

## Supplementary information

### Stacking of the mutagenic base analog 5-bromouracil: energy landscapes of pyrimidine dimers in gas phase and water

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**Section S1.** Methodological details

**Section S2.** Potential energy profiles

**Section S3.** Geometrical parameters and interaction energies of all optimised minima and transition states.

**Section S4.** Cartesian coordinates of all optimised minima and transition states.

## Section S1. Methodological details

### Computation of geometrical parameters

The dimer twist angle  $\tau_{\text{twist}}$  is the final optimised value of the O2(A)–X(A)–X(B)–O2(B) torsion angle. The vertical distance between the two stacked bases,  $\delta_{\text{vert}}$ , was calculated as the scalar product of the vector connecting the midpoints of the base rings ( $\vec{m}_1\vec{m}_2$ ; calculated as the average of the atomic coordinates of the C2, C4 and C6 atoms) and the plane vector of one of the bases (where a plane is defined by the C2, C4 and C6 atoms). This corresponds to the component of  $\vec{m}_1\vec{m}_2$  that is perpendicular to the base plane. As the two bases are not completely parallel in the optimised structures, this scalar product depends on which base's plane vector is used. The vertical distance presented herein is therefore computed as the average of the two values obtained when using the first or the second base's plane vector. The horizontal distance  $\delta_{\text{hor}}$  is calculated as the component of the vector connecting the two midpoints ( $\vec{m}_1\vec{m}_2$ ) that is in the plane of one base. Like for the vertical separation, the horizontal separation is calculated as the average of the two values obtained when using the first or the second base's plane vector. The angle between the two planes of the optimised stacked dimers,  $\alpha_{\text{tilt}}$ , is simply the angle between their plane vectors.

**Section S2.** Potential energy profiles of the FTB and FTF C/BrU, C/T, C/U, T/BrU, T/U, BrU/BrU and C/C dimers, in the gas phase and in water.

### S2.1. C/BrU

Figure S.1 (top left) shows the gas-phase FTB stacking of C/BrU. There are two minima, at  $40^\circ$  and  $260^\circ$ , of which the second is much deeper. The two maxima, at  $0^\circ$  and  $120^\circ$ , have similar heights. There are no repulsive regions. The BSSE varies from 3.09 to 3.85 kcal/mol. Figure S.1 (bottom left) shows the aqueous FTB stacking of C/BrU. There are five minima, at  $40^\circ$ ,  $85^\circ$ ,  $155^\circ$ ,  $210^\circ$  and  $\sim 285^\circ$ , the last of which is very wide and flat and is also the deepest. The maxima are at  $0^\circ$ ,  $60^\circ$ ,  $120^\circ$ ,  $175^\circ$  and  $240^\circ$ . Full optimisation of the gas phase structures yielded two minima (with  $\tau = 54^\circ$  and  $261^\circ$ ) and two transition states. As in the rotational scan, the latter of the two minima is considerably deeper, with  $\Delta E_0^{\text{CP}} = -14.0$  kcal/mol for the structure with  $\tau = 261^\circ$ , compared to  $-7.6$  kcal/mol for the structure with  $\tau = 54^\circ$ .

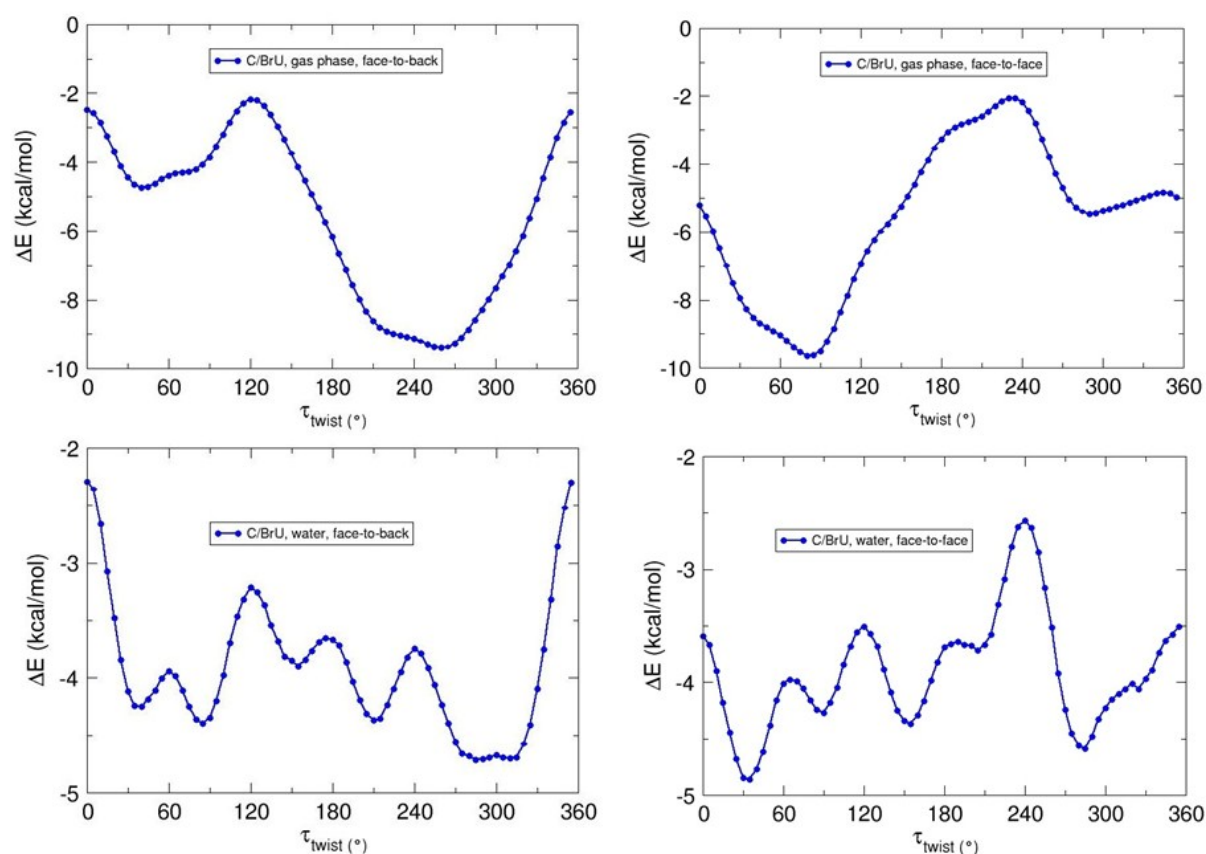


Figure S1. Potential energy profiles of C/BrU

Full optimisation of the aqueous structures initially yielded only four minima, as the optimisations starting from  $\tau = 40^\circ$  and  $85^\circ$  converged to the same structure, with  $\tau = 55^\circ$ . Hence only four transition states could be located. However, the transition states with  $\tau = 329^\circ$  and  $79^\circ$ , which would each be expected to connect the minimum with  $\tau = 55^\circ$  to another minimum, were lower in energy than the  $\tau = 55^\circ$  structure. “Following the imaginary frequency” (performing geometry optimisations on structures obtained from the transition state (TS) by adding or subtracting the magnitudes of the displacement of each atom in the

imaginary vibrational mode) of these two transition states yielded two new minima each, so that eight distinct stacked minima were found in total. Two of these, with  $\tau = 67^\circ$  and  $293^\circ$ , are symmetry-equivalent, and their interaction energies ( $\Delta E_0^{\text{CP}} = -6.4$  kcal/mol for both) are the greatest among these structures.

Figure S.1 (top right) shows the FTF gas-phase rotational profile of C/BrU. There are two minima, at  $80^\circ$  and  $290^\circ$ , with the maxima at  $235^\circ$  and  $345^\circ$ . There are no repulsive regions. Figure S.1 (bottom right) shows the FTF aqueous rotational profile of C/BrU. There are five minima, at  $35^\circ$ ,  $90^\circ$ ,  $155^\circ$ ,  $205^\circ$ , and  $285^\circ$ , with the maxima at  $65^\circ$ ,  $120^\circ$ ,  $190^\circ$ ,  $240^\circ$  and  $355^\circ$ . There are no repulsive regions. Full optimisation of the gas-phase structures yielded two minima, with  $\tau = 76^\circ$  and  $300^\circ$ , and two transition states. The minimum with  $\tau = 76^\circ$  is the more strongly bound. Full optimisation of the aqueous structures initially yielded five minima and five transition states. However, the transition state with  $\tau = 38^\circ$  was essentially isoenergetic with the minimum with  $\tau = 63^\circ$  and lower in energy than the minimum with  $31^\circ$ , while the transition state with  $\tau = 151^\circ$  was essentially isoenergetic with the minimum with  $\tau = 93^\circ$  and lower in energy than the minimum with  $\tau = 176^\circ$ . In each case, “following” the imaginary frequency of the transition state yielded one new minimum and one that had been located already. Hence seven distinct minima were found in total, of which the most strongly bound has  $\tau = 291^\circ$ .

## S2.2. C/T

Figure S.2 (top left) shows the FTB gas-phase energy profile of the C/T dimer. There are two minima, at  $85^\circ$  and  $210^\circ$ , and two maxima, at  $5^\circ$  and  $115^\circ$ . The interaction energies are negative throughout. The BSSE is relatively small and geometry-invariant, ranging from 1.00 to 1.09 kcal/mol. Figure S.2 (bottom left) shows the FTB aqueous energy profile of the C/T dimer. There are five minima, at  $80^\circ$ ,  $160^\circ$ ,  $205^\circ$ ,  $285^\circ$  and  $315^\circ$ , with the maxima at  $0^\circ$ ,  $120^\circ$ ,  $170^\circ$ ,  $240^\circ$  and  $290^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase dimers yielded two minima, the more strongly bound of which had  $\tau = 221^\circ$  and  $\Delta E_0^{\text{CP}} = -10.9$  kcal/mol. Two transition states were also located. However, both were lower in energy than the minimum with  $\tau = 84^\circ$ , and one of them (with  $\tau = 291^\circ$ ) was L-shaped. “Following” the imaginary frequency of the TS with  $\tau = 148^\circ$  yielded two stacked minima: one was new (with  $\tau = 131^\circ$ ), the other was identical to the already-found structure with  $\tau = 221^\circ$ . Carrying out the same procedure for the L-shaped TS with  $\tau = 291^\circ$  yielded two unstacked minima: one also L-shaped, containing an N4H4(C)•••O4(T) hydrogen bond, the other planar, with the bases bound by two hydrogen bonds in non-Watson–Crick fashion. Full optimisation of the aqueous dimers initially yielded four minima, since the starting structures with  $\tau = 285^\circ$  and  $315^\circ$  converged to the same minimum, with  $\tau = 296^\circ$ . Therefore four transition state searches were launched. However, one of these (starting from the guess state with  $\tau = 120^\circ$ ) returned a new energy minimum. Also, “following” the imaginary frequency of the transition state with  $\tau = 230^\circ$  returned two new energy minima. Hence seven minima were found in total, of which the most strongly bound has  $\tau = 296^\circ$  and  $\Delta E_0^{\text{CP}} = -5.8$  kcal/mol.

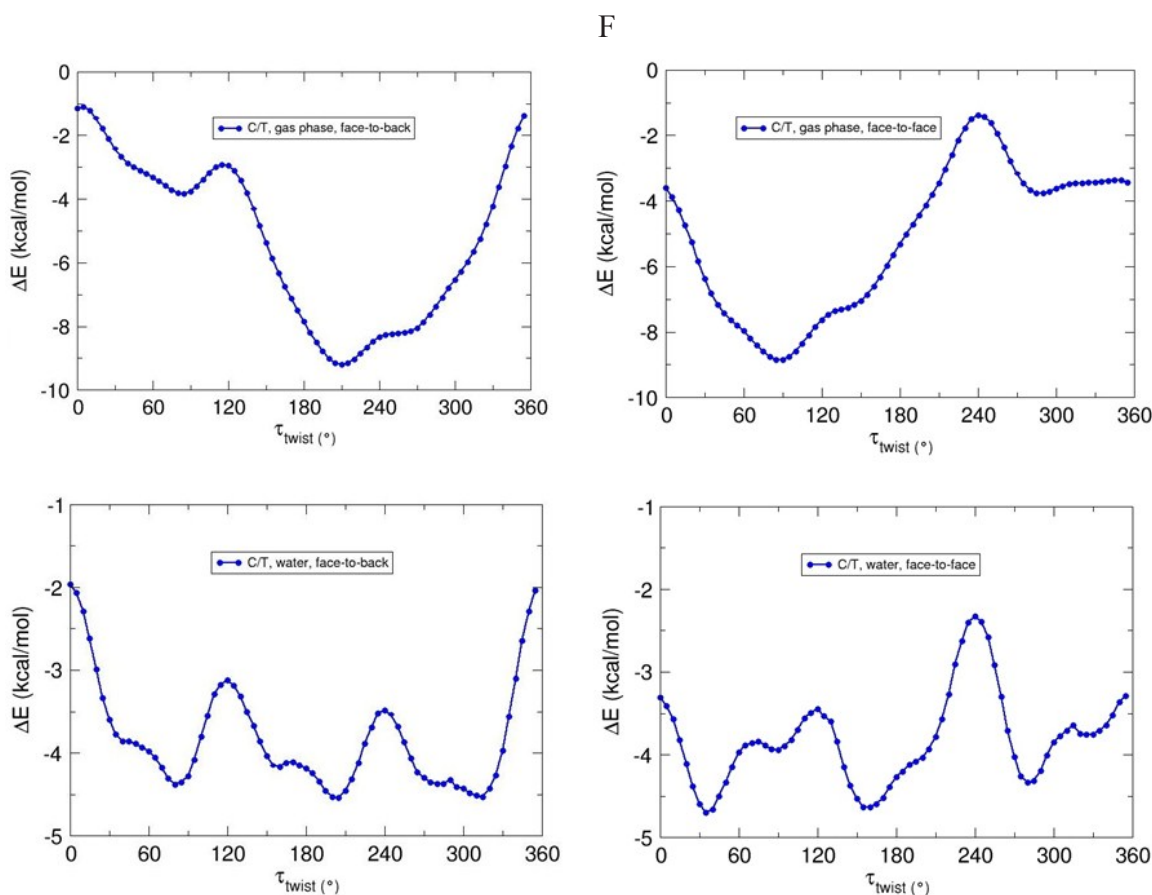


Figure S2. Potential energy profiles of C/T

Figure S.2 (top right) shows the FTF gas-phase rotational profile of stacked C/T. There are two minima, at  $90^\circ$  and  $290^\circ$ . The maxima are at  $240^\circ$  and  $345^\circ$ . The interaction energies are negative throughout. Figure S.2 (bottom right) shows the FTF aqueous rotational profile of stacked C/T. There are five minima, at  $35^\circ$ ,  $90^\circ$ ,  $155^\circ$ ,  $280^\circ$  and  $325^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase structures initially yielded only one minimum (with  $\tau = 83^\circ$ ), because the attempt to locate a minimum starting from  $\tau = 290^\circ$  failed to find a stationary point when using Gaussian's "Tight" convergence criteria. However, with the default criteria, a structure with one imaginary vibrational frequency was located. Then, "following" the imaginary frequency yielded a true minimum, with  $\tau = 318^\circ$ . Two transition states were then located in the attempt to connect the two minima. However, the one with  $\tau = 34^\circ$  was lower in energy than the minimum with  $\tau = 318^\circ$ . "Following" the imaginary frequency of this structure yielded two new minima: one stacked, the other L-shaped, with an N1H1(C)•••O4(T) hydrogen bond. The most strongly bound structure has  $\tau = 83^\circ$  and  $\Delta E_0^{\text{CP}} = -12.1$  kcal/mol. Full optimisation of the aqueous structures initially yielded five minima and five transition states. However, "following" the imaginary frequency of the TS with  $\tau = 233^\circ$  yielded two additional minima. The most strongly bound structure in terms of non-ZPE-corrected energy is the minimum with  $\tau = 298^\circ$ , which has  $\Delta E^{\text{CP}} = -6.2$  kcal/mol. However, after ZPE corrections, the most strongly bound structure is the TS with  $\tau = 328^\circ$ , which has  $\Delta E_0^{\text{CP}} = -5.3$  kcal/mol, compared to 5.2 kcal/mol for the

minimum with  $\tau = 298^\circ$ . This anomalous result is probably due to inaccuracies in the calculation of zero-point corrections, mostly resulting from the use of the harmonic approximation.

### S2.3. C/U

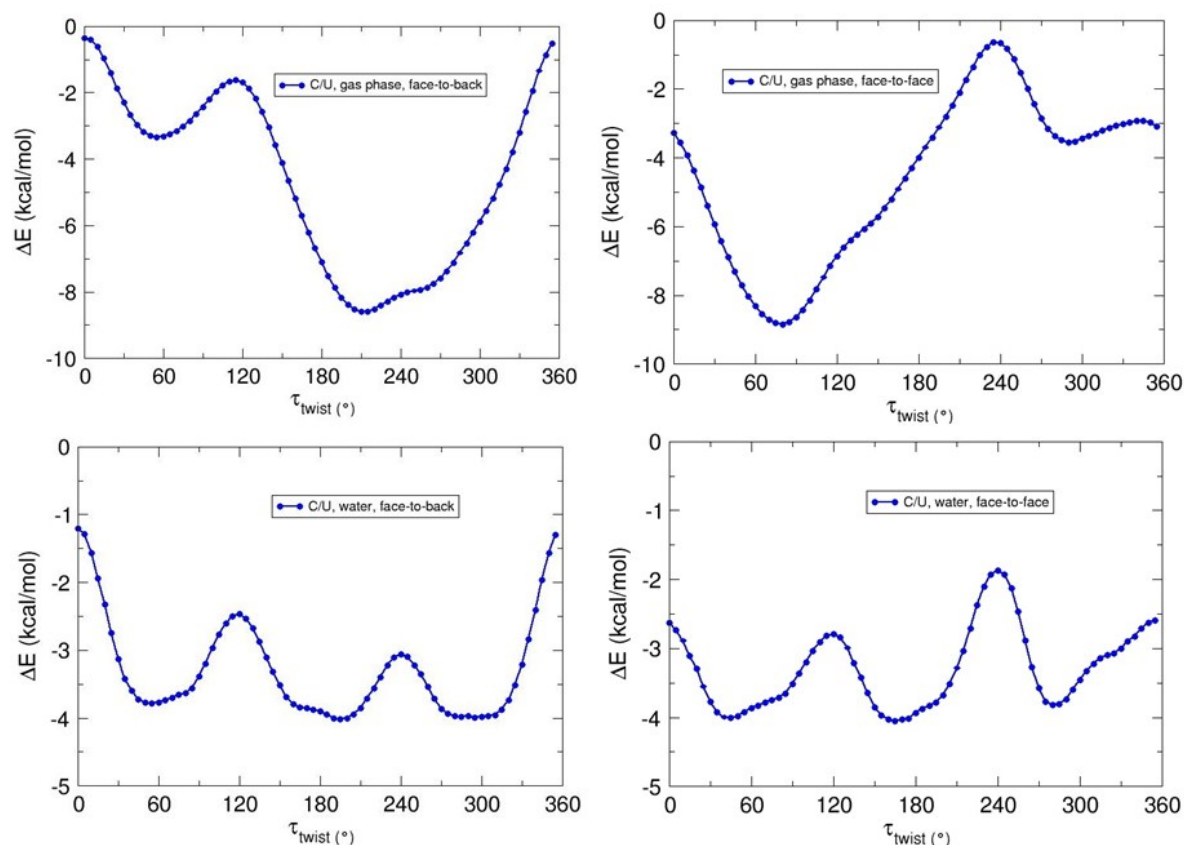


Figure S3. Potential energy profiles of C/U

Figure S.3 (top left) shows the gas-phase FTB energy profile of stacked C/U. There are two minima, at  $55^\circ$  and  $210^\circ$ , with maxima at  $0^\circ$  and  $115^\circ$ . The interaction energies are negative throughout. The BSSE is fairly small and geometry-invariant, ranging from 0.95 to 1.03 kcal/mol. Figure S.3 (bottom left) shows the aqueous FTB energy profile of stacked C/U. There are three minima, at  $55^\circ$ ,  $195^\circ$  and  $295^\circ$ , with maxima at  $0^\circ$ ,  $120^\circ$  and  $240^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase structures yielded two minima and two transition states. The more strongly bound minimum has  $\tau = 220^\circ$  and  $\Delta E_0^{\text{CP}} = -10.2$  kcal/mol. Full optimisation of the aqueous structures initially yielded only two minima, because the attempt to optimise from  $\tau = 55^\circ$  converged to a structure with one imaginary vibrational frequency. However, “following” this frequency yielded two new structures – one, geometrically very similar, also featuring a single imaginary frequency, the other a true minimum, with  $\tau = 60^\circ$ . Using the three obtained minima as inputs, three further TSs were located. The most strongly bound minimum has  $\tau = 295^\circ$  and  $\Delta E_0^{\text{CP}} = -5.0$  kcal/mol.

Figure S.3 (top right) shows the gas-phase FTF energy profile of stacked C/U. There are two minima, at  $80^\circ$  and  $290^\circ$ , with maxima at  $235^\circ$  and  $345^\circ$ . The interaction energies are negative throughout. Figure S.3 (bottom right) shows the aqueous FTF energy profile of stacked C/U. There are three minima, at  $45^\circ$ ,  $165^\circ$  and  $280^\circ$ , with maxima at  $120^\circ$ ,  $240^\circ$  and  $355^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase structures initially yielded two minima and two transition states. However, the TS with  $\tau = 34^\circ$  was lower in energy than the minimum with  $\tau = 320^\circ$  – “following” the negative frequency of this TS yielded one new stacked minimum and one planar structure, which was hydrogen-bonded in non-Watson–Crick geometry. The most strongly bound stacked structure has  $\tau = 82^\circ$  and  $\Delta E_0^{\text{CP}} = -12.6$  kcal/mol. Full optimisation of the aqueous structures initially yielded three minima and three transition states. However, “following” the imaginary frequency of the TS with  $\tau = 232^\circ$  yielded two additional stacked minima. The most strongly bound minimum has  $\tau = 316^\circ$  and  $\Delta E_0^{\text{CP}} = -4.5$  kcal/mol.

