

# Supporting Information for: “Excited-State Relaxation in Uracil versus Hydrated Uracil: Solvatochromatic Shift in the $^1n\pi^*$ State is the Key”

Cartesian coordinates of critical points located on various surfaces are given below.

TABLE I: Cartesian coordinates of  $S_0$ -*min* of gas phase uracil

N	-0.778028	-0.148621	0.129781
N	0.622033	1.665951	-0.083327
C	-0.675020	1.202913	-0.083920
C	1.707862	0.859092	0.110932
C	1.581752	-0.459935	0.317470
C	0.255764	-1.062285	0.336501
O	0.012482	-2.229698	0.509763
O	-1.623675	1.926862	-0.258321
H	-1.711500	-0.519662	0.132806
H	0.723676	2.649633	-0.237770
H	2.662127	1.353679	0.086557
H	2.430646	-1.097078	0.469877

TABLE II: Cartesian coordinates of  $S_{n\pi^*}$ -*min* of gas phase uracil

N	-1.219504	-0.501062	0.011869
N	0.173607	1.322847	-0.205708
C	-1.102600	0.865406	-0.204267
C	1.312707	0.517496	-0.007876
C	1.153748	-0.821958	0.200934
C	-0.117471	-1.316286	0.206920
O	-0.493954	-2.634516	0.401334
O	-2.080102	1.556438	-0.373452
H	-2.152422	-0.864130	0.010264
H	0.265407	2.306317	-0.358007
H	2.259383	1.018800	-0.033768
H	1.998152	-1.466823	0.355037

TABLE III: Cartesian coordinates of  $ci$ - $0\pi$  of gas phase uracil

N	-0.663423	-0.206624	-0.093886
N	0.718001	1.662145	0.265992
C	-0.590246	1.118033	0.254113
C	1.718696	0.879108	-0.178899
C	1.665583	-0.482150	0.264295
C	0.389710	-1.156228	-0.003881
O	0.124395	-2.325474	-0.013794
O	-1.541808	1.824395	0.442620
H	-1.595816	-0.578340	-0.144376
H	0.723978	2.666342	0.182039
H	2.423647	1.301089	-0.881149
H	1.835402	-0.561446	1.337276

TABLE IV: Cartesian coordinates of  $ci-n\pi$  of gas phase uracil

N	-0.757076	-0.078203	0.456403
N	0.674380	1.605618	-0.235641
C	-0.643880	1.144721	-0.148590
C	1.695657	0.954559	0.360117
C	1.567003	-0.518242	0.306608
C	0.296868	-1.028723	0.399242
O	-0.052432	-2.232827	0.351122
O	-1.566603	1.820020	-0.529023
H	-1.687989	-0.454052	0.474317
H	0.749434	2.559250	-0.552504
H	2.575959	1.499951	0.639885
H	2.356798	-1.131222	-0.091585

TABLE V: Cartesian coordinates of  $ci-n\pi$ -p of gas phase uracil

N	-0.001513	0.002892	0.000003
N	2.388296	-0.003709	-0.000001
C	1.196901	0.767216	0.000000
C	2.587089	-1.301969	0.000003
C	1.307594	-2.116947	-0.000001
C	0.080197	-1.464003	-0.000005
O	-0.959221	-2.053545	0.000002
O	1.355855	1.972779	0.000001
H	-0.892400	0.459804	-0.000001
H	3.231428	0.534090	0.000000
H	3.560114	-1.750986	-0.000001
H	1.318358	-3.190377	0.000001

TABLE VI: Cartesian coordinates of  $S_0$ -min of (uracil)(H<sub>2</sub>O)<sub>4</sub>

C	-1.965155	-1.654351	0.153097
N	-2.024816	-0.306923	-0.024301
C	-0.911647	0.454364	-0.183918
N	0.272533	-0.233329	-0.157802
C	0.419869	-1.593177	0.030398
C	-0.812208	-2.326459	0.188154
O	-0.960195	1.666486	-0.339978
O	1.539666	-2.094649	0.052241
H	-0.774984	-3.388778	0.331557
O	-4.673001	0.741489	0.003406
O	4.020599	-0.912400	0.298770
O	2.764685	1.338557	-0.559457
O	1.154548	3.359239	0.608977
H	-2.926952	0.164729	-0.032031
H	1.113877	0.318931	-0.310756
H	-2.918822	-2.138541	0.266048
H	-4.888644	1.340633	0.718151
H	-4.974464	1.173866	-0.795641
H	0.363158	2.892524	0.320690
H	1.870944	2.788063	0.313643
H	3.370236	0.645128	-0.245132
H	3.026366	1.546633	-1.455733
H	3.180707	-1.397840	0.273455
H	4.359709	-0.992257	1.189042

TABLE VII: Cartesian coordinates of  $S_{n\pi^*}$ -min of (uracil)(H<sub>2</sub>O)<sub>4</sub>

