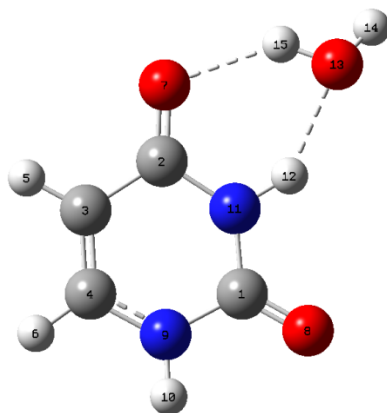


## Supplementary Material B

Geometric parameters of the pre-complex structures (hydrated isomers) of water-assisted tautomerisms in uracil, optimized by MP2/6-311++G(d,p).

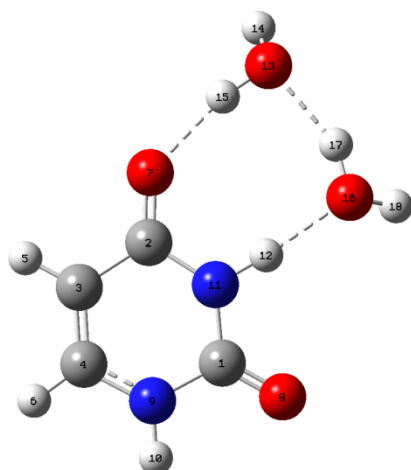
### I-H<sub>2</sub>O for I↔II



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| O | 1  | B7  | 4 | A6  | 3 | D5 0  |
| N | 4  | B8  | 3 | A7  | 2 | D6 0  |
| H | 9  | B9  | 4 | A8  | 3 | D7 0  |
| N | 1  | B10 | 8 | A9  | 9 | D8 0  |
| H | 11 | B11 | 1 | A10 | 8 | D9 0  |
| O | 7  | B12 | 2 | A11 | 1 | D10 0 |
| H | 13 | B13 | 7 | A12 | 2 | D11 0 |
| H | 13 | B14 | 7 | A13 | 2 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.49891420 | A1  | 88.35334270  | D1  | 0.38210196    |
| B2  | 1.45621515 | A2  | 119.50072339 | D2  | 177.71198371  |
| B3  | 1.35494213 | A3  | 118.70196325 | D3  | 179.11545769  |
| B4  | 1.08132389 | A4  | 122.77810031 | D4  | 176.72002539  |
| B5  | 1.08497164 | A5  | 146.85144516 | D5  | 174.61304142  |
| B6  | 1.22963866 | A6  | 150.51778738 | D6  | -3.01643409   |
| B7  | 1.21575878 | A7  | 121.57589856 | D7  | 174.33657160  |
| B8  | 1.37423884 | A8  | 120.78459305 | D8  | -177.89716008 |
| B9  | 1.01051393 | A9  | 124.27142040 | D9  | -3.81632979   |
| B10 | 1.38614866 | A10 | 115.78195241 | D10 | -1.64066326   |
| B11 | 1.02418075 | A11 | 98.72562031  | D11 | 134.90246590  |
| B12 | 2.80530320 | A12 | 126.98720700 | D12 | 175.32752841  |
| B13 | 0.95945455 | A13 | 26.51228622  |     |               |
| B14 | 0.96932990 |     |              |     |               |

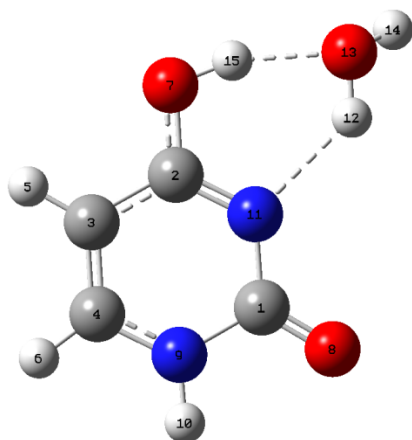
# I-2H<sub>2</sub>O for I↔II



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| O | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 4  | B8  | 3  | A7  | 2 | D6 0  |
| H | 9  | B9  | 4  | A8  | 3 | D7 0  |
| N | 1  | B10 | 8  | A9  | 9 | D8 0  |
| H | 11 | B11 | 1  | A10 | 8 | D9 0  |
| O | 7  | B12 | 2  | A11 | 1 | D10 0 |
| H | 13 | B13 | 7  | A12 | 2 | D11 0 |
| H | 13 | B14 | 7  | A13 | 2 | D12 0 |
| O | 13 | B15 | 7  | A14 | 2 | D13 0 |
| H | 16 | B16 | 13 | A15 | 7 | D14 0 |
| H | 16 | B17 | 13 | A16 | 7 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.48678815 | A1  | 88.52953823  | D1  | -0.39343589   |
| B2  | 1.45608382 | A2  | 119.44451328 | D2  | -177.70328910 |
| B3  | 1.35507813 | A3  | 118.70391297 | D3  | -179.17437334 |
| B4  | 1.08130947 | A4  | 122.87636821 | D4  | -176.20135682 |
| B5  | 1.08501541 | A5  | 147.45832301 | D5  | -173.75000187 |
| B6  | 1.23207514 | A6  | 150.22831771 | D6  | 3.02396592    |
| B7  | 1.21654126 | A7  | 121.35991881 | D7  | -174.15631644 |
| B8  | 1.37311955 | A8  | 120.84390912 | D8  | 178.13535468  |
| B9  | 1.01057723 | A9  | 124.23888982 | D9  | 0.98772719    |
| B10 | 1.38575575 | A10 | 114.90045044 | D10 | -4.77011984   |
| B11 | 1.03401652 | A11 | 133.20883356 | D11 | 137.37733658  |
| B12 | 2.80596016 | A12 | 109.28202918 | D12 | -166.98649307 |
| B13 | 0.95915288 | A13 | 7.98887817   | D13 | -1.00179841   |
| B14 | 0.97298946 | A14 | 79.57701206  | D14 | 163.96779140  |
| B15 | 2.73873524 | A15 | 17.30430012  | D15 | 137.76237004  |
| B16 | 0.97364848 | A16 | 121.73059827 |     |               |
| B17 | 0.95937539 |     |              |     |               |

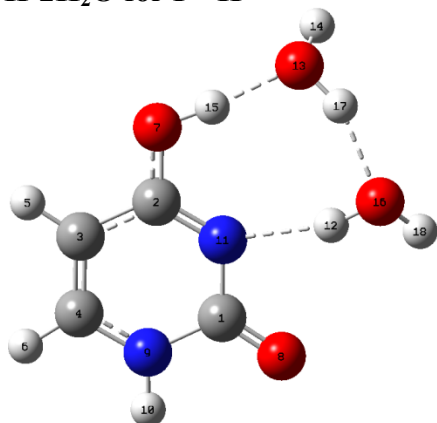
## II-H<sub>2</sub>O for I↔II



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| O | 1  | B7  | 2 | A6  | 7 | D5 0  |
| N | 4  | B8  | 3 | A7  | 2 | D6 0  |
| H | 9  | B9  | 4 | A8  | 3 | D7 0  |
| N | 2  | B10 | 1 | A9  | 8 | D8 0  |
| H | 11 | B11 | 2 | A10 | 1 | D9 0  |
| O | 7  | B12 | 2 | A11 | 1 | D10 0 |
| H | 13 | B13 | 7 | A12 | 2 | D11 0 |
| H | 7  | B14 | 2 | A13 | 1 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.34288308 | A1  | 93.73207390  | D1  | 0.66018014    |
| B2  | 1.43287830 | A2  | 115.83756832 | D2  | -179.61415969 |
| B3  | 1.36154097 | A3  | 121.38427291 | D3  | 179.61364321  |
| B4  | 1.08082031 | A4  | 123.50320185 | D4  | 179.72583512  |
| B5  | 1.08493218 | A5  | 150.29355859 | D5  | -1.99141367   |
| B6  | 1.32944977 | A6  | 153.38917449 | D6  | 0.02051693    |
| B7  | 1.21918783 | A7  | 119.80602936 | D7  | -178.95829575 |
| B8  | 1.36063919 | A8  | 120.92960991 | D8  | -2.32101056   |
| B9  | 1.01197836 | A9  | 30.66662682  | D9  | -177.63179240 |
| B10 | 1.31580089 | A10 | 108.80239547 | D10 | -3.32672739   |
| B11 | 2.02808904 | A11 | 97.12075156  | D11 | 107.22781566  |
| B12 | 2.70491508 | A12 | 134.30066567 | D12 | -1.07176171   |
| B13 | 0.96027774 | A13 | 108.26364376 |     |               |
| B14 | 0.98705384 |     |              |     |               |

## II-2H<sub>2</sub>O for I↔II

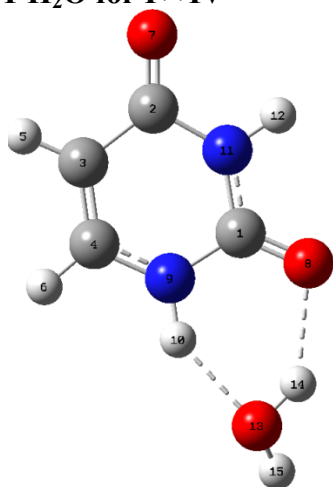


C

|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| O | 1  | B7  | 2  | A6  | 7 | D5 0  |
| N | 4  | B8  | 3  | A7  | 2 | D6 0  |
| H | 9  | B9  | 4  | A8  | 3 | D7 0  |
| N | 2  | B10 | 1  | A9  | 8 | D8 0  |
| H | 11 | B11 | 2  | A10 | 1 | D9 0  |
| O | 7  | B12 | 2  | A11 | 1 | D10 0 |
| H | 13 | B13 | 7  | A12 | 2 | D11 0 |
| H | 7  | B14 | 2  | A13 | 1 | D12 0 |
| O | 13 | B15 | 7  | A14 | 2 | D13 0 |
| H | 13 | B16 | 7  | A15 | 2 | D14 0 |
| H | 16 | B17 | 13 | A16 | 7 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.34434816 | A1  | 93.12853470  | D1  | 0.43857123    |
| B2  | 1.43542310 | A2  | 116.27866515 | D2  | 179.93684721  |
| B3  | 1.36081437 | A3  | 121.09359553 | D3  | 179.74396967  |
| B4  | 1.08094496 | A4  | 123.53939944 | D4  | -179.85447302 |
| B5  | 1.08482957 | A5  | 150.96867159 | D5  | -0.12732658   |
| B6  | 1.32024413 | A6  | 152.52655948 | D6  | -0.52565910   |
| B7  | 1.22287624 | A7  | 119.80373247 | D7  | 179.95589238  |
| B8  | 1.36207700 | A8  | 121.07650087 | D8  | -0.62001621   |
| B9  | 1.01191760 | A9  | 30.55952277  | D9  | -162.05226205 |
| B10 | 1.31785752 | A10 | 135.99474994 | D10 | 0.99950791    |
| B11 | 1.92882363 | A11 | 114.50095213 | D11 | 111.85309376  |
| B12 | 2.65084371 | A12 | 120.71312818 | D12 | 1.44213772    |
| B13 | 0.95989258 | A13 | 110.95134789 | D13 | -14.96692106  |
| B14 | 0.99705862 | A14 | 97.19265215  | D14 | -12.57263758  |
| B15 | 2.69641683 | A15 | 111.69626201 | D15 | 121.13800576  |
| B16 | 0.97830170 | A16 | 144.48916801 |     |               |
| B17 | 0.95992389 |     |              |     |               |

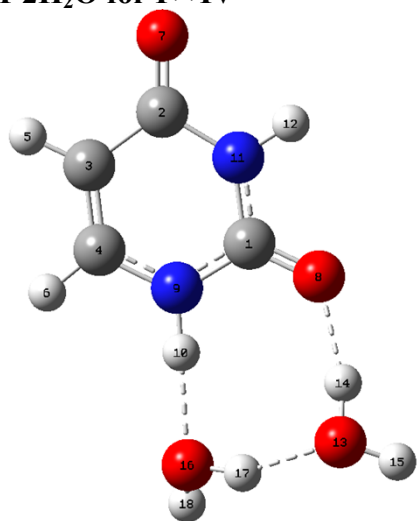
# I-H<sub>2</sub>O for I↔IV



|   |    |     |   |     |    |       |
|---|----|-----|---|-----|----|-------|
| C |    |     |   |     |    |       |
| C | 1  | B1  |   |     |    |       |
| C | 2  | B2  | 1 | A1  |    |       |
| C | 3  | B3  | 2 | A2  | 1  | D1 0  |
| H | 3  | B4  | 2 | A3  | 1  | D2 0  |
| H | 4  | B5  | 3 | A4  | 2  | D3 0  |
| O | 2  | B6  | 1 | A5  | 4  | D4 0  |
| O | 1  | B7  | 4 | A6  | 3  | D5 0  |
| N | 4  | B8  | 3 | A7  | 2  | D6 0  |
| H | 9  | B9  | 4 | A8  | 3  | D7 0  |
| N | 1  | B10 | 8 | A9  | 9  | D8 0  |
| H | 11 | B11 | 1 | A10 | 8  | D9 0  |
| O | 8  | B12 | 1 | A11 | 11 | D10 0 |
| H | 13 | B13 | 8 | A12 | 1  | D11 0 |
| H | 13 | B14 | 8 | A13 | 1  | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.51080863 | A1  | 87.55320799  | D1  | 0.59605819    |
| B2  | 1.45760539 | A2  | 119.70121857 | D2  | 177.75756667  |
| B3  | 1.35563624 | A3  | 118.60422834 | D3  | 178.94141710  |
| B4  | 1.08151732 | A4  | 122.58087403 | D4  | 176.46041534  |
| B5  | 1.08491844 | A5  | 145.84343003 | D5  | 174.68340884  |
| B6  | 1.22022716 | A6  | 151.65610557 | D6  | -2.85626757   |
| B7  | 1.22662256 | A7  | 122.23252186 | D7  | 175.05619200  |
| B8  | 1.37487658 | A8  | 121.54904315 | D8  | -178.04535287 |
| B9  | 1.02043080 | A9  | 123.06585364 | D9  | -3.50329038   |
| B10 | 1.38108474 | A10 | 115.19744717 | D10 | 176.28242506  |
| B11 | 1.01461868 | A11 | 96.22343267  | D11 | 178.55862746  |
| B12 | 2.81432689 | A12 | 26.80718409  | D12 | 137.12096169  |
| B13 | 0.96985570 | A13 | 126.89973039 |     |               |
| B14 | 0.95958463 |     |              |     |               |