## S2.4. T/BrU

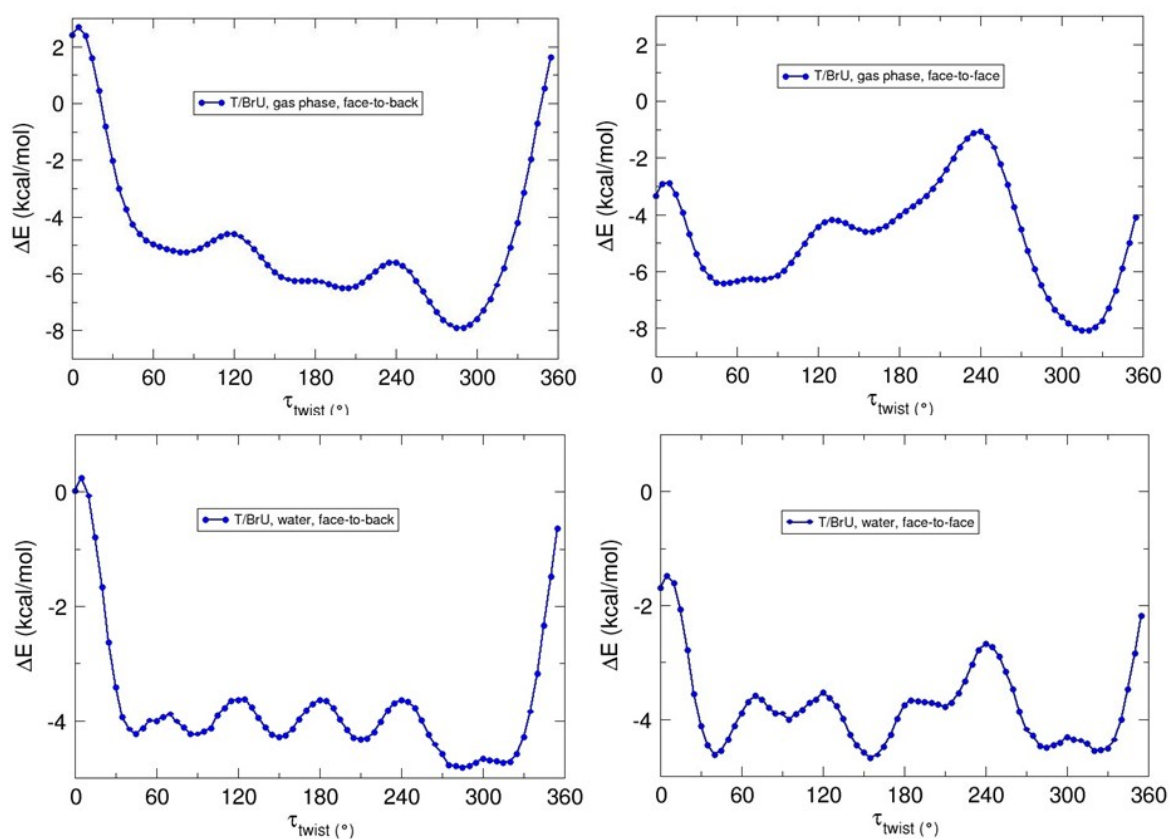


Figure S4. Potential energy profiles of T/BrU

Figure S.4 (top left) shows the FTB gas-phase rotational profile of T/BrU. There are three minima, at  $85^\circ$ ,  $205^\circ$  and  $285^\circ$ , with maxima at  $5^\circ$ ,  $115^\circ$  and  $240^\circ$ . The region around the maximum at  $5^\circ$  is repulsive. The BSSE ranges from 3.33 to 3.93 kcal/mol. Figure S.4 (bottom left) shows the FTB aqueous rotational profile of T/BrU. The six minima are at  $45^\circ$ ,  $90^\circ$ ,  $150^\circ$ ,  $210^\circ$ ,  $285^\circ$  and  $315^\circ$ , with the maxima at  $5^\circ$ ,  $70^\circ$ ,  $125^\circ$ ,  $180^\circ$ ,  $240^\circ$  and  $305^\circ$ . As in the gas phase, the region around the maximum at  $5^\circ$  is repulsive. Full optimisation of the gas-

phase structures yielded three minima and three transition states, the most strongly interacting dimer being the minimum with  $\tau = 288^\circ$ , for which  $\Delta E_0^{\text{CP}} = -11.1$  kcal/mol. Full optimisation of the aqueous structures yielded only four minima, as the starting structures with  $\tau = 90^\circ$  and  $150^\circ$  both converged to a minimum with  $\tau = 112^\circ$ , while those with  $\tau = 285^\circ$  and  $315^\circ$  both found a minimum with  $\tau = 291^\circ$ . Therefore only four transition states were located. The one with  $\tau = 264^\circ$  was lower in energy than the minimum with  $\tau = 223^\circ$ , but “following” the frequency of this TS did not yield any new minima. The global minimum has  $\tau = 291^\circ$  and  $\Delta E_0^{\text{CP}} = -5.9$  kcal/mol.

Figure S.4 (top right) shows the FTF gas-phase rotational profile of T/BrU. There are three minima, at  $\sim 50^\circ$ ,  $155^\circ$  and  $320^\circ$ , the first one being very wide and flat. The interaction energies are attractive throughout. Figure S.4 (bottom right) shows the FTF aqueous rotational profile of T/BrU. There are six minima, at  $40^\circ$ ,  $95^\circ$ ,  $155^\circ$ ,  $210^\circ$ ,  $285^\circ$  and  $320^\circ$ , with maxima at  $5^\circ$ ,  $70^\circ$ ,  $120^\circ$ ,  $185^\circ$ ,  $240^\circ$  and  $300^\circ$ . The interaction energies are attractive throughout. Full optimisation of the gas-phase structures yielded three minima. However, the minimum obtained by starting with  $\tau = 155^\circ$  was not stacked but L-shaped, with an N1H1(Br)•••O2(T) hydrogen bond. The most strongly bound structure was the stacked minimum with  $\tau = 312^\circ$  and  $\Delta E_0^{\text{CP}} = -11.2$  kcal/mol. Full optimisation of the structures in water initially yielded five minima, since the starting structures with  $\tau = 285^\circ$  and  $320^\circ$  both converged to a structure with  $\tau = 292^\circ$ . Therefore five transition states were located. However, the TS with  $\tau = 149^\circ$  had a lower ZPE-corrected energy than the minimum with  $\tau = 105^\circ$ ; “following” its imaginary frequency yielded a sixth stacked minimum with  $\tau = 176^\circ$ . The most stable structure has  $\tau = 292^\circ$  and  $\Delta E_0^{\text{CP}} = -5.7$  kcal/mol.



## S2.5. T/U

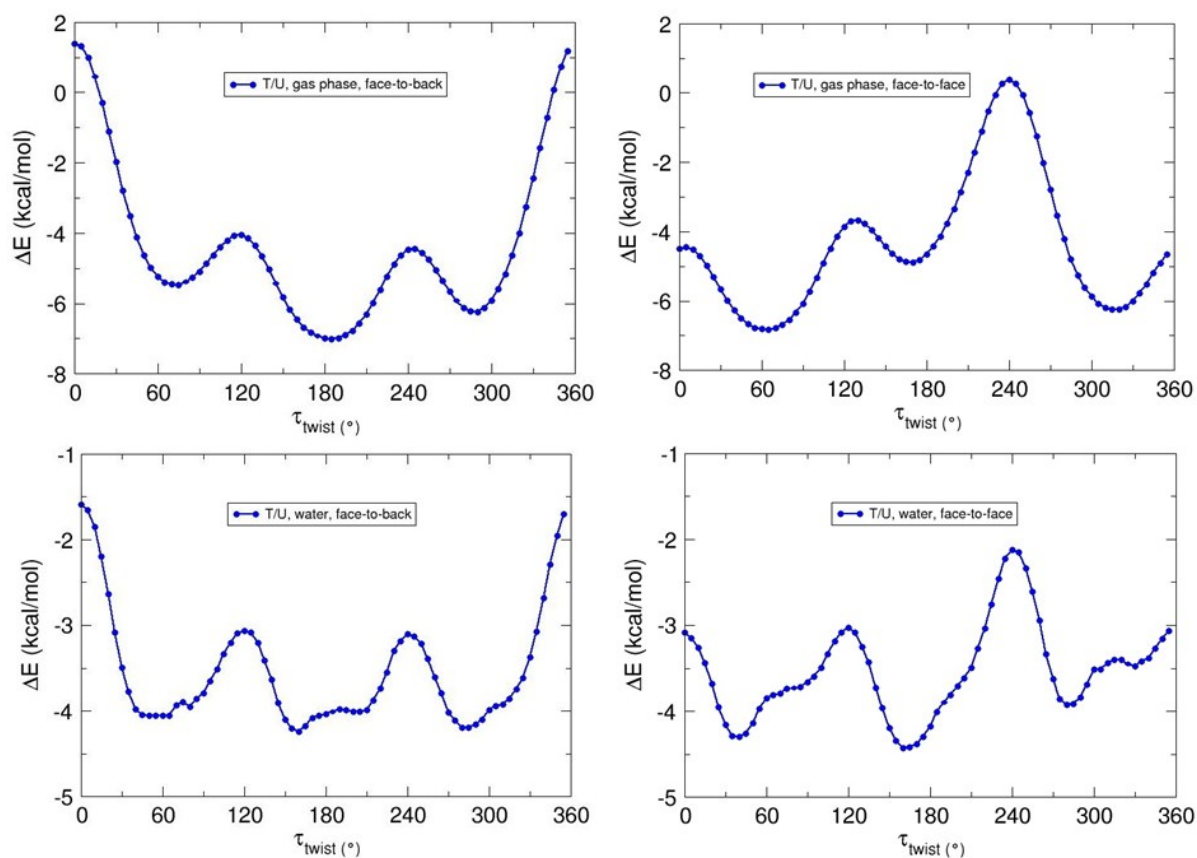


Figure S.5. Potential energy profiles of T/U

Figure S.5 (top left) shows the FTB gas-phase rotational energy profile of stacked T/U. There are three minima, at 75°, 185° and 290°, with the maxima at 0°, 120° and 245°. Interaction energies are positive around the maximum at 0°. The BSSE varies from 0.93 to 1.01 kcal/mol. Figure S.5 (bottom left) shows the FTF gas-phase rotational energy profile of stacked T/U. There are three minima, all rather broad, at ~60°, ~180° and ~285°, with the maxima at 0°, 120° and 240°. Interaction energies are negative throughout. Full optimisation of the gas-phase structures yielded three minima and three transition states. The most strongly bound minimum has  $\tau = 182^{\circ}$  and  $\Delta E_0^{\text{CP}} = -9.1$  kcal/mol. For the aqueous structures, we decided to attempt optimisations from both of the shallow sub-minima, with  $\tau = 160^{\circ}$  and  $205^{\circ}$ , within the broader minimum centred on  $\tau = 180^{\circ}$ . Hence four geometry optimisations were launched, yielding four distinct minima. Four transition states were subsequently located. The strongest interaction energy is for the dimer with  $\tau = 66^{\circ}$ , which has  $\Delta E_0^{\text{CP}} = -4.9$  kcal/mol.

Figure S.5 (top right) shows the FTF gas-phase rotational energy profile of stacked T/U. There are three minima, at 65°, 170° and 315°, with the maxima at 0°, 130° and 240°. Interaction energies are slightly positive around the maximum at 240°. Figure S.5 (bottom right) shows the FTF aqueous rotational energy profile of stacked T/U. There are four minima, at 40°, 160°, 280° and 330°, with the maxima at 120°, 240°, 320° and 355°.

Interaction energies are negative throughout. Full optimisation of the gas-phase structures yielded three minima and three transition states. The most strongly bound minimum has  $\tau = 309^\circ$  and  $\Delta E_0^{\text{CP}} = -9.3$  kcal/mol. Full optimisation of the aqueous structures yielded four minima and four transition states. The most strongly bound minimum has  $\tau = 296^\circ$  and  $\Delta E_0^{\text{CP}} = -4.8$  kcal/mol.

## S2.6 BrU/BrU

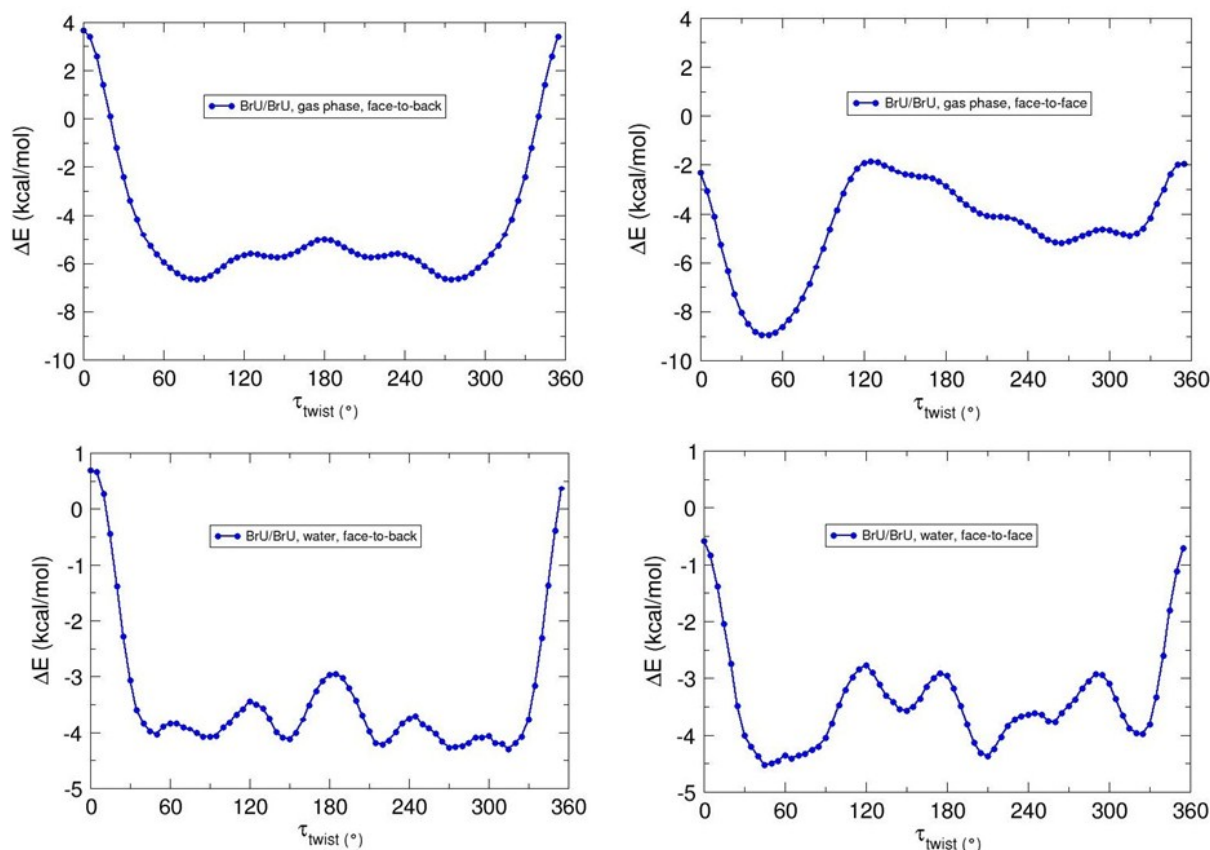


Figure S.6. Potential energy profiles of BrU/BrU

Figure S.6 (top left) shows the face-to-back gas-phase interaction energy of BrU/BrU as a function of  $\tau$ . Due to the identical monomers, the rotational profile is symmetric about  $\tau = 180^\circ$ . There are four minima, at  $\tau = 85^\circ, 145^\circ, 215^\circ$  and  $275^\circ$ , and four maxima, at  $\tau = 0^\circ, 125^\circ, 180^\circ$  and  $235^\circ$ . The BSSE (not shown) ranges from 5.58 to 6.79 kcal/mol: almost double that of U/BrU. The interaction energy at the highest maximum ( $0^\circ$ ) is strongly repulsive: here,  $\Delta E^{\text{CP}} = +3.7$  kcal/mol (but this value would be negative if the counterpoise correction were neglected). At this geometry, all the substituents on one base (including Br and C=O) are situated exactly above the corresponding substituents on the other base, at a distance of 3.4 Å. Full optimisation of the gas-phase structures yielded just three energy minima, because the optimisations starting from  $\tau = 145^\circ$  and  $\tau = 215^\circ$  both converged to the same structure, with  $\tau = 180^\circ$  and  $\Delta E_0^{\text{CP}} = -10.20$  kcal/mol. The other two minima form a symmetry-equivalent pair, with optimised  $\tau$  angles of  $73^\circ$  and  $287^\circ$ , and  $\Delta E_0^{\text{CP}} = -9.50$  kcal/mol for both. Three transition states were also found, of which two form a symmetry-equivalent pair.

Figure S.6 (bottom left) shows the face-to-back interaction energy of BrU/BrU in water PCM solvent. As in the gas phase, the profile is symmetric. However, it is flatter (compare the two y-axes). There are six minima, at 50°, 90°, 150°, 220°, 270° and 315°, and six maxima, at 0°, 65°, 120°, 185°, 245° and 300°. In water, the optimisations yielded six structures, falling into three symmetry-equivalent pairs. The ZPE-corrected interaction energies of all six optimised dimers fall within the narrow range of -5.0 to -5.4 kcal/mol, the pair with  $\tau = 61^\circ/299^\circ$  having the greatest value. Transition state searches between adjacent optimised minima all successfully yielded structures with one imaginary frequency. However, the transition state found by using the minima with  $\tau = 242^\circ$  and  $\tau = 260^\circ$  had an optimised  $\tau$  value of 273°, and was identical to the transition state found by using the minima with  $\tau = 260^\circ$  and  $\tau = 299^\circ$ . “Following the frequency” of this TS yielded the latter pair of minima, confirming that it links those two structures, rather than the former pair.

Figure S.6 (top right) shows the FTF gas-phase stacking of BrU/BrU. Unlike in the FTB case, there is no symmetry. The three minima are at 50°, 265° and 315°, the three maxima at 125°, 295° and 355°. There are no regions of repulsive interaction. The BSSE ranges from 5.50 to 6.82 kcal/mol. Figure S.6 (bottom right) shows the FTF aqueous stacking of BrU/BrU. Excluding a very shallow minimum at 65°, there are five minima, at 45°, 150°, 210°, 260° and 325°. The corresponding maxima are at 0°, 120°, 175°, 245° and 290°. Again there are no repulsive regions. Optimisation of the gas-phase structures yielded only two minima, as the starting structures with  $\tau = 265^\circ$  and  $315^\circ$  converged to the same minimum, with  $\tau = 295^\circ$  and  $\Delta E_0^{\text{CP}} = -8.3$  kcal/mol. The other minimum, with  $\tau = 49^\circ$  and  $\Delta E_0^{\text{CP}} = -11.8$  kcal/mol, has the greatest interaction energy of any gas-phase BrU/BrU dimer found in this study. Two transition states were located, but the one found by starting from  $\tau = 125^\circ$  was L-shaped rather than stacked, and probably does not connect the two minima. Optimisation of the aqueous structures initially yielded five distinct minima, of which the most strongly bound had  $\tau = 56^\circ$  and  $\Delta E_0^{\text{CP}} = -5.6$  kcal/mol. However, the minimum with  $\tau = 121^\circ$  (obtained from the starting structure with  $\tau = 150^\circ$ ) could only be found by using Gaussian’s default convergence criteria – when “Tight” criteria were used, only structures with one imaginary frequency were found when starting a minimum search from  $\tau = 150^\circ$ . Subsequently, five transition states were located in the usual way. However, the guess structures with  $\tau = 120^\circ$  and  $175^\circ$  both yielded the same TS, with optimised  $\tau = 120^\circ$ . Furthermore, this TS was lower in energy ( $\Delta E_0^{\text{CP}} = -5.0$  kcal/mol) than the minimum with  $\tau = 121^\circ$  ( $\Delta E_0^{\text{CP}} = -4.8$  kcal/mol), which was one of the minima it was expected to connect. Nevertheless, “following the frequency” of this TS with displacements in one direction yielded the minimum with  $\tau = 121^\circ$  (using “Tight” optimisation criteria). With displacements in the other direction, a sixth energy minimum was found, which, despite its relatively large angle between planes (12°) and horizontal separation (2.66 Å) had a stronger interaction energy than the other five structures ( $\Delta E_0^{\text{CP}} = -5.9$  kcal/mol).

## S2.7. C/C

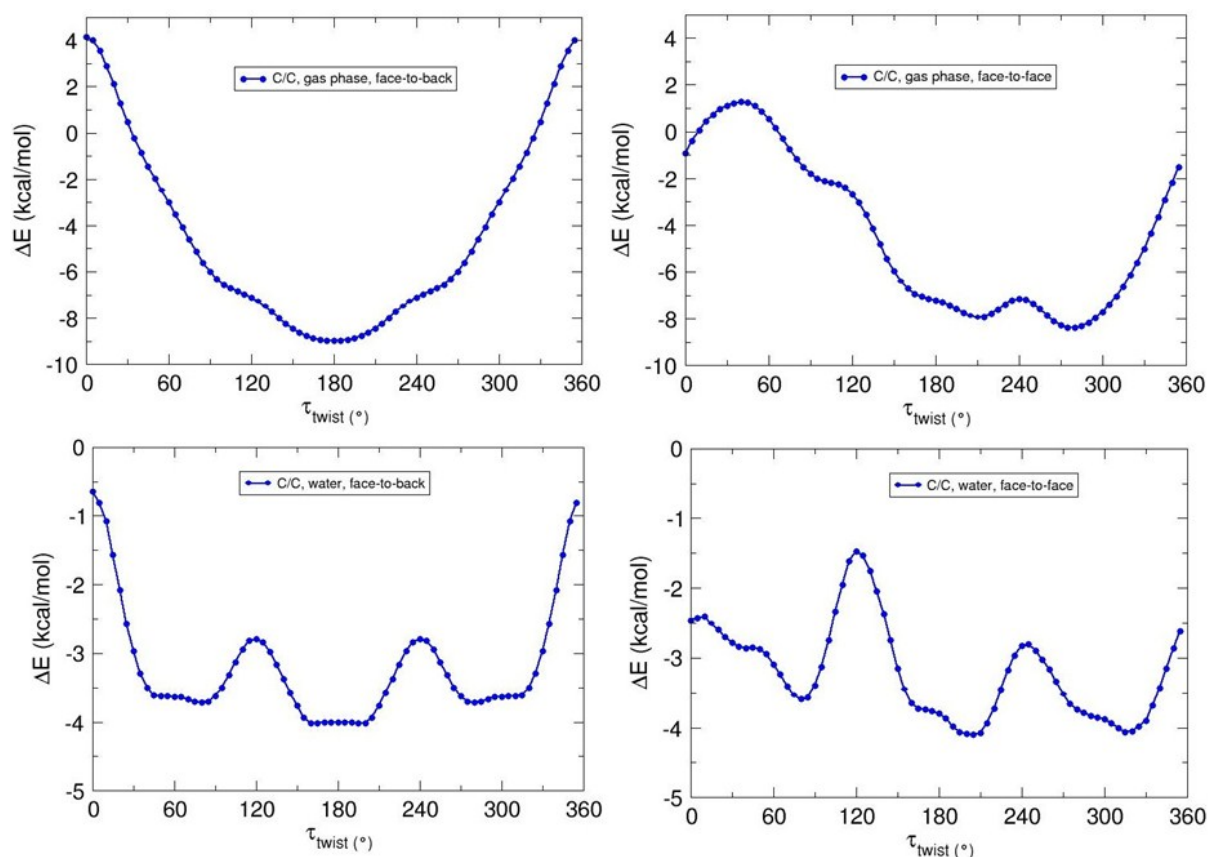


Figure S.7. Potential energy profiles of BrU/BrU

Figure S.7 (top left) shows the FTB gas-phase energy profile of the C/C stacked dimer. In contrast to all other dimers explored in this study, there is only one energy minimum, at  $\tau = 180^\circ$ . The profile is symmetric about this minimum. The maximum is at  $\tau = 0^\circ$ . A large part of the energy profile around the maximum is positive (repulsive). The BSSE is relatively small and geometry-insensitive, varying from 1.01 to 1.07 kcal/mol. Figure S.7 (bottom left) shows the FTB aqueous energy profile of the C/C stacked dimer. There are three minima, at  $80^\circ$ ,  $\sim 180^\circ$  and  $280^\circ$ , the second of which is especially broad and flat. The maxima are at  $0^\circ$ ,  $120^\circ$  and  $240^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase minimum yielded a significantly tilted structure (angle between planes =  $17^\circ$ ) with  $\Delta E_0^{\text{CP}} = -11.1$  kcal/mol. For the aqueous structures, we decided to start optimisations from both of the very shallow sub-minima at  $160^\circ$  and  $200^\circ$  within the broad minimum centred on  $180^\circ$ . These optimisations converged to distinct but symmetry-equivalent, heavily tilted structures with  $\tau = 137^\circ$  and  $223^\circ$ , angle between planes =  $26^\circ$  and  $\Delta E_0^{\text{CP}} = -4.1$  kcal/mol. The starting structures with  $\tau = 80^\circ$  and  $280^\circ$  converged to symmetry-equivalent, also heavily tilted minima with  $\tau = 104^\circ$  and  $256^\circ$ , angle between planes =  $17^\circ$  and  $\Delta E_0^{\text{CP}} = -4.4$  kcal/mol. Four transition states were located.