C	-1.983303	-1.757352	0.168810
N	-2.017339	-0.352672	0.017502
C	-0.943690	0.394980	-0.271847
N	0.256350	-0.276860	-0.361059
C	0.314457	-1.646990	-0.180221
C	-0.796739	-2.412757	0.031236
O	-0.991565	1.617303	-0.419628
O	1.601914	-2.116916	-0.509139
H	-0.732300	-3.482678	0.106425
O	-4.707885	0.763292	0.122188
O	4.159626	-0.897277	0.581390
O	2.800116	1.206098	-0.573536
O	1.133967	3.282153	0.427745
H	-2.911852	0.120429	0.025883
H	1.109379	0.263940	-0.468267
H	-2.911381	-2.216543	0.448844
H	-4.907492	1.387824	0.819099
H	-5.071022	1.143922	-0.677065
H	0.345645	2.797233	0.154932
H	1.855730	2.693654	0.186195
H	3.407525	0.574270	-0.157841
H	3.133778	1.369517	-1.455128
H	3.474850	-1.559786	0.471339
H	4.381238	-0.894782	1.512138

TABLE VIII: Cartesian coordinates of  $ci$ -0 $\pi$  of (uracil)(H<sub>2</sub>O)<sub>4</sub>

C	-1.933538	-1.611650	0.551930
N	-2.087411	-0.392464	-0.015264
C	-0.930448	0.352742	-0.222334
N	0.265660	-0.267662	0.047198
C	0.446216	-1.658476	0.093650
C	-0.828129	-2.364791	0.034438
O	-1.001365	1.524115	-0.544329
O	1.567537	-2.122661	0.041349
H	-0.979304	-2.649143	-1.006710
O	-4.636959	0.880979	0.166739
O	4.073834	-0.919378	0.391007
O	2.755077	1.324120	-0.414810
O	1.019098	3.426868	0.315586
H	-2.946732	0.151391	0.081143
H	1.094293	0.307502	-0.086845
H	-2.569591	-1.871135	1.384568
H	-4.864960	1.543881	0.818348
H	-5.036034	1.172509	-0.653005
H	0.265626	2.907104	0.023087
H	1.765588	2.831025	0.191618
H	3.358110	0.641171	-0.074707
H	2.958760	1.418920	-1.344852
H	3.254282	-1.430150	0.334350
H	4.425782	-1.061630	1.268542

TABLE IX: Cartesian coordinates of  $ci-n\pi$  of (uracil)(H<sub>2</sub>O)<sub>4</sub>

C	-1.960413	-1.575559	0.534946
N	-2.047167	-0.294577	0.083488
C	-0.946449	0.485781	-0.169121
N	0.257991	-0.134891	-0.094100
C	0.368568	-1.542043	-0.105439
C	-0.732637	-2.280977	0.210036
O	-1.062255	1.684808	-0.398950
O	1.510487	-1.996052	-0.491496
H	-0.715417	-3.350406	0.108490
O	-4.671573	0.844109	0.034411
O	4.015888	-0.977887	0.388605
O	2.792316	1.296351	-0.534394
O	1.123366	3.361789	0.554498
H	-2.944415	0.193208	0.092248
H	1.075285	0.407532	-0.351193
H	-2.790765	-1.986367	1.074348
H	-5.001468	1.434390	0.711595
H	-4.990010	1.195924	-0.796848
H	0.322802	2.909247	0.271786
H	1.830892	2.759015	0.304296
H	3.377331	0.603911	-0.185804
H	3.106589	1.505981	-1.413069
H	3.214157	-1.504151	0.289242
H	4.289926	-1.071174	1.300151

TABLE X: Cartesian coordinates of  $ci-n\pi-p$  of (uracil)(H<sub>2</sub>O)<sub>4</sub>

C	-2.107234	-1.573483	0.150471
N	-2.006473	-0.256821	-0.031414
C	-0.869413	0.505671	-0.192016
N	0.321430	-0.270155	-0.148901
C	0.338820	-1.721038	0.044945
C	-0.847932	-2.351763	0.190408
O	-0.876295	1.726643	-0.355542
O	1.502830	-2.234742	0.054254
H	-0.791305	-3.414103	0.330094
O	-4.684494	0.737784	-0.025043
O	4.031428	-0.904305	0.298390
O	2.760351	1.335163	-0.560372
O	1.152696	3.359136	0.608341
H	-2.910704	0.193420	-0.045515
H	1.176378	0.269570	-0.265148
H	-3.058755	-2.055756	0.263955
H	-4.890642	1.342404	0.717358
H	-4.976146	1.177163	-0.797159
H	0.362171	2.886950	0.320178
H	1.870396	2.789316	0.314437
H	3.371973	0.649260	-0.245552
H	3.025100	1.546324	-1.455185
H	3.212761	-1.405654	0.282747
H	4.361846	-0.990886	1.191385