Supporting Information: Intersystem Crossing Enables 4-Thiothymidine to Act as a Photosensitizer in Photodynamic Therapy: An Ab Initio QM/MM Study

Ganglong Cui* and Walter Thiel*

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Email: ganglong.cui@bnu.edu.cn and thiel@kofo.mpg.de

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

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1 System Setup

Initial Cartesian coordinates of 4-thiothymidine (an RNA monomer analogue) were prepared using GaussView 4.0. To explicitly consider solvation effects, 4-thiothymidine was solvated in a spherical water box with a radius of 25 Å. This solvated system was relaxed by performing constrained molecular mechanics (MM) minimizations (1000 steps) and 5-ps molecular dynamics (MD) runs, in which the outermost water molecules were frozen (i.e., those more than 20 Å away from the center of mass of 4-thiothymidine). In the MM minimizations and dynamics runs, 4-thiothymidine was modeled by the CHARMM22 force field [1] (modified based on the parameters of thymidine, see section 11) and water molecules were represented by the TIP3P model [2]. All MM computations were carried out using the CHARMM package (version c31b1). [3] Removal of the frozen water molecules in the final MD snapshot generated the starting structure for the following QM/MM computations.

2 QM/MM Computational Protocol

The QM subsystem contained the 4-thiopyrimidine chromophore of 4-thiothymidine; the MM subsystem consisted of the ribose group and the solvent water molecules (see Fig. 1).

Figure 1: The QM/MM computational protocol used in this work. 4-thiothymidine was solvated in a spherical water box of 20 Å. All atoms up to 10 Å away from any atom of 4-thiothymidine were allowed to move in the geometry optimizations (1133 atoms), and the remaining 2196 atoms were frozen at the positions adopted in the final MD snapshot. The QM subsystem (4-thiopyrimidine chromophore) was described using the ab initio CASPT2//CASSCF method, while the MM subsystem (the remaining part) was treated by the CHARMM force field (ribose) and TIP3P model (water). A hydrogen link atom was used at the QM/MM boundary (black line). Color code: Sulfur in yellow; nitrogen in blue; oxygen in red; carbon in gray; and hydrogen in white. Also shown is the atomic numbering.

In all QM/MM geometry optimizations including those for intersection points (see below), all water molecules within 10 Å from any atom of the 4-thiothymidine monomer were allowed to move (active region, 1133 atoms) while the other atoms were kept fixed (2196 atoms).
All QM/MM computations were done with the locally modified ChemShell version 3.5 [4]. An electronic embedding scheme [5] was adopted in the QM/MM calculations with the MM point charges being incorporated into the one-electron Hamiltonian during the QM calculations. A hydrogen link atom with the charge-shift scheme [6, 7] was employed to treat the QM/MM boundary. No cutoffs were introduced for the nonbonding MM and QM/MM interactions (electrostatic and van der Waals). The built-in DL_POLY module in ChemShell [8] was used to compute the MM energies and gradients. The MOLPRO2010 package [9] was employed to compute energies, gradients, derivative coupling vectors, and spin-orbit couplings of the QM subsystem.

The state-averaged complete-active-space self-consistent field (SA-CASSCF) method was chosen as the QM electronic structure method. At the SA-CASSCF level, full QM/MM geometry optimizations are expensive for higher excited states, and in particular for intersection points (see the following section). To balance computational accuracy and efficiency, we adopted an active space of 10 electrons in 8 orbitals. In all CASSCF computations, equal state weights were used for the $S_0$, $S_1$, and $S_2$ states, and for the $T_1$ and $T_2$ states, respectively. To account for dynamic correlation, the second-order CASSCF perturbation approach (CASPT2) [10–12] was employed to re-evaluate the energies of all optimized structures. To minimize intruder-state issues in the CASPT2 computations, an energy-level shift of 0.2 a.u. was applied. [13] The 6-31G* basis set [14, 15] was used in all QM computations.

