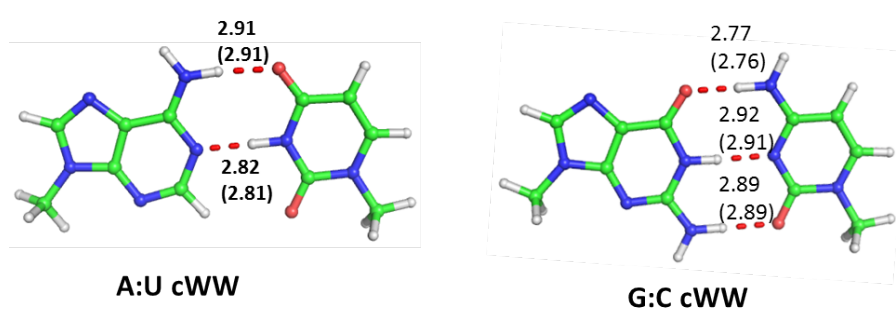


## **Structural and Energetic Characterization of the Emissive RNA Alphabet Based on the Isothiazolo[4,3-*d*]pyrimidine Heterocycle Core**

Mohit Chawla,<sup>1</sup> Albert Poater,<sup>1,2</sup> Romina Oliva,<sup>3</sup> and Luigi Cavallo<sup>1\*</sup>

<sup>1</sup>King Abdullah University of Science and Technology (KAUST), Physical Sciences and Engineering Division, KAUST Catalysis Center, Thuwal 23955-6900, Saudi Arabia. <sup>2</sup>Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Campus Montilivi, 17071 Girona, Catalonia, Spain. <sup>3</sup>Department of Sciences and Technologies, University Parthenope of Naples, Centro Direzionale Isola C4, I-80143, Naples, Italy.

**Impact of the dispersion damping function on optimized geometries:**



**Figure S1:** Comparison of the H-bond distances, in Å, obtained using the D3BJ or the D3 damping approach for dispersion interaction in the geometry optimization (numbers in parentheses).

## Electron density Difference Maps:

To further validate our analysis, we calculated the electron density difference maps using two other alternative protocols. The original map, (A) and the two new maps (B) and (C) are compared below. We describe again the protocol we used to get the map in the original manuscript.

Figure (S2A) is the map described in the manuscript: We took the optimized geometry of the <sup>tz</sup>A base, and we replaced the C9 carbon of <sup>tz</sup>A with a nitrogen, plus we replaced the S8 atom of <sup>tz</sup>A with a carbon, and we added a H atom to C8. Then, we re-optimized the structure freezing the atoms in 6-membered ring plus the N7 atom. With this approach, the heavy atom skeleton of the 6-membered ring of the <sup>tz</sup>A and A bases is identical and can be perfectly superimposed. As remarked by the reviewer, this might bias the analysis since the geometry of the 6-membered ring of <sup>tz</sup>A is imposed to the A base. In this respect, we also have to apologize, since this protocol is

Figure (S2B): We basically reversed the protocol we followed to build the map (A) above. In short, we took the optimized geometry of the A base, and we replaced the N9 carbon of A with a carbon, plus we replaced the C8 carbon with S8 atom, and we deleted a H atom from S8. Then, we re-optimized the structure freezing the atoms in 6-membered ring plus the N7 atom. With this approach, the heavy atom skeleton of the 6-membered ring of the <sup>tz</sup>A and A bases is identical and can be perfectly superimposed. Of course, in this case the geometry of the 6-membered ring of the A base is imposed to <sup>tz</sup>A base.

Figure (S2C): Since two fully relaxed geometries cannot be used to obtain meaningful electron density difference maps, we superimposed the identical atoms in the optimized geometries of both A and <sup>tz</sup>A, and before calculating the electron density difference map, we averaged the coordinates for N1, C2, C6 and N6 atoms, to perfectly superimpose these atoms. With this approach the used geometry is basically middle way between the A and <sup>tz</sup>A geometries.

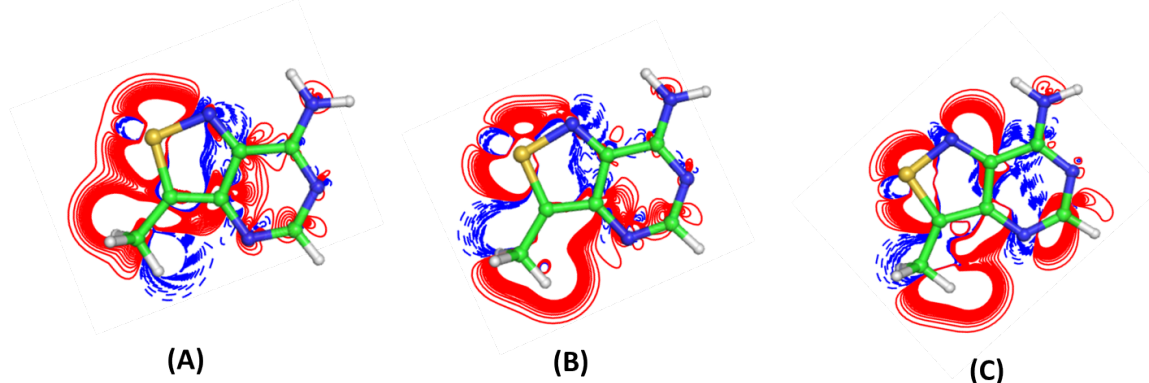
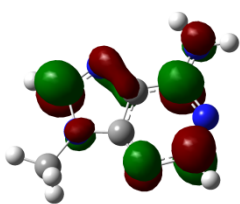
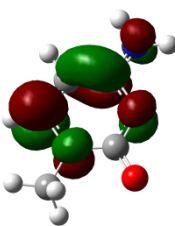
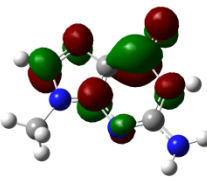
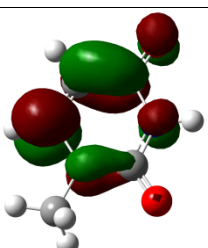
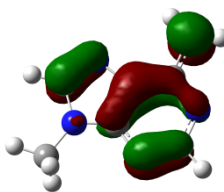
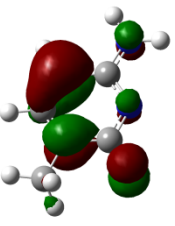
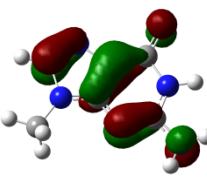
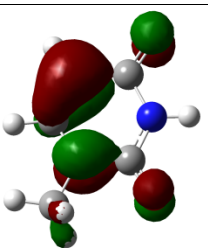
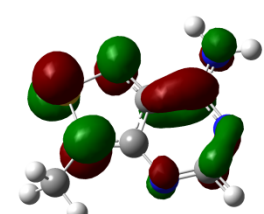
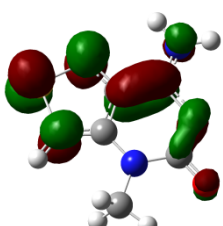
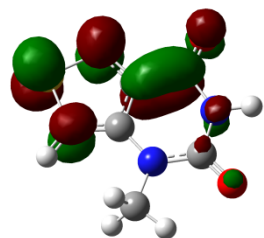
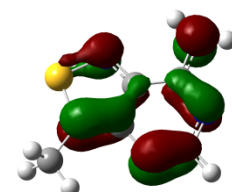
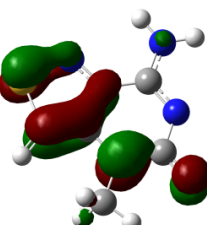
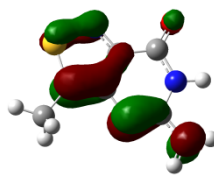
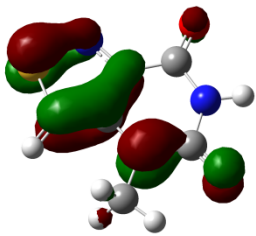
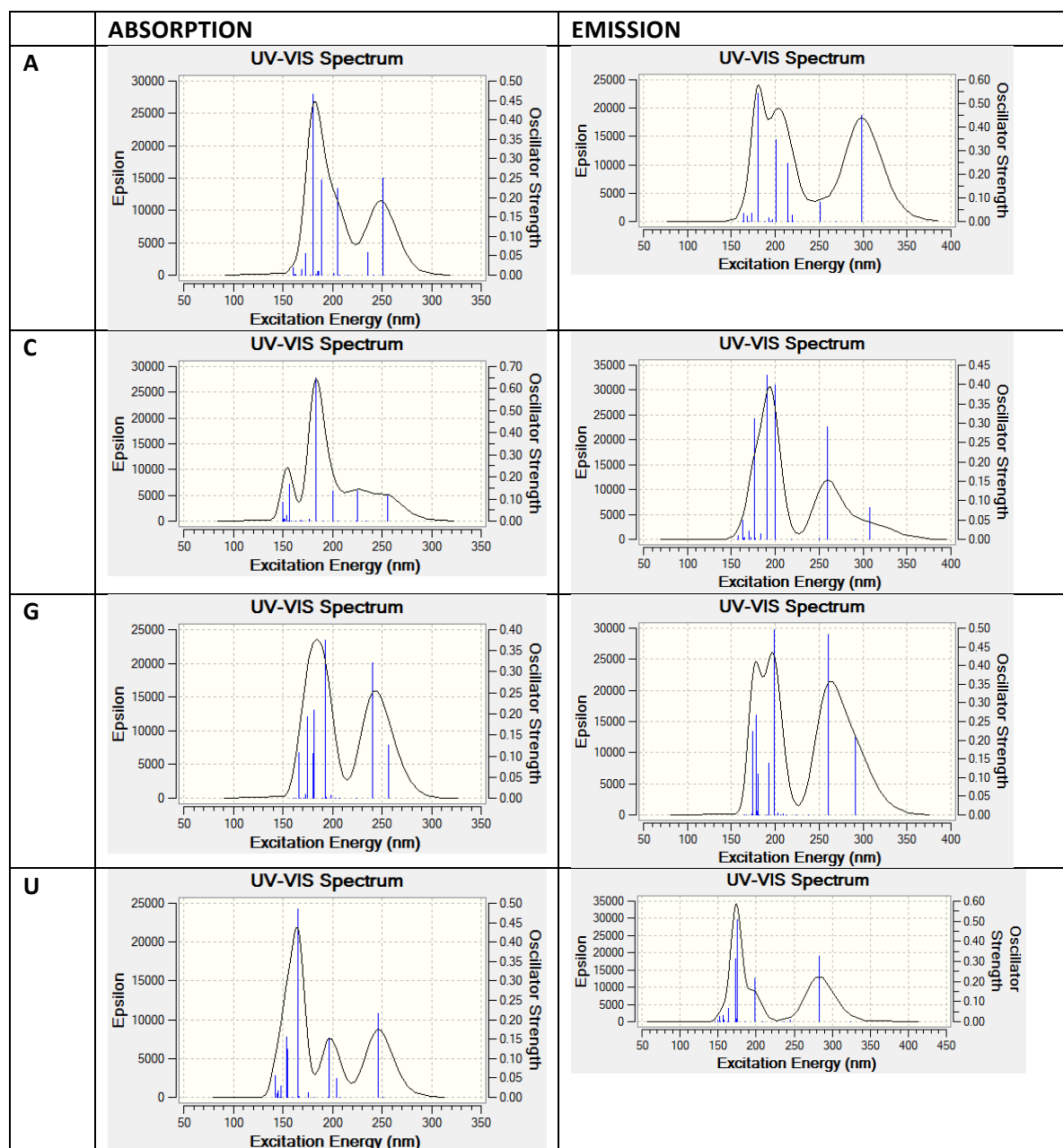


