H          -2.935588         -1.761905          1.427851
H           1.675789          2.198828         -0.177831
O           2.431886          1.744837         -0.635496
H           2.560425          0.927421         -0.114578
H          -1.901670          1.275403         -1.545799
O          -1.388170          2.073761         -1.785461
H          -0.649557          1.699731         -2.311073
H           1.344759          0.205042         -3.155922
O           0.880419          0.639136         -2.425277
H           1.582224          1.114480         -1.872352
H           0.048026          3.662208          0.511016
O           0.089695          2.700546          0.401784
H          -0.522033          2.511121         -0.364270
```

ω	I	ω	I	ω	I
3939.4631	87.265	1409.151	9.580	498.580	68.906
3923.7630	70.440	1257.392	25.157	436.284	29.356
3780.3709	341.934	1218.440	83.588	420.682	26.170
3770.4325	287.655	1105.458	4.335	407.347	40.728
3726.6164	247.010	1014.445	16.673	394.953	35.087
3660.5597	345.245	1005.252	0.119	384.301	76.038
3658.1031	128.868	999.671	12.981	287.958	38.047
3395.4526	759.908	973.741	99.707	272.751	41.090
3357.0854	645.372	933.803	17.115	269.517	71.629
3270.5549	3.765	892.545	117.519	250.869	28.863
3236.6031	508.098	840.625	11.213	229.712	12.369
3213.4757	0.973	795.703	26.060	217.257	5.212
1815.1406	534.875	790.408	42.708	207.185	1.243
1781.9672	790.341	777.277	261.763	194.861	0.465
1711.5626	46.516	747.597	21.950	162.231	3.854
1683.2880	61.687	717.401	376.115	158.995	0.258
1669.6717	185.341	597.636	52.680	118.377	0.213
1640.6074	108.084	585.692	46.033	92.682	1.811
1638.5817	72.212	574.912	5.956	73.107	1.385
1530.0724	132.358	559.034	51.602	67.580	0.284
1470.9927	16.950	541.255	108.120	42.100	1.740
1449.3780	118.496	532.353	10.657	34.373	6.140

Table S6: Vibrational frequencies and IR intensities for uracil-$(H_2O)_4$, 3D isomer 4b

Uracil-$(H_2O)_5$ / isomer 5a: E =-797.061030836 Hartree; ZPE=133.77568 kcal/mol.
IP: 9.47 eV (vert.) and 8.34 eV (adiab.) / EA: -0.38 eV (vert.) and 0.63 eV (adiab.)

```
C           1.272082        -2.279663        -0.292013
C          -0.071819        -2.279995        -0.125195
N          -0.775213        -1.134477         0.127275
C          -0.167680         0.100227         0.221660
N           1.200390         0.093058         0.050674
C           1.997893        -1.028120        -0.194185
O          -0.794959         1.137314         0.452004
O           3.224185        -0.929424        -0.315072
H          -0.677314        -3.178753        -0.178207
H          -1.800606        -1.206093         0.292410
H           1.661969         1.029769         0.082712
H           1.830794        -3.184156        -0.489832
H          -3.633324        -1.842244         1.462131
O          -3.416254        -1.768572         0.520669
H          -4.064004        -1.089553         0.178149
H          -4.409588         0.968238        -0.328971
O          -5.051505         0.210010        -0.255911
H          -5.391840         0.094507        -1.155660
H          -3.306317         2.899558         0.059203
O          -3.178291         2.128077        -0.512293
H          -2.324607         1.739156        -0.207117
H           3.452687         2.250148         0.119951
O           2.511560         2.567328         0.105329
H           2.372395         2.976868         0.972342
O           4.867603         1.247618         0.127839
```

H	5.334024	1.346828	-0.715970
H	4.354153	0.410804	0.021084

ω	I	ω	I	ω	I
3945.2933	121.454	1419.270	18.650	417.903	92.269
3942.1304	113.622	1267.620	73.924	399.290	46.925
3940.8407	86.555	1246.867	129.579	373.845	62.377
3936.9056	89.168	1120.369	0.627	336.026	135.223
3931.4923	83.468	1032.562	5.801	285.892	116.454
3588.4753	804.541	1024.295	1.691	282.780	97.310
3574.8091	1367.900	999.552	14.080	280.001	53.404
3505.5361	457.488	962.260	128.968	259.792	130.105
3460.6996	1203.417	950.975	53.233	250.842	18.751
3378.4442	847.932	908.551	84.547	238.465	60.220
3270.6994	1.205	848.956	49.868	236.476	16.314
3251.4961	1060.622	840.957	103.070	191.974	6.242
3212.6926	6.083	805.836	3.761	190.175	9.909
3175.6897	1170.757	800.719	13.700	186.815	2.222
1794.2572	711.220	787.128	166.112	168.013	10.710
1772.3657	1129.412	749.849	2.611	157.215	0.606
1709.2737	67.255	682.788	181.591	152.756	35.298
1670.6015	67.695	669.860	100.164	78.802	2.460
1658.7113	45.896	584.346	8.089	71.771	0.105
1647.6833	94.863	575.409	22.165	62.834	3.125
1634.5275	59.173	544.177	87.829	53.871	0.429
1626.3502	102.959	489.276	34.691	37.668	0.844
1558.3270	68.554	441.513	6.725	32.496	0.569
1504.2323	37.026	438.732	39.978	27.051	0.103
1470.6626	125.617	426.046	0.715	24.199	0.665

Table S6: Vibrational frequencies and IR intensities for uracil-$(H_2O)_5$, planar isomer 5a

Uracil-$(H_2O)_5$ / isomer 5b: E =-797.063650842 Hartree; ZPE=134.69333 kcal/mol.