3 Full QM/MM Conical Intersection Optimizations

Gradient difference and derivative coupling vectors are required for optimizing minimum-energy conical intersections in the gradient projection method of Bearpark et al. [16] and the Lagrange-Newton method of Manaa and Yarkony. [17]

However, rigorous computation of these vectors remains expensive at the QM/MM level. The derivative coupling vector between electronic states I and J with same spin can be partitioned into QM and MM terms:

$$h_{IJ}(r_{qm}, r_{mm}) = \langle \Psi_I(r_{qm}, r_{mm}) | \frac{\partial}{\partial r_{qm}} | \Psi_J(r_{qm}, r_{mm}) >$$  \hspace{1cm} (1)

and

$$h_{IJ}(r_{qm}, r_{mm}) = \langle \Psi_I(r_{qm}, r_{mm}) | \frac{\partial}{\partial r_{mm}} | \Psi_J(r_{qm}, r_{mm}) > .$$  \hspace{1cm} (2)

The computation of the QM contribution is affordable at the SA-CASSCF level as long as the QM region is small (tens of atoms), whereas the explicit computation of the MM contributions is very expensive (involving usually thousands of MM atoms). Thus, it is impractical to use these rigorous formulations for optimizing
conical intersections at the QM/MM level. To circumvent this bottleneck, several approximate treatments have been proposed, e.g. the sequential QM conical intersection optimization and MM minimization based on the electrostatic potential (ESP) fitting approximation. [18]

In this work, we adopted the penalty function method of Ciminelli et al. [19] implemented in the DL-FIND module of the ChemShell-3.5 package. [20] Its objective function is defined as

\[ f(R) = \frac{E_I + E_J}{2} + c_1 c_2^2 \ln \left[ 1 + \left( \frac{E_I - E_J}{c_2} \right)^2 \right] \] (3)

in which \( E_I \) and \( E_J \) are the QM/MM energies of electronic states I and J. \( c_1 \) and \( c_2 \) are two parameters, for which we used the recommended values of 5.0 (kcal/mol)\(^{-1} \) and 5.0 kcal/mol. [19] Because this method only needs the gradients of the electronic states involved, the expensive computation of derivative coupling vectors is avoided. Full QM/MM conical intersection optimization based on the penalty function method was found to be a practical approach for the large condensed-phase systems studied presently.

The QM/MM-based penalty function method was also employed to optimize the crossing points between electronic states with different spin.

4 Convergence Criteria

In minimizations, the following convergence thresholds had to be satisfied: (1) energy converged to within \( 5.0 \times 10^{-5} \) hartree; (2) maximum force component less than \( 4.5 \times 10^{-3} \) hartree/bohr; (3) root-mean-square force less than \( 3.0 \times 10^{-3} \) hartree/bohr; (4) maximum step size component less than \( 1.8 \times 10^{-3} \) bohr; (5) root-mean-square step size less than \( 1.2 \times 10^{-3} \) bohr.

For the optimization of conical intersections and crossing points, we adopted a more rigorous energy threshold and loosened the other thresholds by a factor of 2: (1) energy converged to within \( 1.0 \times 10^{-5} \) hartree; (2) maximum force component less than \( 9.0 \times 10^{-3} \) hartree/bohr; (3) root-mean-square force less than \( 6.0 \times 10^{-3} \) hartree/bohr; (4) maximum step size component less than \( 3.6 \times 10^{-3} \) bohr; (5) root-mean-square step size less than \( 2.4 \times 10^{-3} \) bohr.

5 Energy Gaps at Intersection Points

Table 1 lists the computed energy gaps at the conical intersections and crossing points optimized with the QM/MM penalty function method (see above). It is evident that the two involved electronic states are essentially degenerate at the QM(CASSCF)/MM level (used for geometry optimization), and they remain close in energy in the single-point QM(CASPT2///CASSCF)/MM calculations.
6 Geometric Parameters of S1S0-MIN

As discussed in the main text, the differences in the electronic and geometric structures of the S1 state of 4-thiothymine and thymine cause their qualitatively different photophysics. Fig. 2 shows that the S1/S0 conical intersection (S1S0-MIN) of 4-thiothymine is structurally different from that of thymine. The X4'-C4-C5-C5' dihedral angle is 12° (X=S) in 4-thiothymine and ca. 95° (X=O) in thymine (see Table 2) indicating that the methyl substituent is coplanar with the ring in the former and essentially perpendicular in the latter. The H6 atom is distorted out of the ring plane more strongly in 4-thiothymine than in thymine, as reflected in the C4-C5-C6-H6' dihedral angles of 95.7° and ca. 130°, respectively. Finally, S1S0-MIN has a very elongated C4-S4' bond in 4-thiothymine (1.98 Å, larger than the typical C-S single bond length of 1.82 Å) while the C4-O4' bond remains short (ca. 1.2 Å, in the range of a typical C=O double bond).