Figure S.7 (top right) shows the FTF gas-phase energy profile of the C/C stacked dimer. There are two minima, at  $210^\circ$  and  $280^\circ$ , and two maxima, at  $40^\circ$  and  $240^\circ$ . The region

around the first maximum is repulsive. Figure S.7 (bottom right) shows the FTF aqueous energy profile of the C/C stacked dimer. There are four minima, at  $40^\circ$ ,  $80^\circ$ ,  $205^\circ$  and  $315^\circ$ , the first of which is very shallow. The maxima are at  $10^\circ$ ,  $45^\circ$ ,  $120^\circ$  and  $245^\circ$ . The interaction energies are negative throughout. Full optimisation of the gas-phase structure with  $\tau = 210^\circ$  yielded a stacked energy minimum with  $\tau = 152^\circ$  and  $\Delta E_0^{\text{CP}} -12.6$  kcal/mol. However, full optimisation of the structure with  $\tau = 280^\circ$  yielded a planar, hydrogen-bonded (non-Watson–Crick) minimum with  $\Delta E_0^{\text{CP}} = -20.9$  kcal/mol. We attempted to locate a stacked minimum corresponding to  $\tau = 280^\circ$  by repeating the geometry optimisations with MP2/6-31+G(d) and B97-D/6-31+G(d), but these procedures followed the same path as M06-2X. Following these findings, no transition state searches were attempted. Full optimisation of the aqueous structures initially yielded only three minima, because the attempt to optimise the structure with  $\tau = 80^\circ$  to a minimum in fact converged to a structure with one imaginary (negative) vibrational frequency. However, “following” the motion of this vibration yielded a true minimum, as confirmed by the absence of negative vibrational frequencies in the resulting structure, which has a  $\tau$  angle of  $102^\circ$ . The structure with the greatest ZPE-corrected interaction energy has  $\tau = 310^\circ$  and  $\Delta E_0^{\text{CP}} = -4.4$  kcal/mol.

Note that the aqueous profiles are much flatter than the gas-phase profiles for all species, due to solvent screening. This is illustrated in Figure S.8, which shows the T/BrU FTF profiles in both phases on the same scale.

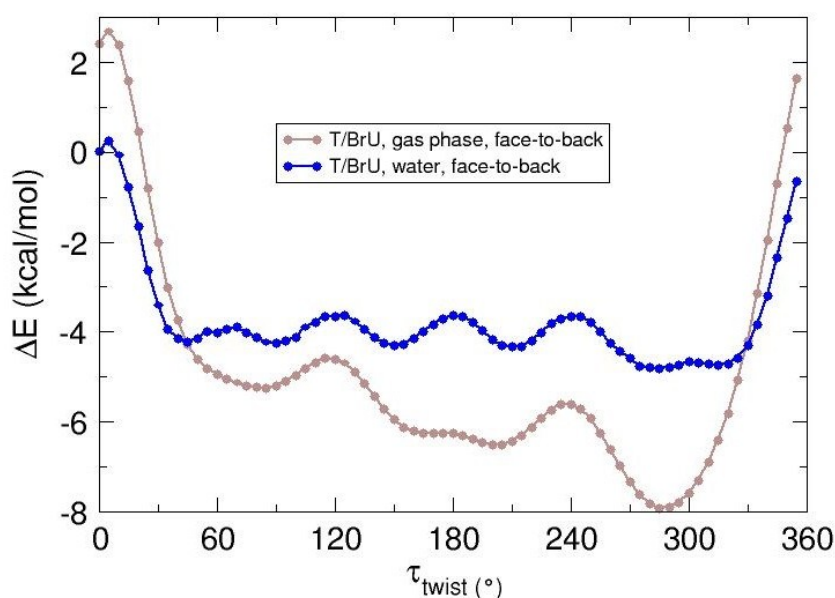


Figure S.8: T/BrU FTF gas-phase and aqueous profiles shown on the same scale.

**Section S3.** Geometrical parameters and interaction energies of all optimised minima and transition states.

**Table S1** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	1	14	3.25	1.27	1	-6.7	-5.9	
40	54	15	3.13	0.99	0	-8.5	-7.6	-3.8
120	77	6	3.03	1.80	1	-7.5	-6.8	
260	261	18	3.08	0.95	0	-15.2	-14.0	-9.1

**Table S2** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	329	12	3.07	1.45	1	-6.0	-5.4	
0 <sup>a</sup>	7	3	3.08	1.56	0	-5.8	-5.1	-5.0
0 <sup>a</sup>	67	10	3.04	1.16	0	-7.1	-6.4	-5.9
40 & 85	55	9	3.16	0.67	0	-5.2	-4.7	-4.1
120	79	8	3.17	0.56	1	-5.2	-4.9	
120 <sup>b</sup>	65	7	3.14	1.27	0	-4.8	-4.3	-3.8
120 <sup>b</sup>	89	10	3.13	0.91	0	-5.4	-4.8	-4.2
155	119	1	3.16	1.22	0	-5.0	-4.4	-3.8
175	153	3	3.19	1.07	1	-4.5	-4.2	
210	241	5	3.16	1.16	0	-5.6	-5.0	-4.4
240	242	5	3.17	1.00	1	-5.5	-5.0	
285	293	10	3.04	1.16	0	-7.1	-6.4	-5.9

<sup>a, b</sup> These minima were obtained by “following” the imaginary frequencies of the transition states listed above them

**Table S3** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
290	300	10	3.07	1.03	0	-10.4	-9.3	-4.3
345	355	2	3.13	1.12	1	-9.1	-8.3	
80	76	16	3.03	1.53	0	-14.9	-13.4	-10.1
235	308	20	3.08	2.18	1	-8.2	-7.3	

**Table S4** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	239	3	3.17	1.28	1	-5.2	-4.6	
285	291	8	3.07	1.13	0	-6.6	-5.9	-5.5
355	5	1	3.13	1.13	1	-5.3	-4.8	
35	31	7	3.13	1.11	0	-5.4	-5.0	-4.3
65	38	8	3.12	1.17	1	-5.5	-5.2	
65 <sup>a</sup>	63	10	3.09	1.42	0	-5.5	-4.8	-4.3
90	93	6	3.14	1.00	0	-4.9	-4.5	-3.8
120	151	8	3.19	0.49	1	-5.0	-4.5	
120 <sup>a</sup>	133	15	3.09	1.14	0	-5.7	-5.1	-4.5
155	176	5	3.19	1.33	0	-4.8	-4.1	-3.5
190	203	5	3.24	0.97	1	-4.4	-4.0	
205	232	3	3.17	1.32	0	-5.2	-4.7	-4.1

<sup>a</sup> These minima were obtained by “following” the imaginary frequencies of the transition states listed above them

**Table S5** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/T minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
5 <sup>a</sup>	n/a	45	n/a	n/a	1	-11.0	-10.0	
5 <sup>b</sup>	n/a	52	n/a	n/a	0	-13.9	-12.5	-10.8
5 <sup>c</sup>	n/a	n/a	n/a	n/a	0	-20.1	-19.5	-18.2
85	84	15	2.90	2.52	0	-8.1	-7.1	-5.3
115	148	6	3.06	1.55	1	-8.8	-7.9	
115 <sup>d</sup>	132	4	3.00	1.69	0	-9.0	-8.0	-6.1
210	221	10	3.13	0.76	0	-12.1	-10.9	-9.2

<sup>a</sup> L-shaped transition state.

<sup>b</sup> L-shaped minimum, found by “following” the imaginary frequency of the transition state listed above it.

<sup>c</sup> Planar H-bonded minimum, found by “following” the imaginary frequency of the transition state listed above it.

<sup>d</sup> Stacked minimum, found by “following” the imaginary frequency of the transition state listed above it.

**Table S6** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/T minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	48	6	3.20	1.48	1	-4.5	-3.7	
80	61	6	3.12	1.11	0	-5.1	-4.4	-3.8
120	124	2	3.18	1.05	0	-4.9	-4.2	-3.6
160	150	3	3.21	0.88	0	-5.2	-4.5	-3.9
170	167	1	3.25	0.05	1	-4.5	-3.9	
205	210	6	3.19	0.84	0	-5.6	-4.8	-4.2
240	230	7	3.19	1.03	1	-5.6	-4.8	
240 <sup>a</sup>	224	8	3.19	1.03	0	-5.6	-4.6	-4.1
240 <sup>a</sup>	250	6	3.18	1.22	0	-5.8	-4.8	-4.4
285 & 315	296	12	3.07	1.11	0	-6.7	-5.8	-5.3

<sup>a</sup> These minima were obtained by “following” the imaginary frequency of the transition state listed above them



**Table S7** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/T minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	275	16	3.11	1.14	1	-6.9	-5.8	
290	310	13	3.10	1.19	1	-8.0	-7.0	
290 <sup>a</sup>	318	14	3.08	1.52	0	-8.1	-7.0	-5.1
345	34	14	3.06	2.42	1	-9.4	-8.6	
345 <sup>b</sup>	68	21	3.13	1.00	0	-12.6	-11.6	-9.7
345 <sup>b, c</sup>	n/a	80	n/a	n/a	0	-11.0	-10.1	-8.7
90	83	16	2.92	2.22	0	-13.4	-12.1	-10.3

<sup>a, b</sup> These minima were obtained by “following” the imaginary frequency of the transition state listed above them

<sup>c</sup> L-shaped minimum

**Table S8** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/T minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	233	2	3.16	1.31	1	-5.6	-4.7	
240 <sup>a</sup>	248	12	3.06	1.51	0	-6.0	-5.1	-4.7
240 <sup>a</sup>	229	3	3.18	1.26	0	-5.7	-4.7	-4.4
280	298	10	3.10	1.06	0	-6.2	-5.2	-4.8
315	328	9	3.12	1.05	1	-5.9	-5.3	
325	333	7	3.12	0.99	0	-5.9	-5.1	-4.6
355	13	6	3.18	1.12	1	-4.9	-4.4	
35	54	11	3.12	1.22	0	-5.7	-4.7	-4.3
75	71	11	3.11	1.56	1	-4.8	-4.2	
90	57	2	3.13	1.21	0	-5.2	-4.4	-3.9
120	148	12	3.18	0.72	1	-5.1	-4.3	
155	164	4	3.22	0.88	0	-5.7	-4.7	-4.3

<sup>a</sup> These minima were obtained by “following” the imaginary frequency of the transition state listed above them

**Table S9** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/U minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	355	21	3.33	1.31	1	-5.3	-4.5	
55	53	19	3.13	1.22	0	-7.0	-6.0	-4.2
115	107	7	3.14	1.44	1	-6.4	-5.5	
210	220	10	3.15	0.76	0	-11.3	-10.2	-8.5

**Table S10** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/U minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	7	7	3.19	1.34	1	-3.5	-2.8	
55	60	14	3.22	0.40	1	-4.6	-4.0	
55 <sup>a</sup>	58	12	3.22	0.38	1	-4.6	-4.1	
55 <sup>a</sup>	60	6	3.13	1.21	0	-4.8	-4.1	-3.5
120	149	3	3.23	0.84	1	-4.2	-3.6	
195	216	7	3.21	0.92	0	-4.9	-4.2	-3.6
240	233	1	3.19	1.02	1	-4.7	-4.0	
295	295	13	3.08	1.16	0	-6.0	-5.0	-4.5

<sup>a</sup> These structures were obtained by “following” the imaginary frequency of the transition state listed above them

**Table S11** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/U minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
290	320	15	3.06	1.66	0	-8.1	-7.0	-5.2
245	34	4	3.02	2.11	1	-9.5	-8.6	
245 <sup>a</sup>	17	9	3.01	2.10	0	-9.5	-8.5	-6.8
245 <sup>a,b</sup>	n/a	n/a	n/a	n/a	0	-20.4	-19.4	-18.0
80	82	17	2.91	2.26	0	-13.9	-12.6	-10.8
235	225	21	3.26	1.81	1	-6.0	-5.0	

<sup>a</sup> These minima were obtained by “following” the imaginary frequency of the transition state listed above them.

<sup>b</sup> Planar hydrogen-bonded minimum.

**Table S12** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/U minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	232	3	3.16	1.40	1	-4.5	-3.9	
240 <sup>a</sup>	254	19	3.13	1.48	0	-5.4	-4.5	-4.0
240 <sup>a</sup>	227	3	3.18	1.32	0	-4.8	-3.9	-3.5
280	316	18	3.10	1.43	0	-5.5	-4.5	-4.1
355	27	4	3.18	1.24	1	-4.2	-3.6	
45	52	16	3.22	0.58	0	-4.8	-4.2	-3.6
120	153	8	3.21	0.60	1	-4.4	-3.7	
165	168	5	3.22	0.86	0	-4.8	-3.8	-3.4

<sup>a</sup> These minima were obtained by “following” the imaginary frequency of the transition state listed above them.

**Table S13** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back T/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
5	34	16	3.13	2.60	1	-4.1	-3.7	
85	102	4	3.04	1.43	0	-8.3	-7.8	-4.0
115	130	14	3.23	1.02	1	-7.5	-7.1	
205	182	3	3.12	1.50	0	-10.1	-9.5	-3.6
240	241	4	3.19	0.96	1	-8.3	-7.8	
285	288	12	3.04	0.92	0	-11.9	-11.1	-5.5

**Table S14** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back T/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
5	340	5	3.26	0.69	1	-4.5	-4.2	
45	58	7	3.10	0.91	0	-5.7	-5.3	-4.6
70	86	3	3.24	0.92	1	-3.8	-3.6	
90 & 150	112	3	3.16	1.21	0	-5.6	-5.2	-4.6
180	208	4	3.23	0.64	1	-5.3	-5.0	
210	223	1	3.18	0.96	0	-5.4	-5.1	-4.4
240	264	2	3.15	1.14	1	-5.7	-5.3	
285 & 315	291	6	3.07	1.10	0	-6.3	-5.9	-5.3

**Table S15** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face T/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	267	15	3.13	2.50	1	-6.5	-6.1	
320	312	11	3.05	0.82	0	-12.0	-11.2	-6.1
10	38	9	3.12	1.96	1	-7.5	-7.0	
50	63	15	3.06	1.23	0	-10.3	-9.6	-3.7
130	83	13	3.05	1.86	1	-8.0	-7.4	
155 <sup>a</sup>	n/a	87	n/a	n/a	0	-11.0	-10.3	-8.3

<sup>a</sup> L-shaped minimum.

**Table S16** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face T/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	218	6	3.21	0.99	1	-4.7	-4.4	
285 & 320	292	6	3.08	1.15	0	-5.9	-5.7	-4.9
5	24	2	3.23	0.74	1	-3.9	-3.8	
40	63	7	3.09	1.50	0	-5.3	-4.9	-4.3
70	149	3	3.21	0.86	1	-5.2	-4.9	
70 <sup>a</sup>	176	2	3.20	1.34	0	-5.0	-4.5	-3.9
95	105	2	3.13	1.25	0	-5.2	-4.7	-4.0
120	104	2	3.18	1.16	1	-5.1	-4.8	
155	114	3	3.15	1.24	0	-5.7	-5.2	-4.6
185	206	6	3.22	1.00	1	-4.8	-4.5	
210	224	4	3.17	1.15	0	-5.2	-4.6	-4.0

<sup>a</sup> This minimum was obtained by “following” the imaginary frequency of the transition state listed above it

**Table S17** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back T/U minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	349	4	3.17	1.55	1	-3.2	-2.8	
75	71	16	3.09	0.87	0	-8.9	-8.1	-6.1
120	134	24	3.33	1.25	1	-7.3	-6.8	
185	182	6	3.09	1.23	0	-9.9	-9.1	-7.4
245	210	10	3.16	0.92	1	-7.4	-6.8	
290	288	17	3.09	0.91	0	-9.6	-8.8	-6.8

**Table S18** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back T/U minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	332	7	3.24	1.00	1	-4.2	-3.6	
60	66	11	3.10	0.95	0	-5.6	-4.9	-4.3
120	113	4	3.18	1.00	1	-4.7	-4.1	
160	175	4	3.17	1.20	0	-5.2	-4.5	-4.0
190	198	2	3.24	0.12	1	-4.3	-3.9	
205	215	1	3.20	0.88	0	-5.1	-4.5	-3.9
240	231	2	3.19	1.05	1	-4.9	-4.3	
285	292	11	3.10	0.96	0	-5.3	-4.6	-4.0

**Table S19** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face T/U minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	271	14	3.13	2.47	1	-5.1	-4.6	
315	309	15	3.07	0.88	0	-10.2	-9.3	-7.4
0	47	11	3.11	2.18	1	-7.4	-6.9	
65	67	19	3.16	0.90	0	-9.8	-8.8	-7.1
130	166	15	3.15	1.18	1	-6.7	-6.1	
170	174	19	3.27	0.61	0	-6.9	-6.4	-4.4

**Table S20** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face T/U minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
240	256	6	3.11	1.41	1	-4.8	-4.1	
280	296	11	3.09	1.04	0	-5.5	-4.8	-4.3
320	316	12	3.12	0.91	1	-5.2	-4.5	
330	333	7	3.11	0.87	0	-5.4	-4.6	-4.1
355	19	3	3.22	1.01	1	-4.5	-4.0	
40	58	9	3.14	1.26	0	-5.0	-4.3	-3.8
120	140	7	3.23	0.93	1	-4.8	-4.1	
160	169	9	3.20	0.25	0	-4.9	-4.3	-3.7

**Table S21** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back BrU/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	326	14	3.12	2.66	1	-5.6	-5.2	
85	73	12	3.05	0.94	0	-10.2	-9.5	-1.5
125	134	4	3.18	0.88	1	-8.6	-8.2	
145 & 215	180	0	3.15	1.90	0	-10.8	-10.2	-0.5
235	226	4	3.18	0.88	1	-8.6	-8.2	
275	287	12	3.05	0.94	0	-10.2	-9.5	-1.5

**Table S22** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back BrU/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	25	7	3.21	1.20	1	-4.0	-4.1	
50	61	4	3.09	1.10	0	-5.6	-5.4	-4.7
65	87	4	3.15	0.80	1	-5.0	-5.1	
90	100	3	3.15	1.28	0	-5.1	-5.0	-4.2
120	87	6	3.17	1.87	1	-4.6	-4.7	
150	118	2	3.15	1.24	0	-5.4	-5.3	-4.5
185	122	7	3.17	1.70	1	-5.1	-5.1	
220	242	2	3.15	1.24	0	-5.4	-5.3	-4.5
270	260	3	3.15	1.28	0	-5.1	-5.0	-4.2
245 & 300	273	4	3.15	0.80	1	-5.0	-5.1	
315	299	4	3.09	1.10	0	-5.6	-5.4	-4.7

**Table S23** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face BrU/BrU minima and transition states in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
50	56	10	3.04	0.79	0	-12.4	-11.8	-4.3
125 <sup>a</sup>	n/a	54	n/a	n/a	1	-5.5	-5.2	
265 & 315	299	15	3.07	1.32	0	-8.8	-8.3	-0.4
355	312	8	3.10	2.11	1	-7.8	-7.5	

<sup>a</sup> L-shaped transition state.

**Table S24** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face BrU/BrU minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	342	1	3.19	0.91	1	-3.7	-3.9	
45	62	4	3.10	1.08	0	-5.6	-5.6	-4.8
120 & 175	127	6	3.13	1.48	1	-5.0	-5.0	
120 <sup>a</sup>	121	12	3.03	2.66	0	-6.0	-5.9	-5.1
150	127	5	3.13	1.38	0	-4.9	-4.8	-4.1
210	243	2	3.15	1.23	0	-5.0	-4.9	-4.1
245	226	4	3.21	1.86	1	-4.1	-4.1	
260	251	2	3.16	1.28	0	-4.9	-4.8	-4.0
290	273	4	3.17	1.12	1	-4.1	-4.1	
325	302	5	3.10	1.51	0	-4.8	-4.8	-4.0

<sup>a</sup> This minimum was obtained by “following” the imaginary frequency of the transition state listed above it

**Table S25** Interaction energy (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/C minimum in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
180	140	17	3.19	1.17	0	-12.6	-11.1	-9.6

**Table S26** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-back C/C minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
0	334	4	3.28	1.04	1	-3.3	-2.5	
80	104	17	3.15	1.08	0	-5.6	-4.4	-4.1
120	126	3	3.19	1.10	1	-4.8	-3.8	
160	137	26	3.31	1.68	0	-5.5	-4.1	-3.9
180	200	1	3.19	1.03	1	-4.8	-4.2	
200	223	26	3.31	1.68	0	-5.5	-4.1	-3.9
240	222	6	3.21	0.93	1	-4.9	-3.9	
280	256	17	3.15	1.08	0	-5.6	-4.4	-4.1



**Table S27** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/C minima in the gas phase calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
210	152	20	3.23	0.71	0	-14.5	-12.6	-11.0
280 <sup>a</sup>	n/a	n/a	n/a	n/a	0	-22.0	-20.9	-19.6

<sup>a</sup> Planar, hydrogen-bonded minimum.