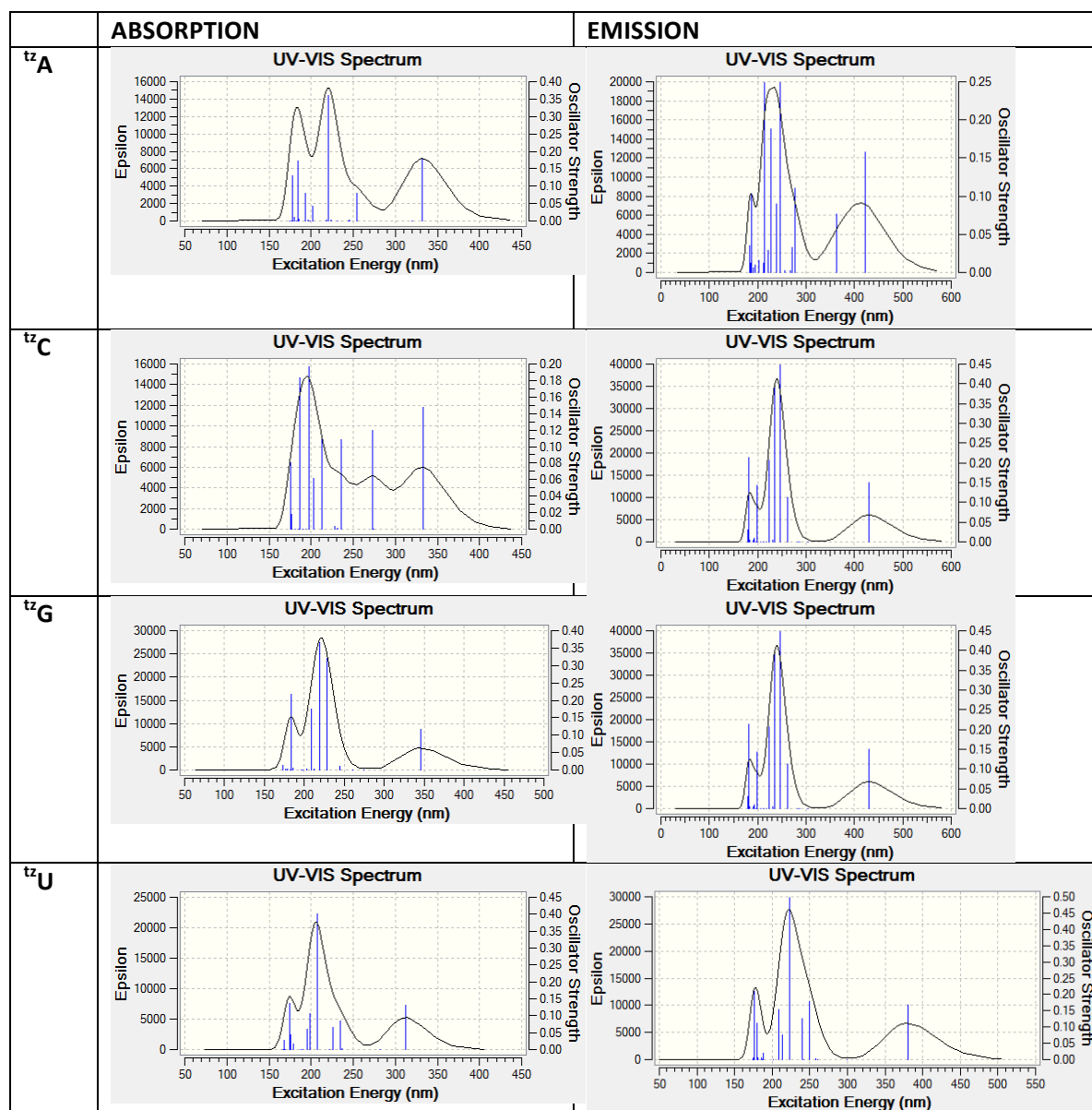
Figure S2: The above density difference maps clearly indicate that the electron density at the Watson-Crick edge is scarcely dependent on the specific approach (either A, B, or C) we have utilized to obtain these maps, further supporting results based on the  $E_{\text{mod}}$  values, which indicate that the modification does not perturb the H-bond base pairing at the Watson-Crick edge.

|   |                                                                                     |                                                                                     |                                                                                      |                                                                                       |
|---|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L |    |    |    |    |
| H |    |    |    |    |
|   | A                                                                                   | C                                                                                   | G                                                                                    | U                                                                                     |
| L |   |   |   |   |
| H |  |  |  |  |
|   | <sup>tz</sup> A                                                                     | <sup>tz</sup> C                                                                     | <sup>tz</sup> G                                                                      | <sup>tz</sup> U                                                                       |

**Figure S3.** Frontier molecular orbitals (H = HOMO, L = LUMO).



**Figure S4A.** Calculated absorption and emission spectra of natural bases.



**Figure S4B.** Calculated absorption and emission spectra of isothiazolo modified bases.

**Table S1:** NICS(0), NICS(1) and HOMA aromaticity values for natural and modified nucleosides.

|                               | 6 membered ring |         |       | 5 membered ring |         |
|-------------------------------|-----------------|---------|-------|-----------------|---------|
|                               | NICS(0)         | NICS(1) | HOMA  | NICS(0)         | NICS(1) |
| <sup>tz</sup> A               | -2.638          | -5.805  | 0.790 | -13.722         | -11.560 |
| <sup>tz</sup> G               | 0.331           | -2.353  | 0.606 | -13.022         | -10.483 |
| <sup>tz</sup> C               | -0.137          | -2.046  | 0.552 | -12.687         | -10.389 |
| <sup>tz</sup> U               | 0.352           | -1.112  | 0.489 | -13.072         | -10.558 |
| A                             | -6.106          | -7.725  | 0.976 | -11.159         | -4.014  |
| G                             | -1.422          | -3.081  | 0.722 | -               | -       |
| C                             | -3.027          | -3.288  | 0.797 | -10.703         | -8.779  |
| U                             | -1.229          | -1.805  | 0.620 | -               | -       |
| C <sub>6</sub> H <sub>6</sub> | -8.227          | -10.370 | 0.995 | -               | -       |

**Table S2:** Coordinates and absolute energies (in a.u.) of the H-bonded base pairs studied in the present work.

33

AU SCF Done: -961.162576415 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.441806 | -1.750925 | 0.015013  |
| N | -0.614210 | -0.050609 | 0.008849  |
| C | -1.115993 | -1.295685 | 0.004777  |
| N | -2.391722 | -1.659470 | 0.000266  |
| C | -3.204962 | -0.596617 | -0.002289 |
| C | -2.828861 | 0.744427  | 0.000368  |
| C | -1.445308 | 1.011014  | 0.005753  |
| N | -0.936066 | 2.248503  | 0.008038  |
| N | -3.934576 | 1.568753  | -0.008914 |
| C | -4.946731 | 0.741058  | -0.016071 |
| N | -4.578431 | -0.585918 | -0.016641 |
| C | 5.076560  | -2.047008 | -0.007724 |
| N | 4.289461  | -0.817442 | -0.003978 |
| C | 2.897402  | -0.962143 | 0.000800  |
| O | 2.374221  | -2.060475 | 0.001642  |
| N | 2.192366  | 0.215500  | 0.004316  |
| C | 2.709973  | 1.501931  | 0.003138  |
| O | 1.966713  | 2.480154  | 0.006065  |
| C | 4.156190  | 1.564718  | -0.001786 |
| C | 4.868764  | 0.421433  | -0.005088 |
| H | 4.632486  | 2.530416  | -0.002823 |
| H | -4.884050 | -2.600607 | -0.370470 |
| H | -0.372463 | -2.084297 | 0.005635  |
| H | -1.566621 | 3.029325  | 0.002563  |
| H | -5.986346 | 1.028399  | -0.027185 |
| H | 4.846354  | -2.643097 | 0.873297  |
| H | 5.949670  | 0.424305  | -0.008863 |
| H | 0.071716  | 2.397066  | 0.008273  |
| H | 1.149717  | 0.115978  | 0.007407  |
| H | 6.132011  | -1.788343 | -0.011079 |
| H | 4.840408  | -2.641586 | -0.888201 |
| H | -6.317315 | -1.578885 | -0.608292 |
| H | -5.762164 | -1.974554 | 1.033196  |

AU-solvent

33

AU-s SCF Done: -961.181251018 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.472560 | -1.741974 | -0.000424 |
| N | -0.629782 | -0.060356 | 0.000529  |
| C | -1.137882 | -1.300701 | 0.000489  |
| N | -2.415248 | -1.662493 | 0.000260  |
| C | -3.228299 | -0.595944 | 0.000054  |
| C | -2.844223 | 0.743688  | 0.000051  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.459210 | 1.005842  | 0.000301  |
| N | -0.938052 | 2.237302  | 0.000377  |
| N | -3.949655 | 1.570179  | -0.000186 |
| C | -4.965993 | 0.742726  | -0.000392 |
| N | -4.599338 | -0.581187 | -0.000299 |
| C | 5.117098  | -2.034440 | -0.000289 |
| N | 4.312813  | -0.812119 | -0.000214 |
| C | 2.929829  | -0.961662 | 0.000123  |
| O | 2.400264  | -2.062850 | 0.000361  |
| N | 2.214866  | 0.210255  | 0.000203  |
| C | 2.727349  | 1.497472  | -0.000016 |
| O | 1.968261  | 2.471434  | 0.000102  |
| C | 4.165997  | 1.569400  | -0.000358 |
| C | 4.886508  | 0.428620  | -0.000445 |
| H | 4.644882  | 2.535466  | -0.000542 |
| H | -5.290433 | -2.348780 | -0.885896 |
| H | -0.399428 | -2.095069 | 0.000650  |
| H | -1.550633 | 3.036725  | -0.000018 |
| H | -6.007767 | 1.029077  | -0.000646 |
| H | 4.893309  | -2.628681 | 0.883310  |
| H | 5.968780  | 0.439162  | -0.000696 |
| H | 0.071817  | 2.368028  | 0.000276  |
| H | 1.177699  | 0.106240  | 0.000378  |
| H | 6.167683  | -1.759545 | -0.000668 |
| H | 4.892738  | -2.628938 | -0.883569 |
| H | -6.505586 | -1.403839 | -0.001633 |
| H | -5.292175 | -2.347758 | 0.886113  |