Table 2: Selected Key Geometric Parameters of S1S0-MIN from Present and Previous Electronic Structure Computations.

<table>
<thead>
<tr>
<th>Method</th>
<th>4-thiothymine</th>
<th>C4-C5-C6-H6'</th>
<th>C4-S4'</th>
<th>S4'-C4-C5-C5'</th>
</tr>
</thead>
<tbody>
<tr>
<td>QM(SA-3-CAS(10,8):6-31G*)/MM</td>
<td>95.7</td>
<td>1.98</td>
<td>1.2</td>
<td></td>
</tr>
<tr>
<td>thymine</td>
<td>C4-C5-C6-H6</td>
<td>C4-O4'</td>
<td>O4'-C4-C5-C5</td>
<td></td>
</tr>
<tr>
<td>OM2/MRCl</td>
<td>126.5</td>
<td>1.224</td>
<td>92.8</td>
<td></td>
</tr>
<tr>
<td>CASCF(14,10)/ANO-S</td>
<td>126.6</td>
<td>1.200</td>
<td>87.7</td>
<td></td>
</tr>
<tr>
<td>MR-CISD(4,4)/SA-3-CAS(12,9)/3-21G</td>
<td>125.5</td>
<td>1.204</td>
<td>105.0</td>
<td></td>
</tr>
<tr>
<td>SA-2-CAS(6,6)/3-21G</td>
<td>130.5</td>
<td>1.235</td>
<td>101.1</td>
<td></td>
</tr>
<tr>
<td>SA-2-CAS(6,6)/6-31G*</td>
<td>129.3</td>
<td>1.213</td>
<td>94.5</td>
<td></td>
</tr>
<tr>
<td>SA-2-CAS(6,6)/cc-pVDZ</td>
<td>133.6</td>
<td>1.183</td>
<td>87.9</td>
<td></td>
</tr>
</tbody>
</table>

*aFrom Lan, Z.G.; Fabiano, E; Thiel, W. [21]

*bFrom Merchán, M.; González-Luque, R.; Climent, T.; Serrano-Andrés, L.; Rodríguez, E.; Reguero, M.; Peláez D. [22]

*cFrom Zechmann, G.; Barbatti, M. [23]


7 Single-point QM Energies

To evaluate the effects of the MM environment (ribose and solvent water molecules) on the energetics, we have performed single-point CASPT2 calculations for the QM part of each QM(CASSCF)/MM optimized structure. The single-point energies are compiled in Table 3. The adiabatic energies of T1-MIN, S1-MIN, and T2-MIN do not differ much at the QM and QM/MM levels (by less than 5 kcal/mol), and they remain close to each other in both cases. The adiabatic energy of S2-MIN is affected more strongly by the MM environment (lowered by
12.1 kcal/mol). The influence of the MM environment is more pronounced in the case of the conical intersections and crossing points: in the single-point QM calculations, the two relevant states remain close to each other only for S1T1-MIN and T2T1-MIN, but they considerably differ in energy in the other cases. For instance, the S₂-T₂ energy gap of S₂T₂-MIN increases from 1.3 kcal/mol at the QM(CASPT2//CASSCF)/MM level to 23.3 kcal/mol in the single-point CASPT2 calculation of the QM region. This demonstrates the importance of environmental effects on the geometric structures and energies of crossing points.

Table 3: Relative Energies (in kcal/mol) from QM(CASPT2//CASSCF)/MM Optimizations and from CASPT2 Single-Point Calculations of the QM Regions of QM(CASSCF)/MM Optimized Structures (see Section 12 for Full Cartesian Coordinates)