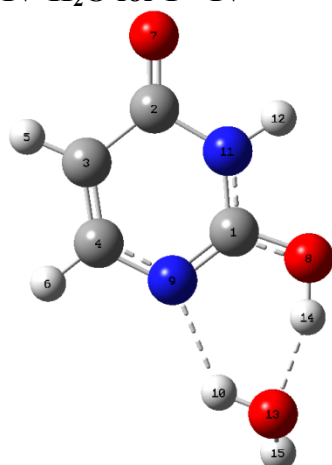
# I-2H<sub>2</sub>O for I↔IV



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| O | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 4  | B8  | 3  | A7  | 2 | D6 0  |
| H | 9  | B9  | 4  | A8  | 3 | D7 0  |
| N | 1  | B10 | 8  | A9  | 9 | D8 0  |
| H | 11 | B11 | 1  | A10 | 8 | D9 0  |
| O | 8  | B12 | 1  | A11 | 9 | D10 0 |
| H | 13 | B13 | 8  | A12 | 1 | D11 0 |
| H | 13 | B14 | 8  | A13 | 1 | D12 0 |
| O | 13 | B15 | 8  | A14 | 1 | D13 0 |
| H | 16 | B16 | 13 | A15 | 8 | D14 0 |
| H | 16 | B17 | 13 | A16 | 8 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.51122733 | A1  | 87.37664873  | D1  | 0.34452474    |
| B2  | 1.45626687 | A2  | 119.60881646 | D2  | 177.96855207  |
| B3  | 1.35616622 | A3  | 118.67770201 | D3  | 179.07594362  |
| B4  | 1.08155831 | A4  | 122.61558195 | D4  | 177.42367844  |
| B5  | 1.08504423 | A5  | 145.82269211 | D5  | 175.86092986  |
| B6  | 1.22057442 | A6  | 152.37951622 | D6  | -2.39705438   |
| B7  | 1.23003431 | A7  | 122.54767245 | D7  | 176.86181332  |
| B8  | 1.37479225 | A8  | 119.63459918 | D8  | -178.21802265 |
| B9  | 1.02873285 | A9  | 122.27891471 | D9  | -2.97935528   |
| B10 | 1.37973988 | A10 | 115.27413529 | D10 | -24.90346825  |
| B11 | 1.01453019 | A11 | 123.21163127 | D11 | -165.16761817 |
| B12 | 2.77981925 | A12 | 9.77422449   | D12 | 172.56618879  |
| B13 | 0.97380574 | A13 | 114.39291896 | D13 | 28.42679815   |
| B14 | 0.95909591 | A14 | 83.53972484  | D14 | 166.08407838  |
| B15 | 2.72553250 | A15 | 15.11133935  | D15 | 117.81837573  |
| B16 | 0.97616617 | A16 | 115.32036802 |     |               |
| B17 | 0.95990832 |     |              |     |               |

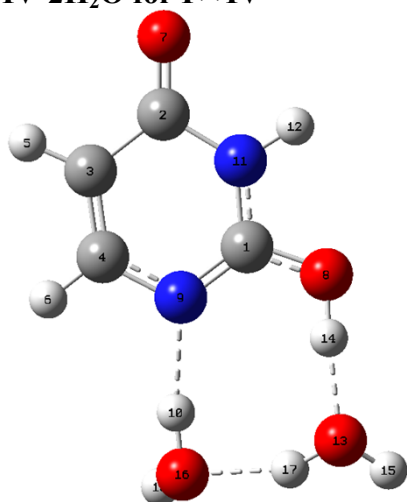
# IV-H<sub>2</sub>O for I↔IV



|   |    |     |   |     |   |
|---|----|-----|---|-----|---|
| C |    |     |   |     |   |
| C | 1  | B1  |   |     |   |
| C | 2  | B2  | 1 | A1  |   |
| C | 3  | B3  | 2 | A2  | 1 |
| H | 3  | B4  | 2 | A3  | 1 |
| H | 4  | B5  | 3 | A4  | 2 |
| O | 2  | B6  | 1 | A5  | 4 |
| O | 1  | B7  | 4 | A6  | 3 |
| N | 1  | B8  | 8 | A7  | 4 |
| H | 9  | B9  | 1 | A8  | 8 |
| N | 1  | B10 | 9 | A9  | 4 |
| H | 11 | B11 | 1 | A10 | 9 |
| O | 8  | B12 | 1 | A11 | 9 |
| H | 8  | B13 | 1 | A12 | 9 |
| H | 13 | B14 | 8 | A13 | 1 |
|   |    |     |   | D1  | 0 |
|   |    |     |   | D2  | 0 |
|   |    |     |   | D3  | 0 |
|   |    |     |   | D4  | 0 |
|   |    |     |   | D5  | 0 |
|   |    |     |   | D6  | 0 |
|   |    |     |   | D7  | 0 |
|   |    |     |   | D8  | 0 |
|   |    |     |   | D9  | 0 |
|   |    |     |   | D10 | 0 |
|   |    |     |   | D11 | 0 |
|   |    |     |   | D12 | 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.45306808 | A1  | 84.29261142  | D1  | -0.06542459   |
| B2  | 1.44990258 | A2  | 120.05311542 | D2  | 179.86248178  |
| B3  | 1.36506859 | A3  | 118.19436325 | D3  | 179.93681695  |
| B4  | 1.08299011 | A4  | 120.19081668 | D4  | -179.98418804 |
| B5  | 1.08680897 | A5  | 147.48077461 | D5  | 179.79612762  |
| B6  | 1.22179010 | A6  | 156.00102056 | D6  | -0.29830269   |
| B7  | 1.32753479 | A7  | 122.65673744 | D7  | 1.79593919    |
| B8  | 1.31079378 | A8  | 105.63468013 | D8  | -0.32219215   |
| B9  | 2.03125634 | A9  | 123.74541978 | D9  | 179.75435572  |
| B10 | 1.35702146 | A10 | 118.43894839 | D10 | -2.88790206   |
| B11 | 1.01520781 | A11 | 96.13774318  | D11 | -1.38743873   |
| B12 | 2.67124024 | A12 | 107.82283252 | D12 | 108.22801220  |
| B13 | 0.98799414 | A13 | 131.80320355 |     |               |
| B14 | 0.96045788 |     |              |     |               |

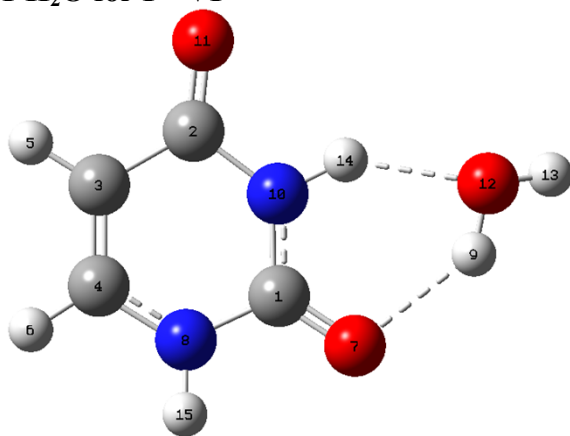
# IV-2H<sub>2</sub>O for I↔IV



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| O | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 1  | B8  | 8  | A7  | 4 | D6 0  |
| H | 9  | B9  | 1  | A8  | 8 | D7 0  |
| N | 1  | B10 | 9  | A9  | 4 | D8 0  |
| H | 11 | B11 | 1  | A10 | 9 | D9 0  |
| O | 8  | B12 | 1  | A11 | 9 | D10 0 |
| H | 8  | B13 | 1  | A12 | 9 | D11 0 |
| H | 13 | B14 | 8  | A13 | 1 | D12 0 |
| O | 13 | B15 | 8  | A14 | 1 | D13 0 |
| H | 13 | B16 | 8  | A15 | 1 | D14 0 |
| H | 16 | B17 | 13 | A16 | 8 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.45959849 | A1  | 84.47297390  | D1  | -0.38478675   |
| B2  | 1.44949352 | A2  | 119.86778852 | D2  | 179.59052469  |
| B3  | 1.36438739 | A3  | 118.36222372 | D3  | 179.72875040  |
| B4  | 1.08292427 | A4  | 120.13480085 | D4  | -179.48465961 |
| B5  | 1.08737872 | A5  | 147.30011516 | D5  | 179.46168031  |
| B6  | 1.22189444 | A6  | 156.88047151 | D6  | -1.02942730   |
| B7  | 1.31927951 | A7  | 123.64852690 | D7  | -10.53575361  |
| B8  | 1.31300616 | A8  | 129.89533090 | D8  | -0.80149735   |
| B9  | 1.84957959 | A9  | 123.06895496 | D9  | 179.49522204  |
| B10 | 1.35899037 | A10 | 118.01570469 | D10 | -9.05579258   |
| B11 | 1.01515247 | A11 | 114.09178297 | D11 | -7.82262363   |
| B12 | 2.62132219 | A12 | 111.40648201 | D12 | 149.79781711  |
| B13 | 0.99813521 | A13 | 121.29641233 | D13 | 19.57206168   |
| B14 | 0.95998049 | A14 | 95.25884306  | D14 | 24.40945759   |
| B15 | 2.68812993 | A15 | 111.04000329 | D15 | 92.53672985   |
| B16 | 0.97818216 | A16 | 132.66215334 |     |               |
| B17 | 0.95977565 |     |              |     |               |

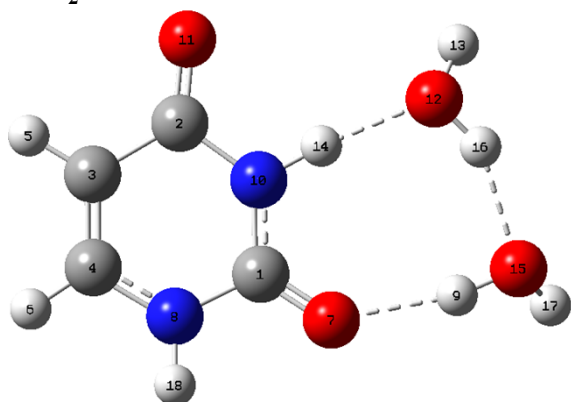
# I-H<sub>2</sub>O for I↔VI



|   |    |     |   |     |    |
|---|----|-----|---|-----|----|
| C |    |     |   |     |    |
| C | 1  | B1  |   |     |    |
| C | 2  | B2  | 1 | A1  |    |
| C | 3  | B3  | 2 | A2  | 1  |
| H | 3  | B4  | 2 | A3  | 1  |
| H | 4  | B5  | 3 | A4  | 2  |
| O | 1  | B6  | 4 | A5  | 3  |
| N | 4  | B7  | 3 | A6  | 2  |
| H | 7  | B8  | 1 | A7  | 8  |
| N | 1  | B9  | 7 | A8  | 8  |
| O | 2  | B10 | 1 | A9  | 7  |
| O | 7  | B11 | 1 | A10 | 10 |
| H | 12 | B12 | 7 | A11 | 1  |
| H | 10 | B13 | 1 | A12 | 7  |
| H | 8  | B14 | 4 | A13 | 3  |
|   |    |     |   | D1  | 0  |
|   |    |     |   | D2  | 0  |
|   |    |     |   | D3  | 0  |
|   |    |     |   | D4  | 0  |
|   |    |     |   | D5  | 0  |
|   |    |     |   | D6  | 0  |
|   |    |     |   | D7  | 0  |
|   |    |     |   | D8  | 0  |
|   |    |     |   | D9  | 0  |
|   |    |     |   | D10 | 0  |
|   |    |     |   | D11 | 0  |
|   |    |     |   | D12 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.50053042 | A1  | 87.83823808  | D1  | 0.32151945    |
| B2  | 1.46129148 | A2  | 119.83938163 | D2  | 177.79863549  |
| B3  | 1.35342833 | A3  | 118.55038806 | D3  | 179.22987921  |
| B4  | 1.08161785 | A4  | 122.95145659 | D4  | 174.83134998  |
| B5  | 1.08479598 | A5  | 149.97456867 | D5  | -2.93988789   |
| B6  | 1.22603626 | A6  | 121.51172103 | D6  | -178.23457930 |
| B7  | 1.37838843 | A7  | 109.66026599 | D7  | -177.93209594 |
| B8  | 2.02140384 | A8  | 124.36362896 | D8  | 2.52002396    |
| B9  | 1.37776846 | A9  | 146.42479834 | D9  | 5.17535436    |
| B10 | 1.21987724 | A10 | 96.68609145  | D10 | -132.77104838 |
| B11 | 2.82299990 | A11 | 128.01938023 | D11 | -3.64044522   |
| B12 | 0.95947582 | A12 | 114.79583305 | D12 | 174.06563540  |
| B13 | 1.02378835 | A13 | 120.87887181 |     |               |
| B14 | 1.01033825 |     |              |     |               |