#### A-tzU cWW

35

AtzU SCF Done: -1451.66555024 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -6.625216 | 1.293488  | 0.000508  |
| N | -1.633222 | 0.146926  | -0.000188 |
| C | -2.272212 | 1.328456  | -0.000019 |
| N | -3.580421 | 1.545669  | 0.000169  |
| C | -4.270464 | 0.399188  | 0.000198  |
| C | -3.745389 | -0.890910 | 0.000045  |
| C | -2.341372 | -1.000270 | -0.000166 |
| N | -1.699455 | -2.175081 | -0.000365 |
| N | -4.750684 | -1.834626 | 0.000131  |
| C | 3.737071  | 2.910455  | 0.000343  |
| N | 3.101831  | 1.601199  | 0.000129  |
| C | 1.713859  | 1.512430  | 0.000100  |
| O | 0.994143  | 2.492438  | 0.000228  |
| N | 1.181164  | 0.231014  | -0.000113 |
| C | 1.833910  | -0.980664 | -0.000282 |
| O | 1.234781  | -2.042532 | -0.000454 |
| C | 3.301636  | -0.839943 | -0.000233 |
| C | 3.884437  | 0.462611  | -0.000028 |
| H | -6.096419 | 2.243018  | 0.000586  |
| H | -1.621562 | 2.194822  | -0.000039 |
| H | -2.239276 | -3.021187 | -0.000193 |
| H | 4.359638  | 3.026520  | -0.888371 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.684152 | -2.212056 | -0.000343 |
| H | 0.131688  | 0.199355  | -0.000110 |
| H | 4.359622  | 3.026234  | 0.889106  |
| H | 2.959460  | 3.665611  | 0.000457  |
| H | -7.252570 | 1.233557  | 0.889411  |
| H | -7.252639 | 1.233746  | -0.888360 |
| N | 4.131451  | -1.861217 | -0.000373 |
| C | 5.254461  | 0.373160  | -0.000019 |
| S | 5.676907  | -1.292551 | -0.000251 |
| H | 5.985201  | 1.162964  | 0.000110  |
| N | -5.634176 | 0.233458  | 0.000364  |
| C | -5.850069 | -1.126647 | 0.000372  |
| H | -6.850207 | -1.530522 | 0.000365  |

# A-tzU cWW Water

35

AtzU-s SCF Done: -1451.68537563 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -6.652571 | 1.289861  | 0.000670  |
| N | -1.645816 | 0.147807  | -0.000265 |
| C | -2.284921 | 1.326788  | -0.000038 |
| N | -3.593451 | 1.546741  | 0.000201  |
| C | -4.288613 | 0.400262  | 0.000202  |
| C | -3.760754 | -0.889861 | -0.000017 |
| C | -2.356155 | -1.000469 | -0.000262 |
| N | -1.707068 | -2.170396 | -0.000491 |
| N | -4.769385 | -1.831551 | 0.000079  |
| C | 3.762447  | 2.907965  | 0.000370  |
| N | 3.114098  | 1.601066  | 0.000100  |
| C | 1.736615  | 1.512634  | -0.000080 |
| O | 1.004690  | 2.490264  | 0.000034  |
| N | 1.197013  | 0.231311  | -0.000292 |
| C | 1.848614  | -0.975856 | -0.000402 |
| O | 1.245185  | -2.042082 | -0.000561 |
| C | 3.310744  | -0.838594 | -0.000206 |
| C | 3.895101  | 0.458904  | 0.000039  |
| H | -6.136438 | 2.245700  | 0.000841  |
| H | -1.635467 | 2.194878  | -0.000058 |
| H | -2.229447 | -3.031511 | -0.000405 |
| H | 4.385553  | 3.014042  | -0.888108 |
| H | -0.692064 | -2.193030 | -0.000555 |
| H | 0.152009  | 0.202148  | -0.000362 |
| H | 4.385334  | 3.013785  | 0.889032  |
| H | 2.995341  | 3.672826  | 0.000385  |
| H | -7.277627 | 1.219410  | 0.889509  |
| H | -7.277710 | 1.219775  | -0.888141 |
| N | 4.139773  | -1.864122 | -0.000221 |
| C | 5.265257  | 0.368046  | 0.000204  |
| S | 5.685966  | -1.292925 | -0.000010 |
| H | 6.005721  | 1.152140  | 0.000405  |
| N | -5.650608 | 0.235699  | 0.000414  |
| C | -5.870394 | -1.120313 | 0.000308  |
| H | -6.873777 | -1.520910 | 0.000437  |

# tzA:U cWW- gas phase

32

tzAU SCF Done: -1303.99689887 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.175949 | -2.076794 | 0.000052  |
| N | -0.324164 | -0.134049 | 0.000127  |
| C | -0.830291 | -1.401169 | 0.000166  |
| N | -2.080188 | -1.772801 | 0.000117  |
| C | -2.973440 | -0.733780 | 0.000022  |
| C | -2.574114 | 0.634982  | -0.000030 |
| C | -1.153735 | 0.900151  | 0.000017  |
| N | -0.690587 | 2.149657  | -0.000053 |
| N | -3.523115 | 1.558541  | -0.000119 |
| C | 5.448053  | -1.951436 | -0.000244 |
| N | 4.616722  | -0.750866 | -0.000006 |
| C | 3.231058  | -0.946897 | 0.000040  |
| O | 2.746965  | -2.062287 | -0.000008 |
| N | 2.483682  | 0.205416  | 0.000168  |
| C | 2.954026  | 1.509016  | 0.000109  |
| O | 2.174986  | 2.460325  | 0.000189  |
| C | 4.396050  | 1.625075  | -0.000040 |
| C | 5.149944  | 0.508118  | -0.000098 |
| H | 4.836735  | 2.607485  | -0.000082 |
| H | -4.502451 | -2.932397 | -0.000156 |
| H | -0.071086 | -2.175517 | 0.000234  |
| H | -1.350178 | 2.907418  | -0.000106 |
| H | 5.235421  | -2.555023 | 0.879990  |
| H | 6.229998  | 0.550892  | -0.000203 |
| H | 0.314831  | 2.330714  | 0.000030  |
| H | 1.447212  | 0.068253  | 0.000192  |
| H | 6.493414  | -1.654852 | 0.000775  |
| H | 5.236816  | -2.553839 | -0.881644 |
| H | -5.816899 | -2.138503 | -0.880949 |
| H | -5.816494 | -2.138630 | 0.881338  |
| C | -4.358045 | -0.830369 | -0.000032 |
| S | -4.979420 | 0.767938  | -0.000142 |

# tzA:U cWW- Water

32

tzAU-s SCF Done: -1304.01241927 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.209491 | 2.064029  | -0.000159 |
| N | -0.335914 | 0.143661  | 0.000059  |
| C | -0.846954 | 1.404409  | 0.000038  |
| N | -2.099051 | 1.775598  | -0.000010 |
| C | -2.992509 | 0.733637  | -0.000040 |
| C | -2.586744 | -0.633092 | -0.000013 |
| C | -1.165076 | -0.895264 | 0.000040  |
| N | -0.691133 | -2.137874 | 0.000079  |
| N | -3.535569 | -1.557801 | -0.000037 |
| C | 5.481567  | 1.942914  | 0.000118  |
| N | 4.636733  | 0.748127  | 0.000031  |
| C | 3.259808  | 0.945063  | 0.000197  |
| O | 2.767231  | 2.062984  | 0.000245  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 2.505530  | -0.202224 | 0.000069  |
| C | 2.973510  | -1.505659 | -0.000054 |
| O | 2.181294  | -2.453679 | -0.000113 |
| C | 4.408427  | -1.627129 | -0.000106 |
| C | 5.167662  | -0.511469 | -0.000070 |
| H | 4.853746  | -2.609107 | -0.000205 |
| H | -4.551406 | 2.931230  | 0.000150  |
| H | -0.092721 | 2.184780  | 0.000068  |
| H | -1.333046 | -2.915415 | 0.000063  |
| H | 5.276805  | 2.544577  | -0.883025 |
| H | 6.248967  | -0.559086 | -0.000139 |
| H | 0.316731  | -2.302569 | 0.000125  |
| H | 1.473763  | -0.062507 | 0.000138  |
| H | 6.522357  | 1.633070  | -0.000535 |
| H | 5.277703  | 2.543863  | 0.883964  |
| H | -5.851769 | 2.115321  | 0.880307  |
| H | -5.851238 | 2.115567  | -0.880999 |
| C | -4.377996 | 0.826723  | -0.000094 |
| S | -4.994718 | -0.771596 | -0.000090 |

#### tzAtzU cWW Gas Phase

34

tzAtzU SCF Done: -1794.49971316 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.382539  | 1.665836  | -0.001184 |
| N | 1.346074  | 0.268297  | 0.000962  |
| C | 1.988722  | 1.473303  | 0.000589  |
| N | 3.271708  | 1.704154  | 0.000096  |
| C | 4.045615  | 0.573521  | -0.000101 |
| C | 3.498097  | -0.742710 | 0.000217  |
| C | 2.057662  | -0.849884 | 0.000808  |
| N | 1.462802  | -2.043103 | 0.001261  |
| N | 4.339514  | -1.765296 | -0.000095 |
| C | -4.126249 | 2.865603  | -0.000202 |
| N | -3.444209 | 1.579756  | -0.000044 |
| C | -2.054564 | 1.541241  | 0.000609  |
| O | -1.368464 | 2.544447  | 0.000777  |
| N | -1.476848 | 0.278295  | 0.001062  |
| C | -2.085335 | -0.955299 | 0.000664  |
| O | -1.447760 | -1.995595 | 0.000876  |
| C | -3.556416 | -0.867410 | 0.000009  |
| C | -4.185224 | 0.413534  | -0.000297 |
| H | 5.807141  | 2.590235  | -0.001102 |
| H | 1.318323  | 2.325306  | 0.000728  |
| H | 2.036048  | -2.868100 | 0.000643  |
| H | -4.752723 | 2.958794  | 0.888356  |
| H | 0.446831  | -2.115190 | 0.001120  |
| H | -0.428997 | 0.284859  | 0.001227  |
| H | -4.751992 | 2.958975  | -0.889260 |
| H | -3.376481 | 3.648407  | 0.000147  |
| H | 7.025878  | 1.656463  | -0.882526 |
| H | 7.026487  | 1.656787  | 0.879731  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.432567  | 0.517029  | -0.000649 |
| S | 5.873757  | -1.139925 | -0.000742 |
| N | -4.349290 | -1.917810 | -0.000337 |
| C | -5.551172 | 0.274963  | -0.000899 |
| S | -5.913563 | -1.404706 | -0.001047 |
| H | -6.309535 | 1.038313  | -0.001382 |