<table>
<thead>
<tr>
<th>Structure</th>
<th>relaxed QM/MM Energy</th>
<th>unrelaxed QM Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>S₀-MIN</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>S₁ (vertical)</td>
<td>69.2</td>
<td>62.8</td>
</tr>
<tr>
<td>S₂ (vertical)</td>
<td>94.6</td>
<td>92.4</td>
</tr>
<tr>
<td>T₁-MIN</td>
<td>52.8</td>
<td>57.5</td>
</tr>
<tr>
<td>S₁-MIN</td>
<td>58.6</td>
<td>56.9</td>
</tr>
<tr>
<td>T₂-MIN</td>
<td>55.8</td>
<td>55.2</td>
</tr>
<tr>
<td>S₂-MIN</td>
<td>71.8</td>
<td>83.9</td>
</tr>
<tr>
<td>S₁S₀-MIN</td>
<td>91.7(S₀)/94.6(S₁)</td>
<td>74.5(S₀)/87.6(S₁)</td>
</tr>
<tr>
<td>T₁S₀-MIN</td>
<td>91.4(S₀)/92.6(T₁)</td>
<td>86.8(S₀)/92.9(T₁)</td>
</tr>
<tr>
<td>S₁T₁-MIN</td>
<td>60.0(T₁)/59.7(S₁)</td>
<td>57.7(T₁)/59.9(S₁)</td>
</tr>
<tr>
<td>S₂S₁-MIN</td>
<td>72.5(S₁)/74.3(S₂)</td>
<td>61.4(S₁)/83.8(S₂)</td>
</tr>
<tr>
<td>S₂T₂-MIN</td>
<td>71.7(T₂)/73.0(S₂)</td>
<td>60.4(T₂)/83.7(S₂)</td>
</tr>
<tr>
<td>T₂T₁-MIN</td>
<td>60.2(T₁)/60.5(T₂)</td>
<td>54.1(T₁)/56.3(T₂)</td>
</tr>
</tbody>
</table>
8 Spin-Orbit Couplings

Spin-orbit couplings (SOCs) were calculated at the CASSCF(10,8)/6-31G* level with and without MM point charges. The atomic mean-field approximation (AMFI) method [25, 26] implemented in MOLPRO2010 package [27] was employed. Table 4 compiles the computed SOC values.

The SOC values were found to be quite sensitive to the absence or presence of MM point charges. They are influenced by polarization effects from the surrounding water molecules and the nearby ribose group, which thus affect the electronic properties and the mechanistic photophysics of 4-thiouridine. The effects of the water molecules and ribose group on the spin-orbit couplings are state-specific and non-additive (see Table 4).

<table>
<thead>
<tr>
<th>structure</th>
<th>X, Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2T2-MIN</td>
<td>[S2]</td>
<td>13.2 / 1.2 / 5.1 / 3.0 81.0 / 2.2 / 76.2 / 3.1</td>
</tr>
<tr>
<td>S1T1-MIN</td>
<td>[S1]</td>
<td>13.7 / 12.9 / 2.0 / 1.8 82.7 / 71.1 / 11.8 / 10.2</td>
</tr>
<tr>
<td>S2-MIN</td>
<td>[S2]</td>
<td>6.6 / 5.3 / 12.4 / 0.8 22.5 / 2.3 / 45.2 / 93.2</td>
</tr>
<tr>
<td>S2-MIN</td>
<td>[S2]</td>
<td>13.1 / 1.2 / 5.3 / 2.8 80.6 / 2.1 / 77.1 / 3.0</td>
</tr>
<tr>
<td>S1-MIN</td>
<td>[S1]</td>
<td>13.7 / 0.9 / 0.6 / 0.7 82.7 / 40.1 / 63.2 / 60.6</td>
</tr>
</tbody>
</table>

mediate the coupling between a singlet with M_s=0 and triplet substates with M_s=+1 and M_s=-1. Their absolute values are identical in the AMFI approximation. They are smaller than the Z components at the QM level and are generally further reduced by inclusion of the MM point charges.

The Z components of the SOC matrix elements mediate the coupling between a singlet with M_s=0 and the triplet substate with M_s=0. Their absolute values (A) are usually quite large (around 80 cm\(^{-1}\) in all cases except for [S2]|\(\hat{\mathcal{H}}\)|T₂> in S2T2-MIN). Including the ribose MM charges (B) lowers [S2]|\(\hat{\mathcal{H}}\)|T₂> dramatically in S2T2-MIN and S2-MIN, and both values remain low at the full QM/MM level (D). By contrast, [S1]|\(\hat{\mathcal{H}}\)|T₁> in S1T1-MIN is mostly reduced when incorporating the water MM charges (C), whereas [S1]|\(\hat{\mathcal{H}}\)|T₁> in S1-MIN remains sizable at all QM/MM levels, e.g. 60.6 cm\(^{-1}\) at (D). Finally, [S₂]|\(\hat{\mathcal{H}}\)|T₁> in S2-MIN increases dramatically when including the MM point charges, up to the full QM/MM value of 93.2 cm\(^{-1}\) at (D).