# I-2H<sub>2</sub>O for I↔VI

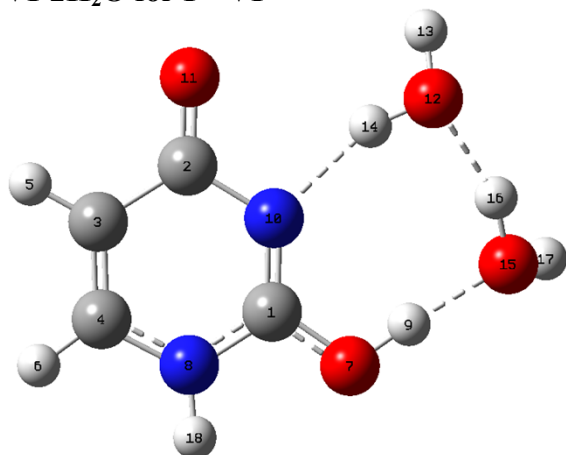


| C |    |     |    |     |    |
|---|----|-----|----|-----|----|
| C | 1  | B1  |    |     |    |
| C | 2  | B2  | 1  | A1  |    |
| C | 3  | B3  | 2  | A2  | 1  |
| H | 3  | B4  | 2  | A3  | 1  |
| H | 4  | B5  | 3  | A4  | 2  |
| O | 1  | B6  | 4  | A5  | 3  |
| N | 4  | B7  | 3  | A6  | 2  |
| H | 7  | B8  | 1  | A7  | 8  |
| N | 1  | B9  | 7  | A8  | 8  |
| O | 2  | B10 | 1  | A9  | 7  |
| O | 10 | B11 | 1  | A10 | 7  |
| H | 12 | B12 | 10 | A11 | 1  |
| H | 10 | B13 | 1  | A12 | 7  |
| O | 12 | B14 | 10 | A13 | 1  |
| H | 12 | B15 | 10 | A14 | 1  |
| H | 15 | B16 | 12 | A15 | 10 |
| H | 8  | B17 | 4  | A16 | 3  |
|   |    |     |    | D1  | 0  |
|   |    |     |    | D2  | 0  |
|   |    |     |    | D3  | 0  |
|   |    |     |    | D4  | 0  |
|   |    |     |    | D5  | 0  |
|   |    |     |    | D6  | 0  |
|   |    |     |    | D7  | 0  |
|   |    |     |    | D8  | 0  |
|   |    |     |    | D9  | 0  |
|   |    |     |    | D10 | 0  |
|   |    |     |    | D11 | 0  |
|   |    |     |    | D12 | 0  |
|   |    |     |    | D13 | 0  |
|   |    |     |    | D14 | 0  |
|   |    |     |    | D15 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.49010992 | A1  | 87.99163824  | D1  | 0.08323289    |
| B2  | 1.46153849 | A2  | 119.77871102 | D2  | 177.86289800  |
| B3  | 1.35318303 | A3  | 118.57082350 | D3  | 179.37845360  |
| B4  | 1.08168588 | A4  | 123.09681283 | D4  | 175.48546076  |
| B5  | 1.08480630 | A5  | 149.12093123 | D5  | -2.79827248   |
| B6  | 1.22907388 | A6  | 121.29128117 | D6  | 168.88768047  |
| B7  | 1.37814681 | A7  | 134.72566064 | D7  | -178.04667425 |
| B8  | 1.85539281 | A8  | 124.75455417 | D8  | 2.95269966    |
| B9  | 1.37132922 | A9  | 146.57241032 | D9  | -5.79734916   |
| B10 | 1.22075182 | A10 | 112.19292675 | D10 | 148.08969262  |
| B11 | 2.81949453 | A11 | 127.16997958 | D11 | -4.63467738   |
| B12 | 0.95944202 | A12 | 116.12683122 | D12 | 14.15289662   |
| B13 | 1.03391055 | A13 | 91.22442597  | D13 | 20.50272038   |
| B14 | 2.74462325 | A14 | 107.93076527 | D14 | 98.50547785   |
| B15 | 0.97299418 | A15 | 138.49192440 | D15 | 174.25972220  |
| B16 | 0.95910462 | A16 | 120.91522965 |     |               |
| B17 | 1.01029651 |     |              |     |               |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.34678709 | A1  | 87.64128473  | D1  | -1.32429505   |
| B2  | 1.46975761 | A2  | 120.23331597 | D2  | 179.24509914  |
| B3  | 1.35438226 | A3  | 118.73826696 | D3  | -179.34013951 |
| B4  | 1.08294210 | A4  | 124.21507861 | D4  | -178.11687198 |
| B5  | 1.08417257 | A5  | 154.22965727 | D5  | -2.08607369   |
| B6  | 1.33008527 | A6  | 112.62758676 | D6  | -179.64715220 |
| B7  | 1.36465755 | A7  | 107.34303604 | D7  | -179.66623167 |
| B8  | 0.99020366 | A8  | 122.74473166 | D8  | 3.38883656    |
| B9  | 1.30044065 | A9  | 149.36914501 | D9  | 2.97419869    |
| B10 | 1.22377387 | A10 | 95.58193732  | D10 | -107.07903240 |
| B11 | 2.66387296 | A11 | 133.54851138 | D11 | -2.84868377   |
| B12 | 0.96034747 | A12 | 82.11609899  | D12 | -177.36989976 |
| B13 | 0.97497286 | A13 | 118.39333845 |     |               |
| B14 | 1.01021607 |     |              |     |               |

# VI-2H<sub>2</sub>O for I↔VI

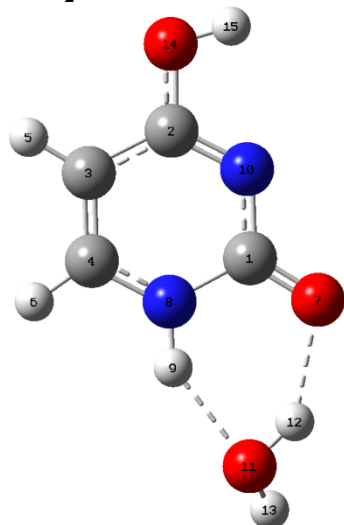


C

|   |    |     |    |     |    |       |
|---|----|-----|----|-----|----|-------|
| C | 1  | B1  |    |     |    |       |
| C | 2  | B2  | 1  | A1  |    |       |
| C | 3  | B3  | 2  | A2  | 1  | D1 0  |
| H | 3  | B4  | 2  | A3  | 1  | D2 0  |
| H | 4  | B5  | 3  | A4  | 2  | D3 0  |
| O | 1  | B6  | 2  | A5  | 3  | D4 0  |
| N | 1  | B7  | 7  | A6  | 4  | D5 0  |
| H | 7  | B8  | 1  | A7  | 8  | D6 0  |
| N | 1  | B9  | 7  | A8  | 8  | D7 0  |
| O | 2  | B10 | 1  | A9  | 10 | D8 0  |
| O | 10 | B11 | 1  | A10 | 7  | D9 0  |
| H | 12 | B12 | 10 | A11 | 1  | D10 0 |
| H | 12 | B13 | 10 | A12 | 1  | D11 0 |
| O | 7  | B14 | 1  | A13 | 10 | D12 0 |
| H | 15 | B15 | 7  | A14 | 1  | D13 0 |
| H | 15 | B16 | 7  | A15 | 1  | D14 0 |
| H | 8  | B17 | 1  | A16 | 10 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.34905832 | A1  | 88.17020358  | D1  | -0.57654341   |
| B2  | 1.46630417 | A2  | 119.80229384 | D2  | 179.44399018  |
| B3  | 1.35496815 | A3  | 119.03079716 | D3  | -179.82800463 |
| B4  | 1.08282331 | A4  | 124.14697028 | D4  | -179.26328004 |
| B5  | 1.08423746 | A5  | 154.88792636 | D5  | -1.02895847   |
| B6  | 1.32055410 | A6  | 112.61213746 | D6  | 177.71450923  |
| B7  | 1.36709571 | A7  | 110.31705436 | D7  | -179.60265314 |
| B8  | 1.00210775 | A8  | 123.64142369 | D8  | 0.88485831    |
| B9  | 1.30225367 | A9  | 148.52598752 | D9  | -16.47176263  |
| B10 | 1.22741745 | A10 | 127.98144947 | D10 | 164.45064679  |
| B11 | 2.85101148 | A11 | 115.71383052 | D11 | -166.25776345 |
| B12 | 0.95996030 | A12 | 12.90662334  | D12 | -1.22161713   |
| B13 | 0.97627540 | A13 | 112.70366293 | D13 | 13.74562600   |
| B14 | 2.61497443 | A14 | 110.85634562 | D14 | -109.57475676 |
| B15 | 0.98072526 | A15 | 120.39374633 | D15 | -179.02753669 |
| B16 | 0.96002370 | A16 | 118.10600288 |     |               |
| B17 | 1.01030358 |     |              |     |               |

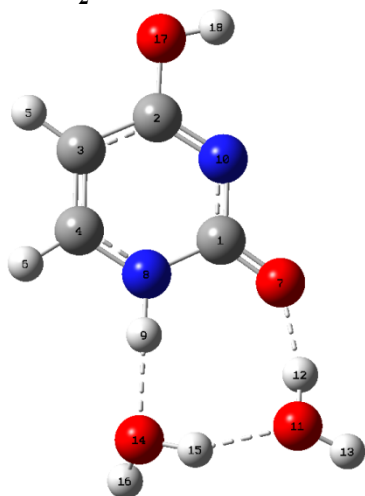
# **II-H<sub>2</sub>O for II↔VIII**



|   |    |     |   |     |    |
|---|----|-----|---|-----|----|
| C |    |     |   |     |    |
| C | 1  | B1  |   |     |    |
| C | 2  | B2  | 1 | A1  |    |
| C | 3  | B3  | 2 | A2  | 1  |
| H | 3  | B4  | 2 | A3  | 1  |
| H | 4  | B5  | 3 | A4  | 2  |
| O | 1  | B6  | 2 | A5  | 3  |
| N | 4  | B7  | 3 | A6  | 2  |
| H | 8  | B8  | 4 | A7  | 3  |
| N | 2  | B9  | 1 | A8  | 7  |
| O | 7  | B10 | 1 | A9  | 10 |
| H | 11 | B11 | 7 | A10 | 1  |
| H | 11 | B12 | 7 | A11 | 1  |
| O | 2  | B13 | 1 | A12 | 7  |
| H | 14 | B14 | 2 | A13 | 1  |
|   |    |     |   | D1  | 0  |
|   |    |     |   | D2  | 0  |
|   |    |     |   | D3  | 0  |
|   |    |     |   | D4  | 0  |
|   |    |     |   | D5  | 0  |
|   |    |     |   | D6  | 0  |
|   |    |     |   | D7  | 0  |
|   |    |     |   | D8  | 0  |
|   |    |     |   | D9  | 0  |
|   |    |     |   | D10 | 0  |
|   |    |     |   | D11 | 0  |
|   |    |     |   | D12 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.32071253 | A1  | 94.44675267  | D1  | -0.53819365   |
| B2  | 1.42534700 | A2  | 114.96747723 | D2  | 179.32319037  |
| B3  | 1.36520167 | A3  | 122.07921000 | D3  | -179.86831977 |
| B4  | 1.08072824 | A4  | 123.44490938 | D4  | -177.98294185 |
| B5  | 1.08497277 | A5  | 153.12450157 | D5  | -0.31884381   |
| B6  | 1.22868092 | A6  | 120.11173884 | D6  | 178.75493419  |
| B7  | 1.35597650 | A7  | 121.27193613 | D7  | 2.29445112    |
| B8  | 1.02278409 | A8  | 31.23148334  | D8  | 176.24024031  |
| B9  | 1.30886736 | A9  | 99.24051527  | D9  | -178.59991281 |
| B10 | 2.76683026 | A10 | 23.14883833  | D10 | 136.81960079  |
| B11 | 0.97361397 | A11 | 122.92488679 | D11 | 1.89376237    |
| B12 | 0.95945187 | A12 | 149.21495224 | D12 | -0.06481274   |
| B13 | 1.34409956 | A13 | 105.52987227 |     |               |
| B14 | 0.96920941 |     |              |     |               |