IP: 9.44 eV (vert.) and 8.65 eV (adiab.) / EA: -0.29 eV (vert.) and 0.51 eV (adiab.)

C	-0.625927	-2.347803	1.212545
C	0.727383	-2.266669	1.234952
N	1.421901	-1.441502	0.396150
C	0.791749	-0.609467	-0.506728
N	-0.587505	-0.671172	-0.498129
C	-1.375082	-1.470452	0.336674
O	1.422912	0.132858	-1.262536
O	-2.609058	-1.398032	0.307589
H	1.337305	-2.851986	1.915123
H	2.423342	-1.190068	0.548667
H	-1.056650	0.064690	-1.049147
H	-1.174553	-3.007589	1.870522
H	3.275870	0.698019	0.997628
O	3.761030	-0.053790	0.565220
H	3.643829	0.146379	-0.379245
H	-4.432399	1.100453	0.253280
O	-4.080312	0.749982	-0.578789
H	-3.652198	-0.103999	-0.322833
H	1.091560	1.989522	-1.131001

O	0.769591	2.773001	-0.641880
H	-0.200149	2.657405	-0.698103
H	-1.883204	1.934875	-2.397519
O	-1.771874	1.739757	-1.454814
H	-2.690865	1.546255	-1.113422
H	2.664250	2.748755	1.861136
O	2.168947	1.968720	1.570848
H	1.584717	2.307002	0.841249

ω	I	ω	I	ω	I
3938.2346	117.341	1418.388	15.025	430.250	18.454
3936.6368	74.103	1260.836	60.458	425.003	43.730
3923.9589	95.610	1252.934	44.947	405.850	70.631
3898.4146	80.547	1116.617	0.237	385.760	20.453
3793.2848	299.061	1032.641	9.585	328.035	32.884
3741.8452	227.576	1013.305	6.756	320.479	98.433
3634.7377	379.000	1001.742	5.019	284.045	48.484
3541.6635	1130.155	899.359	120.275	269.806	45.821
3475.3522	825.139	889.419	162.020	262.459	147.234
3400.7292	745.454	870.783	82.417	247.481	17.752
3368.3785	474.719	833.001	25.279	230.018	9.769
3336.8561	478.394	803.494	1.620	209.142	8.156
3256.7445	3.366	792.130	3.814	203.739	0.379
3211.7108	1.489	878.887	112.561	196.167	8.047
1802.3717	599.902	738.940	24.223	179.105	0.189
1766.4746	973.508	713.399	38.938	159.249	9.385
1703.1612	57.299	703.692	666.423	150.225	3.866
1689.8762	31.649	661.842	130.226	123.375	2.468
1662.6731	162.245	588.117	0.827	100.701	2.484
1657.1330	67.458	574.837	2.490	93.049	13.481
1650.3817	133.467	564.508	28.104	71.088	3.967
1630.9666	64.758	536.685	63.605	62.575	1.121
1556.8107	76.893	475.655	81.522	59.193	2.989
1484.1336	57.954	450.731	73.562	40.179	0.683
1468.2196	83.792	437.471	61.330	33.220	0.096

Table S7: Vibrational frequencies and IR intensities for uracil-$(H_2O)_5$, chain isomer 5b

Uracil-$(H_2O)_5$ / isomer 5c: E =-797.061924336 Hartree; ZPE=134.81736 kcal/mol.
IP: 9.48 eV (vert.) and 8.78 eV (adiab.) / EA: -0.20 eV (vert.) and 0.88 eV (adiab.)