tzA:tzU cWW Water

34

tzAtzU-s SCF Done: -1794.51676510 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -6.404220 | 1.663075  | 0.000985  |
| N | -1.356325 | 0.267237  | -0.000909 |
| C | -1.997056 | 1.468215  | -0.000692 |
| N | -3.281233 | 1.704040  | -0.000227 |
| C | -4.059634 | 0.573751  | 0.000086  |
| C | -3.511956 | -0.742483 | -0.000098 |
| C | -2.071041 | -0.852757 | -0.000626 |
| N | -1.470028 | -2.039925 | -0.000823 |
| N | -4.357949 | -1.762196 | 0.000242  |
| C | 4.148903  | 2.863045  | 0.000390  |
| N | 3.454734  | 1.579695  | 0.000017  |
| C | 2.075442  | 1.539952  | -0.000452 |
| O | 1.377223  | 2.541697  | -0.000475 |
| N | 1.491528  | 0.277563  | -0.000741 |
| C | 2.099999  | -0.951284 | -0.000675 |
| O | 1.459614  | -1.996338 | -0.001000 |
| C | 3.565777  | -0.865565 | -0.000155 |
| C | 4.195205  | 0.410631  | 0.000183  |
| H | -5.840491 | 2.594361  | 0.000791  |
| H | -1.327588 | 2.321910  | -0.000932 |
| H | -2.025817 | -2.881096 | -0.000485 |
| H | 4.775459  | 2.946844  | -0.887995 |
| H | -0.453813 | -2.098740 | -0.001003 |
| H | 0.447513  | 0.285455  | -0.000937 |
| H | 4.774812  | 2.946686  | 0.889245  |
| H | 3.409239  | 3.654487  | 0.000192  |
| H | -7.047716 | 1.646685  | 0.881898  |
| H | -7.048343 | 1.646705  | -0.879471 |
| C | -5.447318 | 0.520056  | 0.000631  |
| S | -5.891714 | -1.134400 | 0.000896  |
| N | 4.358410  | -1.919557 | 0.000068  |
| C | 5.561297  | 0.271882  | 0.000683  |
| S | 5.923423  | -1.402804 | 0.000636  |
| H | 6.328350  | 1.029969  | 0.001034  |

G:C cWW Gas Phase

35

GC SCF Done: -1016.55829586 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.177651  | -1.873432 | 0.000712  |
| N | 4.371713  | -0.656981 | 0.000438  |
| C | 2.965665  | -0.805937 | 0.000287  |
| O | 2.506393  | -1.949056 | 0.000416  |
| N | 2.203781  | 0.310283  | 0.000012  |
| C | 2.746963  | 1.527564  | -0.000112 |
| N | 1.928341  | 2.578868  | -0.000357 |
| C | 4.170882  | 1.699818  | 0.000019  |
| C | 4.927771  | 0.579863  | 0.000292  |
| C | -5.526976 | -1.474330 | 0.000295  |
| N | -0.693541 | -0.045948 | -0.000384 |
| C | -1.229588 | -1.307045 | -0.000395 |
| N | -0.359383 | -2.334261 | -0.000693 |
| N | -2.529326 | -1.539642 | -0.000228 |
| C | -3.257801 | -0.408538 | -0.000095 |
| C | -2.823065 | 0.916782  | -0.000099 |
| C | -1.418403 | 1.157382  | -0.000265 |
| O | -0.817845 | 2.236069  | -0.000269 |
| N | -3.898748 | 1.782324  | 0.000065  |
| C | -4.942408 | 1.004532  | 0.000127  |
| N | -4.623773 | -0.343078 | 0.000027  |
| H | 4.949565  | -2.471523 | 0.880694  |
| H | 2.307984  | 3.507491  | -0.000441 |
| H | 4.625059  | 2.677794  | -0.000086 |
| H | 6.008013  | 0.616662  | 0.000412  |
| H | -5.364223 | -2.091764 | -0.882489 |
| H | 0.650942  | -2.204368 | -0.000297 |
| H | -0.748229 | -3.258277 | -0.000271 |
| H | -5.970916 | 1.329246  | 0.000225  |
| H | -5.366663 | -2.089645 | 0.885025  |
| H | -6.551153 | -1.108151 | -0.001547 |
| H | 6.230425  | -1.601643 | 0.000891  |
| H | 4.949911  | -2.471700 | -0.879241 |
| H | 0.901544  | 2.452719  | -0.000383 |
| H | 0.331759  | 0.056148  | -0.000419 |

G:C cWW Water

35

GC SCF Done: -1016.58401367 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.159882  | -1.901142 | 0.000751  |
| N | 4.361674  | -0.676714 | 0.000418  |
| C | 2.963718  | -0.802136 | 0.000408  |
| O | 2.478158  | -1.942395 | 0.000682  |
| N | 2.210026  | 0.320280  | 0.000072  |
| C | 2.777426  | 1.531209  | -0.000245 |
| N | 1.977169  | 2.598445  | -0.000551 |
| C | 4.198312  | 1.682739  | -0.000235 |
| C | 4.939689  | 0.552260  | 0.000096  |
| C | -5.535768 | -1.488053 | 0.000004  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -0.692644 | -0.021909 | -0.000261 |
| C | -1.218187 | -1.291336 | -0.000363 |
| N | -0.342123 | -2.306631 | -0.000653 |
| N | -2.520220 | -1.534305 | -0.000282 |
| C | -3.262495 | -0.414152 | -0.000098 |
| C | -2.833574 | 0.911721  | 0.000011  |
| C | -1.433829 | 1.164238  | -0.000105 |
| O | -0.855021 | 2.260575  | -0.000010 |
| N | -3.915915 | 1.773316  | 0.000222  |
| C | -4.957981 | 0.985570  | 0.000156  |
| N | -4.628946 | -0.354498 | -0.000052 |
| H | 4.930568  | -2.495138 | 0.883068  |
| H | 2.373538  | 3.525097  | -0.000752 |
| H | 4.663504  | 2.656862  | -0.000483 |
| H | 6.021676  | 0.572705  | 0.000128  |
| H | -5.372957 | -2.101661 | -0.884799 |
| H | 0.669485  | -2.161549 | -0.000348 |
| H | -0.713622 | -3.242511 | -0.000471 |
| H | -5.990508 | 1.302310  | 0.000232  |
| H | -5.374879 | -2.100201 | 0.886184  |
| H | -6.558335 | -1.119266 | -0.001408 |
| H | 6.212947  | -1.633629 | 0.000785  |
| H | 4.930722  | -2.495524 | -0.881347 |
| H | 0.960175  | 2.486503  | -0.000482 |
| H | 0.336274  | 0.089162  | -0.000353 |

#### tzG:C cWW Gas Phase

34

tzGC SCF Done: -1359.39504629 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.498723  | -1.789841 | 0.000793  |
| N | 4.665719  | -0.591204 | 0.000468  |
| C | 3.263643  | -0.772885 | 0.000201  |
| O | 2.830226  | -1.924994 | 0.000263  |
| N | 2.475486  | 0.326717  | -0.000111 |
| C | 2.992505  | 1.554300  | -0.000151 |
| N | 2.150712  | 2.589281  | -0.000461 |
| C | 4.410965  | 1.759973  | 0.000108  |
| C | 5.193456  | 0.657285  | 0.000412  |
| C | -5.289718 | -1.842744 | 0.000391  |
| N | -0.410049 | -0.129262 | -0.000500 |
| C | -0.935626 | -1.414724 | -0.000530 |
| N | -0.022442 | -2.406158 | -0.000897 |
| N | -2.211382 | -1.676949 | -0.000293 |
| C | -3.040371 | -0.584954 | -0.000089 |
| C | -2.592352 | 0.773391  | -0.000109 |
| C | -1.152841 | 1.031506  | -0.000307 |
| O | -0.616111 | 2.136640  | -0.000321 |
| N | -3.509299 | 1.727235  | 0.000026  |
| H | 5.283461  | -2.392412 | 0.880845  |
| H | 2.507161  | 3.526858  | -0.000476 |
| H | 4.842453  | 2.748101  | 0.000068  |
| H | 6.272530  | 0.718917  | 0.000626  |
| H | -5.079424 | -2.458578 | -0.875959 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.981541  | -2.239586 | -0.000477 |
| H | -0.376299 | -3.344359 | -0.000500 |
| H | -5.082090 | -2.456544 | 0.878820  |
| H | -6.349587 | -1.591263 | -0.001456 |
| H | 6.545119  | -1.494774 | 0.000973  |
| H | 5.283827  | -2.392635 | -0.879196 |
| H | 1.132837  | 2.438496  | -0.000591 |
| H | 0.614156  | -0.005450 | -0.000580 |
| S | -4.987869 | 0.994654  | 0.000340  |
| C | -4.424037 | -0.628311 | 0.000167  |

#### tzG:C cWW Water

34

tzGC-s SCF Done: -1359.41666604 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.480539  | -1.816289 | 0.000814  |
| N | 4.653687  | -0.610670 | 0.000458  |
| C | 3.259743  | -0.770020 | 0.000168  |
| O | 2.801884  | -1.921300 | 0.000203  |
| N | 2.477881  | 0.334026  | -0.000177 |
| C | 3.016985  | 1.557584  | -0.000228 |
| N | 2.193058  | 2.607185  | -0.000597 |
| C | 4.433388  | 1.743677  | 0.000064  |
| C | 5.202175  | 0.631666  | 0.000400  |
| C | -5.289434 | -1.856096 | 0.000286  |
| N | -0.406836 | -0.100994 | -0.000520 |
| C | -0.918382 | -1.394212 | -0.000517 |
| N | 0.002109  | -2.371991 | -0.000914 |
| N | -2.196316 | -1.669225 | -0.000256 |
| C | -3.038712 | -0.587795 | -0.000030 |
| C | -2.601901 | 0.770622  | -0.000049 |
| C | -1.165532 | 1.043554  | -0.000310 |
| O | -0.651737 | 2.162752  | -0.000344 |
| N | -3.527546 | 1.718845  | 0.000087  |
| H | 5.264732  | -2.415299 | 0.883085  |
| H | 2.566381  | 3.543286  | -0.000625 |
| H | 4.874317  | 2.728991  | 0.000018  |
| H | 6.283346  | 0.678059  | 0.000640  |
| H | -5.080886 | -2.471118 | -0.877140 |
| H | 1.007413  | -2.188434 | -0.000645 |
| H | -0.331603 | -3.321954 | -0.000576 |
| H | -5.083467 | -2.469247 | 0.879647  |
| H | -6.348807 | -1.604208 | -0.001486 |
| H | 6.526966  | -1.524048 | 0.000999  |
| H | 5.265117  | -2.415559 | -0.881374 |
| H | 1.181922  | 2.472127  | -0.000788 |
| H | 0.621842  | 0.033166  | -0.000691 |
| S | -5.003073 | 0.974153  | 0.000557  |
| C | -4.424126 | -0.641701 | 0.000166  |