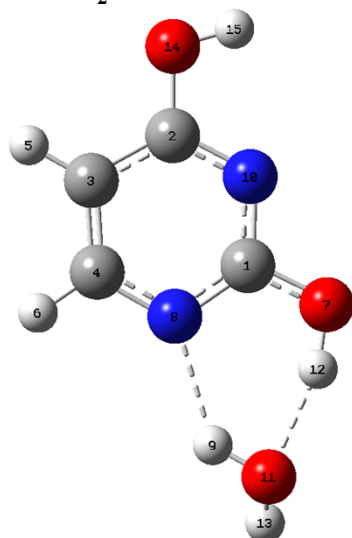
# **II-2H<sub>2</sub>O for II↔VIII**



|   |    |     |    |     |    |
|---|----|-----|----|-----|----|
| C |    |     |    |     |    |
| C | 1  | B1  |    |     |    |
| C | 2  | B2  | 1  | A1  |    |
| C | 3  | B3  | 2  | A2  | 1  |
| H | 3  | B4  | 2  | A3  | 1  |
| H | 4  | B5  | 3  | A4  | 2  |
| O | 1  | B6  | 2  | A5  | 3  |
| N | 4  | B7  | 3  | A6  | 2  |
| H | 8  | B8  | 4  | A7  | 3  |
| N | 2  | B9  | 1  | A8  | 7  |
| O | 7  | B10 | 1  | A9  | 10 |
| H | 11 | B11 | 7  | A10 | 1  |
| H | 11 | B12 | 7  | A11 | 1  |
| O | 11 | B13 | 7  | A12 | 1  |
| H | 14 | B14 | 11 | A13 | 7  |
| H | 14 | B15 | 11 | A14 | 7  |
| O | 2  | B16 | 1  | A15 | 7  |
| H | 17 | B17 | 2  | A16 | 1  |
|   |    |     |    | D1  | 0  |
|   |    |     |    | D2  | 0  |
|   |    |     |    | D3  | 0  |
|   |    |     |    | D4  | 0  |
|   |    |     |    | D5  | 0  |
|   |    |     |    | D6  | 0  |
|   |    |     |    | D7  | 0  |
|   |    |     |    | D8  | 0  |
|   |    |     |    | D9  | 0  |
|   |    |     |    | D10 | 0  |
|   |    |     |    | D11 | 0  |
|   |    |     |    | D12 | 0  |
|   |    |     |    | D13 | 0  |
|   |    |     |    | D14 | 0  |
|   |    |     |    | D15 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.31980501 | A1  | 94.29439524  | D1  | -0.90407440   |
| B2  | 1.42339125 | A2  | 114.85412603 | D2  | 179.17116850  |
| B3  | 1.36604936 | A3  | 122.12012205 | D3  | -179.72576989 |
| B4  | 1.08076671 | A4  | 123.55797141 | D4  | -177.63363927 |
| B5  | 1.08511333 | A5  | 152.56124468 | D5  | -0.06474855   |
| B6  | 1.23169329 | A6  | 120.36894567 | D6  | 179.86902768  |
| B7  | 1.35537114 | A7  | 119.24987576 | D7  | 2.48450435    |
| B8  | 1.03037388 | A8  | 31.22309013  | D8  | 153.52712528  |
| B9  | 1.30989247 | A9  | 124.43242221 | D9  | -158.00092538 |
| B10 | 2.74092517 | A10 | 8.57148358   | D10 | 178.83582140  |
| B11 | 0.97719617 | A11 | 113.17158889 | D11 | 34.49144986   |
| B12 | 0.95897489 | A12 | 83.74749490  | D12 | 164.00625920  |
| B13 | 2.71219771 | A13 | 15.03202396  | D13 | 113.18156884  |
| B14 | 0.97741437 | A14 | 114.63701149 | D14 | 2.25563791    |
| B15 | 0.95991442 | A15 | 149.14529269 | D15 | -0.10505843   |
| B16 | 1.34445180 | A16 | 105.49862547 |     |               |
| B17 | 0.96913284 |     |              |     |               |

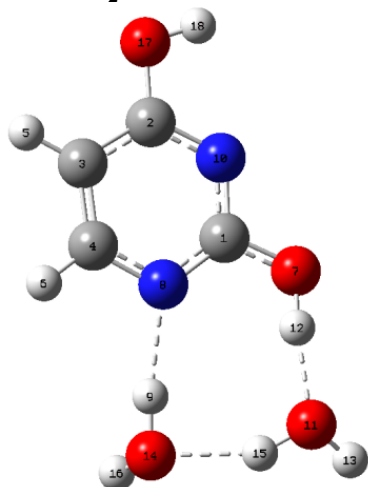
# VIII-H<sub>2</sub>O for II↔VIII



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 1  | B6  | 2 | A5  | 3 | D4 0  |
| N | 1  | B7  | 7 | A6  | 2 | D5 0  |
| H | 8  | B8  | 1 | A7  | 7 | D6 0  |
| N | 2  | B9  | 1 | A8  | 7 | D7 0  |
| O | 7  | B10 | 1 | A9  | 8 | D8 0  |
| H | 7  | B11 | 1 | A10 | 8 | D9 0  |
| H | 11 | B12 | 7 | A11 | 1 | D10 0 |
| O | 2  | B13 | 1 | A12 | 7 | D11 0 |
| H | 14 | B14 | 2 | A13 | 1 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.26453899 | A1  | 91.27467120  | D1  | -0.22947007   |
| B2  | 1.40306964 | A2  | 115.12134289 | D2  | 179.84292918  |
| B3  | 1.38350457 | A3  | 121.86705678 | D3  | -179.90391363 |
| B4  | 1.08229041 | A4  | 120.76417812 | D4  | -179.54339370 |
| B5  | 1.08729459 | A5  | 146.34658112 | D5  | -179.84670138 |
| B6  | 1.33133974 | A6  | 119.02624010 | D6  | 0.87002345    |
| B7  | 1.34149379 | A7  | 108.31189460 | D7  | 0.41658168    |
| B8  | 2.02656758 | A8  | 32.11653174  | D8  | -2.25377804   |
| B9  | 1.32543129 | A9  | 97.50187005  | D9  | -1.13378426   |
| B10 | 2.74371302 | A10 | 108.35855825 | D10 | 105.91592600  |
| B11 | 0.98077589 | A11 | 131.50328979 | D11 | 0.43216233    |
| B12 | 0.96019542 | A12 | 149.80607031 | D12 | -0.21635490   |
| B13 | 1.34526127 | A13 | 105.85170373 |     |               |
| B14 | 0.96821725 |     |              |     |               |

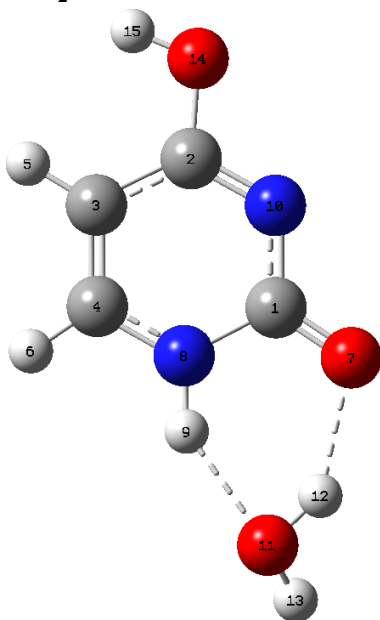
# VIII-2H<sub>2</sub>O for II↔VIII



|   |    |     |    |     |   |
|---|----|-----|----|-----|---|
| C |    |     |    |     |   |
| C | 1  | B1  |    |     |   |
| C | 2  | B2  | 1  | A1  |   |
| C | 3  | B3  | 2  | A2  | 1 |
| H | 3  | B4  | 2  | A3  | 1 |
| H | 4  | B5  | 3  | A4  | 2 |
| O | 1  | B6  | 2  | A5  | 3 |
| N | 1  | B7  | 7  | A6  | 2 |
| H | 8  | B8  | 1  | A7  | 7 |
| N | 2  | B9  | 1  | A8  | 7 |
| O | 7  | B10 | 1  | A9  | 8 |
| H | 7  | B11 | 1  | A10 | 8 |
| H | 11 | B12 | 7  | A11 | 1 |
| O | 11 | B13 | 7  | A12 | 1 |
| H | 11 | B14 | 7  | A13 | 1 |
| H | 14 | B15 | 11 | A14 | 7 |
| O | 2  | B16 | 1  | A15 | 7 |
| H | 17 | B17 | 2  | A16 | 1 |
|   |    |     |    | D1  | 0 |
|   |    |     |    | D2  | 0 |
|   |    |     |    | D3  | 0 |
|   |    |     |    | D4  | 0 |
|   |    |     |    | D5  | 0 |
|   |    |     |    | D6  | 0 |
|   |    |     |    | D7  | 0 |
|   |    |     |    | D8  | 0 |
|   |    |     |    | D9  | 0 |
|   |    |     |    | D10 | 0 |
|   |    |     |    | D11 | 0 |
|   |    |     |    | D12 | 0 |
|   |    |     |    | D13 | 0 |
|   |    |     |    | D14 | 0 |
|   |    |     |    | D15 | 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.26966486 | A1  | 91.42964785  | D1  | -1.00782172   |
| B2  | 1.40341322 | A2  | 114.98545354 | D2  | 179.37588420  |
| B3  | 1.38238353 | A3  | 121.97414808 | D3  | -179.50160820 |
| B4  | 1.08224355 | A4  | 120.81956480 | D4  | -177.92852422 |
| B5  | 1.08782534 | A5  | 146.04338380 | D5  | -179.34075504 |
| B6  | 1.32403947 | A6  | 119.65576504 | D6  | -15.71143936  |
| B7  | 1.34287863 | A7  | 130.97009340 | D7  | 1.58676221    |
| B8  | 1.86134235 | A8  | 31.98842642  | D8  | -9.81822446   |
| B9  | 1.32438208 | A9  | 114.90433154 | D9  | -8.36186631   |
| B10 | 2.68570039 | A10 | 110.87398932 | D10 | 155.41028625  |
| B11 | 0.98797690 | A11 | 120.72074921 | D11 | 24.84815024   |
| B12 | 0.95980996 | A12 | 94.03051093  | D12 | 30.68936693   |
| B13 | 2.71369887 | A13 | 111.26647418 | D13 | 86.26692340   |
| B14 | 0.97496230 | A14 | 131.49494379 | D14 | 2.22914339    |
| B15 | 0.95975064 | A15 | 149.69349855 | D15 | -0.70680528   |
| B16 | 1.34522380 | A16 | 105.81095525 |     |               |
| B17 | 0.96828402 |     |              |     |               |

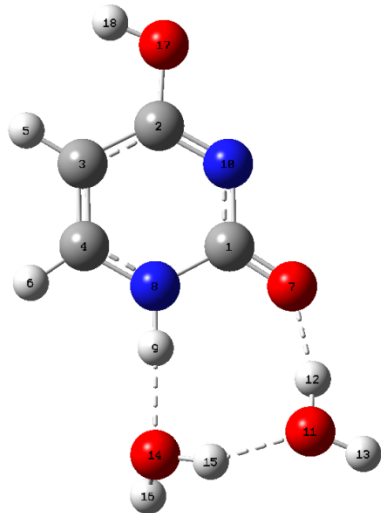
### III-H<sub>2</sub>O for III↔IX



|   |    |     |   |     |    |
|---|----|-----|---|-----|----|
| C |    |     |   |     |    |
| C | 1  | B1  |   |     |    |
| C | 2  | B2  | 1 | A1  |    |
| C | 3  | B3  | 2 | A2  | 1  |
| H | 3  | B4  | 2 | A3  | 1  |
| H | 4  | B5  | 3 | A4  | 2  |
| O | 1  | B6  | 2 | A5  | 3  |
| N | 4  | B7  | 3 | A6  | 2  |
| H | 8  | B8  | 4 | A7  | 3  |
| N | 2  | B9  | 1 | A8  | 7  |
| O | 7  | B10 | 1 | A9  | 10 |
| H | 11 | B11 | 7 | A10 | 1  |
| H | 11 | B12 | 7 | A11 | 1  |
| O | 2  | B13 | 1 | A12 | 7  |
| H | 14 | B14 | 2 | A13 | 1  |
|   |    |     |   | D1  | 0  |
|   |    |     |   | D2  | 0  |
|   |    |     |   | D3  | 0  |
|   |    |     |   | D4  | 0  |
|   |    |     |   | D5  | 0  |
|   |    |     |   | D6  | 0  |
|   |    |     |   | D7  | 0  |
|   |    |     |   | D8  | 0  |
|   |    |     |   | D9  | 0  |
|   |    |     |   | D10 | 0  |
|   |    |     |   | D11 | 0  |
|   |    |     |   | D12 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.31530546 | A1  | 93.90898583  | D1  | -0.95904285   |
| B2  | 1.43165165 | A2  | 115.49226234 | D2  | 179.06983257  |
| B3  | 1.36621860 | A3  | 123.18142022 | D3  | -179.63080703 |
| B4  | 1.08298096 | A4  | 123.38788927 | D4  | -177.12959882 |
| B5  | 1.08511993 | A5  | 153.17393353 | D5  | -0.07945563   |
| B6  | 1.22824008 | A6  | 119.88729375 | D6  | 178.70710112  |
| B7  | 1.35145749 | A7  | 121.41694925 | D7  | 3.20190671    |
| B8  | 1.02321442 | A8  | 31.23538056  | D8  | 176.81900440  |
| B9  | 1.30472009 | A9  | 99.53351426  | D9  | -178.72627530 |
| B10 | 2.76538792 | A10 | 23.08414660  | D10 | 136.51070954  |
| B11 | 0.97388992 | A11 | 122.82632960 | D11 | 2.76026585    |
| B12 | 0.95947462 | A12 | 146.24087284 | D12 | 179.74128414  |
| B13 | 1.35166176 | A13 | 108.72557124 |     |               |
| B14 | 0.96317589 |     |              |     |               |