C	-1.691083	-1.816798	0.230183
C	-0.899770	-2.368326	1.158373
N	0.450195	-2.153374	1.173056
C	1.090379	-1.310137	0.292933
N	0.264225	-0.744624	-0.644445
C	-1.105791	-0.957879	-0.783318
O	2.289078	-1.119775	0.345837
O	-1.719562	-0.451420	-1.702985
H	-1.274984	-3.017529	1.936171
H	1.036193	-2.538932	1.894364
H	0.706281	-0.094001	-1.297912
H	-2.753712	-1.985663	0.203357
H	-0.516759	1.269836	1.680113

O	0.309254	0.924428	2.086675
H	0.275552	1.166988	3.013757
H	2.102410	1.825357	-2.597341
O	1.463900	1.624353	-1.910949
H	1.913404	1.767512	-1.038355
H	-1.653644	2.076145	-0.153543
O	-1.861722	1.816298	0.778052
H	-2.546058	2.413346	1.083198
H	-0.298687	2.286703	-1.900112
O	-1.261520	2.299070	-1.778211
H	-1.540562	1.416289	-2.066065
H	1.757030	1.606189	1.130729
O	2.513077	1.673051	0.520311
H	2.831056	0.758830	0.490721

ω	I	ω	I	ω	I
3945.1251	78.384	1410.232	10.790	436.964	53.950
3931.5031	86.817	1254.528	19.505	421.839	11.779
3926.2399	72.321	1219.681	86.386	413.785	40.103
3783.9880	236.926	1105.956	4.937	410.682	35.331
3746.8037	373.919	1016.120	18.873	405.368	67.340
3706.3609	300.343	1009.174	4.663	310.112	48.221
3659.8911	128.661	998.946	9.294	305.135	6.192
3636.6647	341.209	974.727	141.078	300.312	23.216
3412.1004	721.495	939.078	26.787	242.920	143.043
3404.6082	557.655	888.121	88.076	239.526	34.142
3272.0596	8.383	842.255	77.410	231.845	7.393
3260.2315	1490.187	824.199	110.479	218.541	8.752
3225.3520	1.750	794.444	3.403	199.861	1.952
3213.9489	225.011	787.469	21.462	188.005	6.891
1815.9264	447.656	760.047	295.255	181.568	13.767
1791.2342	840.705	745.300	40.822	161.281	1.492
1711.1135	59.993	738.486	206.025	155.527	2.676
1688.6531	82.790	590.366	16.559	118.829	0.256
1680.8854	210.766	576.336	5.901	91.944	0.678
1666.9080	99.022	570.471	50.722	77.739	3.986
1656.2590	106.905	566.312	107.474	65.057	0.682
1648.6119	59.545	553.511	63.846	64.579	1.356
1528.3126	126.889	535.219	43.865	53.085	1.249
1466.8735	11.073	521.882	108.847	50.366	5.280
1447.3920	105.486	474.214	25.685	37.123	1.433

Table S8: Vibrational frequencies and IR intensities for uracil-$(H_2O)_5$, 3D isomer 5c

3 Infrared absorption spectra of the pentahydrates

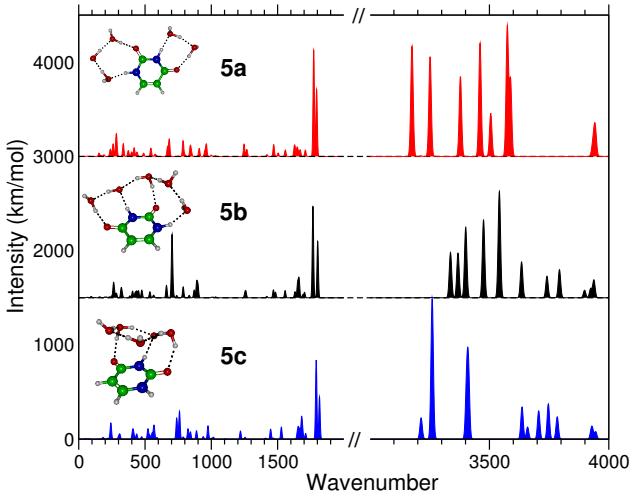

Figure S1: Infrared absorption spectra of the three isomers of uracil-$(H_2O)_5$.

4 Charge transfer cross-sections for protons impinging toward the -z direction

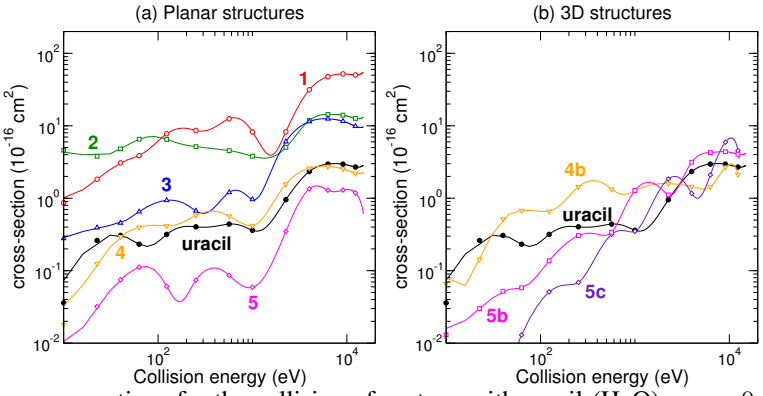

Figure S2: Charge transfer cross sections for the collision of protons with uracil-$(H_2O)_n$, $n = 0$–5, on the -z side of uracil (see main text for definition).

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