#### G:tzC cWW Gas Phase

37

GtzC SCF Done: -1507.06460904 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.940099 | 2.815783  | -0.000327 |
| N | -3.264147 | 1.526861  | -0.000168 |
| C | -1.861107 | 1.453887  | -0.000120 |
| O | -1.206914 | 2.494738  | -0.000233 |
| N | -1.247175 | 0.229679  | 0.000048  |
| C | -1.908295 | -0.912451 | 0.000134  |
| N | -1.266970 | -2.068029 | 0.000253  |
| C | -3.366343 | -0.892446 | 0.000093  |
| C | -4.011348 | 0.373803  | -0.000059 |
| C | 6.676511  | 0.882580  | 0.000170  |
| N | 1.685169  | 0.177200  | 0.000159  |
| C | 2.400566  | 1.346571  | 0.000087  |
| N | 1.688740  | 2.489282  | 0.000251  |
| N | 3.719652  | 1.386481  | -0.000042 |
| C | 4.275260  | 0.161202  | -0.000101 |
| C | 3.650918  | -1.086254 | -0.000016 |
| C | 2.227076  | -1.118747 | 0.000109  |
| O | 1.476453  | -2.099711 | 0.000179  |
| N | 4.587910  | -2.100057 | -0.000140 |
| H | -4.566682 | 2.912751  | 0.888311  |
| H | -1.807441 | -2.916251 | 0.000305  |
| H | 6.604767  | 1.519142  | -0.881078 |
| H | 0.671452  | 2.503587  | -0.000044 |
| H | 2.205924  | 3.348044  | -0.000150 |
| H | 6.610511  | 1.512738  | 0.886511  |
| H | 7.635434  | 0.369383  | -0.004793 |
| H | -4.566651 | 2.912548  | -0.889009 |
| H | -3.187310 | 3.594958  | -0.000403 |
| H | -0.229266 | -2.100082 | 0.000218  |
| H | 0.657426  | 0.228121  | 0.000185  |
| N | -4.137184 | -1.960873 | 0.000186  |
| C | -5.376476 | 0.210696  | -0.000076 |
| S | -5.713817 | -1.474673 | 0.000101  |
| H | -6.149355 | 0.959307  | -0.000175 |
| N | 5.616474  | -0.103568 | -0.000334 |
| C | 5.734120  | -1.483498 | -0.000251 |
| H | 6.703966  | -1.955268 | -0.000399 |

# G:tzC cWW Water

37

GtzC-s SCF Done: -1507.08878340 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.926882 | 2.818706  | 0.000448  |
| N | -3.253206 | 1.525149  | 0.000515  |
| C | -1.862510 | 1.437297  | 0.001120  |
| O | -1.187364 | 2.472639  | 0.001194  |
| N | -1.253192 | 0.208366  | 0.000887  |
| C | -1.929458 | -0.926772 | 0.000366  |
| N | -1.296009 | -2.089107 | 0.000204  |
| C | -3.383504 | -0.893384 | -0.000087 |
| C | -4.013538 | 0.377373  | -0.000026 |
| C | 6.689143  | 0.906971  | -0.000887 |
| N | 1.685613  | 0.152940  | 0.000267  |
| C | 2.388071  | 1.334465  | -0.000461 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 1.665131  | 2.463326  | -0.000928 |
| N | 3.711219  | 1.387350  | -0.000770 |
| C | 4.284626  | 0.172154  | -0.000364 |
| C | 3.669255  | -1.078494 | 0.000326  |
| C | 2.248562  | -1.126662 | 0.000714  |
| O | 1.518754  | -2.130031 | 0.001328  |
| N | 4.616437  | -2.086832 | 0.000567  |
| H | -4.553644 | 2.912791  | 0.888281  |
| H | -1.832841 | -2.943682 | -0.000121 |
| H | 6.615600  | 1.538839  | -0.884787 |
| H | 0.644917  | 2.457301  | -0.000425 |
| H | 2.162491  | 3.341026  | -0.001174 |
| H | 6.620039  | 1.534977  | 0.886153  |
| H | 7.647592  | 0.394109  | -0.004411 |
| H | -4.552928 | 2.913085  | -0.887859 |
| H | -3.176026 | 3.598848  | 0.000879  |
| H | -0.269144 | -2.123664 | 0.000632  |
| H | 0.653684  | 0.192881  | 0.000413  |
| N | -4.168884 | -1.954020 | -0.000648 |
| C | -5.380719 | 0.234013  | -0.000594 |
| S | -5.737888 | -1.442680 | -0.001044 |
| H | -6.151068 | 0.988724  | -0.000727 |
| N | 5.628043  | -0.083608 | -0.000626 |
| C | 5.760817  | -1.457211 | 0.000020  |
| H | 6.737161  | -1.918908 | -0.000051 |

#### tzG:tzC cWW Gas Phase

36

tzGtzC SCF Done: -1849.90108880 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.290261  | 2.761980  | 0.000783  |
| N | 3.578865  | 1.491762  | 0.000525  |
| C | 2.175090  | 1.458303  | -0.000003 |
| O | 1.549161  | 2.515254  | -0.000157 |
| N | 1.526156  | 0.249805  | -0.000270 |
| C | 2.157161  | -0.907890 | -0.000376 |
| N | 1.486210  | -2.048463 | -0.000717 |
| C | 3.614327  | -0.928707 | -0.000107 |
| C | 4.294100  | 0.318689  | 0.000352  |
| C | -6.484055 | 1.307373  | 0.000353  |
| N | -1.408815 | 0.305436  | -0.000727 |
| C | -2.111908 | 1.503696  | -0.000609 |
| N | -1.347190 | 2.613932  | -0.000980 |
| N | -3.411197 | 1.582176  | -0.000301 |
| C | -4.077422 | 0.383506  | -0.000022 |
| C | -3.440835 | -0.897279 | -0.000060 |
| C | -1.980041 | -0.948541 | -0.000457 |
| O | -1.292632 | -1.967410 | -0.000521 |
| N | -4.212894 | -1.971795 | 0.000330  |
| H | 4.919070  | 2.841261  | -0.887902 |
| H | 2.002517  | -2.911453 | -0.000613 |
| H | -6.361811 | 1.949425  | 0.874550  |
| H | -0.331063 | 2.586953  | -0.000579 |
| H | -1.827956 | 3.493832  | -0.000433 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.369977 | 1.942069  | -0.880351 |
| H | -7.496752 | 0.906136  | 0.006594  |
| H | 4.918942  | 2.840930  | 0.889583  |
| H | 3.559560  | 3.561849  | 0.000868  |
| H | 0.454184  | -2.051751 | -0.000710 |
| H | -0.378902 | 0.329971  | -0.000796 |
| S | -5.779978 | -1.456894 | 0.000776  |
| C | -5.453197 | 0.229733  | 0.000448  |
| N | 4.354836  | -2.018657 | -0.000230 |
| C | 5.654184  | 0.117365  | 0.000568  |
| S | 5.944003  | -1.576528 | 0.000200  |
| H | 6.447766  | 0.844039  | 0.000961  |

tzG:tzC cWW Water

36

tzGtzC-s SCF Done: -1849.92052254 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.273263 | 2.765993  | -0.000634 |
| N | -3.564475 | 1.490967  | -0.000290 |
| C | -2.172933 | 1.441447  | 0.000057  |
| O | -1.526170 | 2.494520  | 0.000068  |
| N | -1.528562 | 0.229150  | 0.000379  |
| C | -2.174756 | -0.923178 | 0.000352  |
| N | -1.511763 | -2.069526 | 0.000622  |
| C | -3.628773 | -0.929543 | 0.000020  |
| C | -4.293487 | 0.322964  | -0.000297 |
| C | 6.486630  | 1.329543  | -0.000412 |
| N | 1.405100  | 0.277400  | 0.000658  |
| C | 2.092934  | 1.486754  | 0.000525  |
| N | 1.316565  | 2.582473  | 0.000798  |
| N | 3.396057  | 1.579889  | 0.000252  |
| C | 4.078980  | 0.391077  | 0.000049  |
| C | 3.455821  | -0.892483 | 0.000167  |
| C | 1.996275  | -0.961490 | 0.000517  |
| O | 1.331702  | -1.999021 | 0.000656  |
| N | 4.238932  | -1.961489 | -0.000155 |
| H | -4.901987 | 2.842762  | 0.887393  |
| H | -2.024391 | -2.938813 | 0.000577  |
| H | 6.364607  | 1.970225  | -0.875739 |
| H | 0.297451  | 2.535539  | 0.000456  |
| H | 1.775933  | 3.478450  | 0.000259  |
| H | 6.372615  | 1.963126  | 0.881195  |
| H | 7.499606  | 0.930001  | -0.006499 |
| H | -4.901694 | 2.842435  | -0.888895 |
| H | -3.544118 | 3.566409  | -0.000659 |
| H | -0.488133 | -2.076816 | 0.000737  |
| H | 0.370067  | 0.290348  | 0.000729  |
| S | 5.803956  | -1.431492 | -0.000512 |
| C | 5.458286  | 0.249744  | -0.000402 |
| N | -4.384668 | -2.011632 | 0.000013  |
| C | -5.656184 | 0.142134  | -0.000566 |
| S | -5.966758 | -1.543611 | -0.000533 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -6.446836 | 0.875583 | -0.000829 |
|---|-----------|----------|-----------|

#### A:A tHW Gas

36

AA-t-1jj2 SCF Done: -1013.67143104 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.538731  | 0.591820  | -0.181004 |
| N | 1.414091  | 0.787674  | -0.097214 |
| C | 2.341696  | 1.735539  | -0.292982 |
| N | 3.663015  | 1.612674  | -0.309062 |
| C | 4.035459  | 0.345159  | -0.096201 |
| C | 3.194988  | -0.743390 | 0.117142  |
| C | 1.808884  | -0.485060 | 0.109704  |
| N | 0.894386  | -1.441741 | 0.304471  |
| N | 3.921986  | -1.902858 | 0.290152  |
| C | 5.166496  | -1.515211 | 0.185226  |
| N | 5.309300  | -0.166561 | -0.053612 |
| C | -5.368156 | -2.361611 | -0.279960 |
| N | -3.536449 | 2.393754  | 0.191681  |
| C | -4.781039 | 1.918320  | 0.117134  |
| N | -5.183287 | 0.653386  | -0.004017 |
| C | -4.141456 | -0.179048 | -0.038901 |
| C | -2.791122 | 0.158767  | 0.033931  |
| C | -2.498038 | 1.536278  | 0.149259  |
| N | -1.255197 | 2.028917  | 0.225490  |
| N | -2.010010 | -0.981727 | -0.023736 |
| C | -2.868048 | -1.965119 | -0.132493 |
| N | -4.173660 | -1.551014 | -0.145450 |
| H | 6.354531  | 1.447489  | -0.825985 |
| H | 1.953285  | 2.734142  | -0.460102 |
| H | 1.216925  | -2.385128 | 0.424277  |
| H | 6.028732  | -2.158396 | 0.264609  |
| H | -5.786824 | -2.269525 | -1.282034 |
| H | -5.566645 | 2.664186  | 0.158386  |
| H | -0.411823 | 1.462254  | 0.115468  |
| H | -2.611756 | -3.010310 | -0.201424 |
| H | 7.310394  | -0.035448 | -0.622574 |
| H | 6.879324  | 0.953172  | 0.789941  |
| H | -5.118117 | -3.402347 | -0.086902 |
| H | -6.113688 | -2.027113 | 0.438123  |
| H | -0.105187 | -1.247631 | 0.208152  |
| H | -1.168760 | 3.028456  | 0.284006  |

#### A:A tHW Water

36

AA-t-1jj-s SCF Done: -1013.69101355 A.U.