9 Local Hydrogen-Bonding Networks

We have examined the local hydrogen-bonding (HB) networks of all optimized structures near the S4’ and O2’ acceptor atoms and the N3H3’ donor moiety. The corresponding parts of the QM/MM optimized structures are shown in Figures 3–13, and the relevant HB distances are listed in Table 5. The HB networks near O2’ and N3H3’ are rather stable: there are always three HBs and one HB, respectively, which are strong having HB distances
Table 5: Hydrogen-Bond Distances (in Å) around Acceptor Atoms (O\textsuperscript{2}' and S\textsubscript{4}') and Donor Moiety (N\textsubscript{3}-H\textsubscript{3}')

<table>
<thead>
<tr>
<th></th>
<th>HB (O\textsuperscript{2}')</th>
<th>HB (H\textsubscript{3}')</th>
<th>HB (S\textsubscript{4}')</th>
</tr>
</thead>
<tbody>
<tr>
<td>S0-MIN</td>
<td>1.57 1.62 1.67</td>
<td>1.52</td>
<td>2.15 2.20 2.40</td>
</tr>
<tr>
<td>S1-MIN</td>
<td>1.55 1.62 1.65</td>
<td>1.52</td>
<td>2.36 2.45 2.55</td>
</tr>
<tr>
<td>S2-MIN</td>
<td>1.56 1.62 1.67</td>
<td>1.52</td>
<td>2.21 2.31 2.80</td>
</tr>
<tr>
<td>T1-MIN</td>
<td>1.55 1.61 1.66</td>
<td>1.52</td>
<td>2.18 2.22 2.50</td>
</tr>
<tr>
<td>T2-MIN</td>
<td>1.56 1.61 1.61</td>
<td>1.53</td>
<td>2.43 2.82 -</td>
</tr>
<tr>
<td>S1S0-MIN</td>
<td>1.53 1.61 1.66</td>
<td>1.52</td>
<td>2.23 2.28 2.40</td>
</tr>
<tr>
<td>S1T1-MIN</td>
<td>1.56 1.62 1.65</td>
<td>1.52</td>
<td>2.25 2.43 -</td>
</tr>
<tr>
<td>S2S1-MIN</td>
<td>1.56 1.62 1.67</td>
<td>1.52</td>
<td>2.21 2.30 2.80</td>
</tr>
<tr>
<td>S2T2-MIN</td>
<td>1.56 1.62 1.68</td>
<td>1.52</td>
<td>2.20 2.31 2.80</td>
</tr>
<tr>
<td>T2T1-MIN</td>
<td>1.56 1.62 1.63</td>
<td>1.52</td>
<td>2.44 2.80 2.88</td>
</tr>
<tr>
<td>S0T1-MIN</td>
<td>1.56 1.63 1.64</td>
<td>1.50</td>
<td>2.17 2.18 2.61</td>
</tr>
</tbody>
</table>

of typically 1.5–1.6 Å that vary only slightly for a given HB (maximum fluctuation of 0.07 Å). By contrast, the number of HBs varies near the S\textsubscript{4}' acceptor atom: for example, there are only two (rather than three) HBs in T2-MIN and S1T1-MIN. Moreover, the distances and orientations of the HBs around S\textsubscript{4}' differ significantly between the different structures (e.g. within a range of 0.6 Å for the second HB). Thus, the HB network near S\textsubscript{4}' appears to be quite variable.