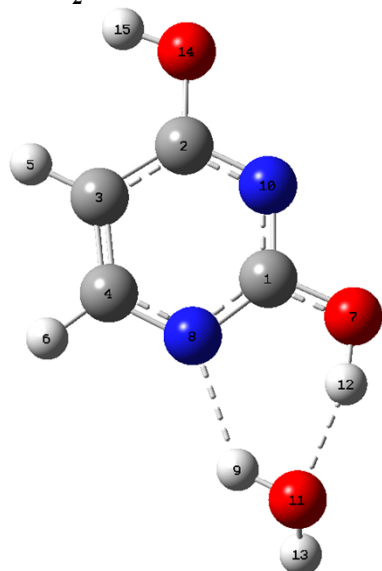
### III-2H<sub>2</sub>O for III↔IX



|   |    |     |    |     |    |       |
|---|----|-----|----|-----|----|-------|
| C |    |     |    |     |    |       |
| C | 1  | B1  |    |     |    |       |
| C | 2  | B2  | 1  | A1  |    |       |
| C | 3  | B3  | 2  | A2  | 1  | D1 0  |
| H | 3  | B4  | 2  | A3  | 1  | D2 0  |
| H | 4  | B5  | 3  | A4  | 2  | D3 0  |
| O | 1  | B6  | 2  | A5  | 3  | D4 0  |
| N | 4  | B7  | 3  | A6  | 2  | D5 0  |
| H | 8  | B8  | 4  | A7  | 3  | D6 0  |
| N | 2  | B9  | 1  | A8  | 7  | D7 0  |
| O | 7  | B10 | 1  | A9  | 10 | D8 0  |
| H | 11 | B11 | 7  | A10 | 1  | D9 0  |
| H | 11 | B12 | 7  | A11 | 1  | D10 0 |
| O | 11 | B13 | 7  | A12 | 1  | D11 0 |
| H | 14 | B14 | 11 | A13 | 7  | D12 0 |
| H | 14 | B15 | 11 | A14 | 7  | D13 0 |
| O | 2  | B16 | 1  | A15 | 7  | D14 0 |
| H | 17 | B17 | 2  | A16 | 1  | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.31413589 | A1  | 93.75978370  | D1  | -1.39975608   |
| B2  | 1.42943819 | A2  | 115.37813934 | D2  | 178.92077510  |
| B3  | 1.36715454 | A3  | 123.21882347 | D3  | -179.44857061 |
| B4  | 1.08304121 | A4  | 123.51287590 | D4  | -176.66538888 |
| B5  | 1.08526718 | A5  | 152.63686711 | D5  | 0.19750428    |
| B6  | 1.23131348 | A6  | 120.12925148 | D6  | 179.66217080  |
| B7  | 1.35086127 | A7  | 119.37656348 | D7  | 3.43227929    |
| B8  | 1.03087887 | A8  | 31.24143358  | D8  | 152.71056191  |
| B9  | 1.30589819 | A9  | 124.27891556 | D9  | -157.07880261 |
| B10 | 2.73702564 | A10 | 8.77594135   | D10 | -178.71585684 |
| B11 | 0.97743382 | A11 | 113.49677949 | D11 | 36.07214039   |
| B12 | 0.95895308 | A12 | 83.72986318  | D12 | 163.82580398  |
| B13 | 2.70891182 | A13 | 14.99479209  | D13 | 111.68805587  |
| B14 | 0.97770763 | A14 | 114.29678515 | D14 | 3.30470476    |
| B15 | 0.95995855 | A15 | 146.20099154 | D15 | 179.97224094  |
| B16 | 1.35203357 | A16 | 108.66523834 |     |               |
| B17 | 0.96320941 |     |              |     |               |

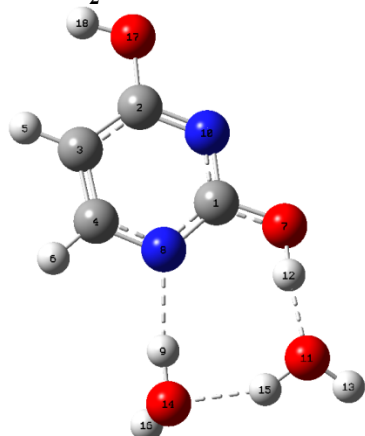
# IX-H<sub>2</sub>O for III↔IX



|   |    |     |   |     |    |       |
|---|----|-----|---|-----|----|-------|
| C |    |     |   |     |    |       |
| C | 1  | B1  |   |     |    |       |
| C | 2  | B2  | 1 | A1  |    |       |
| C | 3  | B3  | 2 | A2  | 1  | D1 0  |
| H | 3  | B4  | 2 | A3  | 1  | D2 0  |
| H | 4  | B5  | 3 | A4  | 2  | D3 0  |
| O | 1  | B6  | 2 | A5  | 3  | D4 0  |
| N | 4  | B7  | 3 | A6  | 2  | D5 0  |
| H | 8  | B8  | 4 | A7  | 3  | D6 0  |
| N | 2  | B9  | 1 | A8  | 7  | D7 0  |
| O | 7  | B10 | 1 | A9  | 10 | D8 0  |
| H | 7  | B11 | 1 | A10 | 10 | D9 0  |
| H | 11 | B12 | 7 | A11 | 1  | D10 0 |
| O | 2  | B13 | 1 | A12 | 7  | D11 0 |
| H | 14 | B14 | 2 | A13 | 1  | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.25944834 | A1  | 90.84315816  | D1  | -0.35477442   |
| B2  | 1.40630220 | A2  | 115.58647587 | D2  | 179.82052996  |
| B3  | 1.38550899 | A3  | 122.86295433 | D3  | -179.80128173 |
| B4  | 1.08456694 | A4  | 120.71743757 | D4  | -179.31946088 |
| B5  | 1.08752349 | A5  | 146.41892774 | D5  | 0.22554515    |
| B6  | 1.33088638 | A6  | 123.08956201 | D6  | 178.71785748  |
| B7  | 1.34445206 | A7  | 135.91174065 | D7  | 0.60818723    |
| B8  | 2.03183235 | A8  | 32.10783714  | D8  | 178.02389339  |
| B9  | 1.32300582 | A9  | 97.83116940  | D9  | 178.95913508  |
| B10 | 2.75118385 | A10 | 108.46916846 | D10 | 105.89137914  |
| B11 | 0.98015126 | A11 | 131.03931584 | D11 | 0.67266151    |
| B12 | 0.96018794 | A12 | 146.60440110 | D12 | 179.99319317  |
| B13 | 1.35139990 | A13 | 108.47495730 |     |               |
| B14 | 0.96343411 |     |              |     |               |

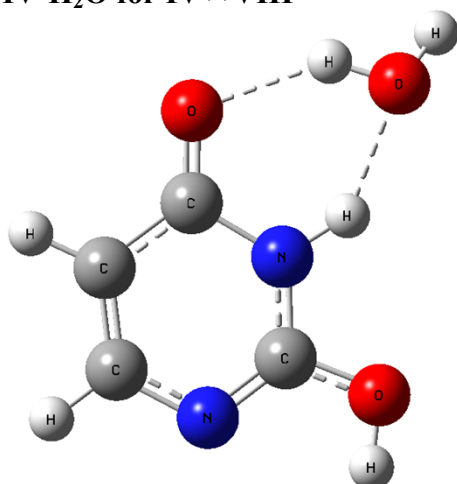
# IX-2H<sub>2</sub>O for III↔IX



|   |    |     |    |     |    |
|---|----|-----|----|-----|----|
| C |    |     |    |     |    |
| C | 1  | B1  |    |     |    |
| C | 2  | B2  | 1  | A1  |    |
| C | 3  | B3  | 2  | A2  | 1  |
| H | 3  | B4  | 2  | A3  | 1  |
| H | 4  | B5  | 3  | A4  | 2  |
| O | 1  | B6  | 2  | A5  | 3  |
| N | 4  | B7  | 3  | A6  | 2  |
| H | 8  | B8  | 4  | A7  | 3  |
| N | 2  | B9  | 1  | A8  | 7  |
| O | 7  | B10 | 1  | A9  | 10 |
| H | 7  | B11 | 1  | A10 | 10 |
| H | 11 | B12 | 7  | A11 | 1  |
| O | 11 | B13 | 7  | A12 | 1  |
| H | 11 | B14 | 7  | A13 | 1  |
| H | 14 | B15 | 11 | A14 | 7  |
| O | 2  | B16 | 1  | A15 | 7  |
| H | 17 | B17 | 2  | A16 | 1  |
|   |    |     |    | D1  | 0  |
|   |    |     |    | D2  | 0  |
|   |    |     |    | D3  | 0  |
|   |    |     |    | D4  | 0  |
|   |    |     |    | D5  | 0  |
|   |    |     |    | D6  | 0  |
|   |    |     |    | D7  | 0  |
|   |    |     |    | D8  | 0  |
|   |    |     |    | D9  | 0  |
|   |    |     |    | D10 | 0  |
|   |    |     |    | D11 | 0  |
|   |    |     |    | D12 | 0  |
|   |    |     |    | D13 | 0  |
|   |    |     |    | D14 | 0  |
|   |    |     |    | D15 | 0  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.26411100 | A1  | 90.99131574  | D1  | -1.45577620   |
| B2  | 1.40683002 | A2  | 115.45884579 | D2  | 179.31399560  |
| B3  | 1.38430273 | A3  | 122.95290914 | D3  | -179.11245916 |
| B4  | 1.08451431 | A4  | 120.81222606 | D4  | -177.27219910 |
| B5  | 1.08801497 | A5  | 146.18806495 | D5  | 0.76583034    |
| B6  | 1.32375353 | A6  | 123.14701618 | D6  | -166.65481656 |
| B7  | 1.34619493 | A7  | 112.08252939 | D7  | 2.09792505    |
| B8  | 1.86229260 | A8  | 31.99491552  | D8  | 170.00310403  |
| B9  | 1.32195259 | A9  | 114.85881998 | D9  | 171.50256372  |
| B10 | 2.69158168 | A10 | 110.80474837 | D10 | 157.29922377  |
| B11 | 0.98720669 | A11 | 120.42009008 | D11 | 26.66858617   |
| B12 | 0.95983254 | A12 | 93.72978132  | D12 | 32.82040743   |
| B13 | 2.71886311 | A13 | 111.27842742 | D13 | 84.60588319   |
| B14 | 0.97449210 | A14 | 130.80954879 | D14 | 2.92159007    |
| B15 | 0.95977672 | A15 | 146.52737108 | D15 | 179.90977688  |
| B16 | 1.35143230 | A16 | 108.47012933 |     |               |
| B17 | 0.96345627 |     |              |     |               |

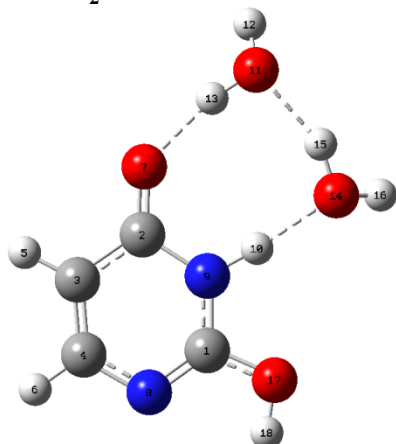
# IV-H<sub>2</sub>O for IV↔VIII



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| N | 1  | B7  | 4 | A6  | 3 | D5 0  |
| N | 1  | B8  | 8 | A7  | 4 | D6 0  |
| H | 9  | B9  | 1 | A8  | 8 | D7 0  |
| O | 7  | B10 | 2 | A9  | 1 | D8 0  |
| H | 11 | B11 | 7 | A10 | 2 | D9 0  |
| H | 11 | B12 | 7 | A11 | 2 | D10 0 |
| O | 1  | B13 | 8 | A12 | 4 | D11 0 |
| H | 14 | B14 | 1 | A13 | 8 | D12 0 |

|     |            |     |              |     |              |
|-----|------------|-----|--------------|-----|--------------|
| B1  | 2.42229154 | A1  | 84.43053788  | D1  | 0.26073241   |
| B2  | 1.44462857 | A2  | 119.94016423 | D2  | 179.78913323 |
| B3  | 1.36751558 | A3  | 118.15035100 | D3  | 179.75697798 |
| B4  | 1.08298171 | A4  | 120.45076455 | D4  | 179.27904143 |
| B5  | 1.08667708 | A5  | 148.56428103 | D5  | 179.96549145 |
| B6  | 1.23261963 | A6  | 33.67884163  | D6  | -0.31787585  |
| B7  | 1.30293876 | A7  | 125.53528341 | D7  | 178.97919778 |
| B8  | 1.35234751 | A8  | 120.31851083 | D8  | -2.94899184  |
| B9  | 1.02667063 | A9  | 97.98457370  | D9  | 135.28069856 |
| B10 | 2.78183123 | A10 | 125.30356130 | D10 | 177.96956213 |
| B11 | 0.95952021 | A11 | 25.11943562  | D11 | 179.98357738 |
| B12 | 0.97175584 | A12 | 120.90761163 | D12 | -0.20098580  |
| B13 | 1.34163415 | A13 | 105.47784084 |     |              |
| B14 | 0.96730744 |     |              |     |              |