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 6.533336 | -0.633287 | 0.117619  |
| N | 1.400935 | -0.755902 | 0.098821  |
| C | 2.314922 | -1.726727 | 0.230923  |
| N | 3.639369 | -1.622488 | 0.227931  |
| C | 4.029573 | -0.349846 | 0.066263  |
| C | 3.200656 | 0.759604  | -0.081289 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.810135  | 0.522096  | -0.059910 |
| N | 0.898370  | 1.489795  | -0.193522 |
| N | 3.946889  | 1.912550  | -0.223808 |
| C | 5.188872  | 1.498083  | -0.163198 |
| N | 5.309150  | 0.140855  | 0.011464  |
| C | -5.350419 | 2.387260  | 0.176295  |
| N | -3.545805 | -2.407060 | -0.154831 |
| C | -4.790878 | -1.922456 | -0.114529 |
| N | -5.187938 | -0.654002 | -0.025398 |
| C | -4.142423 | 0.179992  | 0.021084  |
| C | -2.794518 | -0.171716 | -0.014205 |
| C | -2.502802 | -1.550625 | -0.103567 |
| N | -1.258314 | -2.040444 | -0.144242 |
| N | -2.004411 | 0.960987  | 0.050390  |
| C | -2.856996 | 1.955317  | 0.123738  |
| N | -4.164521 | 1.550927  | 0.111186  |
| H | 6.576610  | -1.139140 | 1.080916  |
| H | 1.911550  | -2.726798 | 0.355882  |
| H | 1.204588  | 2.445101  | -0.285337 |
| H | 6.064431  | 2.126513  | -0.238681 |
| H | -5.940766 | 2.133039  | 1.055073  |
| H | -5.580378 | -2.665859 | -0.159577 |
| H | -0.424373 | -1.455681 | -0.059914 |
| H | -2.593460 | 3.001004  | 0.187056  |
| H | 7.382717  | 0.038730  | 0.025488  |
| H | 6.575906  | -1.379004 | -0.674602 |
| H | -5.043418 | 3.428190  | 0.236498  |
| H | -5.960717 | 2.241006  | -0.713307 |
| H | -0.100166 | 1.281640  | -0.119882 |
| H | -1.145339 | -3.041440 | -0.190909 |

#### tzA:A tHW Gas

35

tzAA-t-1jj2 SCF Done: -1356.50330060 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.687932  | 0.507864  | -0.435506 |
| N | 1.578268  | 0.826987  | -0.132952 |
| C | 2.505185  | 1.706957  | -0.538859 |
| N | 3.821816  | 1.553223  | -0.596844 |
| C | 4.189633  | 0.335791  | -0.181900 |
| C | 3.347540  | -0.680772 | 0.262068  |
| C | 1.968767  | -0.396235 | 0.275245  |
| N | 1.045904  | -1.277790 | 0.686563  |
| N | 4.067586  | -1.807785 | 0.598728  |
| C | 5.309267  | -1.471364 | 0.364782  |
| N | 5.456794  | -0.188532 | -0.114067 |
| C | -5.560200 | -2.046739 | -0.430678 |
| N | -3.287887 | 2.593419  | 0.350583  |
| C | -4.573910 | 2.176366  | 0.239967  |
| N | -5.034238 | 0.968840  | 0.034634  |
| C | -4.058841 | 0.017001  | -0.057458 |
| C | -2.666058 | 0.310282  | 0.054960  |
| C | -2.314682 | 1.701106  | 0.253394  |
| N | -1.040430 | 2.092227  | 0.346149  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -1.824061 | -0.711908 | -0.031422 |
| H | 6.481241  | 1.239516  | -1.212640 |
| H | 2.120366  | 2.667969  | -0.861224 |
| H | 1.344162  | -2.208389 | 0.917793  |
| H | 6.166098  | -2.109773 | 0.512123  |
| H | -6.361389 | -1.316450 | -0.329569 |
| H | -5.310791 | 2.967018  | 0.330741  |
| H | -0.233960 | 1.488335  | 0.166338  |
| H | 7.426622  | -0.205051 | -0.795804 |
| H | 7.083707  | 1.027511  | 0.437677  |
| H | -5.636920 | -2.511365 | -1.415256 |
| H | -5.702003 | -2.828193 | 0.317393  |
| H | 0.061211  | -1.081846 | 0.526586  |
| H | -0.881812 | 3.078235  | 0.467399  |
| S | -2.719098 | -2.090440 | -0.271916 |
| C | -4.257503 | -1.343798 | -0.256099 |

#### tzA:A tHW Water

35

tzAA-t-1jj2-s SCF Done: -1356.52034264 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -6.688373 | 0.553260  | 0.396588  |
| N | -1.566734 | 0.781297  | 0.155443  |
| C | -2.481230 | 1.687108  | 0.528613  |
| N | -3.802610 | 1.557178  | 0.567132  |
| C | -4.188161 | 0.337749  | 0.166037  |
| C | -3.356695 | -0.701495 | -0.247402 |
| C | -1.971917 | -0.442814 | -0.243299 |
| N | -1.051681 | -1.337071 | -0.627790 |
| N | -4.097515 | -1.816293 | -0.585486 |
| C | -5.338375 | -1.448405 | -0.379275 |
| N | -5.463354 | -0.158184 | 0.075812  |
| C | 5.565383  | -2.052613 | 0.373522  |
| N | 3.280311  | 2.606317  | -0.349279 |
| C | 4.568736  | 2.189551  | -0.279669 |
| N | 5.036750  | 0.980623  | -0.091281 |
| C | 4.064141  | 0.025063  | 0.033991  |
| C | 2.671170  | 0.320314  | -0.032292 |
| C | 2.308408  | 1.708810  | -0.223372 |
| N | 1.033304  | 2.092000  | -0.278080 |
| N | 1.830359  | -0.701284 | 0.085149  |
| H | -6.672510 | 0.877580  | 1.435796  |
| H | -2.081241 | 2.647754  | 0.836959  |
| H | -1.335656 | -2.278469 | -0.847405 |
| H | -6.210222 | -2.066597 | -0.537631 |
| H | 6.338253  | -1.510824 | -0.170136 |
| H | 5.303218  | 2.981357  | -0.393761 |
| H | 0.239042  | 1.466755  | -0.115962 |
| H | -7.532541 | -0.113350 | 0.240138  |
| H | -6.795174 | 1.426936  | -0.244470 |
| H | 5.866835  | -2.095610 | 1.422608  |
| H | 5.515655  | -3.073675 | -0.002459 |
| H | -0.068906 | -1.133606 | -0.471796 |
| H | 0.844208  | 3.076412  | -0.400843 |

|   |          |           |          |
|---|----------|-----------|----------|
| S | 2.730002 | -2.079545 | 0.292030 |
| C | 4.266448 | -1.337198 | 0.225746 |

# G:G tHW Gas Phase

38

GG-t-1jj2 SCF Done: -1164.21872153 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.654108  | 3.264478  | 0.006334  |
| N | 4.136071  | -1.773337 | -0.064017 |
| C | 5.105963  | -0.803346 | -0.110243 |
| N | 6.406655  | -1.233703 | -0.125721 |
| N | 4.848899  | 0.478144  | -0.093419 |
| C | 3.527136  | 0.751938  | -0.007069 |
| C | 2.471805  | -0.147308 | 0.041987  |
| C | 2.733710  | -1.546352 | 0.008799  |
| O | 1.960124  | -2.491386 | 0.036196  |
| N | 1.279078  | 0.523720  | 0.114144  |
| C | 1.589960  | 1.791915  | 0.106176  |
| N | 2.952141  | 1.993863  | 0.033843  |
| C | -6.311390 | -1.466708 | -0.159205 |
| N | -1.501093 | -0.022732 | 0.144768  |
| C | -2.030089 | -1.277890 | 0.141961  |
| N | -1.158248 | -2.311812 | 0.263146  |
| N | -3.322747 | -1.520060 | 0.057720  |
| C | -4.052237 | -0.386934 | -0.014957 |
| C | -3.624466 | 0.939785  | -0.018702 |
| C | -2.216443 | 1.195990  | 0.063518  |
| O | -1.604105 | 2.256274  | 0.068890  |
| N | -4.702281 | 1.796552  | -0.109831 |
| C | -5.741653 | 1.012975  | -0.159453 |
| N | -5.416952 | -0.330520 | -0.102843 |
| H | 4.252707  | 3.343841  | -0.899533 |
| H | 6.613335  | -2.117885 | -0.559429 |
| H | -0.479712 | 0.091021  | 0.180699  |
| H | 0.866271  | 2.591955  | 0.143265  |
| H | -6.246616 | -1.968054 | -1.125702 |
| H | -1.539904 | -3.228879 | 0.121200  |
| H | -6.769557 | 1.331608  | -0.231535 |
| H | 2.921854  | 4.067089  | 0.026635  |
| H | 4.311180  | 3.352241  | 0.870110  |
| H | -6.047971 | -2.182473 | 0.617445  |
| H | -7.331844 | -1.123747 | -0.002123 |
| H | -0.160241 | -2.196046 | 0.147604  |
| H | 7.073889  | -0.504334 | -0.316962 |
| H | 4.399361  | -2.747498 | -0.031765 |

# G:G tHW Water

38

GG-t-1jj2-s SCF Done: -1164.25837797 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.844693 | 3.236104  | -0.048352 |
| N | -4.034898 | -1.820984 | 0.047187  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.065684 | -0.911436 | 0.047990  |
| N | -6.319923 | -1.408625 | 0.039171  |
| N | -4.874134 | 0.392200  | 0.023140  |
| C | -3.573543 | 0.734397  | -0.011004 |
| C | -2.465714 | -0.104575 | -0.016324 |
| C | -2.664829 | -1.510084 | 0.016799  |
| O | -1.823359 | -2.411133 | 0.021554  |
| N | -1.305340 | 0.637156  | -0.049785 |
| C | -1.698990 | 1.884504  | -0.064063 |
| N | -3.068587 | 2.007112  | -0.042211 |
| C | 6.287941  | -1.548916 | 0.001139  |
| N | 1.496360  | 0.066329  | -0.030037 |
| C | 1.981040  | -1.213920 | -0.063781 |
| N | 1.080411  | -2.211065 | -0.130094 |
| N | 3.274383  | -1.499296 | -0.048381 |
| C | 4.050447  | -0.401086 | -0.000910 |
| C | 3.664579  | 0.936503  | 0.034271  |
| C | 2.269237  | 1.239284  | 0.019757  |
| O | 1.716277  | 2.340783  | 0.044242  |
| N | 4.774614  | 1.760841  | 0.079368  |
| C | 5.791544  | 0.940020  | 0.071494  |
| N | 5.418866  | -0.386874 | 0.023463  |
| H | -4.454570 | 3.298835  | 0.851246  |
| H | -6.492254 | -2.375714 | 0.271068  |
| H | 0.472759  | 0.219036  | -0.042891 |
| H | -1.042306 | 2.740493  | -0.087168 |
| H | 6.090331  | -2.185328 | 0.862535  |
| H | 1.433775  | -3.155533 | -0.096573 |
| H | 6.833539  | 1.222554  | 0.098413  |
| H | -3.161540 | 4.080622  | -0.081223 |
| H | -4.496040 | 3.263314  | -0.920146 |
| H | 6.122788  | -2.127250 | -0.906811 |
| H | 7.321946  | -1.214679 | 0.031125  |
| H | 0.075819  | -2.074559 | -0.060984 |
| H | -7.074746 | -0.755931 | 0.187725  |
| H | -4.253130 | -2.815383 | 0.062488  |