Figure 3: S0-MIN
Figure 4: S1-MIN

Figure 5: S2-MIN
Figure 6: T1-MIN

Figure 7: T2-MIN
Figure 8: S1S0-MIN

Figure 9: S1T1-MIN
Figure 12: TIS0-MIN

Figure 13: T2T1-MIN
References


11. Force Fields

Topological file

MASS 4 HT  1.00800 H ! TIPS3P WATER HYDROGEN
MASS 75 OT  15.99940 O ! TIPS3P WATER OXYGEN
MASS 201 NC=O  14.006700
MASS 202 C=C  12.011000
MASS 203 C=O  12.011000
MASS 204 CR  12.011000
MASS 205 HCMM  1.007940
MASS 206 OR  15.999400
MASS 207 HNCO  1.007940
MASS 208 O=C  15.999400
MASS 209 HOR  1.007940
MASS 210 S=C  32.066000

AUTOGENERATE ANGLES DIHE
DEFA FIRS NONE LAST NONE

RESI LIG  0.000
GROUP
ATOM N1 NC=O -0.4691
ATOM C4 C=C -0.0410
ATOM C5 C=C -0.1238
ATOM C7 C=O  0.4256
ATOM N2 NC=O -0.4900
ATOM C8 C=O  0.6900
ATOM C1 CR  0.2800
ATOM H1 HCMM  0.0000
ATOM H2 HCMM  0.0000
ATOM C2 CR  0.2800
ATOM H3 HCMM  0.0000
ATOM O1 OR  -0.5600
ATOM C3 CR  0.5801
ATOM H4 HCMM  0.0000
ATOM H5 HCMM  0.1500
ATOM C6 CR  0.1382
ATOM H6 HCMM  0.0000
ATOM H7 HCMM  0.0000
ATOM H8 HCMM  0.0000
ATOM H9 HNCO  0.3700
ATOM O2 O=C -0.5700
ATOM C9 CR  0.2800
ATOM H10 HCMM  0.0000
ATOM C10 CR  0.2800
ATOM H11 HCMM  0.0000
ATOM O3 OR  -0.6800
ATOM O4 OR  -0.6800
ATOM H12 HOR  0.4000
ATOM H13 HOR  0.4000
ATOM O5 OR  -0.6800
ATOM H14 HOR  0.4000
ATOM S1 S=C -0.3800
BOND H7 C6
BOND H8 C6
BOND C6 H6
BOND C6 C5
BOND S1   C7
BOND C5   C7
BOND C5   C4
BOND C7   N2
BOND H5   C4
BOND C4   N1
BOND N2   H9
BOND N2   C8
BOND N1   C8
BOND N1   C3
BOND C8   O2
BOND H4   C3
BOND C3   O1
BOND C3   C10
BOND O1   C2
BOND H12  O4
BOND H1   C1
BOND O4   C10
BOND C10  H11
BOND C10  C9
BOND C2   C1
BOND C2   H3
BOND C2   C9
BOND C1   O5
BOND C1   H2
BOND O5   H14
BOND H13  O3
BOND C9   O3
BOND C9   H10
IMPH N1   C8   C3   C4
IMPH C4   C5   N1   H5
IMPH C5   C7   C4   C6
IMPH C7   S1   C5   N2
IMPH C3   O1   N1   C10
IMPH C3   O1   N1   H4
IMPH C2   C1   O1   C9
IMPH C2   C1   O1   H3
IMPH C1   O5   C2   H1
IMPH C1   H1   C2   H2
IMPH C6   H7   C5   H8
IMPH C6   H7   C5   H6
IMPH N2   C8   C7   H9
IMPH C8   N2   N1   O2
IMPH C9   C10  C2   O3
IMPH C9   C10  C2   H10
IMPH C10  C9   C3   O4
IMPH C10  O4   C3   H11
IC N1   C4   C5   C7 1.37 121.23 0.04 120.79 1.44
IC N1   C4   C5   C6 1.37 121.23 -179.96 121.64 1.50
IC N1   C8   N2   C7 1.37 115.23 -0.04 126.50 1.38
IC N1   C8   N2   H9 1.37 115.23 179.99 116.76 1.09
IC N1   C3   O1   C2 1.53 109.58 -127.70 109.99 1.46
IC N1   C3   O1   C2 1.53 109.58 -127.70 109.99 1.46
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RESI TIP3 0.000 ! tip3p water model, generate using noangle nodihedral

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ATOM H2 HT 0.417
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ANGLE H1 OH2 H2 ! required
ACCEPTOR OH2
PATCHING FIRS NONE LAST NONE

Parameter file

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CR CR 306.432 1.5080  
HOR OR 560.905 0.9720  
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HT HT 0.000 1.5139 ! ALLOW WAT

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HT 0.000000 -0.046000 0.224500 ! ALLOW WAT

12. Cartesian Coordinates of All Optimized Structures

XYZ format (Angstrom)
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