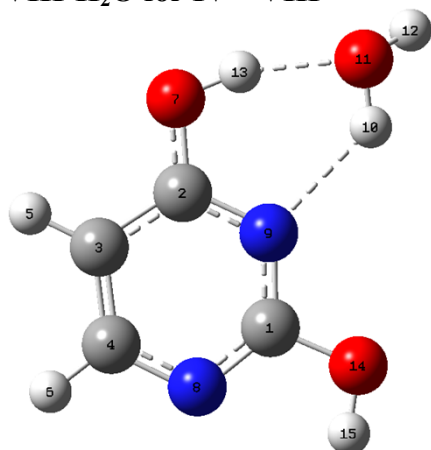
# IV-2H<sub>2</sub>O for IV↔VIII



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| N | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 1  | B8  | 8  | A7  | 4 | D6 0  |
| H | 9  | B9  | 1  | A8  | 8 | D7 0  |
| O | 7  | B10 | 2  | A9  | 1 | D8 0  |
| H | 11 | B11 | 7  | A10 | 2 | D9 0  |
| H | 11 | B12 | 7  | A11 | 2 | D10 0 |
| O | 11 | B13 | 7  | A12 | 2 | D11 0 |
| H | 14 | B14 | 11 | A13 | 7 | D12 0 |
| H | 14 | B15 | 11 | A14 | 7 | D13 0 |
| O | 1  | B16 | 8  | A15 | 4 | D14 0 |
| H | 17 | B17 | 1  | A16 | 8 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.41085874 | A1  | 84.62025141  | D1  | -0.10679182   |
| B2  | 1.44321723 | A2  | 119.87011652 | D2  | 179.89853733  |
| B3  | 1.36800836 | A3  | 118.16353453 | D3  | 179.96570927  |
| B4  | 1.08297842 | A4  | 120.53190033 | D4  | -179.57092215 |
| B5  | 1.08677739 | A5  | 149.22519770 | D5  | -179.84187668 |
| B6  | 1.23530714 | A6  | 33.65506448  | D6  | -0.28595885   |
| B7  | 1.30457065 | A7  | 125.84338254 | D7  | 178.65964115  |
| B8  | 1.35218588 | A8  | 118.91946643 | D8  | -14.47153272  |
| B9  | 1.03770841 | A9  | 130.95805033 | D9  | 152.92641581  |
| B10 | 2.76978015 | A10 | 110.20091049 | D10 | -159.79670934 |
| B11 | 0.95919579 | A11 | 7.83298898   | D11 | 14.40746028   |
| B12 | 0.97528723 | A12 | 80.90526183  | D12 | 162.92902643  |
| B13 | 2.71965144 | A13 | 15.67325061  | D13 | 131.18393119  |
| B14 | 0.97627271 | A14 | 119.27447191 | D14 | -179.84780857 |
| B15 | 0.95949618 | A15 | 120.55364754 | D15 | -1.14563885   |
| B16 | 1.34213078 | A16 | 105.29585740 |     |               |
| B17 | 0.96729420 |     |              |     |               |

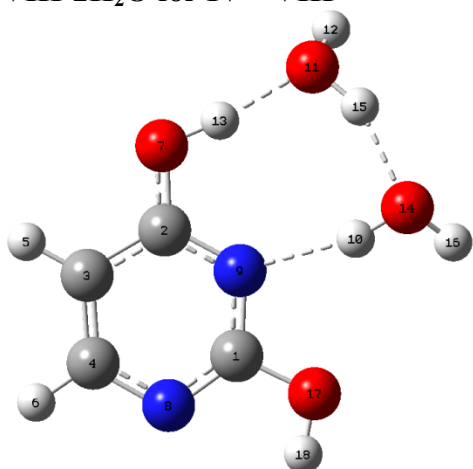
# VIII-H<sub>2</sub>O for IV↔VIII



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| N | 1  | B7  | 4 | A6  | 3 | D5 0  |
| N | 2  | B8  | 1 | A7  | 8 | D6 0  |
| H | 9  | B9  | 2 | A8  | 1 | D7 0  |
| O | 7  | B10 | 2 | A9  | 1 | D8 0  |
| H | 11 | B11 | 7 | A10 | 2 | D9 0  |
| H | 7  | B12 | 2 | A11 | 1 | D10 0 |
| O | 1  | B13 | 8 | A12 | 4 | D11 0 |
| H | 14 | B14 | 1 | A13 | 8 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.26712233 | A1  | 89.82026021  | D1  | 0.06290204    |
| B2  | 1.40660266 | A2  | 116.19100861 | D2  | 179.91784462  |
| B3  | 1.38306294 | A3  | 120.97543549 | D3  | 179.90567522  |
| B4  | 1.08259469 | A4  | 120.92107761 | D4  | 179.95811505  |
| B5  | 1.08708280 | A5  | 151.23469726 | D5  | -179.99653339 |
| B6  | 1.33184822 | A6  | 32.92528197  | D6  | 179.99810634  |
| B7  | 1.32885112 | A7  | 32.05163701  | D7  | -177.93139583 |
| B8  | 1.33698382 | A8  | 108.87864377 | D8  | -3.01174387   |
| B9  | 2.08278111 | A9  | 97.91064570  | D9  | 109.72859273  |
| B10 | 2.72217425 | A10 | 133.96470008 | D10 | -1.13268336   |
| B11 | 0.96034210 | A11 | 108.52377062 | D11 | -179.87357362 |
| B12 | 0.98388738 | A12 | 117.62438018 | D12 | -0.28866086   |
| B13 | 1.34825980 | A13 | 105.38892913 |     |               |
| B14 | 0.96662569 |     |              |     |               |

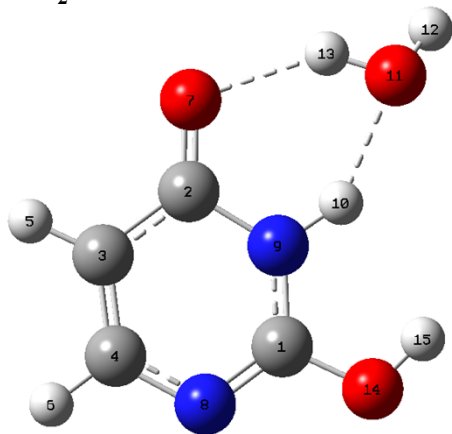
# VIII-2H<sub>2</sub>O for IV↔VIII



|   |    |     |    |     |   |
|---|----|-----|----|-----|---|
| C |    |     |    |     |   |
| C | 1  | B1  |    |     |   |
| C | 2  | B2  | 1  | A1  |   |
| C | 3  | B3  | 2  | A2  | 1 |
| H | 3  | B4  | 2  | A3  | 1 |
| H | 4  | B5  | 3  | A4  | 2 |
| O | 2  | B6  | 1  | A5  | 4 |
| N | 1  | B7  | 4  | A6  | 3 |
| N | 1  | B8  | 8  | A7  | 4 |
| H | 9  | B9  | 1  | A8  | 8 |
| O | 7  | B10 | 2  | A9  | 1 |
| H | 11 | B11 | 7  | A10 | 2 |
| H | 7  | B12 | 2  | A11 | 1 |
| O | 11 | B13 | 7  | A12 | 2 |
| H | 11 | B14 | 7  | A13 | 2 |
| H | 14 | B15 | 11 | A14 | 7 |
| O | 1  | B16 | 8  | A15 | 4 |
| H | 17 | B17 | 1  | A16 | 8 |
|   |    |     |    | D1  | 0 |
|   |    |     |    | D2  | 0 |
|   |    |     |    | D3  | 0 |
|   |    |     |    | D4  | 0 |
|   |    |     |    | D5  | 0 |
|   |    |     |    | D6  | 0 |
|   |    |     |    | D7  | 0 |
|   |    |     |    | D8  | 0 |
|   |    |     |    | D9  | 0 |
|   |    |     |    | D10 | 0 |
|   |    |     |    | D11 | 0 |
|   |    |     |    | D12 | 0 |
|   |    |     |    | D13 | 0 |
|   |    |     |    | D14 | 0 |
|   |    |     |    | D15 | 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.26943674 | A1  | 89.25382299  | D1  | 0.16166927    |
| B2  | 1.40974441 | A2  | 116.65805079 | D2  | -179.95832044 |
| B3  | 1.38148685 | A3  | 120.61233645 | D3  | 179.83691201  |
| B4  | 1.08266302 | A4  | 120.99170226 | D4  | -179.67074359 |
| B5  | 1.08698133 | A5  | 152.14322259 | D5  | -179.62459247 |
| B6  | 1.32330215 | A6  | 33.14519636  | D6  | 0.13144487    |
| B7  | 1.32569705 | A7  | 128.58486117 | D7  | 168.21275162  |
| B8  | 1.33873639 | A8  | 108.40300779 | D8  | 1.66282153    |
| B9  | 1.94658533 | A9  | 115.75965053 | D9  | 114.03816643  |
| B10 | 2.66327484 | A10 | 120.76339285 | D10 | 1.87960715    |
| B11 | 0.95984217 | A11 | 111.47823315 | D11 | -14.54541199  |
| B12 | 0.99276177 | A12 | 96.92428735  | D12 | -11.83853387  |
| B13 | 2.70293983 | A13 | 112.82456017 | D13 | 118.56479870  |
| B14 | 0.97637681 | A14 | 143.29324832 | D14 | -179.90167936 |
| B15 | 0.95977301 | A15 | 117.72660159 | D15 | -1.85070467   |
| B16 | 1.35231706 | A16 | 105.56489031 |     |               |
| B17 | 0.96657447 |     |              |     |               |

# V-H<sub>2</sub>O for V↔X

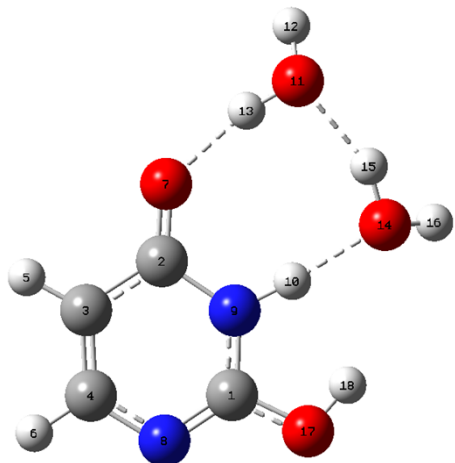


C

|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| N | 1  | B7  | 4 | A6  | 3 | D5 0  |
| N | 1  | B8  | 8 | A7  | 4 | D6 0  |
| H | 9  | B9  | 1 | A8  | 8 | D7 0  |
| O | 7  | B10 | 2 | A9  | 1 | D8 0  |
| H | 11 | B11 | 7 | A10 | 2 | D9 0  |
| H | 11 | B12 | 7 | A11 | 2 | D10 0 |
| O | 1  | B13 | 8 | A12 | 4 | D11 0 |
| H | 14 | B14 | 1 | A13 | 8 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.43938606 | A1  | 84.47078439  | D1  | 0.03787576    |
| B2  | 1.43996873 | A2  | 119.56260009 | D2  | 179.69421115  |
| B3  | 1.36937885 | A3  | 118.42297101 | D3  | -179.98640017 |
| B4  | 1.08297215 | A4  | 120.03344500 | D4  | 178.77257225  |
| B5  | 1.08693876 | A5  | 147.71848174 | D5  | 178.96931749  |
| B6  | 1.23409399 | A6  | 33.62340837  | D6  | -0.54806021   |
| B7  | 1.29938547 | A7  | 124.60565669 | D7  | -178.55050719 |
| B8  | 1.36100665 | A8  | 121.94574877 | D8  | -0.53591018   |
| B9  | 1.02616491 | A9  | 97.89834622  | D9  | 136.53264082  |
| B10 | 2.78303417 | A10 | 124.00139289 | D10 | -178.47162162 |
| B11 | 0.95987283 | A11 | 24.40103876  | D11 | -179.08404857 |
| B12 | 0.97374420 | A12 | 117.91116639 | D12 | -168.42813305 |
| B13 | 1.34678613 | A13 | 109.76540948 |     |               |
| B14 | 0.96412143 |     |              |     |               |

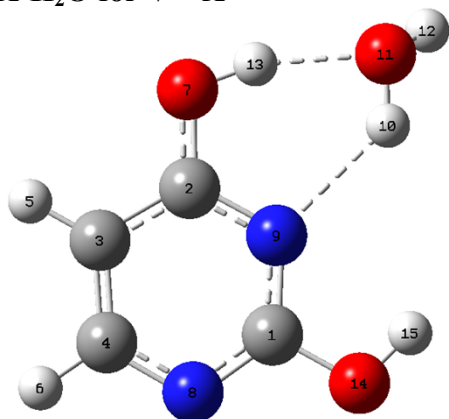
# V-2H<sub>2</sub>O for V↔X



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| N | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 1  | B8  | 8  | A7  | 4 | D6 0  |
| H | 9  | B9  | 1  | A8  | 8 | D7 0  |
| O | 7  | B10 | 2  | A9  | 1 | D8 0  |
| H | 11 | B11 | 7  | A10 | 2 | D9 0  |
| H | 11 | B12 | 7  | A11 | 2 | D10 0 |
| O | 11 | B13 | 7  | A12 | 2 | D11 0 |
| H | 14 | B14 | 11 | A13 | 7 | D12 0 |
| H | 14 | B15 | 11 | A14 | 7 | D13 0 |
| O | 1  | B16 | 8  | A15 | 4 | D14 0 |
| H | 17 | B17 | 1  | A16 | 8 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.41085874 | A1  | 84.62025141  | D1  | -0.10679182   |
| B2  | 1.44321723 | A2  | 119.87011652 | D2  | 179.89853733  |
| B3  | 1.36800836 | A3  | 118.16353453 | D3  | 179.96570927  |
| B4  | 1.08297842 | A4  | 120.53190033 | D4  | -179.57092215 |
| B5  | 1.08677739 | A5  | 149.22519770 | D5  | -179.84187668 |
| B6  | 1.23530714 | A6  | 33.65506448  | D6  | -0.28595885   |
| B7  | 1.30457065 | A7  | 125.84338254 | D7  | 178.65964115  |
| B8  | 1.35218588 | A8  | 118.91946643 | D8  | -14.47153272  |
| B9  | 1.03770841 | A9  | 130.95805033 | D9  | 152.92641581  |
| B10 | 2.76978015 | A10 | 110.20091049 | D10 | -159.79670934 |
| B11 | 0.95919579 | A11 | 7.83298898   | D11 | 14.40746028   |
| B12 | 0.97528723 | A12 | 80.90526183  | D12 | 162.92902643  |
| B13 | 2.71965144 | A13 | 15.67325061  | D13 | 131.18393119  |
| B14 | 0.97627271 | A14 | 119.27447191 | D14 | -179.84780857 |
| B15 | 0.95949618 | A15 | 120.55364754 | D15 | 170.24240511  |
| B16 | 1.34213078 | A16 | 105.29585740 |     |               |
| B17 | 0.96729420 |     |              |     |               |