# tzG:G tHW Gas Phase

37

tzGG-t-1jj2 SCF Done: -1507.05147062 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.172258  | 3.143766  | -0.004353 |
| N | 3.852341  | -2.023150 | -0.080956 |
| C | 4.944525  | -1.168159 | -0.150021 |
| N | 6.170526  | -1.791096 | -0.182249 |
| N | 4.856113  | 0.117303  | -0.133756 |
| C | 3.582646  | 0.633428  | -0.020902 |
| C | 2.406582  | -0.166564 | 0.040744  |
| C | 2.520732  | -1.621329 | 0.009376  |
| O | 1.621899  | -2.442853 | 0.060289  |
| N | 1.251396  | 0.464200  | 0.128740  |
| C | -6.473332 | -1.360579 | -0.151336 |
| N | -1.594739 | -0.168053 | 0.168974  |
| C | -2.191294 | -1.394821 | 0.181784  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -1.376506 | -2.468747 | 0.336897  |
| N | -3.492519 | -1.567233 | 0.083322  |
| C | -4.160798 | -0.398968 | -0.023552 |
| C | -3.663496 | 0.902409  | -0.044620 |
| C | -2.245800 | 1.087026  | 0.055675  |
| O | -1.578261 | 2.111053  | 0.054308  |
| N | -4.692038 | 1.812785  | -0.172415 |
| C | -5.770428 | 1.084201  | -0.225571 |
| N | -5.517952 | -0.273488 | -0.142248 |
| H | 5.161988  | 2.806708  | -0.308106 |
| H | 6.238682  | -2.659963 | -0.687735 |
| H | -0.577178 | -0.097049 | 0.219848  |
| H | -6.197673 | -2.095512 | -0.906158 |
| H | -1.802398 | -3.366310 | 0.194935  |
| H | -6.778292 | 1.454697  | -0.326287 |
| H | 3.833067  | 3.911530  | -0.700052 |
| H | 4.259334  | 3.605427  | 0.981224  |
| H | -6.503281 | -1.857879 | 0.818370  |
| H | -7.459499 | -0.962649 | -0.380241 |
| H | -0.375688 | -2.391173 | 0.213298  |
| H | 6.928945  | -1.153422 | -0.365656 |
| H | 3.997173  | -3.021267 | -0.032257 |
| C | 3.244938  | 1.975420  | 0.026065  |
| S | 1.533136  | 2.091790  | 0.134885  |

#### tzG:G tHW Water

37

tzGG-t-1jj2-s SCF Done: -1507.08839063 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.259594  | 3.114526  | 0.000076  |
| N | 3.824523  | -2.045431 | -0.064921 |
| C | 4.940586  | -1.219245 | -0.127920 |
| N | 6.134954  | -1.857340 | -0.168623 |
| N | 4.875579  | 0.078428  | -0.107656 |
| C | 3.615380  | 0.614039  | -0.012547 |
| C | 2.421612  | -0.157960 | 0.047446  |
| C | 2.516354  | -1.614143 | 0.019191  |
| O | 1.585580  | -2.410386 | 0.064047  |
| N | 1.274292  | 0.497848  | 0.124724  |
| C | -6.464463 | -1.456072 | -0.093018 |
| N | -1.606082 | -0.074583 | 0.104890  |
| C | -2.153932 | -1.330487 | 0.139134  |
| N | -1.299827 | -2.362901 | 0.258922  |
| N | -3.456356 | -1.551776 | 0.079902  |
| C | -4.175960 | -0.417729 | -0.013203 |
| C | -3.723940 | 0.898781  | -0.051623 |
| C | -2.317976 | 1.135123  | 0.009813  |
| O | -1.709210 | 2.205486  | -0.010956 |
| N | -4.788786 | 1.775202  | -0.152994 |
| C | -5.844247 | 1.004847  | -0.174899 |
| N | -5.539359 | -0.337682 | -0.093140 |
| H | 5.034728  | 2.935514  | -0.745483 |
| H | 6.181515  | -2.822654 | -0.461733 |
| H | -0.585868 | 0.029511  | 0.141050  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.262676 | -2.113163 | -0.937681 |
| H | -1.685640 | -3.291246 | 0.195729  |
| H | -6.869249 | 1.337018  | -0.247905 |
| H | 3.760463  | 4.053870  | -0.232751 |
| H | 4.756387  | 3.224667  | 0.966496  |
| H | -6.365308 | -2.028466 | 0.828134  |
| H | -7.478672 | -1.072536 | -0.170367 |
| H | -0.293579 | -2.250032 | 0.184739  |
| H | 6.940432  | -1.285505 | -0.375805 |
| H | 3.953636  | -3.056173 | -0.072833 |
| C | 3.309134  | 1.966292  | 0.026386  |
| S | 1.604841  | 2.118638  | 0.126433  |

# A:U tHW Gas Phase

33

AU-t-1ehz SCF Done: -961.162938000 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.659603  | -1.923645 | -0.000153 |
| N | 3.929290  | -0.659225 | -0.000052 |
| C | 2.538570  | -0.730042 | 0.000028  |
| O | 1.962626  | -1.811876 | -0.000022 |
| N | 1.889983  | 0.468590  | 0.000191  |
| C | 2.461005  | 1.742802  | 0.000103  |
| O | 1.756352  | 2.739304  | 0.000224  |
| C | 3.913008  | 1.729813  | -0.000129 |
| C | 4.568763  | 0.554831  | -0.000197 |
| C | -3.770288 | 2.742963  | -0.000185 |
| N | -3.224274 | -2.357009 | -0.000031 |
| C | -4.307601 | -1.574178 | -0.000145 |
| N | -4.375621 | -0.242721 | -0.000156 |
| C | -3.157299 | 0.301057  | -0.000028 |
| C | -1.942847 | -0.379086 | 0.000104  |
| C | -2.005636 | -1.787216 | 0.000100  |
| N | -0.916514 | -2.571591 | 0.000286  |
| N | -0.897422 | 0.520388  | 0.000163  |
| C | -1.461025 | 1.703289  | 0.000083  |
| N | -2.828760 | 1.640004  | -0.000020 |
| H | 4.401270  | -2.508094 | 0.880880  |
| H | 4.438248  | 2.670074  | -0.000278 |
| H | 5.648253  | 0.503328  | -0.000377 |
| H | -4.404141 | 2.695235  | -0.884286 |
| H | -5.256995 | -2.097171 | -0.000261 |
| H | 0.027378  | -2.202649 | 0.000107  |
| H | 0.846206  | 0.426217  | 0.000230  |
| H | -0.913985 | 2.633239  | 0.000107  |
| H | -3.217490 | 3.679086  | 0.000297  |
| H | -4.404935 | 2.694767  | 0.883314  |
| H | 4.401864  | -2.507674 | -0.881644 |
| H | 5.725452  | -1.712515 | 0.000271  |
| H | -1.057248 | -3.565870 | -0.000134 |

## A:U tHW Water

33

AU-t-lehz-s SCF Done: -961.181544343 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.642012 | -1.953854 | 0.000497  |
| N | -3.929770 | -0.675332 | 0.000138  |
| C | -2.544802 | -0.716999 | -0.000030 |
| O | -1.936914 | -1.784655 | 0.000288  |
| N | -1.915721 | 0.495112  | -0.000220 |
| C | -2.516127 | 1.751759  | -0.000395 |
| O | -1.824279 | 2.766067  | -0.000368 |
| C | -3.960317 | 1.712068  | -0.000150 |
| C | -4.594771 | 0.522792  | 0.000071  |
| C | 3.829115  | 2.730403  | 0.000412  |
| N | 3.207662  | -2.369383 | -0.000087 |
| C | 4.304015  | -1.603245 | 0.000154  |
| N | 4.391926  | -0.273711 | 0.000194  |
| C | 3.180332  | 0.293556  | 0.000076  |
| C | 1.955809  | -0.368955 | -0.000110 |
| C | 1.994205  | -1.779346 | -0.000227 |
| N | 0.894184  | -2.542660 | -0.000477 |
| N | 0.922488  | 0.546243  | -0.000172 |
| C | 1.509765  | 1.719512  | -0.000021 |
| N | 2.875011  | 1.634725  | 0.000148  |
| H | -4.375723 | -2.530553 | -0.882910 |
| H | -4.510992 | 2.639310  | -0.000142 |
| H | -5.674610 | 0.451667  | 0.000247  |
| H | 4.459344  | 2.677695  | 0.886585  |
| H | 5.246229  | -2.141732 | 0.000139  |
| H | -0.040817 | -2.148908 | -0.000469 |
| H | -0.876201 | 0.468685  | -0.000201 |
| H | 0.991026  | 2.666407  | -0.000003 |
| H | 3.283877  | 3.670601  | 0.000067  |
| H | 4.460056  | 2.677457  | -0.885235 |
| H | -4.375929 | -2.529980 | 0.884346  |
| H | -5.709781 | -1.756117 | 0.000310  |
| H | 1.001341  | -3.546925 | -0.000430 |

## tzA:U tHW Gas Phase

32

tzAU-t-lehz SCF Done: -1303.99186122 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.878379 | 1.865738  | -0.000099 |
| N | -4.101078 | 0.628756  | -0.000120 |
| C | -2.716964 | 0.751533  | 0.000164  |
| O | -2.177621 | 1.851718  | 0.000398  |
| N | -2.022937 | -0.423033 | 0.000173  |
| C | -2.546577 | -1.721994 | -0.000160 |
| O | -1.804616 | -2.686967 | -0.000175 |
| C | -3.998108 | -1.758785 | -0.000466 |
| C | -4.695861 | -0.608968 | -0.000439 |
| C | 4.254471  | -2.425403 | -0.000060 |
| N | 2.942232  | 2.630923  | -0.000464 |
| C | 4.122241  | 1.960695  | -0.000801 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 4.335114  | 0.670145  | -0.000513 |
| C | 3.191368  | -0.076603 | 0.000092  |
| C | 1.884977  | 0.494193  | 0.000323  |
| C | 1.814417  | 1.939237  | 0.000167  |
| N | 0.642178  | 2.584434  | 0.000681  |
| N | 0.860629  | -0.351176 | 0.000493  |
| H | -4.642395 | 2.458622  | 0.881434  |
| H | -4.488343 | -2.717688 | -0.000729 |
| H | -5.776368 | -0.596486 | -0.000676 |
| H | 5.183837  | -1.858336 | -0.000938 |
| H | 4.999714  | 2.598101  | -0.001368 |
| H | -0.263245 | 2.128416  | 0.000660  |
| H | -0.994462 | -0.338771 | 0.000330  |
| H | 4.237775  | -3.069606 | -0.880609 |
| H | 4.238819  | -3.068629 | 0.881216  |
| H | -4.642566 | 2.458586  | -0.881708 |
| H | -5.935289 | 1.614297  | 0.000008  |
| H | 0.671610  | 3.589280  | 0.000178  |
| C | 3.113834  | -1.465058 | 0.000119  |
| S | 1.462708  | -1.901477 | 0.000352  |