**Table S28** Interaction energies (in kcal/mol) and structural parameters (distances in Å, angles in degrees) of the face-to-face C/C minima and transition states in water PCM solvent calculated at the M06-2X/6-31+G(d) level of theory

$\tau_{\text{twist}}$ (initial)	$\tau_{\text{twist}}$ (final)	Angle between planes	Vertical separation	Horizontal separation	Im. Freq.	$\Delta E^{\text{CP}}$	$\Delta E_0^{\text{CP}}$	$\Delta H^{\text{CP}}$
10	340	2	3.16	1.22	1	-4.3	-3.6	
40	19	1	3.20	1.00	0	-4.8	-4.1	-3.5
45	41	6	3.22	1.20	1	-3.9	-3.0	
80	86	7	3.23	0.45	1	-3.8	-3.1	
80	110	18	3.12	1.55	0	-5.2	-3.4	-3.6
120	158	9	3.20	1.17	1	-4.4	-3.5	
205	188	4	3.21	1.04	0	-5.2	-4.2	-3.8
245	214	5	3.23	0.69	1	-4.2	-3.3	
315	309	17	3.20	0.72	0	-5.1	-4.4	-3.8

#### Section S4. Cartesian coordinates of all optimised minima and transition states.

The Cartesian coordinates are given in xyz format (first line: number of atoms; second line: title; following lines: atom symbol and Cartesian coordinates in Hartree). The title line gives information on the system (ftb/ftf: face-to-back or face-to-face; gas/water: gas-phase or continuum water; min/max – minimum or transition state optimisation; plus/minus: starting structures obtained from the transition state by adding or subtracting the magnitudes of the displacement of each atom in the imaginary vibrational mode). The value after min or max shows the starting twist angle. The optimised twist angle is given as well. Angles are in degrees. The start and optimised twist angles conform to those listed in Tables S1 – S28 (Section S2).

24

BrU-BrU-ftb-gas-max0: Optimised twist = 326.26 deg.

```
O -4.81911200 -1.68304300 -0.20757200
C -3.93468700 -0.85764300 -0.20457900
N -3.79170400 0.09673300 0.79196000
H -4.43586000 0.00537600 1.56685700
N -2.98591000 -0.73972000 -1.20498900
H -3.07359300 -1.40406300 -1.96824100
C -2.76563600 0.99865900 0.83477500
H -2.75131800 1.66236400 1.69226400
C -1.89287700 0.12868700 -1.26819500
O -1.10167900 0.06974300 -2.18457200
C -1.83027100 1.05824200 -0.13325100
Br -0.41609200 2.26942100 -0.08190100
C 2.29063900 -0.57108000 0.39481500
C 1.73695800 -0.18395200 1.55707600
N 0.48506400 -0.60721400 1.93883900
C -0.31968100 -1.41821000 1.16077900
N 0.28443100 -1.81889800 -0.00887900
C 1.55396000 -1.47280200 -0.50310300
Br 3.97667000 0.00032600 -0.13753800
H 2.24348700 0.48048500 2.24758400
H 0.07219700 -0.28499400 2.80395700
O -1.44982300 -1.73450300 1.48564300
O 1.94875500 -1.91441400 -1.55507800
H -0.27389000 -2.41029500 -0.61783800
```

24

BrU-BrU-ftb-gas-max125: Optimised twist = 134.25 deg.

```
O -1.87264200 -2.51674500 1.53774600
C -0.84436500 -2.11918700 1.03382900
N -0.58446500 -2.18329400 -0.32451700
H -1.35246800 -2.51403800 -0.89633800
N 0.19184700 -1.55383500 1.75550900
H 0.05052900 -1.50833800 2.75996500
C 0.54157400 -1.66235800 -0.90847200
H 0.59049900 -1.72860500 -1.98935100
C 1.36151100 -0.95180300 1.27345800
O 2.12168600 -0.38836400 2.03080600
C 1.51301500 -1.07734200 -0.17959800
Br 3.03860500 -0.35809100 -0.96413600
C -1.63041100 0.94852800 -0.04772400
C -1.47200100 1.25092000 1.25725200
```

N	-0.35771300	1.90103200	1.71542300
C	0.67035800	2.34824400	0.89145000
N	0.48942800	1.98462900	-0.43373500
C	-0.56509200	1.27233900	-1.00467100
Br	-3.15954900	0.10149200	-0.68984100
H	-2.21612200	0.98882300	2.00212800
H	-0.24063700	2.11217700	2.69867300
O	1.61220800	2.98629200	1.29500400
O	-0.54606200	0.95824400	-2.17755800
H	1.25848800	2.21977700	-1.05575300

24

BrU-BrU-ftb-gas-max235: Optimised twist = 225.76 deg.

O	-1.61227500	2.98629900	1.29542400
C	-0.67046400	2.34827100	0.89175100
N	0.35763600	1.90093900	1.71562400
H	0.24062100	2.11199000	2.69890100
N	-0.48960800	1.98479800	-0.43348300
H	-1.25868800	2.22003800	-1.05544000
C	1.47189400	1.25086900	1.25732300
H	2.21604600	0.98867400	2.00213400
C	0.56488600	1.27258200	-1.00456100
O	0.54581300	0.95865500	-2.17749100
C	1.63024000	0.94863300	-0.04769800
Br	3.15934600	0.10166600	-0.68999100
C	-1.51282100	-1.07743800	-0.17967000
C	-0.54134300	-1.66245400	-0.90849700
N	0.58463600	-2.18344600	-0.32448100
C	0.84443900	-2.11940900	1.03388800
N	-0.19179400	-1.55402700	1.75551300
C	-1.36139700	-0.95192600	1.27339700
Br	-3.03835900	-0.35816600	-0.96428700
H	-0.59019900	-1.72866700	-1.98938100
H	1.35266200	-2.51421500	-0.89625500
O	1.87265600	-2.51705000	1.53786300
O	-2.12158700	-0.38845300	2.03070400
H	-0.05054800	-1.50857800	2.75998100

24

BrU-BrU-ftb-gas-min145: Optimised twist = 180.00 deg.

O	3.06257200	-2.43697800	0.17827000
C	1.89252200	-2.12945400	0.18067000
N	1.17840000	-1.85068600	1.33491800
H	1.72397600	-1.81557300	2.18743500
N	1.12617200	-2.01162700	-0.96770400
H	1.63035200	-2.14818700	-1.83881900
C	-0.15473500	-1.54255600	1.34882300
H	-0.58868500	-1.36056800	2.32570700
C	-0.20714300	-1.61604200	-1.08287700
O	-0.70557100	-1.41706700	-2.17356600
C	-0.87641900	-1.45968000	0.21215900
Br	-2.69874400	-1.07698800	0.21653700
C	0.87641800	1.45967700	-0.21215600
C	0.15473700	1.54255200	-1.34882300
N	-1.17840000	1.85067400	-1.33492000
C	-1.89252100	2.12945500	-0.18067500
N	-1.12617600	2.01161900	0.96770100
C	0.20714100	1.61604400	1.08287800
Br	2.69874400	1.07698600	-0.21653400
H	0.58869000	1.36056300	-2.32570500

H -1.72397300 1.81557500 -2.18744000  
O -3.06256700 2.43699500 -0.17827900  
O 0.70556900 1.41708100 2.17356900  
H -1.63035300 2.14820200 1.83881400  
24

BrU-BrU-ftb-gas-min215: Optimised twist = 180.00 deg.

O -3.06268700 -2.43687700 -0.17825000  
C -1.89262400 -2.12940200 -0.18065400  
N -1.17849200 -1.85068300 -1.33490700  
H -1.72406500 -1.81557100 -2.18742600  
N -1.12626800 -2.01159300 0.96771600  
H -1.63045100 -2.14812300 1.83883300  
C 0.15465300 -1.54259400 -1.34881800  
H 0.58860700 -1.36063200 -2.32570400  
C 0.20706100 -1.61605100 1.08288300  
O 0.70549400 -1.41708500 2.17357000  
C 0.87633900 -1.45972200 -0.21215400  
Br 2.69867600 -1.07708000 -0.21653800  
C -0.87633800 1.45971400 0.21215200  
C -0.15466000 1.54258400 1.34882000  
N 1.17848500 1.85066900 1.33491900  
C 1.89262100 2.12940700 0.18067400  
N 1.12627700 2.01158000 -0.96770400  
C -0.20705300 1.61605100 -1.08288200  
Br -2.69867600 1.07707500 0.21652200  
H -0.58862300 1.36062400 2.32570300  
H 1.72404900 1.81557800 2.18744400  
O 3.06267800 2.43691000 0.17827800  
O -0.70548700 1.41710400 -2.17357300  
H 1.63046300 2.14812900 -1.83881700  
24

BrU-BrU-ftb-gas-min275: Optimised twist = 286.99 deg.

O -2.53781300 -2.73100800 -1.39916200  
C -2.24402600 -1.57136500 -1.20097500  
N -2.90349600 -0.78132700 -0.26981800  
H -3.59147900 -1.26493200 0.29589300  
N -1.22787500 -0.90846500 -1.86057200  
H -0.68839700 -1.47736900 -2.50925100  
C -2.46466000 0.46038600 0.10614100  
H -3.01170400 0.92980600 0.91619800  
C -0.69008200 0.35184000 -1.56942800  
O 0.27476000 0.77390700 -2.16542100  
C -1.40604700 1.04493500 -0.48782700  
Br -0.77757400 2.71668400 0.03807200  
C 1.63582100 -0.51301100 0.64880000  
C 1.18487000 0.25375600 1.65984500  
N 0.03967700 -0.05947700 2.35287100  
C -0.77113500 -1.13454300 2.04423800  
N -0.25974800 -1.93107400 1.04062200  
C 0.89273000 -1.71911000 0.26406300  
Br 3.17142600 -0.09447600 -0.30394400  
H 1.69468800 1.15837300 1.97003500  
H -0.31710500 0.56545300 3.06472400  
O -1.83843900 -1.33992500 2.59174200  
O 1.17365700 -2.47962400 -0.63437600  
H -0.81289300 -2.75035700 0.79479400  
24

BrU-BrU-ftb-gas-min85: Optimised twist = 73.01 deg.

O	1.83843200	-1.33991300	2.59175900
C	0.77113000	-1.13453000	2.04425300
N	-0.03967800	-0.05945900	2.35287900
H	0.31709900	0.56546800	3.06473600
N	0.25974000	-1.93106500	1.04064200
H	0.81288500	-2.75034900	0.79481600
C	-1.18487000	0.25377500	1.65985000
H	-1.69468400	1.15839600	1.97003300
C	-0.89273400	-1.71910000	0.26407800
O	-1.17366100	-2.47961700	-0.63435900
C	-1.63582100	-0.51299600	0.64880700
Br	-3.17142200	-0.09445800	-0.30394400
C	1.40605100	1.04491900	-0.48783500
C	2.46465800	0.46035700	0.10613100
N	2.90347600	-0.78136400	-0.26982800
C	2.24399400	-1.57139200	-1.20098400
N	1.22785000	-0.90847800	-1.86058000
C	0.69007400	0.35183300	-1.56943300
Br	0.77760500	2.71667800	0.03806300
H	3.01171100	0.92976800	0.91618700
H	3.59145600	-1.26497600	0.29588000
O	2.53776400	-2.73103900	-1.39917100
O	-0.27476500	0.77391300	-2.16542200
H	0.68836200	-1.47737500	-2.50925600

24

BrU-BrU-ftb-water-max0: Optimised twist = 24.58 deg.

O	4.45228200	-0.53786800	-0.90784200
C	3.40645500	0.04201400	-0.67965300
N	2.60106200	0.56853900	-1.66917100
H	2.93366800	0.46624300	-2.62212600
N	2.91031000	0.23600500	0.59482800
H	3.47360800	-0.15311400	1.34715800
C	1.42388300	1.21630700	-1.42022900
H	0.89197000	1.58428200	-2.29010300
C	1.73932000	0.88935300	0.97317900
O	1.44052300	1.00334100	2.14989200
C	0.95785700	1.36999700	-0.16261100
Br	-0.62116100	2.29340400	0.20155600
C	-1.49217800	-1.09247000	-0.23996500
C	-0.65457500	-1.51334000	-1.20885500
N	0.57733200	-2.03579000	-0.91269000
C	1.02824400	-2.23632200	0.37521700
N	0.16621900	-1.75416000	1.33943500
C	-1.09927500	-1.19407800	1.16410900
Br	-3.19275600	-0.43751400	-0.63305900
H	-0.90351200	-1.45960400	-2.26235700
H	1.16401800	-2.40042200	-1.65618400
O	2.09566800	-2.76313300	0.63571700
O	-1.76349100	-0.84436400	2.12364900
H	0.48466700	-1.84826700	2.30091700

24

BrU-BrU-ftb-water-max120: Optimised twist = 87.46 deg.

O	3.71244100	-0.03463600	-1.92735100
C	2.91225000	-0.23814300	-1.03202700
N	2.79408200	0.57155600	0.07726000
H	3.43178200	1.35881900	0.12664000
N	2.03247400	-1.30378200	-1.03186400
H	2.09419100	-1.92706900	-1.83329900

C	1.90714500	0.34419200	1.09349100
H	1.93661300	1.05047600	1.91479900
C	1.06677300	-1.61642200	-0.07745700
O	0.33270400	-2.57911800	-0.23022600
C	1.04101000	-0.68901700	1.04812500
Br	-0.16420500	-1.02540200	2.42834200
C	-0.93733800	1.08082400	-0.75387500
C	-0.44605100	0.58643800	-1.90930300
N	-0.91167300	-0.58757000	-2.43466100
C	-1.90148500	-1.34905000	-1.84532400
N	-2.40907700	-0.79273400	-0.68730100
C	-2.05373600	0.41177600	-0.08639500
Br	-0.31917900	2.67693800	-0.01831400
H	0.33683200	1.08227200	-2.47304600
H	-0.52109600	-0.94814200	-3.29871300
O	-2.30191400	-2.39936000	-2.31225700
O	-2.65114700	0.82465000	0.89174100
H	-3.16860000	-1.30831500	-0.25009000

24

BrU-BrU-ftb-water-max185: Optimised twist = 121.66 deg.

O	-2.45991300	-2.24579800	1.92281600
C	-1.41287200	-2.00979000	1.34742100
N	-1.14343100	-2.43298200	0.06326300
H	-1.88714400	-2.93874600	-0.40584900
N	-0.37793700	-1.29669100	1.92217700
H	-0.53502100	-0.98409100	2.87730900
C	0.00663900	-2.13018600	-0.60862400
H	0.08266200	-2.51517000	-1.61897800
C	0.83055600	-0.92361200	1.33824100
O	1.64135800	-0.25412400	1.95768800
C	0.98205500	-1.39435100	-0.03429800
Br	2.59465400	-1.04514700	-0.90179300
C	-1.13843100	1.25952300	-0.23192100
C	-1.14320200	1.72247600	1.03630400
N	-0.04024500	2.31525300	1.58062200
C	1.14870600	2.48467600	0.90024200
N	1.10561600	2.03388200	-0.40469000
C	0.03996100	1.43823600	-1.07459800
Br	-2.64877500	0.47704100	-0.99993100
H	-2.00733000	1.63766900	1.68567900
H	-0.05456000	2.63029500	2.54445200
O	2.13418100	2.99912200	1.39604300
O	0.13975000	1.11177000	-2.24537400
H	1.96412700	2.14789700	-0.93784600

24

BrU-BrU-ftb-water-max245-minus: Optimised twist = 259.86 deg.

O	1.31367900	-2.46768000	2.69751400
C	0.51340200	-1.99971000	1.90942400
N	-0.55302500	-1.21029800	2.29099200
H	-0.64640600	-1.03356500	3.28537300
N	0.58122000	-2.21114600	0.54489300
H	1.35351200	-2.79248000	0.22883800
C	-1.48375800	-0.71635400	1.41623100
H	-2.28699200	-0.13500100	1.85572500
C	-0.31621900	-1.79137000	-0.43371400
O	-0.17270500	-2.11895400	-1.59825600
C	-1.39137500	-0.94997800	0.09116200
Br	-2.67038800	-0.33509400	-1.11795900

C	1.17676900	1.05312500	-0.48043500
C	0.14525400	1.75003900	-1.00318200
N	-0.73135700	2.42684300	-0.20214900
C	-0.61919200	2.49743300	1.17012000
N	0.47250200	1.81391200	1.66914500
C	1.40256300	1.05410500	0.96255000
Br	2.42350100	0.17572900	-1.55227800
H	-0.05008300	1.79970300	-2.06821700
H	-1.52121000	2.91314800	-0.61326800
O	-1.40603100	3.10337500	1.87545300
O	2.29650300	0.46583100	1.54751700
H	0.59063100	1.84648100	2.67895600

24

BrU-BrU-ftb-water-max245: Optimised twist = 272.82 deg.

O	0.58900000	3.40674300	-1.82890600
C	0.90854300	2.28562400	-1.47744400
N	1.92362400	2.03736300	-0.57476100
H	2.41323400	2.84914600	-0.21354700
N	0.28863300	1.14136300	-1.94094500
H	-0.45000100	1.28877100	-2.62472400
C	2.26702200	0.78350000	-0.14963600
H	3.07267900	0.73220800	0.57420100
C	0.59002700	-0.18469600	-1.63100300
O	0.01317600	-1.10294200	-2.18496400
C	1.62610200	-0.31212800	-0.60838200
Br	2.10372900	-2.03296100	-0.07398300
C	-1.57061500	-0.20837400	0.72405700
C	-0.78097600	-0.92108100	1.55601400
N	0.16747600	-0.31279600	2.33107700
C	0.40356300	1.04476400	2.32261700
N	-0.44671700	1.74840200	1.49120400
C	-1.47051900	1.24827600	0.68738900
Br	-2.89650600	-1.01057500	-0.30942400
H	-0.84787200	-1.99890800	1.64833600
H	0.77206200	-0.87046300	2.92520200
O	1.28286500	1.57742200	2.97690200
O	-2.16637500	1.99976700	0.02722200
H	-0.33221600	2.75946600	1.50003700

24

BrU-BrU-ftb-water-max245-plus: Optimised twist = 299.47 deg.

O	-3.77075400	-1.01383000	-1.63783700
C	-2.89827000	-0.27925000	-1.20996700
N	-2.98638400	0.37007000	0.00438000
H	-3.83176000	0.20847500	0.54194000
N	-1.72585600	-0.02033700	-1.89114000
H	-1.62813400	-0.48205900	-2.79203100
C	-2.00329400	1.17895700	0.50204600
H	-2.20387900	1.63101900	1.46714300
C	-0.66181900	0.78879500	-1.49506400
O	0.30723200	0.94344600	-2.21691900
C	-0.85144200	1.38172100	-0.17291300
Br	0.48052300	2.51463800	0.47323700
C	1.30723400	-1.03737600	0.44572100
C	1.13470600	-0.53257500	1.68590700
N	-0.02893700	-0.72038500	2.37636100
C	-1.09741000	-1.44321300	1.88822500
N	-0.87267300	-1.98407400	0.63668700
C	0.27424600	-1.87375100	-0.15424800

Br 2.88495500 -0.75709000 -0.50247900  
H 1.89113900 0.06148600 2.18483400  
H -0.14510400 -0.31579100 3.29978800  
O -2.14497700 -1.58081100 2.49459800  
O 0.33528200 -2.43070900 -1.23671300  
H -1.61500200 -2.57884800 0.27451400  
24

BrU-BrU-ftb-water-max300: Optimised twist = 272.82 deg.

O 0.58989600 3.40687900 -1.82846400  
C 0.90917600 2.28564400 -1.47713100  
N 1.92420000 2.03704400 -0.57447500  
H 2.41401400 2.84867000 -0.21318400  
N 0.28899300 1.14158200 -1.94075400  
H -0.44961800 1.28924200 -2.62450400  
C 2.26729500 0.78305400 -0.14948600  
H 3.07293800 0.73148900 0.57434800  
C 0.59006100 -0.18458400 -1.63094900  
O 0.01298100 -1.10263100 -2.18500400  
C 1.62610500 -0.31237100 -0.60834100  
Br 2.10331900 -2.03336800 -0.07409800  
C -1.57074800 -0.20817100 0.72399200  
C -0.78127200 -0.92106000 1.55594800  
N 0.16731500 -0.31299400 2.33101800  
C 0.40372300 1.04450900 2.32254800  
N -0.44639800 1.74834400 1.49113800  
C -1.47032300 1.24845600 0.68733100  
Br -2.89680800 -1.01007200 -0.30950700  
H -0.84841400 -1.99887200 1.64826800  
H 0.77177600 -0.87080000 2.92513900  
O 1.28315900 1.57696600 2.97681800  
O -2.16601000 2.00011000 0.02717000  
H -0.33167100 2.75938200 1.49998500  
24

BrU-BrU-ftb-water-max65-minus: Optimised twist = 60.53 deg.

O 2.14498100 -1.58078600 2.49459600  
C 1.09740900 -1.44320100 1.88822900  
N 0.02893800 -0.72037000 2.37636400  
H 0.14511600 -0.31575000 3.29977900  
N 0.87266200 -1.98408200 0.63670300  
H 1.61499600 -2.57884600 0.27452400  
C -1.13470500 -0.53255900 1.68591000  
H -1.89113100 0.06151700 2.18482900  
C -0.27425700 -1.87375600 -0.15423500  
O -0.33529000 -2.43071400 -1.23669900  
C -1.30724200 -1.03737700 0.44573200  
Br -2.88496300 -0.75708800 -0.50246800  
C 0.85145300 1.38172600 -0.17293000  
C 2.00330000 1.17895100 0.50203400  
N 2.98638200 0.37004800 0.00437700  
C 2.89826100 -0.27927700 -1.20996600  
N 1.72585400 -0.02035000 -1.89114600  
C 0.66182000 0.78878600 -1.49507200  
Br -0.48050400 2.51465300 0.47322000  
H 2.20388400 1.63101300 1.46713200  
H 3.83177200 0.20847800 0.54192300  
O 3.77073500 -1.01387300 -1.63783000  
O -0.30723800 0.94343000 -2.21692000  
H 1.62810900 -0.48211600 -2.79201100



24

BrU-BrU-ftb-water-max65: Optimised twist = 87.18 deg.