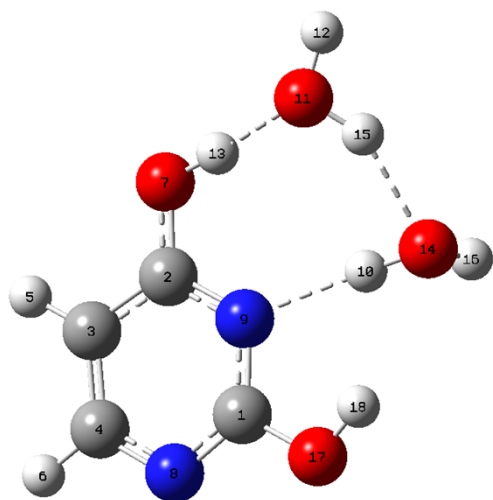
# X-H<sub>2</sub>O for V↔X



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 2  | B6  | 1 | A5  | 4 | D4 0  |
| N | 1  | B7  | 4 | A6  | 3 | D5 0  |
| N | 2  | B8  | 1 | A7  | 8 | D6 0  |
| H | 9  | B9  | 2 | A8  | 1 | D7 0  |
| O | 7  | B10 | 2 | A9  | 1 | D8 0  |
| H | 11 | B11 | 7 | A10 | 2 | D9 0  |
| H | 7  | B12 | 2 | A11 | 1 | D10 0 |
| O | 1  | B13 | 8 | A12 | 4 | D11 0 |
| H | 14 | B14 | 1 | A13 | 8 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.27860072 | A1  | 89.47643980  | D1  | -0.36270402   |
| B2  | 1.40290178 | A2  | 116.23342691 | D2  | 179.77850655  |
| B3  | 1.38493453 | A3  | 120.82776204 | D3  | -179.70074990 |
| B4  | 1.08258253 | A4  | 120.59347465 | D4  | 179.82176161  |
| B5  | 1.08738753 | A5  | 151.71589241 | D5  | 179.73597422  |
| B6  | 1.33343018 | A6  | 33.07795883  | D6  | -179.18721472 |
| B7  | 1.32510782 | A7  | 32.03830226  | D7  | 176.82812608  |
| B8  | 1.34083227 | A8  | 106.83326766 | D8  | 1.47327724    |
| B9  | 2.12092347 | A9  | 98.91848956  | D9  | 109.13053375  |
| B10 | 2.72603483 | A10 | 129.84679476 | D10 | 0.92979682    |
| B11 | 0.96073677 | A11 | 109.15710635 | D11 | 179.63437322  |
| B12 | 0.98162420 | A12 | 115.29282650 | D12 | -176.38575599 |
| B13 | 1.34920377 | A13 | 106.54706785 |     |               |
| B14 | 0.96430161 |     |              |     |               |

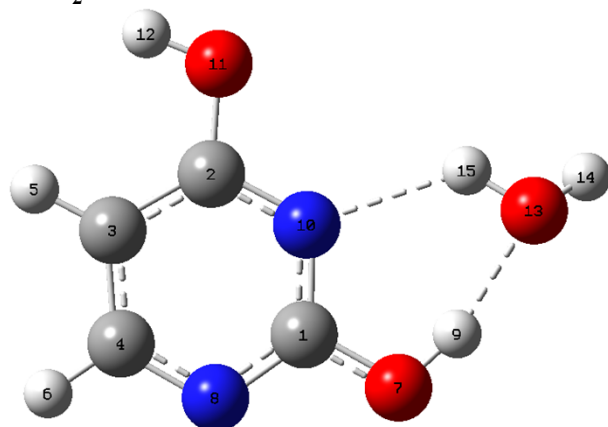
# X-2H<sub>2</sub>O for V↔X



|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C |    |     |    |     |   |       |
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 2  | B6  | 1  | A5  | 4 | D4 0  |
| N | 1  | B7  | 4  | A6  | 3 | D5 0  |
| N | 2  | B8  | 1  | A7  | 8 | D6 0  |
| H | 9  | B9  | 2  | A8  | 1 | D7 0  |
| O | 7  | B10 | 2  | A9  | 1 | D8 0  |
| H | 11 | B11 | 7  | A10 | 2 | D9 0  |
| H | 7  | B12 | 2  | A11 | 1 | D10 0 |
| O | 11 | B13 | 7  | A12 | 2 | D11 0 |
| H | 11 | B14 | 7  | A13 | 2 | D12 0 |
| H | 14 | B15 | 11 | A14 | 7 | D13 0 |
| O | 1  | B16 | 8  | A15 | 4 | D14 0 |
| H | 17 | B17 | 1  | A16 | 8 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.28791326 | A1  | 89.34195470  | D1  | -0.55658128   |
| B2  | 1.40312138 | A2  | 116.25239811 | D2  | 179.06238946  |
| B3  | 1.38586319 | A3  | 120.89304752 | D3  | -179.64637485 |
| B4  | 1.08260047 | A4  | 120.45241198 | D4  | 178.89327628  |
| B5  | 1.08747810 | A5  | 151.12832485 | D5  | 179.02882737  |
| B6  | 1.32897292 | A6  | 33.09888241  | D6  | -177.53693210 |
| B7  | 1.32513669 | A7  | 31.70197647  | D7  | 158.63914366  |
| B8  | 1.34002267 | A8  | 127.85955903 | D8  | -10.20874026  |
| B9  | 1.83268716 | A9  | 111.94366353 | D9  | 165.29612382  |
| B10 | 2.70824149 | A10 | 123.70690371 | D10 | -8.41384196   |
| B11 | 0.96009021 | A11 | 110.30120760 | D11 | 31.63268775   |
| B12 | 0.98727170 | A12 | 92.60840252  | D12 | 36.34061842   |
| B13 | 2.76663330 | A13 | 112.60907626 | D13 | 86.06663875   |
| B14 | 0.97229925 | A14 | 128.23497057 | D14 | 179.69103101  |
| B15 | 0.96078710 | A15 | 115.73089723 | D15 | -174.52630092 |
| B16 | 1.34732903 | A16 | 107.62326934 |     |               |
| B17 | 0.96734140 |     |              |     |               |

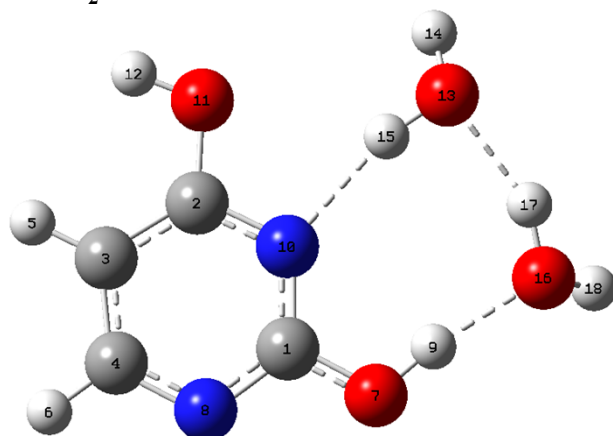
# XI-H<sub>2</sub>O for XI↔XII



|   |    |     |   |     |   |
|---|----|-----|---|-----|---|
| C |    |     |   |     |   |
| C | 1  | B1  |   |     |   |
| C | 2  | B2  | 1 | A1  |   |
| C | 3  | B3  | 2 | A2  | 1 |
| H | 3  | B4  | 2 | A3  | 1 |
| H | 4  | B5  | 3 | A4  | 2 |
| O | 1  | B6  | 4 | A5  | 3 |
| N | 1  | B7  | 7 | A6  | 4 |
| H | 7  | B8  | 1 | A7  | 8 |
| N | 2  | B9  | 1 | A8  | 7 |
| O | 2  | B10 | 1 | A9  | 7 |
| H | 11 | B11 | 2 | A10 | 1 |
| O | 7  | B12 | 1 | A11 | 8 |
| H | 13 | B13 | 7 | A12 | 1 |
| H | 13 | B14 | 7 | A13 | 1 |
|   |    |     |   | D1  | 0 |
|   |    |     |   | D2  | 0 |
|   |    |     |   | D3  | 0 |
|   |    |     |   | D4  | 0 |
|   |    |     |   | D5  | 0 |
|   |    |     |   | D6  | 0 |
|   |    |     |   | D7  | 0 |
|   |    |     |   | D8  | 0 |
|   |    |     |   | D9  | 0 |
|   |    |     |   | D10 | 0 |
|   |    |     |   | D11 | 0 |
|   |    |     |   | D12 | 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.27604617 | A1  | 90.43210771  | D1  | -0.24836442   |
| B2  | 1.39828889 | A2  | 115.46737378 | D2  | 179.90517749  |
| B3  | 1.39248677 | A3  | 122.74673791 | D3  | -179.78510055 |
| B4  | 1.08449997 | A4  | 120.21873624 | D4  | 179.56528224  |
| B5  | 1.08796340 | A5  | 148.03828093 | D5  | -0.27673832   |
| B6  | 1.33049613 | A6  | 115.53010193 | D6  | -178.80837596 |
| B7  | 1.33795060 | A7  | 108.45310691 | D7  | 0.52672815    |
| B8  | 0.98046599 | A8  | 31.95489631  | D8  | 0.60061166    |
| B9  | 1.32804750 | A9  | 146.03932494 | D9  | -179.61438001 |
| B10 | 1.35433212 | A10 | 108.44910605 | D10 | -177.22523331 |
| B11 | 0.96358512 | A11 | 98.55929002  | D11 | -109.19258905 |
| B12 | 2.75130039 | A12 | 133.02491685 | D12 | -4.94687745   |
| B13 | 0.96018458 | A13 | 82.42320159  |     |               |
| B14 | 0.96973472 |     |              |     |               |

# XI-2H<sub>2</sub>O for XI↔XII

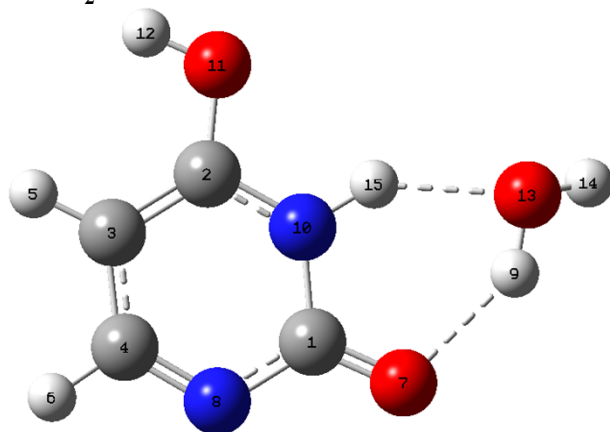


C

|   |    |     |    |     |   |       |
|---|----|-----|----|-----|---|-------|
| C | 1  | B1  |    |     |   |       |
| C | 2  | B2  | 1  | A1  |   |       |
| C | 3  | B3  | 2  | A2  | 1 | D1 0  |
| H | 3  | B4  | 2  | A3  | 1 | D2 0  |
| H | 4  | B5  | 3  | A4  | 2 | D3 0  |
| O | 1  | B6  | 4  | A5  | 3 | D4 0  |
| N | 4  | B7  | 3  | A6  | 2 | D5 0  |
| H | 7  | B8  | 1  | A7  | 8 | D6 0  |
| N | 2  | B9  | 1  | A8  | 7 | D7 0  |
| O | 2  | B10 | 1  | A9  | 7 | D8 0  |
| H | 11 | B11 | 2  | A10 | 1 | D9 0  |
| O | 10 | B12 | 2  | A11 | 1 | D10 0 |
| H | 13 | B13 | 10 | A12 | 2 | D11 0 |
| H | 13 | B14 | 10 | A13 | 2 | D12 0 |
| O | 7  | B15 | 1  | A14 | 8 | D13 0 |
| H | 16 | B16 | 7  | A15 | 1 | D14 0 |
| H | 16 | B17 | 7  | A16 | 1 | D15 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.27840521 | A1  | 90.88440038  | D1  | 0.39159729    |
| B2  | 1.39554232 | A2  | 115.14768520 | D2  | -179.67021864 |
| B3  | 1.39358361 | A3  | 122.88082529 | D3  | 179.67358447  |
| B4  | 1.08434317 | A4  | 120.18616914 | D4  | -179.20427517 |
| B5  | 1.08810024 | A5  | 147.48719739 | D5  | -0.61600394   |
| B6  | 1.32205050 | A6  | 123.87887790 | D6  | 177.70274228  |
| B7  | 1.33640148 | A7  | 111.24217096 | D7  | -1.49732389   |
| B8  | 0.98797588 | A8  | 31.97150209  | D8  | -0.11696405   |
| B9  | 1.32927678 | A9  | 145.53110953 | D9  | -176.64406790 |
| B10 | 1.35837062 | A10 | 108.63549108 | D10 | -170.15602623 |
| B11 | 0.96349042 | A11 | 111.87745067 | D11 | -31.55487644  |
| B12 | 2.91977247 | A12 | 111.52338295 | D12 | 6.80045840    |
| B13 | 0.95971575 | A13 | 9.08230377   | D13 | 177.83847908  |
| B14 | 0.97363838 | A14 | 116.63711553 | D14 | 10.76993768   |
| B15 | 2.68459938 | A15 | 113.93181715 | D15 | -116.08515997 |
| B16 | 0.97465795 | A16 | 120.43682554 |     |               |
| B17 | 0.95968309 |     |              |     |               |