#### tzA:U tHW Water

32

tzAU-t-lehz-s SCF Done: -1304.00927992 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.870962 | 1.890452  | 0.000009  |
| N | -4.104033 | 0.643365  | 0.000014  |
| C | -2.724270 | 0.745012  | 0.000134  |
| O | -2.156842 | 1.833836  | 0.000238  |
| N | -2.044816 | -0.441098 | 0.000125  |
| C | -2.588554 | -1.724965 | 0.000024  |
| O | -1.850947 | -2.704556 | -0.000114 |
| C | -4.032601 | -1.744603 | -0.000198 |
| C | -4.716402 | -0.583021 | -0.000164 |
| C | 4.267034  | -2.433819 | -0.000014 |
| N | 2.948346  | 2.635189  | -0.000149 |
| C | 4.129957  | 1.968624  | -0.000344 |
| N | 4.348130  | 0.677790  | -0.000293 |
| C | 3.206110  | -0.077331 | -0.000101 |
| C | 1.899084  | 0.491729  | 0.000065  |
| C | 1.819158  | 1.937336  | 0.000038  |
| N | 0.645342  | 2.570252  | 0.000230  |
| N | 0.875894  | -0.353640 | 0.000262  |
| H | -4.629573 | 2.477197  | 0.883879  |
| H | -4.543917 | -2.694084 | -0.000368 |
| H | -5.798254 | -0.558262 | -0.000289 |
| H | 5.203467  | -1.878954 | -0.000786 |
| H | 5.006629  | 2.609416  | -0.000386 |
| H | -0.253215 | 2.097548  | 0.000265  |
| H | -1.019120 | -0.365359 | 0.000172  |
| H | 4.243501  | -3.077985 | -0.880261 |
| H | 4.244381  | -3.076931 | 0.881034  |
| H | -4.629666 | 2.477151  | -0.883921 |
| H | -5.929058 | 1.646525  | 0.000070  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 0.650234 | 3.579805  | 0.000149  |
| C | 3.133390 | -1.465787 | -0.000001 |
| S | 1.481450 | -1.900943 | 0.000090  |

#### A:C tHW Gas Phase

34

AC-t-1N32 SCF Done: -941.269596200 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.537308 | 1.148522  | 0.003169  |
| N | -4.427325 | 0.203279  | 0.001569  |
| C | -3.111384 | 0.750960  | 0.002509  |
| O | -2.986252 | 1.965825  | 0.004625  |
| N | -2.069487 | -0.122965 | 0.000984  |
| C | -2.259397 | -1.432965 | -0.001762 |
| N | -1.173991 | -2.220469 | -0.003658 |
| C | -3.575351 | -2.001923 | -0.002752 |
| C | -4.615972 | -1.135980 | -0.000996 |
| C | 5.138651  | -1.802018 | 0.020620  |
| N | 2.387020  | 2.512568  | -0.001494 |
| C | 3.700761  | 2.288570  | -0.005099 |
| N | 4.350510  | 1.123562  | -0.005138 |
| C | 3.493541  | 0.100697  | -0.003116 |
| C | 2.102096  | 0.165833  | 0.000011  |
| C | 1.535427  | 1.465034  | 0.000231  |
| N | 0.223263  | 1.695243  | 0.002029  |
| N | 1.566007  | -1.111747 | -0.002312 |
| C | 2.606530  | -1.907983 | -0.005982 |
| N | 3.802333  | -1.241619 | -0.010616 |
| H | -5.481612 | 1.786736  | 0.883011  |
| H | -1.277819 | -3.217556 | -0.005387 |
| H | -3.738695 | -3.067849 | -0.004803 |
| H | -5.642893 | -1.474737 | -0.001577 |
| H | 5.787277  | -1.208986 | -0.619988 |
| H | 4.323089  | 3.176579  | -0.007789 |
| H | -0.478397 | 0.954783  | 0.002422  |
| H | -0.234679 | -1.806438 | -0.003337 |
| H | 2.566856  | -2.985680 | -0.011082 |
| H | -6.475337 | 0.598116  | 0.002819  |
| H | -5.482301 | 1.789002  | -0.875082 |
| H | 5.108430  | -2.827605 | -0.341010 |
| H | 5.543938  | -1.786783 | 1.032708  |
| H | -0.101704 | 2.646366  | 0.001525  |

#### A:C tHW Water

34

AC-t-1N32-s SCF Done: -941.292956955 A.U.

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -5.546199 | 1.146991 | 0.000103  |
| N | -4.426375 | 0.210087 | 0.000298  |
| C | -3.120046 | 0.747157 | -0.001015 |
| O | -2.984400 | 1.971881 | -0.002070 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -2.073464 | -0.116425 | -0.001043 |
| C | -2.265339 | -1.435289 | 0.000396  |
| N | -1.185863 | -2.223630 | 0.000332  |
| C | -3.580044 | -1.998466 | 0.001907  |
| C | -4.619541 | -1.132932 | 0.001752  |
| C | 5.124321  | -1.836220 | 0.000099  |
| N | 2.405211  | 2.519539  | 0.001118  |
| C | 3.721314  | 2.288092  | 0.001871  |
| N | 4.362674  | 1.120309  | 0.001554  |
| C | 3.502337  | 0.094609  | 0.000299  |
| C | 2.111485  | 0.174279  | -0.000565 |
| C | 1.550471  | 1.472043  | -0.000125 |
| N | 0.235560  | 1.703685  | -0.000962 |
| N | 1.561439  | -1.094784 | -0.001887 |
| C | 2.594677  | -1.903084 | -0.001780 |
| N | 3.796266  | -1.247925 | -0.000456 |
| H | -5.500373 | 1.784412  | 0.881078  |
| H | -1.290574 | -3.225653 | 0.001583  |
| H | -3.740605 | -3.065925 | 0.003069  |
| H | -5.648225 | -1.469689 | 0.002775  |
| H | 5.674534  | -1.520759 | -0.884870 |
| H | 4.348411  | 3.174112  | 0.002856  |
| H | -0.467676 | 0.961430  | -0.001339 |
| H | -0.248029 | -1.814592 | -0.000585 |
| H | 2.543962  | -2.982141 | -0.002622 |
| H | -6.476655 | 0.585548  | 0.001008  |
| H | -5.501228 | 1.782983  | -0.881947 |
| H | 5.029067  | -2.918964 | -0.001051 |
| H | 5.673042  | -1.522516 | 0.886623  |
| H | -0.089202 | 2.657630  | -0.000353 |

#### tzA:C tHW Gas Phase

33

tzAC-t-1N32 SCF Done: -1284.10218738 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -5.716043 | 1.134802  | 0.000300  |
| N | -4.599045 | 0.196929  | 0.000124  |
| C | -3.287795 | 0.753912  | 0.000122  |
| O | -3.168066 | 1.969249  | 0.000256  |
| N | -2.241459 | -0.114664 | -0.000031 |
| C | -2.423146 | -1.424764 | -0.000383 |
| N | -1.325208 | -2.196927 | -0.000668 |
| C | -3.732387 | -2.004047 | -0.000534 |
| C | -4.778466 | -1.143419 | -0.000244 |
| C | 5.355330  | -1.363886 | -0.000175 |
| N | 2.082994  | 2.706488  | -0.000210 |
| C | 3.429796  | 2.573760  | -0.000481 |
| N | 4.154938  | 1.482809  | -0.000516 |
| C | 3.415566  | 0.334370  | -0.000170 |
| C | 1.986615  | 0.319061  | 0.000184  |
| C | 1.328281  | 1.614851  | 0.000092  |
| N | 0.003435  | 1.714774  | 0.000383  |
| N | 1.396809  | -0.870853 | 0.000644  |
| H | -5.664272 | 1.774282  | 0.879353  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.399117 | -3.196356 | -0.000767 |
| H | -3.888486 | -3.070904 | -0.000838 |
| H | -5.803104 | -1.488716 | -0.000301 |
| H | 5.965216  | -0.461875 | -0.000342 |
| H | 3.972673  | 3.513116  | -0.000702 |
| H | -0.636009 | 0.918433  | -0.000021 |
| H | -0.408822 | -1.750908 | -0.000377 |
| H | -6.650090 | 0.577942  | 0.000714  |
| H | -5.664890 | 1.773972  | -0.879027 |
| H | 5.608124  | -1.955717 | -0.881563 |
| H | 5.608362  | -1.955613 | 0.881205  |
| H | -0.414620 | 2.630347  | 0.000076  |
| C | 3.920864  | -0.959190 | -0.000007 |
| S | 2.588789  | -2.031537 | 0.000640  |

tzA:C tHW Water

33

tzAC-t-1N32-s SCF Done: -1284.12246136 A.U.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.724393  | 1.137393  | 0.000149  |
| N | 4.600000  | 0.205252  | 0.000025  |
| C | 3.297107  | 0.749127  | -0.000492 |
| O | 3.164901  | 1.973848  | -0.000209 |
| N | 2.247714  | -0.111663 | -0.000266 |
| C | 2.434133  | -1.429431 | 0.000100  |
| N | 1.345203  | -2.206972 | 0.000226  |
| C | 3.743698  | -2.000506 | 0.000357  |
| C | 4.786925  | -1.138483 | 0.000370  |
| C | -5.358289 | -1.382035 | 0.000566  |
| N | -2.085985 | 2.710506  | 0.000126  |
| C | -3.434813 | 2.581112  | 0.000482  |
| N | -4.161466 | 1.491265  | 0.000535  |
| C | -3.425907 | 0.335633  | 0.000190  |
| C | -1.998943 | 0.322102  | -0.000187 |
| C | -1.335158 | 1.611973  | -0.000203 |
| N | -0.009900 | 1.707183  | -0.000507 |
| N | -1.407169 | -0.866266 | -0.000504 |
| H | 5.681170  | 1.773994  | -0.881456 |
| H | 1.426108  | -3.210910 | 0.000378  |
| H | 3.899116  | -3.068633 | 0.000636  |
| H | 5.814106  | -1.479596 | 0.000668  |
| H | -5.986657 | -0.493134 | 0.000745  |
| H | -3.975768 | 3.522985  | 0.000699  |
| H | 0.632229  | 0.908950  | -0.000475 |
| H | 0.426316  | -1.773948 | -0.000033 |
| H | 6.652184  | 0.571704  | 0.000385  |
| H | 5.680852  | 1.774193  | 0.881599  |
| H | -5.600015 | -1.978867 | 0.881343  |
| H | -5.600501 | -1.978875 | -0.880070 |
| H | 0.409909  | 2.624863  | -0.000408 |
| C | -3.928587 | -0.959891 | 0.000171  |
| S | -2.594024 | -2.028163 | -0.000550 |