O	-1.28329800	1.57675000	2.97677000
C	-0.40379400	1.04440300	2.32250200
N	-0.16721900	-0.31307100	2.33096900
H	-0.77162600	-0.87095400	2.92507300
N	0.44624300	1.74834500	1.49109800
H	0.33140100	2.75937000	1.49995900
C	0.78144100	-0.92101800	1.55589500
H	0.84871400	-1.99882200	1.64821300
C	1.47022100	1.24858300	0.68727800
O	2.16580400	2.00032300	0.02710500
C	1.57082800	-0.20803100	0.72394000
Br	2.89698700	-1.00976900	-0.30955900
C	-1.62610800	-0.31253700	-0.60830000
C	-2.26746300	0.78276600	-0.14938300
N	-1.92457000	2.03683000	-0.57431500
C	-0.90959900	2.28563300	-1.47697200
N	-0.28924800	1.14169000	-1.94066600
C	-0.59010100	-0.18453900	-1.63091900
Br	-2.10305200	-2.03363000	-0.07412600
H	-3.07308400	0.73104000	0.57446200
H	-2.41450800	2.84836200	-0.21297800
O	-0.59049300	3.40693500	-1.82825000
O	-0.01288300	-1.10246700	-2.18502600
H	0.44934000	1.28950000	-2.62440800

24

BrU-BrU-ftb-water-max65-plus: Optimised twist = 100.14 deg.

O	1.40607400	3.10330500	1.87551800
C	0.61922300	2.49739100	1.17017300
N	0.73138100	2.42683300	-0.20209800
H	1.52123100	2.91314800	-0.61321100
N	-0.47247900	1.81387400	1.66918700
H	-0.59059900	1.84641600	2.67900000
C	-0.14524200	1.75005800	-1.00314200
H	0.05009100	1.79974100	-2.06817700
C	-1.40255000	1.05409100	0.96257900
O	-2.29649100	0.46580800	1.54753700
C	-1.17676300	1.05314400	-0.48040700
Br	-2.42350700	0.17578500	-1.55226700
C	1.39136800	-0.94998900	0.09113900
C	1.48375200	-0.71639800	1.41621300
N	0.55301400	-1.21035700	2.29096200
C	-0.51342000	-1.99974900	1.90937300
N	-0.58123700	-2.21115400	0.54483700
C	0.31620400	-1.79135800	-0.43375900
Br	2.67038400	-0.33508300	-1.11796800
H	2.28698900	-0.13506200	1.85572200
H	0.64639800	-1.03365100	3.28534700
O	-1.31370400	-2.46773000	2.69745000
O	0.17268700	-2.11891000	-1.59831000
H	-1.35353400	-2.79247300	0.22876700

24

BrU-BrU-ftb-water-min150: Optimised twist = 117.53 deg.

O	-1.92155600	-2.30148300	2.17351000
C	-0.94616300	-1.99428000	1.51181900
N	-0.78853800	-2.34851100	0.18903200
H	-1.54692100	-2.87972300	-0.22556600

N	0.11131900	-1.26133300	2.01646200
H	0.03987700	-1.00010700	2.99703900
C	0.26713100	-1.95184500	-0.58183900
H	0.25419300	-2.28376700	-1.61370500
C	1.22589000	-0.78556800	1.32874700
O	2.06001200	-0.09854400	1.89484900
C	1.25489600	-1.18380300	-0.07515600
Br	2.72584000	-0.67101500	-1.09670400
C	-1.40376100	0.98318800	-0.19868300
C	-1.44593800	1.36329200	1.09596200
N	-0.41804200	2.06145000	1.66581200
C	0.69933700	2.48212300	0.97097100
N	0.70903800	2.07712800	-0.35026200
C	-0.27227000	1.36795300	-1.03979600
Br	-2.83220900	0.10040100	-1.01438700
H	-2.28216000	1.13183300	1.74650900
H	-0.47064400	2.33909400	2.63994600
O	1.58555000	3.14811700	1.47176400
O	-0.14463700	1.11646300	-2.22563300
H	1.52245800	2.36025300	-0.89143700

24

BrU-BrU-ftb-water-min220: Optimised twist = 242.47 deg.

O	-1.58553600	3.14815600	1.47164000
C	-0.69931900	2.48214500	0.97087800
N	0.41805500	2.06149800	1.66574400
H	0.47066100	2.33920300	2.63986100
N	-0.70900900	2.07709900	-0.35033900
H	-1.52243400	2.36018400	-0.89152800
C	1.44596000	1.36332800	1.09592600
H	2.28218000	1.13190100	1.74648700
C	0.27230000	1.36788800	-1.03983600
O	0.14466600	1.11633600	-2.22565900
C	1.40379100	0.98316900	-0.19870200
Br	2.83224600	0.10035500	-1.01436500
C	-1.25493000	-1.18378800	-0.07512400
C	-0.26718400	-1.95185600	-0.58180300
N	0.78850000	-2.34850100	0.18905900
C	0.94615100	-1.99423800	1.51183400
N	-0.11131000	-1.26125800	2.01647400
C	-1.22589100	-0.78550600	1.32876500
Br	-2.72589100	-0.67101800	-1.09665600
H	-0.25427100	-2.28381800	-1.61365700
H	1.54686300	-2.87974600	-0.22553300
O	1.92155000	-2.30144000	2.17351700
O	-2.05999400	-0.09845400	1.89486100
H	-0.03984700	-1.00000100	2.99704100

24

BrU-BrU-ftb-water-min270: Optimised twist = 259.86 deg.

O	1.31361600	-2.46759900	2.69761200
C	0.51335300	-1.99964200	1.90950000
N	-0.55306100	-1.21019500	2.29103100
H	-0.64644600	-1.03342100	3.28540300
N	0.58117300	-2.21113400	0.54497800
H	1.35345500	-2.79249600	0.22895000
C	-1.48378100	-0.71627000	1.41624500
H	-2.28700800	-0.13488700	1.85571300
C	-0.31625200	-1.79138100	-0.43365100
O	-0.17273700	-2.11901500	-1.59817900

C	-1.39139700	-0.94995000	0.09118600
Br	-2.67039200	-0.33508900	-1.11796500
C	1.17679400	1.05309300	-0.48046700
C	0.14528800	1.75001000	-1.00322800
N	-0.73131300	2.42684200	-0.20220900
C	-0.61914300	2.49746300	1.17005800
N	0.47254500	1.81394300	1.66909600
C	1.40259400	1.05410700	0.96251600
Br	2.42350400	0.17564500	-1.55229300
H	-0.05004800	1.79965600	-2.06826400
H	-1.52115700	2.91315300	-0.61333700
O	-1.40597400	3.10343000	1.87537900
O	2.29653000	0.46583900	1.54749500
H	0.59067900	1.84653600	2.67890600

24

BrU-BrU-ftb-water-min315: Optimised twist = 299.48 deg.

O	-3.77087800	-1.01376300	-1.63773500
C	-2.89837200	-0.27920000	-1.20987900
N	-2.98642900	0.37007900	0.00449300
H	-3.83178400	0.20847700	0.54208300
N	-1.72598600	-0.02027200	-1.89109700
H	-1.62829900	-0.48198600	-2.79199600
C	-2.00331200	1.17894300	0.50214200
H	-2.20385700	1.63098600	1.46725600
C	-0.66191400	0.78881600	-1.49502900
O	0.30712200	0.94346200	-2.21690600
C	-0.85148000	1.38170700	-0.17285300
Br	0.48052200	2.51459200	0.47328300
C	1.30729700	-1.03739100	0.44568500
C	1.13475100	-0.53267000	1.68590100
N	-0.02889300	-0.72054000	2.37633500
C	-1.09736800	-1.44331900	1.88812900
N	-0.87260200	-1.98412300	0.63657500
C	0.27431900	-1.87372800	-0.15434900
Br	2.88500500	-0.75700200	-0.50250300
H	1.89116900	0.06137900	2.18486600
H	-0.14507400	-0.31600000	3.29978400
O	-2.14495400	-1.58092700	2.49446600
O	0.33535900	-2.43060400	-1.23685700
H	-1.61494200	-2.57883900	0.27433000

24

BrU-BrU-ftb-water-min50: Optimised twist = 60.53 deg.

O	2.14493400	-1.58065300	2.49472100
C	1.09737200	-1.44310400	1.88833100
N	0.02890000	-0.72023100	2.37640100
H	0.14507100	-0.31554400	3.29978600
N	0.87263500	-1.98407800	0.63684400
H	1.61497100	-2.57887000	0.27471600
C	-1.13472500	-0.53244900	1.68591100
H	-1.89115600	0.06166400	2.18477800
C	-0.27425800	-1.87377100	-0.15413300
O	-0.33527400	-2.43079000	-1.23656900
C	-1.30724300	-1.03734200	0.44576000
Br	-2.88495100	-0.75709700	-0.50247600
C	0.85147100	1.38170100	-0.17297400
C	2.00333000	1.17891400	0.50196600
N	2.98638200	0.36998100	0.00430100
C	2.89821400	-0.27937600	-1.21002100

N	1.72579500	-0.02043900	-1.89117800
C	0.66179800	0.78874400	-1.49510500
Br	-0.48044400	2.51467800	0.47317100
H	2.20394800	1.63099400	1.46704800
H	3.83178100	0.20840000	0.54183200
O	3.77065600	-1.01400800	-1.63788600
O	-0.30726100	0.94341300	-2.21694500
H	1.62802300	-0.48221400	-2.79203500

24

BrU-BrU-ftb-water-min90: Optimised twist = 100.14 deg.

O	1.40583100	3.10362300	1.87519500
C	0.61904000	2.49757000	1.16990300
N	0.73124700	2.42683900	-0.20235500
H	1.52109000	2.91313200	-0.61350300
N	-0.47263600	1.81404900	1.66897000
H	-0.59079000	1.84671500	2.67877600
C	-0.14531900	1.74992000	-1.00334200
H	0.05004300	1.79948300	-2.06837700
C	-1.40264500	1.05412700	0.96243000
O	-2.29656800	0.46586600	1.54743700
C	-1.17682000	1.05301700	-0.48055000
Br	-2.42349300	0.17546800	-1.55233600
C	1.39143100	-0.94990500	0.09125400
C	1.48382700	-0.71610900	1.41629200
N	0.55313300	-1.20998800	2.29113200
C	-0.51326800	-1.99949300	1.90968200
N	-0.58109600	-2.21111200	0.54517900
C	0.31630500	-1.79141400	-0.43349800
Br	2.67038900	-0.33510800	-1.11796800
H	2.28704200	-0.13466500	1.85570000
H	0.64652100	-1.03312100	3.28548800
O	-1.31351600	-2.46739100	2.69784400
O	0.17278600	-2.11914900	-1.59799700
H	-1.35336900	-2.79252000	0.22921200

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C-BrU-ftb-gas-max0: Optimised twist = 0.93 deg.

O	-1.62845800	3.10613800	-0.74463900
C	-0.69936500	2.35957400	-0.55062100
N	0.31197700	2.64170500	0.36272400
H	0.22206400	3.52969200	0.83971000
N	-0.51656600	1.15071200	-1.20171500
H	-1.26467700	0.87820700	-1.83711700
C	1.38681600	1.82221400	0.58908300
H	2.09936300	2.16184100	1.33257800
C	0.55277600	0.26136600	-1.08853300
O	0.61327600	-0.73916100	-1.77270700
C	1.54139700	0.66368400	-0.07827900
Br	2.98038000	-0.47458300	0.23097200
C	-0.64273300	-1.85196100	0.97719100
C	-0.97757800	-0.84405200	1.81665200
N	-2.06725400	-0.07775900	1.55683900
C	-2.91431200	-0.28569900	0.43737300
N	-2.54522600	-1.28194400	-0.43105200
C	-1.49269400	-2.02739100	-0.17600400
H	0.22321600	-2.47767800	1.15061300
H	-0.40991300	-0.60118500	2.70947500
H	-2.36106900	0.66194700	2.18266500
O	-3.88359800	0.43553600	0.30429300

N -1.21207600 -3.03951900 -1.04034400  
H -0.24257000 -3.31625800 -1.12359700  
H -1.71129100 -2.98505200 -1.92028200

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C-BrU-ftb-gas-max120: Optimised twist = 76.93 deg.

O -1.76092600 -2.55480700 -1.06562900  
C -0.74715300 -1.90498700 -0.88814600  
N -0.51847000 -0.69837600 -1.52881800  
H -1.26086400 -0.38181600 -2.13906400  
N 0.27929400 -2.27957200 -0.05398500  
H 0.10315700 -3.11005500 0.50411600  
C 0.56837700 0.10520500 -1.27665100  
H 0.59118800 1.05349000 -1.80212000  
C 1.42099900 -1.54646200 0.30056800  
O 2.21486800 -1.98176100 1.10164300  
C 1.52537300 -0.26182600 -0.40845400  
Br 2.98356600 0.82795800 -0.03054200  
C -2.81192500 1.79409900 -0.60348000  
C -3.50843000 0.63469900 -0.47016500  
N -3.12070300 -0.28796600 0.43539500  
C -1.97675800 -0.13659700 1.25710900  
N -1.29054000 1.04533200 1.14170300  
C -1.66534900 1.93975000 0.25755000  
H -3.10243200 2.55621700 -1.31522200  
H -4.38244900 0.39357000 -1.06653800  
H -3.54404200 -1.20949500 0.46217800  
O -1.66121100 -1.05679600 1.98749100  
N -0.86712400 3.03434800 0.11153000  
H -1.22795800 3.86718300 -0.33019000  
H -0.15126700 3.15965500 0.81700100

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C-BrU-ftb-gas-min260: Optimised twist = 261.13 deg.

O 2.58012700 -2.36398600 0.41772200  
C 1.43046500 -1.98498900 0.30811100  
N 0.58447600 -1.78175900 1.38261500  
H 1.03995200 -1.79028200 2.28837400  
N 0.83184900 -1.73906400 -0.91299000  
H 1.41965200 -1.89978000 -1.72463100  
C -0.63962500 -1.18101600 1.26145400  
H -1.15369500 -0.96652300 2.19035500  
C -0.38962600 -1.10161900 -1.16239800  
O -0.72123800 -0.82138700 -2.29575700  
C -1.15018500 -0.84111400 0.05966700  
Br -2.79917800 0.01133800 -0.10319100  
C 1.50735800 1.94586000 -1.32829900  
C 0.39629300 2.53170600 -0.81854100  
N 0.04190900 2.31304600 0.47084900  
C 0.75061100 1.44535700 1.32535600  
N 1.86594400 0.84950400 0.81332800  
C 2.22571500 1.07359300 -0.43773400  
H 1.80440400 2.09236500 -2.35834400  
H -0.25297700 3.17845500 -1.39832200  
H -0.81724800 2.69123300 0.85170300  
O 0.31203000 1.24196000 2.45022400  
N 3.31714400 0.41383500 -0.88371100  
H 3.59050000 0.45141600 -1.85344800  
H 3.69801200 -0.32200600 -0.29782600

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C-BrU-ftb-gas-min40: Optimised twist = 53.60 deg.

O	-2.09045200	2.58593600	-0.22423600
C	-1.00761400	2.03892500	-0.22732100
N	-0.02979800	2.32983400	0.71654000
H	-0.27727200	3.04949400	1.38316800
N	-0.61782500	1.08185500	-1.14047200
H	-1.32082800	0.81262100	-1.83014100
C	1.16486300	1.66492900	0.80543000
H	1.81940200	1.96243100	1.61704100
C	0.57926700	0.35091300	-1.16827700
O	0.79391100	-0.47436000	-2.02484100
C	1.49298500	0.69490900	-0.06724700
Br	3.09613600	-0.24471800	0.05638600
C	-1.07276300	-1.03338800	1.74964200
C	-2.16962000	-0.23606400	1.79878500
N	-3.02486100	-0.19248700	0.75124100
C	-2.80065000	-0.89928900	-0.45447100
N	-1.73176800	-1.75277900	-0.47896700
C	-0.89583900	-1.79100700	0.53402700
H	-0.37501400	-1.09927300	2.57497800
H	-2.41365700	0.39026600	2.65094700
H	-3.77069800	0.49286800	0.71037600
O	-3.53798200	-0.67895300	-1.39964500
N	0.19245400	-2.59407800	0.40927800
H	0.98593600	-2.45243500	1.01809200
H	0.40236700	-2.89781600	-0.53495600

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C-BrU-ftb-water-max0-minus: Optimised twist = 66.56 deg.

O	3.03325000	-2.11983400	-0.49150000
C	1.86007200	-1.79357500	-0.43311500
N	1.13015900	-1.39535600	-1.53178400
H	1.64192600	-1.30360300	-2.40274100
N	1.12774800	-1.82068000	0.73697800
H	1.63478000	-2.11680800	1.56679800
C	-0.16242900	-0.96423100	-1.45993300
H	-0.60760800	-0.64223500	-2.39452500
C	-0.18048000	-1.39121200	0.93836700
O	-0.68350000	-1.42493700	2.05012600
C	-0.82780900	-0.92893600	-0.28547300
Br	-2.60467900	-0.37211700	-0.18252200
C	-0.01034000	1.97369200	1.46562000
C	-0.67405500	2.44669000	0.38261300
N	-0.12596500	2.32905900	-0.85249100
C	1.11199500	1.71978300	-1.08178800
N	1.79537300	1.25267100	-0.00227700
C	1.27214500	1.37720600	1.21541900
H	-0.42532400	2.04147700	2.46259300
H	-1.64756200	2.91993300	0.43604800
H	-0.61776900	2.67213200	-1.67011000
O	1.51348100	1.61544300	-2.24515900
N	1.98177700	0.88394300	2.24355800
H	1.67198400	0.98703800	3.19931100
H	2.90926900	0.51681200	2.07500600

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C-BrU-ftb-water-max0: Optimised twist = 328.53 deg.

O	2.31113600	2.85571700	-0.28691300
C	1.28672900	2.20066900	-0.36479900
N	1.02000600	1.33494000	-1.40389900

H	1.77178100	1.19970700	-2.07195000
N	0.26678800	2.28372900	0.56300500
H	0.41565600	2.94409000	1.32151600
C	-0.09797100	0.55195600	-1.46319400
H	-0.16459900	-0.11718400	-2.31385100
C	-0.92170900	1.56148000	0.59578900
O	-1.73906700	1.74318800	1.48322300
C	-1.05072700	0.61473800	-0.50864200
Br	-2.59500100	-0.42855200	-0.58111600
C	0.13789100	-2.25897000	0.97782500
C	0.63640300	-2.78048900	-0.16800400
N	1.71482200	-2.20651900	-0.76218300
C	2.37034800	-1.08977800	-0.23485200
N	1.87613500	-0.55275000	0.91296400
C	0.81002000	-1.09773700	1.49281500
H	-0.73001600	-2.68237800	1.46578900
H	0.21655800	-3.64799200	-0.66365000
H	2.09788700	-2.59352800	-1.61761500
O	3.34076600	-0.63093100	-0.84576400
N	0.35218200	-0.51422300	2.61276300
H	-0.50548900	-0.81419600	3.05397800
H	0.78513000	0.33957800	2.94030500

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C-BrU-ftb-water-max0-plus: Optimised twist = 6.50 deg.

O	-2.33010300	2.93550500	-0.26380500
C	-1.32322100	2.25236100	-0.32127200
N	-1.08789600	1.33312100	-1.32263600
H	-1.81991800	1.23167300	-2.01747400
N	-0.29738300	2.34202600	0.59797800
H	-0.43509900	3.01656100	1.34595000
C	0.04726000	0.57568400	-1.40215300
H	0.10804100	-0.09987700	-2.24834000
C	0.88525900	1.61129600	0.63609500
O	1.69829200	1.78616900	1.52941400
C	1.01890200	0.66921200	-0.47071500
Br	2.58171400	-0.34123600	-0.57189500
C	-0.14644000	-2.52148800	0.30498800
C	-1.03361000	-2.71073900	-0.70072400
N	-2.14972200	-1.93982600	-0.77472200
C	-2.46370900	-0.95990400	0.17378100
N	-1.56078900	-0.73386600	1.16684000
C	-0.45385900	-1.46740900	1.23362000
H	0.75472500	-3.11414200	0.39050700
H	-0.90914700	-3.45630800	-1.47741100
H	-2.82805500	-2.08448900	-1.51402800
O	-3.52267700	-0.33877200	0.05247200
N	0.41610400	-1.18796000	2.21949700
H	1.33155800	-1.61465600	2.24682200
H	0.24811600	-0.38727500	2.81523200

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C-BrU-ftb-water-max120-minus: Optimised twist = 64.82 deg.

O	-3.96956600	-0.13089200	-0.48339500
C	-2.80602300	-0.48733800	-0.40477200
N	-1.99124800	-0.64694000	-1.50659400
H	-2.41919900	-0.47700800	-2.41045400
N	-2.18012100	-0.76657800	0.79126200
H	-2.74906400	-0.64694700	1.62530300
C	-0.67484900	-1.00790200	-1.42518400

H	-0.14649400	-1.09172000	-2.36790600
C	-0.85831100	-1.15797500	0.99981100
O	-0.45039100	-1.40444900	2.12142400
C	-0.08202500	-1.23150800	-0.23426200
Br	1.70423600	-1.75292500	-0.11782900
C	1.19481100	1.91939400	-1.38016000
C	-0.14163500	2.13797100	-1.41622700
N	-0.86184500	2.12890600	-0.26428700
C	-0.28161100	1.92723700	0.99539200
N	1.06112900	1.70955100	1.04194100
C	1.77467400	1.72189300	-0.07852400
H	1.79538900	1.91647600	-2.28036200
H	-0.69541300	2.31781500	-2.33096000
H	-1.85318500	2.34420700	-0.27523400
O	-1.01120700	1.95039000	1.98929400
N	3.10662100	1.57342400	0.03207300
H	3.68351900	1.42847100	-0.78436500
H	3.49356900	1.32150800	0.93219500

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C-BrU-ftb-water-max120: Optimised twist = 79.33 deg.