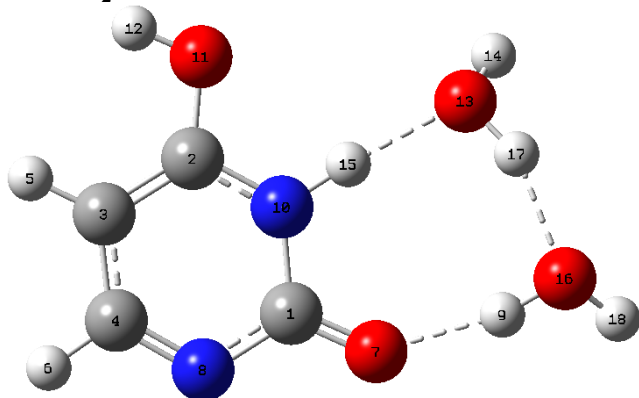
# XII-H<sub>2</sub>O for XI↔XII



|   |    |     |   |     |   |       |
|---|----|-----|---|-----|---|-------|
| C |    |     |   |     |   |       |
| C | 1  | B1  |   |     |   |       |
| C | 2  | B2  | 1 | A1  |   |       |
| C | 3  | B3  | 2 | A2  | 1 | D1 0  |
| H | 3  | B4  | 2 | A3  | 1 | D2 0  |
| H | 4  | B5  | 3 | A4  | 2 | D3 0  |
| O | 1  | B6  | 4 | A5  | 3 | D4 0  |
| N | 4  | B7  | 3 | A6  | 2 | D5 0  |
| H | 7  | B8  | 1 | A7  | 8 | D6 0  |
| N | 2  | B9  | 1 | A8  | 7 | D7 0  |
| O | 2  | B10 | 1 | A9  | 7 | D8 0  |
| H | 11 | B11 | 2 | A10 | 1 | D9 0  |
| O | 7  | B12 | 1 | A11 | 8 | D10 0 |
| H | 13 | B13 | 7 | A12 | 1 | D11 0 |
| H | 10 | B14 | 2 | A13 | 1 | D12 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.43622940 | A1  | 90.53828969  | D1  | -0.58096610   |
| B2  | 1.37621281 | A2  | 115.35478689 | D2  | 179.46140533  |
| B3  | 1.41539479 | A3  | 122.37176542 | D3  | -179.45401893 |
| B4  | 1.08249996 | A4  | 118.18084083 | D4  | 177.75137674  |
| B5  | 1.09009700 | A5  | 154.31215303 | D5  | 0.39920342    |
| B6  | 1.22724303 | A6  | 126.40034331 | D6  | -176.52246777 |
| B7  | 1.31767843 | A7  | 111.47625419 | D7  | 3.33655574    |
| B8  | 1.92016735 | A8  | 28.85597092  | D8  | 1.41507989    |
| B9  | 1.34546299 | A9  | 142.45073195 | D9  | -179.03257420 |
| B10 | 1.34534499 | A10 | 108.54196224 | D10 | -176.48875300 |
| B11 | 0.96392250 | A11 | 99.46967110  | D11 | -134.49399338 |
| B12 | 2.76532260 | A12 | 123.74025745 | D12 | -176.96471496 |
| B13 | 0.95949598 | A13 | 120.03448051 |     |               |
| B14 | 1.02743717 |     |              |     |               |

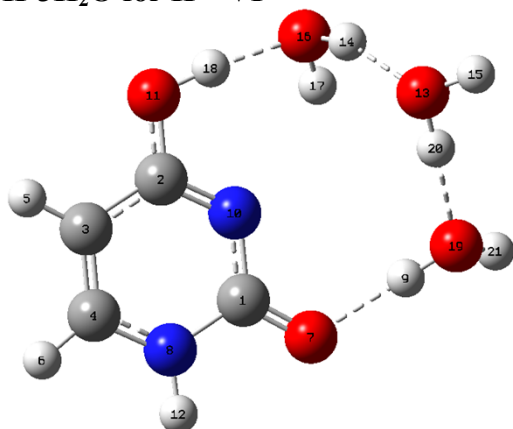
### XII-2H<sub>2</sub>O for XI↔XII



|   |    |     |    |     |    |     |   |
|---|----|-----|----|-----|----|-----|---|
| C | 1  | B1  |    |     |    |     |   |
| C | 2  | B2  | 1  | A1  |    |     |   |
| C | 3  | B3  | 2  | A2  | 1  | D1  | 0 |
| H | 3  | B4  | 2  | A3  | 1  | D2  | 0 |
| H | 4  | B5  | 3  | A4  | 2  | D3  | 0 |
| O | 1  | B6  | 4  | A5  | 3  | D4  | 0 |
| N | 4  | B7  | 3  | A6  | 2  | D5  | 0 |
| H | 7  | B8  | 1  | A7  | 8  | D6  | 0 |
| N | 2  | B9  | 1  | A8  | 7  | D7  | 0 |
| O | 2  | B10 | 1  | A9  | 7  | D8  | 0 |
| H | 11 | B11 | 2  | A10 | 1  | D9  | 0 |
| O | 10 | B12 | 2  | A11 | 1  | D10 | 0 |
| H | 13 | B13 | 10 | A12 | 2  | D11 | 0 |
| H | 10 | B14 | 2  | A13 | 1  | D12 | 0 |
| O | 13 | B15 | 10 | A14 | 2  | D13 | 0 |
| H | 13 | B16 | 10 | A15 | 2  | D14 | 0 |
| H | 16 | B17 | 13 | A16 | 10 | D15 | 0 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.42493217 | A1  | 90.65637323  | D1  | -0.07500127   |
| B2  | 1.37763244 | A2  | 115.32049336 | D2  | 179.81045756  |
| B3  | 1.41301478 | A3  | 122.35349425 | D3  | -179.89254536 |
| B4  | 1.08262332 | A4  | 118.34983730 | D4  | 179.46352398  |
| B5  | 1.09008700 | A5  | 153.65983383 | D5  | -0.10783168   |
| B6  | 1.22968868 | A6  | 126.17343703 | D6  | -155.35676420 |
| B7  | 1.31881996 | A7  | 136.20586540 | D7  | 1.33783687    |
| B8  | 1.79065389 | A8  | 29.03214093  | D8  | 0.76783998    |
| B9  | 1.34501735 | A9  | 142.70847137 | D9  | -177.78045197 |
| B10 | 1.34568300 | A10 | 108.37955190 | D10 | -174.13791218 |
| B11 | 0.96384233 | A11 | 121.39738345 | D11 | -69.92906484  |
| B12 | 2.79476728 | A12 | 128.47376459 | D12 | -177.54909567 |
| B13 | 0.95959577 | A13 | 118.87607084 | D13 | 164.46457011  |
| B14 | 1.03783938 | A14 | 89.73155753  | D14 | 166.63560600  |
| B15 | 2.71485254 | A15 | 104.34815192 | D15 | 122.32613133  |
| B16 | 0.97720262 | A16 | 139.90575961 |     |               |
| B17 | 0.95911983 |     |              |     |               |

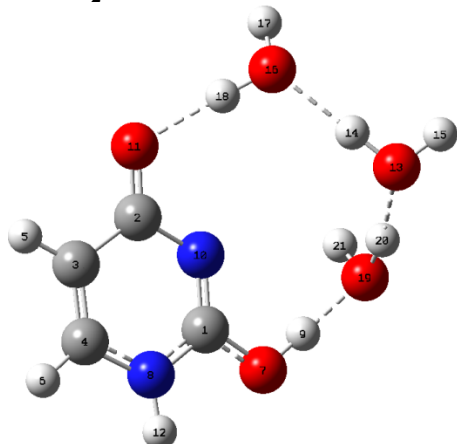
# $\Pi$ -3H<sub>2</sub>O for $\Pi \leftrightarrow VI$



|   |    |     |    |     |    |
|---|----|-----|----|-----|----|
| C |    |     |    |     |    |
| C | 1  | B1  |    |     |    |
| C | 2  | B2  | 1  | A1  |    |
| C | 3  | B3  | 2  | A2  | 1  |
| H | 3  | B4  | 2  | A3  | 1  |
| H | 4  | B5  | 3  | A4  | 2  |
| O | 1  | B6  | 2  | A5  | 3  |
| N | 4  | B7  | 3  | A6  | 2  |
| H | 7  | B8  | 1  | A7  | 8  |
| N | 2  | B9  | 1  | A8  | 7  |
| O | 2  | B10 | 1  | A9  | 7  |
| H | 8  | B11 | 4  | A10 | 3  |
| O | 10 | B12 | 2  | A11 | 1  |
| H | 13 | B13 | 10 | A12 | 2  |
| H | 13 | B14 | 10 | A13 | 2  |
| O | 11 | B15 | 2  | A14 | 1  |
| H | 16 | B16 | 11 | A15 | 2  |
| H | 11 | B17 | 2  | A16 | 1  |
| O | 13 | B18 | 10 | A17 | 2  |
| H | 13 | B19 | 10 | A18 | 2  |
| H | 19 | B20 | 13 | A19 | 10 |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.32862707 | B20 | 0.95969352   | A19 | 123.80916161  |
| B2  | 1.43525272 | A1  | 93.12284514  | D1  | -1.02529252   |
| B3  | 1.36073631 | A2  | 116.25912815 | D2  | 179.05509308  |
| B4  | 1.08114703 | A3  | 121.12915793 | D3  | -179.53839659 |
| B5  | 1.08465739 | A4  | 123.74171895 | D4  | -174.70255795 |
| B6  | 1.23440364 | A5  | 153.29625898 | D5  | 0.23151567    |
| B7  | 1.36318997 | A6  | 119.59371883 | D6  | -152.02804499 |
| B8  | 1.79862938 | A7  | 114.02577849 | D7  | 7.54601280    |
| B9  | 1.32233401 | A8  | 30.67743716  | D8  | 4.22042070    |
| B10 | 1.31740747 | A9  | 150.37942443 | D9  | 177.43888699  |
| B11 | 1.01204057 | A10 | 121.16900817 | D10 | -137.24780032 |
| B12 | 3.86614754 | A11 | 109.75910792 | D11 | -62.03140593  |
| B13 | 1.81510803 | A12 | 56.56755027  | D12 | 154.12563743  |
| B14 | 0.95913516 | A13 | 167.66631255 | D13 | 1.24907006    |
| B15 | 2.60970981 | A14 | 104.46876159 | D14 | 25.91948286   |
| B16 | 0.96490783 | A15 | 92.79282397  | D15 | -0.58309898   |
| B17 | 1.00742177 | A16 | 108.64797746 | D16 | 167.92314805  |
| B18 | 2.76709572 | A17 | 61.36273967  | D17 | 164.50389955  |
| B19 | 0.97702802 | A18 | 63.08123955  | D18 | 120.61414984  |

# VI-3H<sub>2</sub>O for II↔VI



|   |    |     |    |     |    |
|---|----|-----|----|-----|----|
| C |    |     |    |     |    |
| C | 1  | B1  |    |     |    |
| C | 2  | B2  | 1  | A1  |    |
| C | 3  | B3  | 2  | A2  | 1  |
| H | 3  | B4  | 2  | A3  | 1  |
| H | 4  | B5  | 3  | A4  | 2  |
| O | 1  | B6  | 2  | A5  | 3  |
| N | 1  | B7  | 7  | A6  | 4  |
| H | 7  | B8  | 1  | A7  | 8  |
| N | 1  | B9  | 7  | A8  | 8  |
| O | 2  | B10 | 1  | A9  | 10 |
| H | 8  | B11 | 1  | A10 | 10 |
| O | 10 | B12 | 1  | A11 | 7  |
| H | 13 | B13 | 10 | A12 | 1  |
| H | 13 | B14 | 10 | A13 | 1  |
| O | 11 | B15 | 2  | A14 | 1  |
| H | 16 | B16 | 11 | A15 | 2  |
| H | 16 | B17 | 11 | A16 | 2  |
| O | 7  | B18 | 1  | A17 | 10 |
| H | 19 | B19 | 7  | A18 | 1  |
| H | 19 | B20 | 7  | A19 | 1  |

|     |            |     |              |     |               |
|-----|------------|-----|--------------|-----|---------------|
| B1  | 2.32621748 | B20 | 0.96262866   | A19 | 107.88643878  |
| B2  | 1.46247511 | A1  | 88.74669665  | D1  | 3.16069138    |
| B3  | 1.35548171 | A2  | 119.37360322 | D2  | -179.10205981 |
| B4  | 1.08265182 | A3  | 119.19455585 | D3  | 177.98645738  |
| B5  | 1.08425254 | A4  | 124.26265137 | D4  | 176.37407508  |
| B6  | 1.31820623 | A5  | 154.86892051 | D5  | 3.12148924    |
| B7  | 1.36998532 | A6  | 112.59200750 | D6  | -176.45586653 |
| B8  | 1.01113731 | A7  | 109.31424634 | D7  | -179.51843531 |
| B9  | 1.30348452 | A8  | 123.35824714 | D8  | -9.08401346   |
| B10 | 1.23767675 | A9  | 149.50845574 | D9  | 179.62187741  |
| B11 | 1.01064714 | A10 | 118.12160915 | D10 | -38.87411649  |
| B12 | 3.77209110 | A11 | 109.71442132 | D11 | -164.01825247 |
| B13 | 0.97963476 | A12 | 62.87077047  | D12 | -164.43492362 |
| B14 | 0.96001170 | A13 | 167.64524539 | D13 | -24.00601103  |
| B15 | 2.74309790 | A14 | 116.64809036 | D14 | 146.95568879  |
| B16 | 0.96037735 | A15 | 105.92654626 | D15 | 115.68473249  |
| B17 | 0.98127320 | A16 | 2.12763378   | D16 | 4.00574806    |
| B18 | 2.58510010 | A17 | 109.29098190 | D17 | 56.31611948   |
| B19 | 0.98211548 | A18 | 111.45614882 | D18 | -55.88641406  |