

Supplementary Material for "Supersonic jet UV spectrum and nonradiative processes of the thymine analogue 5-methyl-2-hydroxypyrimidine"

Simon Lobsiger, Hans-Martin Frey, Samuel Leutwyler
*Department of Chemistry and Biochemistry, University of Bern,
Freiestrasse 3, CH-3012 Bern, Switzerland*

Table 1: S_0 and S_1 geometries optimized at the TD-B3LYP/TZVP level. The distances are given in Å and the angles in degrees.

| | S_0 | S_1 | S_1-S_0 |
|---|---------|---------|-----------|
| Distances | | | |
| N ¹ -C ² | 1.33129 | 1.32326 | -0.00803 |
| C ² -N ³ | 1.32969 | 1.29607 | -0.03362 |
| N ³ -C ⁴ | 1.32924 | 1.37841 | 0.04917 |
| C ⁴ -C ⁵ | 1.39716 | 1.40631 | 0.00915 |
| C ⁵ -C ⁶ | 1.39090 | 1.38399 | -0.00691 |
| C ⁶ -N ¹ | 1.33379 | 1.38268 | 0.04889 |
| O-H | 0.96796 | 0.96813 | 0.00017 |
| C ² -O | 1.34503 | 1.33658 | -0.00845 |
| C ⁴ -H | 1.08722 | 1.07814 | -0.00908 |
| C ⁵ -C ⁷ | 1.50395 | 1.50139 | -0.00256 |
| C ⁶ -H | 1.08654 | 1.08080 | -0.00574 |
| C ⁷ -H ¹² | 1.09118 | 1.09061 | -0.00057 |
| C ⁷ -H ¹³ | 1.09304 | 1.09311 | 0.00007 |
| C ⁷ -H ¹⁴ | 1.09304 | 1.09312 | 0.00008 |
| Angles | | | |
| N ¹ -C ² -N ³ | 126.833 | 118.058 | -8.775 |
| C ² -N ³ -C ⁴ | 115.582 | 125.881 | 10.298 |
| N ³ -C ⁴ -C ⁵ | 123.790 | 117.206 | -6.584 |
| C ⁴ -C ⁵ -C ⁶ | 114.521 | 116.327 | 1.806 |
| C ⁵ -C ⁶ -N ¹ | 123.176 | 121.285 | -1.891 |
| C ⁶ -N ¹ -C ² | 116.097 | 121.244 | 5.147 |
| C ² -O-H | 106.735 | 107.040 | 0.305 |
| N ¹ -C ² -O | 117.274 | 121.489 | 4.215 |
| N ³ -C ⁴ -H ¹⁰ | 115.759 | 117.871 | 2.112 |
| C ⁴ -C ⁵ -C ⁷ | 122.589 | 121.274 | -1.315 |
| C ⁵ -C ⁶ -H ¹¹ | 120.793 | 122.502 | 1.709 |
| Dihedral angles | | | |
| C ⁴ -C ⁵ -C ⁷ -H ¹⁴ | 60.035 | 59.877 | 0.158 |

Table 2: S_0 and S_1 geometries optimized at the RI-CC2/aug-cc-pVDZ level. The distances are given in Å and the angles in degrees.

| | S_0 | S_1 | S_1-S_0 |
|---|---------|---------|-----------|
| Distances | | | |
| N ¹ -C ² | 1.34959 | 1.34454 | -0.00505 |
| C ² -N ³ | 1.34797 | 1.31528 | -0.03269 |
| N ³ -C ⁴ | 1.35131 | 1.40696 | 0.05565 |
| C ⁴ -C ⁵ | 1.41129 | 1.41977 | 0.00848 |
| C ⁵ -C ⁶ | 1.40579 | 1.40000 | -0.00579 |
| C ⁶ -N ¹ | 1.35496 | 1.40726 | 0.05230 |
| O-H | 0.97501 | 0.97596 | 0.00095 |
| C ² -O | 1.36017 | 1.34797 | -0.0122 |
| C ⁴ -H | 1.09715 | 1.09024 | -0.00691 |
| C ⁵ -C ⁷ | 1.51004 | 1.50839 | -0.00165 |
| C ⁶ -H | 1.09656 | 1.09259 | -0.00397 |
| C ⁷ -H ¹² | 1.10111 | 1.10086 | -0.00025 |
| C ⁷ -H ¹³ | 1.10202 | 1.10216 | 0.00014 |
| C ⁷ -H ¹⁴ | 1.10202 | 1.10216 | 0.00014 |
| Angles | | | |
| N ¹ -C ² -N ³ | 128.216 | 118.955 | -9.261 |
| C ² -N ³ -C ⁴ | 114.528 | 125.480 | 10.952 |
| N ³ -C ⁴ -C ⁵ | 123.914 | 116.823 | -7.091 |
| C ⁴ -C ⁵ -C ⁶ | 114.981 | 116.920 | 1.939 |
| C ⁵ -C ⁶ -N ¹ | 123.272 | 121.693 | -1.579 |
| C ⁶ -N ¹ -C ² | 115.090 | 120.130 | 5.040 |
| C ² -O-H | 105.341 | 105.377 | 0.036 |
| N ¹ -C ² -O | 116.915 | 121.309 | 4.394 |
| N ³ -C ⁴ -H ¹⁰ | 115.555 | 117.595 | 2.040 |
| C ⁴ -C ⁵ -C ⁷ | 122.307 | 120.959 | -1.348 |
| C ⁵ -C ⁶ -H ¹¹ | 120.830 | 122.412 | 1.582 |
| Dihedral angles | | | |
| C ⁴ -C ⁵ -C ⁷ -H ¹⁴ | 60.036 | 59.983 | -0.053 |