O	-2.35005800	-2.37613900	-1.04022100
C	-1.25727500	-1.87236900	-0.83997400
N	-0.56420700	-1.16655200	-1.79831500
H	-1.00774900	-1.08751800	-2.70679600
N	-0.59938800	-1.95143400	0.37019900
H	-1.10095200	-2.42844700	1.11536600
C	0.64631600	-0.56590400	-1.57271900
H	1.07019200	-0.02466000	-2.41061400
C	0.62747700	-1.39074100	0.71936700
O	1.08995600	-1.55017600	1.83535700
C	1.24706400	-0.63782200	-0.36887600
Br	2.88065200	0.18959000	-0.02768100
C	-1.70533000	2.01873800	-1.04977000
C	-2.78891100	1.24069200	-0.81156300
N	-2.87897800	0.53884600	0.34694900
C	-1.89990300	0.58717800	1.34644300
N	-0.79927900	1.35127200	1.11199400
C	-0.69767000	2.03627900	-0.02425300
H	-1.60087500	2.58653900	-1.96489600
H	-3.61182400	1.13012100	-1.50830200
H	-3.67995800	-0.05627900	0.52737500
O	-2.07076200	-0.07797300	2.37177000
N	0.41540700	2.76158700	-0.20985500
H	0.57164800	3.29168400	-1.05518500
H	1.13810000	2.75488500	0.49792400

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C-BrU-ftb-water-max120-plus: Optimised twist = 88.59 deg.

O	-2.18675700	-2.22716900	-1.36187400
C	-1.10853300	-1.72977100	-1.08189900
N	-0.43538800	-0.87024700	-1.92295800
H	-0.88201000	-0.67369000	-2.81170700
N	-0.44487400	-1.97683900	0.10193300
H	-0.92608800	-2.58338500	0.76118000
C	0.75674900	-0.27564700	-1.60662400
H	1.16367000	0.39927200	-2.35032400
C	0.76194800	-1.43189600	0.53784900
O	1.23310400	-1.74524300	1.61733000
C	1.35434400	-0.50488800	-0.42160400



Br	2.93061700	0.36034800	0.06449800
C	-2.13988700	1.91100000	-0.81646400
C	-3.14618500	1.08412200	-0.44224000
N	-3.01029700	0.30711700	0.66244100
C	-1.86658500	0.31738000	1.46725700
N	-0.84026500	1.12890500	1.09068500
C	-0.96128300	1.89004800	0.00670300
H	-2.21348000	2.54064900	-1.69328600
H	-4.08137600	0.99473100	-0.98278900
H	-3.75530500	-0.31965100	0.94520300
O	-1.83331600	-0.41741100	2.45774200
N	0.09207100	2.65008300	-0.33315300
H	0.06650600	3.26918300	-1.13068400
H	0.92012200	2.64408200	0.24889100

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C-BrU-ftb-water-max175: Optimised twist = 152.91 deg.

O	3.84498700	-0.90215000	-0.25099700
C	2.64013700	-1.02278800	-0.11210900
N	2.02185200	-1.06126300	1.11919900
H	2.62804600	-0.98694600	1.92884200
N	1.76540500	-1.13683000	-1.17391900
H	2.18977400	-1.11515600	-2.09778000
C	0.66880900	-1.17257800	1.28275900
H	0.31581800	-1.20190600	2.30687500
C	0.37438800	-1.21813500	-1.13374200
O	-0.27605600	-1.26995800	-2.16408500
C	-0.16423700	-1.23177400	0.22271400
Br	-2.00267800	-1.45969100	0.42990500
C	1.37397500	2.04144500	0.20125500
C	1.08962900	2.02969900	-1.12446500
N	-0.19972300	1.97681400	-1.53953000
C	-1.28701100	1.96700600	-0.65624300
N	-1.01338500	1.97998200	0.67768900
C	0.24748300	1.99096000	1.09268100
H	2.39276600	2.07978800	0.56557700
H	1.84740800	2.05244900	-1.89984500
H	-0.42232200	1.94604200	-2.52812400
O	-2.42666600	1.95326500	-1.12693900
N	0.46565000	1.92004900	2.41945600
H	1.39072800	2.04211300	2.80693100
H	-0.32424000	1.96928400	3.04965300

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C-BrU-ftb-water-max240: Optimised twist = 241.90 deg.

O	-3.07544100	-2.16153100	-0.51815100
C	-1.91325900	-1.80891000	-0.41821200
N	-1.12827300	-1.47554400	-1.50151100
H	-1.57744200	-1.51159100	-2.41007900
N	-1.25451100	-1.70836900	0.79135400
H	-1.80117800	-1.95809800	1.61161700
C	0.17442700	-1.07991000	-1.39823600
H	0.67570700	-0.84187900	-2.32929700
C	0.07185700	-1.34356500	1.02072000
O	0.53194900	-1.34340300	2.15025800
C	0.78688600	-0.98366400	-0.19900200
Br	2.58978100	-0.52473300	-0.05498800
C	-1.26872000	1.63204800	1.54643900
C	0.02655100	2.03167800	1.54541800
N	0.66303900	2.26700600	0.37089100

C	0.05860300	2.07238900	-0.87441300
N	-1.24861300	1.69431700	-0.88784300
C	-1.88495200	1.47362300	0.25765800
H	-1.80234000	1.43005800	2.46596500
H	0.60855900	2.17925500	2.44781800
H	1.64160500	2.53185000	0.35992400
O	0.73360800	2.24213400	-1.89423100
N	-3.16543300	1.07111600	0.18479600
H	-3.69287900	0.82531100	1.01014500
H	-3.58711200	0.91134400	-0.72054800

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C-BrU-ftb-water-min155: Optimised twist = 119.27 deg.

O	2.94619500	-2.57125600	-0.17932800
C	1.80795300	-2.13481200	-0.18646400
N	0.89387800	-2.39166100	0.81263600
H	1.21336800	-2.98157500	1.57307400
N	1.30951100	-1.34171800	-1.19981300
H	1.95471100	-1.14014900	-1.95963700
C	-0.37366300	-1.87907100	0.82793700
H	-0.99021700	-2.16163400	1.67349100
C	0.05178900	-0.74512800	-1.28357800
O	-0.23841100	-0.04359800	-2.23783400
C	-0.81402800	-1.06401600	-0.15263000
Br	-2.55583100	-0.40434500	-0.16471700
C	1.60359900	0.83713500	1.53140200
C	2.39377300	1.13880200	0.47222500
N	1.91775600	1.92018800	-0.52981300
C	0.63914100	2.49232100	-0.50818300
N	-0.17377500	2.17266200	0.53587500
C	0.27239600	1.38316100	1.50665600
H	1.95411400	0.21374000	2.34404200
H	3.41079700	0.77838500	0.36269400
H	2.50546100	2.15792200	-1.32096500
O	0.31518600	3.25160200	-1.42393800
N	-0.57976600	1.08221700	2.50037400
H	-0.31208500	0.48798000	3.27177000
H	-1.52480100	1.44126100	2.47041900

25

C-BrU-ftb-water-min210: Optimised twist = 241.20 deg.

O	-3.41293800	-1.71338600	-0.60989100
C	-2.21653100	-1.50753700	-0.50872700
N	-1.43891400	-1.03794000	-1.54591500
H	-1.92086000	-0.84241500	-2.41637000
N	-1.50751200	-1.72357900	0.65652800
H	-2.04904700	-2.07820400	1.44064700
C	-0.09277700	-0.82745000	-1.44711000
H	0.39885000	-0.46586700	-2.34323300
C	-0.13915400	-1.56492800	0.87311600
O	0.35635800	-1.84106100	1.95267300
C	0.57197700	-1.05350700	-0.29414900
Br	2.42613900	-0.86657700	-0.17982700
C	-0.95225000	1.50488900	1.66388000
C	0.37939300	1.74945900	1.73550300
N	1.05581600	2.14567900	0.62928000
C	0.45308500	2.27998800	-0.62508700
N	-0.88900900	2.06836200	-0.70504300
C	-1.56131500	1.68207300	0.37419200
H	-1.52006800	1.18105800	2.52660800

H	0.95926900	1.64498000	2.64544300
H	2.05846000	2.29177600	0.66456300
O	1.15976100	2.57837200	-1.59250200
N	-2.87158400	1.42058800	0.22451800
H	-3.45427100	1.15367600	1.00505900
H	-3.30878200	1.56410600	-0.67630000

25

C-BrU-ftb-water-min285: Optimised twist = 293.44 deg.

O	-3.03330000	-2.11979500	-0.49149200
C	-1.86011900	-1.79354500	-0.43310800
N	-1.13020800	-1.39532500	-1.53177800
H	-1.64197500	-1.30356600	-2.40273400
N	-1.12779200	-1.82066000	0.73698200
H	-1.63482200	-2.11679000	1.56680300
C	0.16238900	-0.96422500	-1.45993100
H	0.60756900	-0.64223600	-2.39452500
C	0.18044500	-1.39121700	0.93836600
O	0.68346900	-1.42495700	2.05012300
C	0.82777700	-0.92894900	-0.28547500
Br	2.60466000	-0.37217100	-0.18253200
C	0.01041300	1.97369900	1.46561100
C	0.67412400	2.44668400	0.38259600
N	0.12601500	2.32906300	-0.85250100
C	-1.11195700	1.71980400	-1.08178100
N	-1.79533100	1.25270900	-0.00226100
C	-1.27208700	1.37723900	1.21542800
H	0.42541000	2.04147800	2.46257900
H	1.64763900	2.91991100	0.43601800
H	0.61782200	2.67211100	-1.67012800
O	-1.51345600	1.61546700	-2.24514900
N	-1.98171500	0.88399500	2.24357800
H	-1.67190700	0.98708600	3.19932600
H	-2.90921700	0.51687900	2.07504200

25

C-BrU-ftb-water-min310: Optimised twist = 293.44 deg.

O	-3.03329300	-2.11982900	-0.49151300
C	-1.86012000	-1.79355200	-0.43312500
N	-1.13022200	-1.39528900	-1.53178800
H	-1.64198900	-1.30354200	-2.40274500
N	-1.12779100	-1.82066900	0.73696300
H	-1.63480600	-2.11685300	1.56677500
C	0.16237600	-0.96419300	-1.45994200
H	0.60755200	-0.64218400	-2.39453200
C	0.18044800	-1.39123100	0.93834800
O	0.68347900	-1.42499000	2.05010100
C	0.82777200	-0.92894100	-0.28548900
Br	2.60465800	-0.37217200	-0.18255100
C	0.01044400	1.97366000	1.46563000
C	0.67413700	2.44666800	0.38261500
N	0.12600300	2.32908500	-0.85247600
C	-1.11197600	1.71983700	-1.08175000
N	-1.79533200	1.25271400	-0.00222900
C	-1.27207000	1.37722100	1.21545600
H	0.42546400	2.04139700	2.46259000
H	1.64766100	2.91987800	0.43602900
H	0.61778700	2.67217600	-1.67009900
O	-1.51349800	1.61553200	-2.24511200
N	-1.98169500	0.88398500	2.24361000

H -1.67184900 0.98701000 3.19935300  
H -2.90917900 0.51682500 2.07507600  
25

C-BrU-ftb-water-min40: Optimised twist = 54.89 deg.

O -2.32031400 -2.44193900 -0.77487300  
C -1.23383300 -1.90597200 -0.63843900  
N -0.59478500 -1.23076500 -1.65675500  
H -1.07147500 -1.21173300 -2.55190300  
N -0.52947900 -1.91291200 0.54758100  
H -1.01173100 -2.33383200 1.33789700  
C 0.62384900 -0.62361800 -1.51596000  
H 1.02019800 -0.14456700 -2.40372100  
C 0.68845000 -1.29665200 0.82465100  
O 1.17820300 -1.35427100 1.93954300  
C 1.27189800 -0.62343800 -0.33381400  
Br 2.95182500 0.16185500 -0.13322100  
C -1.28033300 2.21486500 -0.97993100  
C -2.44901600 1.56154600 -1.19322400  
N -2.94974100 0.73518400 -0.24025500  
C -2.31674400 0.52054300 0.98969400  
N -1.13549800 1.15848800 1.20812200  
C -0.63533800 1.96892500 0.28066500  
H -0.85678900 2.87980700 -1.72102900  
H -3.02768000 1.65267300 -2.10515500  
H -3.81317600 0.22731900 -0.39802300  
O -2.84117800 -0.24754000 1.80051700  
N 0.52788700 2.58198100 0.56105800  
H 1.03729200 3.08657400 -0.15082700  
H 1.03351500 2.30781700 1.39386700  
25

C-BrU-ftb-water-min85: Optimised twist = 54.89 deg.

O -2.32031900 -2.44192300 -0.77489200  
C -1.23383400 -1.90596400 -0.63845400  
N -0.59477100 -1.23076800 -1.65676900  
H -1.07146000 -1.21172100 -2.55191600  
N -0.52948600 -1.91290900 0.54757000  
H -1.01174200 -2.33383600 1.33788100  
C 0.62386600 -0.62362700 -1.51596500  
H 1.02022800 -0.14458700 -2.40372600  
C 0.68844000 -1.29664800 0.82465100  
O 1.17818100 -1.35426200 1.93954900  
C 1.27190100 -0.62343900 -0.33381100  
Br 2.95182600 0.16185200 -0.13320500  
C -1.28036600 2.21483000 -0.97996500  
C -2.44904900 1.56149700 -1.19321600  
N -2.94975000 0.73516000 -0.24021100  
C -2.31671800 0.52055000 0.98972800  
N -1.13547700 1.15851500 1.20811600  
C -0.63534400 1.96893600 0.28062700  
H -0.85684400 2.87975600 -1.72109100  
H -3.02773200 1.65259400 -2.10513700  
H -3.81317100 0.22726400 -0.39795800  
O -2.84112600 -0.24752400 1.80057700  
N 0.52787700 2.58201400 0.56098200  
H 1.03725500 3.08660600 -0.15092400  
H 1.03352800 2.30787800 1.39378700  
26

C-C-ftb-gas-min180: Optimised twist = 139.98 deg.

O	-3.00838800	-1.66218900	-1.00693900
C	-2.40510000	-0.91868100	-0.25127900
N	-1.75090000	-1.48498900	0.86747900
H	-1.85100800	-2.48787700	0.95938700
N	-2.28575200	0.43660800	-0.41036100
C	-1.53253300	1.13396800	0.41782300
C	-0.78925900	0.55810300	1.50986700
C	-0.93552200	-0.77619000	1.68786100
H	-0.42808600	-1.32992900	2.47103800
H	-0.14241500	1.15681200	2.13834200
N	-1.45074800	2.47378900	0.22095100
H	-0.60660200	2.95510600	0.51518800
H	-1.91795500	2.83086900	-0.60269300
C	2.30615900	-0.91845000	0.02572000
C	1.40080500	-1.41822000	-0.97428300
C	0.68339100	-0.48384300	-1.64625900
N	2.41784400	0.35089000	0.35192700
C	1.62978500	1.27904700	-0.26732300
N	0.85067100	0.82817600	-1.35281300
N	3.06719300	-1.80518000	0.72426200
H	1.28723300	-2.47543700	-1.17650700
H	-0.04194300	-0.72309100	-2.41735100
H	0.25544400	1.52702100	-1.78199200
O	1.55110300	2.45697800	0.05815400
H	3.22496900	-2.73105400	0.35522600
H	3.79411700	-1.41020100	1.30675800

26

C-C-ftb-water-max0: Optimised twist = 333.65 deg.

O	2.33965200	1.29563500	-1.66856400
C	2.00101400	0.39938500	-0.89191000
N	2.52229500	0.40089400	0.40691500
H	3.14887900	1.16292600	0.63974400
N	1.14485400	-0.60674200	-1.22225400
C	0.88241100	-1.56874400	-0.34681200
C	1.45795000	-1.61589200	0.96973500
C	2.27592400	-0.58813900	1.30313600
H	2.75862000	-0.49600200	2.26920500
H	1.23640500	-2.41723900	1.66250800
N	0.05321700	-2.55567000	-0.74120400
H	-0.31637300	-3.21355800	-0.06917100
H	-0.46355100	-2.43247100	-1.60288700
C	-2.27760400	-0.09750500	-0.29923500
C	-2.05168800	-0.68014800	0.99535000
C	-1.21704000	-0.00260000	1.81928100
N	-1.76824500	1.06962500	-0.67457800
C	-0.93981600	1.74661700	0.16619600
N	-0.65960400	1.16470500	1.40768400
N	-3.03013900	-0.76262700	-1.19562900
H	-2.50113900	-1.62063900	1.28630200
H	-0.94901800	-0.34176400	2.81336400
H	-0.04099100	1.68485800	2.01937500
O	-0.42824100	2.83738000	-0.10160300
H	-3.53212700	-1.60169800	-0.94266300
H	-3.25554500	-0.31767100	-2.07542100

26

C-C-ftb-water-max120: Optimised twist = 126.17 deg.

O	-2.25431900	-0.64026000	-2.07820300
C	-1.92797300	-0.04700600	-1.04603200

N	-2.45043600	-0.48509200	0.17471600
H	-3.07462900	-1.28281200	0.13755500
N	-1.07487300	1.01365000	-1.02025700
C	-0.78261500	1.59824000	0.13458700
C	-1.34964200	1.19479200	1.39114200
C	-2.18072000	0.12593900	1.35702500
H	-2.65462600	-0.29452500	2.23648900
H	-1.10199000	1.69698200	2.31709100
N	0.07121900	2.64515800	0.10188400
H	0.52447200	2.93423200	0.95855600
H	0.61475300	2.77062100	-0.74361200
C	0.90643200	-1.31647800	0.90555200
C	0.61390800	-1.93715100	-0.35608100
C	1.17346400	-1.36474200	-1.44977400
N	1.68333700	-0.24416800	1.02928300
C	2.24507900	0.31550700	-0.07615100
N	1.96930300	-0.27604400	-1.31228900
N	0.38759100	-1.83740200	2.03183100
H	-0.03088700	-2.80297900	-0.43362800
H	1.01995400	-1.72748100	-2.45950500
H	2.38504200	0.16390300	-2.12536500
O	2.97782100	1.30994700	-0.04634400
H	-0.27955800	-2.59511800	2.00419900
H	0.51885900	-1.34765200	2.90681100

26

C-C-ftb-water-max180-minus: Optimised twist = 223.11 deg.

O	1.74487600	2.38539600	-0.31977900
C	1.81220900	1.22465000	0.11149600
N	1.11782200	0.90953600	1.28074200
H	0.62171400	1.66916700	1.73400900
N	2.51121200	0.23596100	-0.49874900
C	2.44111900	-1.00653000	-0.02911600
C	1.66095100	-1.36942300	1.12240700
C	1.02023500	-0.35810900	1.75687700
H	0.41556300	-0.49514800	2.64593000
H	1.60070300	-2.39085600	1.47423600
N	3.13147200	-1.95410700	-0.68321600
H	3.15534200	-2.91172500	-0.36394800
H	3.69921700	-1.69611500	-1.47926300
C	-1.52125800	1.10971600	-0.42317100
C	-0.74222400	0.31442100	-1.33234600
C	-1.04321600	-1.00592000	-1.38549700
N	-2.52029200	0.61879100	0.30115200
C	-2.83313200	-0.70406100	0.21762400
N	-2.05450400	-1.50091800	-0.62782600
N	-1.24440300	2.42575300	-0.30501800
H	0.05031300	0.74462700	-1.93117700
H	-0.51744200	-1.71604500	-2.01390600
H	-2.29159500	-2.48572700	-0.66384400
O	-3.75160800	-1.23340000	0.84981600
H	-0.32227900	2.75970800	-0.57629900
H	-1.71494100	2.93256500	0.43472000

26

C-C-ftb-water-max180: Optimised twist = 199.84 deg.

O	2.92881300	1.67619700	-0.44652500
C	2.29046700	0.73495300	0.03547900
N	1.48683400	0.97632600	1.15430300
H	1.46281000	1.93057600	1.49541600

N	2.32027500	-0.53204000	-0.45898000
C	1.56165800	-1.47254900	0.09303900
C	0.72812500	-1.24395500	1.24073200
C	0.72234400	0.01780300	1.73495300
H	0.12461600	0.32467000	2.58554400
H	0.12028900	-2.02808400	1.67359900
N	1.56606800	-2.68854500	-0.48265800
H	1.08361300	-3.47194500	-0.06618900
H	2.19657300	-2.86841900	-1.25271100
C	-1.30804400	1.44851100	-0.38531500
C	-0.67181700	0.78479100	-1.48929100
C	-0.98148600	-0.52318300	-1.66220400
N	-2.15639200	0.84311400	0.43957300
C	-2.44667000	-0.47470200	0.26364700
N	-1.85409800	-1.13093100	-0.82007600
N	-1.02869200	2.74155500	-0.14766000
H	0.02851800	1.29464800	-2.13839100
H	-0.56113900	-1.13844400	-2.44986700
H	-2.07857800	-2.11317900	-0.93106800
O	-3.19955700	-1.11631300	1.00262400
H	-0.42295500	3.27441000	-0.75517400
H	-1.49321900	3.22032500	0.61230400

26

C-C-ftb-water-max180-plus: Optimised twist = 180.00 deg.

O	-3.29559700	-1.17105000	-0.75187400
C	-2.49256900	-0.46463000	-0.13455700
N	-1.79043500	-1.02857000	0.93560000
H	-1.97748800	-2.00463000	1.13579100
N	-2.24445100	0.83882300	-0.43487700
C	-1.34287300	1.51788100	0.26619800
C	-0.61969900	0.95921100	1.37499000
C	-0.87932800	-0.33847500	1.66617400
H	-0.38518000	-0.88334000	2.46282900
H	0.10973100	1.53307300	1.93244500
N	-1.08781700	2.78212100	-0.11540700
H	-0.46963300	3.38041900	0.41364200
H	-1.63553700	3.19489300	-0.85866900
C	1.34285500	-1.51787500	-0.26618700
C	0.61967300	-0.95919600	-1.37496900
C	0.87932100	0.33848300	-1.66616400
N	2.24445100	-0.83882700	0.43487500
C	2.49259100	0.46462000	0.13454100
N	1.79045000	1.02856600	-0.93560700
N	1.08778400	-2.78211100	0.11542600
H	-0.10978000	-1.53304700	-1.93240600
H	0.38516200	0.88335500	-2.46280700
H	1.97755200	2.00461000	-1.13583500
O	3.29564300	1.17102700	0.75184100
H	0.46959900	-3.38040700	-0.41362300
H	1.63550600	-3.19488500	0.85868400

26

C-C-ftb-water-max240: Optimised twist = 222.05 deg.

O	-2.72807900	-1.74999700	-0.25779900
C	-2.17054500	-0.72973400	0.16255200
N	-1.41456900	-0.81673800	1.33559800
H	-1.38077400	-1.72477000	1.78491900
N	-2.24175100	0.47922900	-0.45440600
C	-1.53250300	1.50040900	0.01464300

C	-0.71305700	1.41917700	1.19228700
C	-0.69190500	0.22149900	1.82614400
H	-0.11393500	0.02799400	2.72259300
H	-0.14002300	2.26418600	1.55121300
N	-1.57681000	2.65342700	-0.67491300
H	-1.12150400	3.48963800	-0.33827600
H	-2.18554600	2.72760200	-1.47905500
C	0.99891800	-1.35986500	-0.62234600
C	0.68650800	-0.42303200	-1.66464300
C	1.31473000	0.77651600	-1.60233200
N	1.85630800	-1.10206100	0.35811700
C	2.47220800	0.11100600	0.41712000
N	2.18779300	1.03165300	-0.59574200
N	0.41795500	-2.57829200	-0.63915900
H	-0.02111100	-0.65757000	-2.44905600
H	1.16087000	1.57160800	-2.32283600
H	2.65419400	1.92952900	-0.53330300
O	3.25820100	0.43771800	1.31137900
H	-0.41995700	-2.72883600	-1.18693300
H	0.53820700	-3.16752300	0.17507200

26

C-C-ftb-water-min160: Optimised twist = 136.89 deg.

O	3.75171000	-1.23336900	0.84979300
C	2.83320800	-0.70405100	0.21762100
N	2.05457500	-1.50092700	-0.62780400
H	2.29168700	-2.48573200	-0.66382500
N	2.52034600	0.61879600	0.30114800
C	1.52128500	1.10969900	-0.42315500
C	0.74224700	0.31438300	-1.33230700
C	1.04326300	-1.00595300	-1.38545800
H	0.51749100	-1.71609000	-2.01385600
H	-0.05030800	0.74457300	-1.93112800
N	1.24441000	2.42573100	-0.30500400
H	0.32228000	2.75967200	-0.57628100
H	1.71495500	2.93255900	0.43471800
C	-2.44119100	-1.00651300	-0.02912200
C	-1.66103800	-1.36941300	1.12240900
C	-1.02030400	-0.35810700	1.75687500
N	-2.51124700	0.23597600	-0.49877100
C	-1.81222700	1.22465200	0.11147100
N	-1.11786100	0.90953600	1.28072900
N	-3.13156900	-1.95407700	-0.68321400
H	-1.60081400	-2.39084400	1.47424700
H	-0.41564500	-0.49515300	2.64593500
H	-0.62173700	1.66916000	1.73399000
O	-1.74485900	2.38539300	-0.31981600
H	-3.15546200	-2.91169200	-0.36393900
H	-3.69930200	-1.69607800	-1.47926800

26

C-C-ftb-water-min200: Optimised twist = 223.11 deg.

O	1.74486000	2.38539700	-0.31979000
C	1.81221100	1.22465300	0.11149000
N	1.11783100	0.90953300	1.28073700
H	0.62171300	1.66915800	1.73400300
N	2.51122900	0.23597400	-0.49875300
C	2.44115600	-1.00651700	-0.02911600
C	1.66098500	-1.36942000	1.12240200
C	1.02025200	-0.35811500	1.75686900



H	0.41556800	-0.49516500	2.64591200
H	1.60074300	-2.39085500	1.47422700
N	3.13152900	-1.95408400	-0.68321000
H	3.15541300	-2.91170100	-0.36394100
H	3.69926500	-1.69608600	-1.47926200
C	-1.52127800	1.10971100	-0.42316000
C	-0.74224100	0.31442000	-1.33233700
C	-1.04323300	-1.00592000	-1.38549700
N	-2.52032300	0.61878500	0.30114800
C	-2.83315500	-0.70406900	0.21761900
N	-2.05451900	-1.50092300	-0.62782400
N	-1.24441700	2.42574400	-0.30499300
H	0.05029500	0.74463300	-1.93116600
H	-0.51746400	-1.71604200	-2.01391400
H	-2.29161300	-2.48573100	-0.66385100
O	-3.75163000	-1.23341200	0.84981100
H	-0.32229000	2.75969600	-0.57626800
H	-1.71496100	2.93255600	0.43474200

26

C-C-ftb-water-min280: Optimised twist = 256.21 deg.

O	-2.25617000	1.67852300	-1.00093900
C	-1.94605900	0.63087200	-0.41757400
N	-1.95199300	-0.56359600	-1.13929500
H	-2.19583500	-0.49457600	-2.12058300
N	-1.59994600	0.57716300	0.89506800
C	-1.17397500	-0.57014700	1.41542900
C	-1.08781700	-1.79079900	0.66533200
C	-1.50124200	-1.73291500	-0.62531100
H	-1.49023600	-2.58386700	-1.29568900
H	-0.71996200	-2.70839300	1.10561200
N	-0.82706400	-0.56891300	2.71525100
H	-0.41507500	-1.38166100	3.15033300
H	-0.80259700	0.30808900	3.21800100
C	1.16265000	1.40930300	-0.19265600
C	1.98817700	1.11259500	0.94369700
C	2.51779700	-0.13452800	0.99253100
N	0.94615100	0.54616400	-1.17826300
C	1.49661200	-0.69696900	-1.12912800
N	2.27350000	-1.01469400	-0.01041100
N	0.58171100	2.62704300	-0.29894500
H	2.15528600	1.83339300	1.73324700
H	3.13863700	-0.49096200	1.80640500
H	2.66507600	-1.94913500	0.01755100
O	1.34115600	-1.55217400	-2.00635600
H	0.53895400	3.20093600	0.53340900
H	-0.24751200	2.66875800	-0.88768700

26

C-C-ftb-water-min80: Optimised twist = 103.79 deg.

O	-1.34119800	-1.55213000	-2.00636500
C	-1.49662000	-0.69692600	-1.12913000
N	-2.27350900	-1.01463700	-0.01041100
H	-2.66509800	-1.94907200	0.01755200
N	-0.94611300	0.54618700	-1.17825400
C	-1.16261000	1.40933600	-0.19265500
C	-1.98815700	1.11265200	0.94369000
C	-2.51779700	-0.13446300	0.99252600
H	-3.13864700	-0.49088300	1.80639800
H	-2.15526300	1.83346000	1.73323200

N	-0.58164300	2.62706500	-0.29894000
H	-0.53889700	3.20096700	0.53340800
H	0.24759000	2.66876200	-0.88767000
C	1.17394600	-0.57020900	1.41542000
C	1.08771500	-1.79082700	0.66527900
C	1.50114900	-1.73292100	-0.62536100
N	1.59998200	0.57709600	0.89510100
C	1.94610000	0.63083300	-0.41753700
N	1.95197200	-0.56361300	-1.13930000
N	0.82703800	-0.56900300	2.71524400
H	0.71980200	-2.70841300	1.10552600
H	1.49008700	-2.58384700	-1.29577200
H	2.19583700	-0.49457100	-2.12058100
O	2.25626700	1.67848600	-1.00086800
H	0.41499400	-1.38174300	3.15028900
H	0.80260400	0.30798500	3.21801900

28

C-T-ftb-gas-max115minus: Optimised twist = 131.21 deg.

O	-0.16094300	2.75176100	-0.76142600
C	-0.71591500	1.66352900	-0.76127800
N	-0.26886500	0.58871100	-1.49430300
H	0.58223300	0.74760400	-2.01777200
N	-1.84061200	1.38268800	-0.01797000
H	-2.23099000	2.15676900	0.50977200
C	-0.81551300	-0.68192800	-1.40092300
H	-0.29360500	-1.44588400	-1.96718500
C	-2.49832100	0.14648800	0.11589700
O	-3.49279600	0.06017100	0.80653100
C	-1.88710500	-0.95533300	-0.63651500
C	-2.45497600	-2.32420300	-0.43542600
C	2.87253800	0.63781200	-0.10744000
C	2.11309200	1.39673100	0.72432600
N	1.12943400	0.81767900	1.44800600
C	0.79046700	-0.55461000	1.35243300
N	1.57807700	-1.32252100	0.53196100
C	2.54957900	-0.76265500	-0.15296300
H	3.66503500	1.06870100	-0.70552100
H	2.23493800	2.46810100	0.83549200
H	0.52405900	1.37027100	2.04401600
O	-0.16914100	-0.96066300	1.98128100
N	3.24576700	-1.56933600	-1.00733800
H	4.15621100	-1.27528800	-1.33031100
H	3.11476900	-2.56432900	-0.87471900
H	-2.32291600	-2.62045800	0.61025000
H	-3.52705300	-2.33801600	-0.65239400
H	-1.94932000	-3.05316400	-1.07388200

28

C-T-ftb-gas-max115: Optimised twist = 147.62 deg.

O	-0.16309300	2.89003900	-0.38948700
C	-0.71404600	1.81121300	-0.53541100
N	-0.25350700	0.83277800	-1.38609500
H	0.60786700	1.05028900	-1.87058600
N	-1.85600300	1.44349500	0.14477700
H	-2.25857700	2.15155800	0.75051900
C	-0.80124700	-0.43736600	-1.45724200
H	-0.26904600	-1.12877900	-2.10169600
C	-2.50640800	0.19729700	0.12517300
O	-3.49853500	0.02175800	0.80463500

C	-1.88563700	-0.80303900	-0.74936800
C	-2.45136400	-2.18777800	-0.72976500
C	2.71450300	0.82162900	0.26140800
C	1.81366600	1.14374200	1.22415500
N	0.91386200	0.22177900	1.63735600
C	0.85142700	-1.09853800	1.12445400
N	1.74945300	-1.41023800	0.13489600
C	2.61925700	-0.51091600	-0.26810900
H	3.43294000	1.54233100	-0.10668300
H	1.75284600	2.12687200	1.67727700
H	0.22930400	0.43604300	2.35334900
O	0.01084500	-1.85599100	1.57126900
N	3.43233700	-0.86344700	-1.30739300
H	4.28130400	-0.34043600	-1.46728800
H	3.46554200	-1.85210300	-1.52252200
H	-2.31166900	-2.62276300	0.26505800
H	-3.52367600	-2.17389500	-0.94534500
H	-1.94447200	-2.82358700	-1.45997300

28

C-T-ftb-gas-max115plus: Optimised twist = 221.30 deg.

O	-1.84367900	2.58080400	-0.26174200
C	-1.70000500	1.38247400	-0.44068100
N	-0.94837100	0.85544900	-1.46747600
H	-0.45336100	1.53515800	-2.03081400
N	-2.27188900	0.41903600	0.36378400
H	-2.83356400	0.76757600	1.13431400
C	-0.58646500	-0.47549400	-1.53253300
H	0.12411300	-0.72237800	-2.31566100
C	-1.94947100	-0.94481400	0.40189200
O	-2.39328500	-1.65218500	1.28871500
C	-1.05302300	-1.39634400	-0.66591300
C	-0.65334800	-2.83991100	-0.68810400
C	0.84531900	0.95778900	1.55693800
C	1.05994300	-0.34797000	1.85583900
N	1.78981500	-1.12197200	1.01793000
C	2.24964300	-0.67105000	-0.24132200
N	2.10231500	0.66511200	-0.50682600
C	1.44033100	1.43298800	0.33481400
H	0.27941300	1.60992600	2.20987700
H	0.67362000	-0.82517700	2.75059600
H	1.91368500	-2.11220600	1.19036500
O	2.72271300	-1.48754800	-1.01357600
N	1.32001500	2.74875300	0.02197100
H	0.54198000	3.27990700	0.39218200
H	1.67203400	3.02892300	-0.88419100
H	-0.34560800	-3.16095100	0.31236600
H	-1.49517800	-3.47813400	-0.97605400
H	0.17613500	-3.00185500	-1.38142400

28

C-T-ftb-gas-max5minus: Optimised twist = 180.02 deg.

O	0.67381000	-2.29893900	-0.00049600
C	1.40197500	-1.30611100	-0.00030100
N	0.93207500	-0.02596300	-0.00023000
H	-0.09776100	0.07597200	-0.00014900
N	2.77477100	-1.40104200	-0.00016400
H	3.16058700	-2.33973800	-0.00022600
C	1.75056800	1.07727900	0.00002400
H	1.21598800	2.02304800	0.00010200

C	3.69873300	-0.34405200	0.00004700
O	4.89415600	-0.57970000	0.00013900
C	3.09879300	0.98987900	0.00014500
C	4.02423000	2.16804600	0.00033800
C	-4.20543400	-0.79473000	0.00032400
C	-4.64709100	0.48524400	0.00005400
N	-3.76722300	1.51931800	-0.00027700
C	-2.37167400	1.33091800	-0.00015500
N	-1.93123000	0.04152300	-0.00003400
C	-2.77417300	-0.98196300	0.00023800
H	-4.89147300	-1.63157800	0.00060300
H	-5.69986700	0.74644000	0.00006200
H	-4.07921800	2.48233200	-0.00031400
O	-1.63217000	2.30411500	-0.00019900
N	-2.25001900	-2.21274000	0.00050500
H	-2.84036400	-3.02998300	0.00026900
H	-1.23002000	-2.32635400	0.00007300
H	4.67628500	2.14822500	0.87929700
H	4.67567500	2.14904100	-0.87910000
H	3.45961700	3.10406200	0.00095400

28

C-T-ftb-gas-max5: Optimised twist = 291.28 deg.

O	2.28591100	2.04155700	-1.51522500
C	2.02100400	1.24058200	-0.64329700
N	1.47701900	1.57710100	0.57794500
H	1.03447900	2.49031700	0.60807600
N	2.26900000	-0.12006600	-0.77313500
H	2.74075200	-0.39844800	-1.62763000
C	1.09347900	0.64129100	1.50753700
H	0.60566900	1.05437800	2.38471800
C	1.88900700	-1.14221700	0.09911100
O	2.06064000	-2.31133000	-0.21271500
C	1.28960900	-0.68509800	1.35200700
C	0.88005100	-1.72448700	2.35076900
C	-2.68037800	-1.25612700	-0.71620900
C	-3.40247400	-0.55439700	0.18932100
N	-2.95146800	0.64441900	0.63461100
C	-1.72917000	1.20969800	0.21589500
N	-1.02905700	0.53127000	-0.73701800
C	-1.45648700	-0.64093900	-1.16397100
H	-3.01496000	-2.21293200	-1.09493100
H	-4.34757600	-0.90002800	0.59413200
H	-3.46085400	1.17829700	1.32785400
O	-1.36276000	2.25272700	0.74472600
N	-0.70464300	-1.27061600	-2.09539400
H	-0.81794900	-2.26054300	-2.25645100
H	0.21070900	-0.87861700	-2.27893200
H	0.15633700	-2.41885000	1.91051000
H	1.73943700	-2.32242100	2.67018700
H	0.42982300	-1.25937700	3.23213900

28

C-T-ftb-gas-max5plus: Optimised twist = 267.26 deg.

O	0.10139900	-1.28598000	2.43181600
C	0.85655000	-0.96714200	1.53369400
N	1.23055500	-1.81006000	0.51100700
H	0.64708600	-2.63390000	0.41709100
N	1.45147300	0.28253600	1.45390900
H	1.15157300	0.94380000	2.16344300

C	1.93147700	-1.38104800	-0.59058900
H	2.04997300	-2.12620600	-1.36998300
C	2.06781300	0.82350600	0.33088500
O	2.25220900	2.03669100	0.26183100
C	2.42031600	-0.13004800	-0.71181400
C	3.15414300	0.37786100	-1.91491800
C	-2.97250400	1.38203800	0.07352200
C	-3.67173700	0.24932400	-0.17174600
N	-3.02819700	-0.86999600	-0.58341000
C	-1.63113300	-0.93204700	-0.76128000
N	-0.92474300	0.21133200	-0.52822500
C	-1.54539300	1.30688800	-0.12416800
H	-3.45951600	2.28993000	0.40477900
H	-4.74789200	0.17789500	-0.05641500
H	-3.52451400	-1.73562000	-0.75334900
O	-1.14069600	-2.00085200	-1.10733300
N	-0.79863000	2.40190000	0.11753500
H	-1.22559000	3.26368400	0.41972000
H	0.21021800	2.38728900	-0.01890900
H	2.57855200	1.16703500	-2.40927200
H	4.11915300	0.81072000	-1.63350000
H	3.32726800	-0.42947600	-2.63134000

28

C-T-ftb-gas-min210: Optimised twist = 221.32 deg.

O	-1.83690400	2.58518500	-0.26250400
C	-1.69618400	1.38644400	-0.44109800
N	-0.94512200	0.85727000	-1.46713400
H	-0.44825300	1.53552300	-2.03060400
N	-2.27110300	0.42466700	0.36321600
H	-2.83234100	0.77483900	1.13332200
C	-0.58722800	-0.47473200	-1.53219300
H	0.12283000	-0.72368200	-2.31513000
C	-1.95253100	-0.94007300	0.40159000
O	-2.39866600	-1.64612200	1.28829200
C	-1.05682500	-1.39420600	-0.66575500
C	-0.66112900	-2.83886800	-0.68760000
C	0.84713800	0.95553700	1.55683500
C	1.05892500	-0.35068900	1.85565800
N	1.78753700	-1.12609900	1.01791400
C	2.24856800	-0.67601200	-0.24117500
N	2.10444700	0.66056900	-0.50642300
C	1.44375800	1.42969500	0.33507300
H	0.28238800	1.60880500	2.20963900
H	0.67134200	-0.82723400	2.75022400
H	1.90928000	-2.11661800	1.19025700
O	2.71980000	-1.49345900	-1.01355500
N	1.32650400	2.74581900	0.02251900
H	0.54938200	3.27853500	0.39241800
H	1.67968700	3.02546100	-0.88335500
H	-0.35363000	-3.16033800	0.31281300
H	-1.50484300	-3.47492600	-0.97480000
H	0.16752200	-3.00335300	-1.38130200

28

C-T-ftb-gas-min85: Optimised twist = 84.39 deg.

O	0.68697200	-0.96887000	1.92036100
C	-0.34211000	-0.56928800	1.40026900
N	-0.81696800	0.71324700	1.59765600
H	-0.21919500	1.30619800	2.15724200

N	-1.13817100	-1.33409800	0.58108200
H	-0.73470700	-2.22507900	0.29597100
C	-1.88107100	1.24213800	0.89796200
H	-2.09498100	2.28606600	1.10528600
C	-2.22397100	-0.89049600	-0.18330200
O	-2.79546400	-1.64302300	-0.94739800
C	-2.60794200	0.51273000	0.03194600
C	-3.77673500	1.03478100	-0.74535200
C	2.78540600	1.38296800	0.05035100
C	3.42843000	0.20393400	0.25099400
N	2.89820300	-0.94505600	-0.21732200
C	1.63267100	-1.01397300	-0.83627800
N	1.00034300	0.18029300	-1.07872300
C	1.53483500	1.30117000	-0.65103700
H	3.18479700	2.32036900	0.41483900
H	4.37393400	0.12545800	0.77672900
H	3.31091200	-1.84323900	0.00307000
O	1.17498200	-2.10912000	-1.11287200
N	0.80887700	2.44443100	-0.84457400
H	1.29263800	3.33121100	-0.85131100
H	0.03326900	2.35406000	-1.49018500
H	-3.59880600	0.93297700	-1.82047900
H	-4.67870800	0.45758100	-0.51918500
H	-3.96413700	2.08699500	-0.51286700

28

C-T-ftb-water-max0: Optimised twist = 48.46 deg.

O	-3.45145700	-1.31721400	-0.04770100
C	-2.59016300	-0.48708600	0.20899300
N	-1.88012800	-0.47452300	1.38468300
H	-2.10729900	-1.20188000	2.05266900
N	-2.24905700	0.53442100	-0.64883000
H	-2.72506600	0.53313400	-1.54632300
C	-0.87645800	0.42735700	1.65549600
H	-0.39166100	0.29772400	2.61748200
C	-1.23808100	1.47823300	-0.48103200
O	-1.01948100	2.30342000	-1.36029200
C	-0.51533700	1.39506300	0.78609100
C	0.57872500	2.38460800	1.04471800
C	2.49035300	-0.85560300	0.99277600
C	1.51165300	-1.78998000	1.06723100
N	0.64342000	-1.94708900	0.03646400
C	0.68580300	-1.16126500	-1.12093300
N	1.67808700	-0.23455800	-1.21741200
C	2.54625900	-0.08858300	-0.22200000
H	3.19878200	-0.70670400	1.79699400
H	1.36962900	-2.44173300	1.92186300
H	-0.08805500	-2.64796700	0.08074200
O	-0.16973100	-1.34709700	-1.99098000
N	3.51721500	0.82718000	-0.37663200
H	4.20427100	1.00218200	0.34216200
H	3.55771700	1.37214700	-1.22745700
H	1.30275900	2.37792400	0.22411300
H	0.17783900	3.40109900	1.11957400
H	1.10314900	2.14672100	1.97401500

28

C-T-ftb-water-max120: Optimised twist = 123.54 deg.

O	0.56869500	2.81386200	-1.18869700
C	0.98590100	1.73425200	-0.79335700

N	1.72382600	1.57888200	0.35343300
H	1.91491900	2.42354200	0.87946200
N	0.75458400	0.54987500	-1.45998000
H	0.21888800	0.62316100	-2.32060900
C	2.20262300	0.36415800	0.79162500
H	2.76098100	0.40243500	1.72078300
C	1.21296300	-0.72298000	-1.11291000
O	0.95793700	-1.67875100	-1.83464700
C	1.98468700	-0.78804800	0.12397400
C	2.46006200	-2.12867000	0.59263800
C	-1.50650800	1.28792900	1.10228800
C	-2.20850200	1.31918000	-0.05663500
N	-2.45525200	0.16781300	-0.73026200
C	-2.03639300	-1.08830600	-0.27404700
N	-1.29951700	-1.12753700	0.87033600
C	-1.05250800	-0.00437900	1.53723800
H	-1.28655500	2.18945800	1.65937800
H	-2.59241700	2.23103200	-0.49906700
H	-2.99491400	0.17819700	-1.58838400
O	-2.35360900	-2.08838800	-0.92251900
N	-0.34706800	-0.10343800	2.67721500
H	-0.06348300	0.71447100	3.19742600
H	0.03501100	-1.00069300	2.94581000
H	1.60921100	-2.79748400	0.76131200
H	3.10440800	-2.60108400	-0.15557000
H	3.01981000	-2.03479600	1.52628000

28

C-T-ftb-water-max170: Optimised twist = 166.82 deg.

O	-0.06184900	3.14495800	-0.61617600
C	0.48303700	2.14619400	-0.16795900
N	0.35389700	1.73143600	1.13375600
H	-0.24414000	2.29525900	1.72675600
N	1.28550000	1.32053700	-0.92695500
H	1.39446500	1.58372900	-1.90263300
C	0.98062400	0.61730000	1.64326200
H	0.78200500	0.42290200	2.69179800
C	1.93852100	0.15733800	-0.51398100
O	2.58754700	-0.49617300	-1.32260100
C	1.77249500	-0.18114200	0.89571900
C	2.45705200	-1.40617100	1.42100200
C	-2.20923400	0.44107200	-0.78283200
C	-1.49706000	-0.13666100	-1.78018700
N	-0.79926200	-1.27689100	-1.54385800
C	-0.78258800	-1.91454500	-0.29789700
N	-1.49945900	-1.34690300	0.71057600
C	-2.16516600	-0.21849600	0.49452100
H	-2.76391900	1.35753600	-0.93568100
H	-1.43818800	0.26730100	-2.78451200
H	-0.25153500	-1.70897200	-2.27942600
O	-0.12127300	-2.94867700	-0.17338600
N	-2.80632800	0.33266000	1.54030600
H	-3.39250500	1.14776400	1.43181900
H	-2.82326900	-0.15750200	2.42474500
H	2.10490500	-2.29502800	0.88853500
H	3.54082400	-1.33611700	1.28285500
H	2.24944400	-1.53295300	2.48638500

28

C-T-ftb-water-max240-minus: Optimised twist = 249.83 deg.

O	3.00479100	-1.71514400	-0.46124700
C	2.26063500	-0.74631700	-0.51337100
N	1.36069400	-0.53372400	-1.52676100
H	1.30591100	-1.25531800	-2.23615600
N	2.24472500	0.24248200	0.44869100
H	2.89929300	0.12336600	1.21688700
C	0.52819200	0.55952700	-1.58887000
H	-0.13892700	0.57702500	-2.44461700
C	1.46255300	1.39791500	0.46452400
O	1.58053900	2.20283900	1.38088600
C	0.53843100	1.53751000	-0.65741400
C	-0.33284800	2.75548500	-0.71280700
C	-0.88042400	-0.49369800	1.80905200
C	-1.80417900	0.47407600	1.59323200
N	-2.53665400	0.46851500	0.45145400
C	-2.39001200	-0.50394800	-0.54356400
N	-1.48533500	-1.49662100	-0.32677700
C	-0.75087100	-1.48964600	0.78052900
H	-0.27196500	-0.51276200	2.70397700
H	-1.99985200	1.28060200	2.29091900
H	-3.22243000	1.19404400	0.27504700
O	-3.08065400	-0.41529500	-1.56312600
N	0.16083300	-2.46602700	0.92551900
H	0.77581500	-2.50577100	1.72573400
H	0.28251800	-3.14975200	0.19018400
H	-0.87420200	2.89003600	0.22915200
H	0.26755200	3.65774700	-0.87100200
H	-1.05982900	2.67377900	-1.52498900

28

C-T-ftb-water-max240: Optimised twist = 229.91 deg.

O	2.77573900	-1.95744800	-0.32349300
C	2.16322200	-0.90417100	-0.43094000
N	1.26004400	-0.65181200	-1.43286300
H	1.09665700	-1.40788400	-2.08763400
N	2.31677900	0.14793900	0.44705400
H	2.97501400	-0.00123200	1.20677000
C	0.54227900	0.51726600	-1.53412000
H	-0.14995400	0.55808600	-2.36870500
C	1.63289600	1.36297100	0.43799600
O	1.84953000	2.19264100	1.31378800
C	0.68434300	1.53563900	-0.65826500
C	-0.07517600	2.82447200	-0.74473900
C	-0.71060600	-0.89498900	1.64204700
C	-1.35508600	0.29057000	1.77551600
N	-2.22003300	0.70408900	0.81640600
C	-2.46524200	-0.02510700	-0.35221900
N	-1.85041000	-1.23237300	-0.48323400
C	-1.01466300	-1.65483300	0.46002700
H	-0.01490700	-1.25166500	2.39067300
H	-1.22099200	0.95189300	2.62415900
H	-2.70316600	1.59103000	0.90416100
O	-3.22140900	0.45605500	-1.20082600
N	-0.43358100	-2.85335400	0.28041000
H	0.27407100	-3.20143800	0.91151400
H	-0.60310100	-3.36295500	-0.57661100
H	-0.56807500	3.04834000	0.20663600
H	0.59709200	3.66077700	-0.96418700
H	-0.83492100	2.77272700	-1.52877100



28

C-T-ftb-water-max240-plus: Optimised twist = 223.72 deg.

O	-2.30160800	2.37936200	-0.25103300
C	-1.93360300	1.22215200	-0.40083700
N	-1.07947300	0.82366700	-1.39803400
H	-0.74224000	1.55402800	-2.01465000
N	-2.34181400	0.19077500	0.41803400
H	-2.97502500	0.44627200	1.17068700
C	-0.59620100	-0.45889100	-1.51791900
H	0.10264100	-0.60966300	-2.33416500
C	-1.90159200	-1.13182000	0.39009600
O	-2.30714900	-1.92926600	1.22769100
C	-0.95913300	-1.45258200	-0.67852800
C	-0.44448700	-2.85621700	-0.77384900
C	0.76651300	0.92082200	1.54294400
C	1.14054400	-0.35981100	1.78733700
N	1.98309200	-0.99451400	0.93529200
C	2.47460500	-0.40012300	-0.23240000
N	2.12567100	0.89298000	-0.47684700
C	1.31750400	1.53046700	0.36366600
H	0.09978600	1.45687200	2.20643300
H	0.80195900	-0.92876000	2.64609100
H	2.26688000	-1.95242600	1.10718200
O	3.19439200	-1.06974000	-0.97816300
N	1.00803600	2.80755300	0.07929300
H	0.30653800	3.30996500	0.60524800
H	1.34362200	3.21774300	-0.78225200
H	0.01711100	-3.16475500	0.16990300
H	-1.25902700	-3.55840800	-0.97971100
H	0.29919000	-2.94093000	-1.56995200

28

C-T-ftb-water-min160: Optimised twist = 150.46 deg.

O	-3.26283000	-1.00799800	-1.02598400
C	-2.47523300	-0.35430000	-0.35619200
N	-2.09288300	-0.70022300	0.91545600
H	-2.49839200	-1.55041600	1.28985800
N	-1.88729000	0.80779700	-0.80993100
H	-2.14741700	1.09842300	-1.74855000
C	-1.17662200	0.01376200	1.65315900
H	-0.96003900	-0.39658500	2.63343900
C	-0.94123400	1.59236900	-0.14855000
O	-0.47702000	2.58375700	-0.69945600
C	-0.58189100	1.13429100	1.18994200
C	0.43046000	1.92199000	1.96411000
C	0.46682400	-1.82266400	-0.83878100
C	0.64062000	-0.90553200	-1.82160000
N	1.52723400	0.10698800	-1.65374500
C	2.30931400	0.25231900	-0.50191000
N	2.14865800	-0.66504300	0.48966900
C	1.25709100	-1.63969900	0.34770100
H	-0.23848400	-2.63798400	-0.93736500
H	0.09665000	-0.92279400	-2.75940800
H	1.64802300	0.81203200	-2.37211800
O	3.09720800	1.20067500	-0.44018500
N	1.08101900	-2.47540300	1.38594700
H	0.47855300	-3.28310800	1.31735100
H	1.67137400	-2.38330800	2.20195600
H	1.37956700	1.97062200	1.41983900

H 0.08583100 2.94889400 2.12400200  
H 0.61235100 1.45871600 2.93695200  
28

C-T-ftb-water-min205: Optimised twist = 210.18 deg.

O -2.46778100 2.24377900 -0.06696300  
C -2.02222100 1.12595000 -0.28715600  
N -1.21453800 0.83206000 -1.35714300  
H -0.97180000 1.61139400 -1.95815200  
N -2.28958600 0.03723000 0.51541200  
H -2.87925300 0.21686300 1.32336200  
C -0.64633100 -0.40345700 -1.56267700  
H -0.00061500 -0.47108100 -2.43167000  
C -1.74469000 -1.24197800 0.40838500  
O -2.01499900 -2.09410200 1.24718500  
C -0.86864500 -1.45151100 -0.74032800  
C -0.25908900 -2.80609900 -0.93434500  
C 0.75208700 1.19435400 1.43720400  
C 1.05142900 -0.06034900 1.85542200  
N 1.85503400 -0.85320600 1.10373000  
C 2.37719100 -0.45255600 -0.13160700  
N 2.10769800 0.81539000 -0.54883800  
C 1.33746800 1.60587300 0.19061700  
H 0.11307400 1.85002900 2.01516000  
H 0.67987700 -0.48663800 2.78051100  
H 2.08638600 -1.79126000 1.41073200  
O 3.05340700 -1.25793100 -0.77667100  
N 1.08224900 2.83932100 -0.27901400  
H 0.53916800 3.50652100 0.25012700  
H 1.52748100 3.14865400 -1.13286200  
H 0.33911000 -3.09223300 -0.06282800  
H -1.03478400 -3.56847600 -1.05988600  
H 0.38715400 -2.81466300 -1.81504100  
28

C-T-ftb-water-min285: Optimised twist = 295.67 deg.

O 2.61857700 -1.95030400 0.54771900  
C 2.06545900 -0.99511300 0.02026000  
N 1.47870500 -1.04723500 -1.21881500  
H 1.41845400 -1.96493900 -1.64487300  
N 2.00161100 0.25177900 0.60645000  
H 2.42666200 0.33148500 1.52578900  
C 0.79029400 0.00443900 -1.77249000  
H 0.33293000 -0.20492000 -2.73400300  
C 1.32587300 1.37409800 0.13299400  
O 1.30834200 2.40419400 0.79889200  
C 0.68228900 1.20763100 -1.16655200  
C -0.05258400 2.37335700 -1.75426500  
C -1.97306300 0.89079700 1.13844800  
C -2.60971900 0.72317300 -0.04632700  
N -2.38256000 -0.38962900 -0.78730400  
C -1.49994600 -1.40006400 -0.39084200  
N -0.87034600 -1.25494600 0.80559800  
C -1.09030000 -0.16879000 1.54167600  
H -2.12702500 1.77136900 1.74820400  
H -3.30651300 1.44414200 -0.45836900  
H -2.84684400 -0.51949500 -1.67927300  
O -1.32333900 -2.36061000 -1.14705500  
N -0.43180500 -0.07101200 2.70787400  
H -0.56286800 0.71421700 3.32913900

H 0.16330900 -0.83178600 3.00813500  
H -0.81254600 2.74167100 -1.05745400  
H 0.63033300 3.20443700 -1.95976000  
H -0.54357600 2.08771300 -2.68802100  
28

C-T-ftb-water-min315: Optimised twist = 295.67 deg.

O 2.61831800 -1.95056900 0.54763700  
C 2.06531600 -0.99528800 0.02021900  
N 1.47855900 -1.04728400 -1.21885900  
H 1.41814400 -1.96497100 -1.64493400  
N 2.00161800 0.25158600 0.60646600  
H 2.42669000 0.33119900 1.52580200  
C 0.79026000 0.00449500 -1.77247700  
H 0.33285800 -0.20476600 -2.73399300  
C 1.32601000 1.37400600 0.13306300  
O 1.30860100 2.40407500 0.79900600  
C 0.68240300 1.20767400 -1.16648700  
C -0.05233900 2.37350800 -1.75414800  
C -1.97300300 0.89088600 1.13845200  
C -2.60964800 0.72334300 -0.04634100  
N -2.38255200 -0.38945200 -0.78734900  
C -1.50001700 -1.39995700 -0.39090100  
N -0.87043700 -1.25492400 0.80555900  
C -1.09032500 -0.16877500 1.54166600  
H -2.12690700 1.77145400 1.74822700  
H -3.30638500 1.44437100 -0.45837400  
H -2.84682800 -0.51925600 -1.67933100  
O -1.32345000 -2.36048800 -1.14714400  
N -0.43184700 -0.07108200 2.70787900  
H -0.56289500 0.71411900 3.32918300  
H 0.16319700 -0.83191300 3.00813500  
H -0.81228800 2.74185500 -1.05734100  
H 0.63066500 3.20453500 -1.95957000  
H -0.54332800 2.08796900 -2.68793800  
28

C-T-ftb-water-min80: Optimised twist = 61.08 deg.

O -0.44055300 -2.77741000 -0.95142400  
C 0.29315900 -1.80859900 -0.80839100  
N 0.33116000 -0.75374600 -1.68580200  
H -0.28402200 -0.81766700 -2.48854900  
N 1.15997100 -1.66964100 0.25287600  
H 1.10221700 -2.39259200 0.96450600  
C 1.16658000 0.33115100 -1.53866400  
H 1.08632900 1.07872500 -2.32080900  
C 2.00487600 -0.59421100 0.51822400  
O 2.68548000 -0.58850400 1.53798300  
C 2.00771500 0.46068300 -0.49205700  
C 2.90965500 1.63798400 -0.28618100  
C -2.00424200 1.62316700 -0.75282200  
C -2.69811700 0.46015900 -0.81900200  
N -2.48530200 -0.51010500 0.10365500  
C -1.57278000 -0.37412200 1.15674800  
N -0.85751400 0.78106000 1.22385300  
C -1.06072700 1.73988300 0.32480700  
H -2.15167700 2.41693300 -1.47333600  
H -3.43204800 0.24507700 -1.58701400  
H -2.97903500 -1.39369700 0.04820900  
O -1.45279600 -1.30433100 1.95890400

N	-0.32730500	2.85911700	0.43834500
H	-0.44773200	3.64057100	-0.18953200
H	0.31194500	2.95781600	1.21540500
H	2.70530700	2.11640300	0.67729100
H	3.96052000	1.33052700	-0.27761300
H	2.76736500	2.37649900	-1.07872000

25

C-U-ftb-gas-max0: Optimised twist = 355.35 deg.

O	2.44095700	1.70641200	-1.11978300
C	2.14444000	0.65310500	-0.60709200
N	2.82836600	0.13876600	0.49242600
H	3.59801800	0.70965900	0.81657600
N	1.11273300	-0.16478500	-1.03534300
H	0.54210700	0.20787200	-1.79235000
C	2.55545600	-1.08219500	1.05356400
H	3.18352400	-1.35923100	1.89341900
C	0.78244000	-1.43982600	-0.56331000
O	-0.10428100	-2.08749000	-1.09215200
C	1.57568500	-1.87730700	0.58217300
H	1.35946400	-2.84519600	1.01260700
C	-1.97375300	-0.79471800	1.14661600
C	-1.26992300	0.07559700	1.90701000
N	-0.89910200	1.27655800	1.39532600
C	-1.21680300	1.69141300	0.07778800
N	-1.90484400	0.79193600	-0.69774700
C	-2.27040200	-0.36795300	-0.19932400
H	-2.28547000	-1.76118200	1.52014600
H	-0.97394100	-0.13094000	2.93032400
H	-0.38982700	1.95596700	1.94639200
O	-0.84401800	2.78906100	-0.28893600
N	-3.00086000	-1.19529300	-0.99670600
H	-2.89543000	-2.18848700	-0.83538700
H	-2.99660300	-0.93129700	-1.97499300

25

C-U-ftb-gas-max115: Optimised twist = 106.87 deg.

O	-0.31456600	-1.05512700	2.25864200
C	-0.87299500	-0.31299300	1.46779000
N	-0.58860100	1.03879800	1.38884500
H	0.15128000	1.35738500	2.00025700
N	-1.83455700	-0.72234400	0.57475200
H	-2.05488900	-1.71347300	0.57702600
C	-1.15755200	1.88228500	0.46027000
H	-0.79433400	2.90320200	0.48400000
C	-2.51336300	0.05630600	-0.38477000
O	-3.37024100	-0.44358900	-1.08036400
C	-2.09035400	1.45491500	-0.40782800
H	-2.54080400	2.10971100	-1.14043200
C	2.57993000	0.23994800	0.57990600
C	2.30587500	-1.07815200	0.75912000
N	1.50114800	-1.72222000	-0.11256400
C	0.85379300	-1.08632200	-1.19969600
N	1.12559300	0.24997500	-1.37079700
C	1.92486800	0.86743100	-0.53471900
H	3.22135000	0.78686500	1.25905500
H	2.69510600	-1.66199400	1.58561400
H	1.23232700	-2.68627600	0.04330500
O	0.10171800	-1.74102200	-1.89457600
N	2.07023600	2.22066700	-0.70520700

H 2.90435100 2.66065600 -0.34115300  
H 1.75238300 2.56718700 -1.60293600  
25

C-U-ftb-gas-min210: Optimised twist = 220.06 deg.

O -2.08191300 2.17821000 0.02535700  
C -1.83709700 1.03965900 -0.33468500  
N -1.03464000 0.75141300 -1.42180300  
H -0.60049300 1.55405000 -1.86004900  
N -2.32843400 -0.08189400 0.29825200  
H -2.91427100 0.09500600 1.10839700  
C -0.57335200 -0.51516300 -1.70059700  
H 0.14800800 -0.57997800 -2.50824900  
C -1.89193600 -1.40765500 0.12833000  
O -2.26725200 -2.27466500 0.89437600  
C -0.97913900 -1.58762900 -0.99452300  
H -0.60768700 -2.58176200 -1.20253800  
C 0.70225600 0.62814700 1.60172900  
C 1.03483500 -0.68074600 1.73222900  
N 1.85780300 -1.26257300 0.82877200  
C 2.31636000 -0.60228800 -0.33564500  
N 2.02945300 0.73428800 -0.43667400  
C 1.27380500 1.31546700 0.47302000  
H 0.06034800 1.13116700 2.31365800  
H 0.67318800 -1.30907100 2.53963100  
H 2.07056000 -2.25172500 0.87320300  
O 2.90975500 -1.25328300 -1.17760200  
N 1.02401600 2.64119900 0.32479300  
H 0.19631000 3.04654400 0.74272500  
H 1.37754100 3.07789200 -0.51636300

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C-U-ftb-gas-min55: Optimised twist = 53.24 deg.

O -0.98130000 -2.54285800 -0.34037300  
C -1.36929600 -1.39320200 -0.27338100  
N -2.31083800 -0.99003100 0.66600700  
H -2.66878800 -1.73093000 1.25408000  
N -0.93103000 -0.37254100 -1.08833500  
H -0.22064000 -0.62220200 -1.77681700  
C -2.73965800 0.30622300 0.80557300  
H -3.47718800 0.47126100 1.58343000  
C -1.28680000 0.98749300 -1.01853700  
O -0.79585300 1.79748800 -1.77659900  
C -2.26660900 1.29371500 0.02340800  
H -2.60253400 2.31722000 0.11871300  
C 0.93337900 0.53633500 1.75423100  
C 1.06448000 -0.81355000 1.70778000  
N 1.64107700 -1.40251200 0.63565000  
C 2.05613000 -0.68010800 -0.50812800  
N 1.98193100 0.68481200 -0.43543200  
C 1.42806500 1.25835900 0.60740100  
H 0.48946800 1.03889900 2.60409400  
H 0.72451400 -1.47381500 2.49929100  
H 1.61148100 -2.40869000 0.51411400  
O 2.41575400 -1.30657800 -1.48954400  
N 1.33293500 2.61560600 0.59022200  
H 0.67761900 3.06563000 1.21259400  
H 1.44058300 3.03928400 -0.32423100

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C-U-ftb-water-max0: Optimised twist = 7.05 deg.

O	2.57647300	1.65693400	-0.85002700
C	2.17352700	0.56535000	-0.48239200
N	2.67313800	-0.08517400	0.62509000
H	3.41206800	0.39401700	1.12680600
N	1.17676400	-0.13351100	-1.13225300
H	0.77214000	0.32563000	-1.94455200
C	2.26328500	-1.33379800	1.01790900
H	2.75767700	-1.72691500	1.89824700
C	0.68895700	-1.40649500	-0.81815600
O	-0.18777100	-1.91142900	-1.50738100
C	1.30830500	-2.01102800	0.34849600
H	0.97777500	-2.99161500	0.66224200
C	-1.85061700	-0.70429400	1.25618400
C	-0.92116700	0.07951100	1.85362500
N	-0.52701200	1.23741500	1.26271800
C	-1.05086000	1.68378800	0.04261600
N	-1.97320500	0.89630700	-0.57334100
C	-2.36416500	-0.23809700	-0.00266500
H	-2.17815300	-1.63621900	1.69794800
H	-0.44994800	-0.16383500	2.79917200
H	0.14790400	1.84418500	1.71480400
O	-0.64964100	2.75661900	-0.41551500
N	-3.30894800	-0.95701800	-0.63439300
H	-3.53997600	-1.89181900	-0.32947400
H	-3.58073400	-0.68617900	-1.57026100

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C-U-ftb-water-max120: Optimised twist = 148.93 deg.

O	-3.07558000	0.47646900	1.38480500
C	-2.37648800	0.11824900	0.44944900
N	-2.12157600	0.91136000	-0.64710000
H	-2.55252100	1.82883200	-0.64397800
N	-1.77077900	-1.11886900	0.39282400
H	-1.93808100	-1.72945200	1.18808300
C	-1.31235400	0.52663800	-1.68522900
H	-1.19262200	1.25982600	-2.47391000
C	-0.91291800	-1.59955300	-0.60160700
O	-0.41264300	-2.71175900	-0.48928400
C	-0.70700500	-0.67934500	-1.70548000
H	-0.05664700	-0.97697800	-2.51652900
C	0.58426900	1.32307900	1.23480800
C	0.81356700	0.12848300	1.83333300
N	1.65733500	-0.76537500	1.26067200
C	2.34430700	-0.50972700	0.06746800
N	2.13055900	0.69011000	-0.53711900
C	1.27380400	1.55410400	-0.00497100
H	-0.09076000	2.05449300	1.66085500
H	0.34627800	-0.17379900	2.76393200
H	1.81803100	-1.67017100	1.68859400
O	3.10268400	-1.37700700	-0.37469400
N	1.03080700	2.68673500	-0.68822500
H	0.46365700	3.42640500	-0.29906900
H	1.55947300	2.87993000	-1.52858700

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C-U-ftb-water-max240: Optimised twist = 233.15 deg.

O	-3.02065500	1.24105400	-0.17914900
C	-2.26707000	0.27974300	-0.18653600
N	-1.91292800	-0.39209200	-1.33524900
H	-2.30445100	-0.03463600	-2.19917300

N	-1.69108500	-0.23614200	0.95521600
H	-1.92559600	0.23994300	1.82220800
C	-1.07823900	-1.47816600	-1.34823700
H	-0.88243800	-1.89959200	-2.32705200
C	-0.83885300	-1.34121500	1.05453000
O	-0.41439900	-1.68729700	2.15029900
C	-0.53980200	-1.97640800	-0.21518000
H	0.12339300	-2.83069500	-0.22731000
C	1.26972200	1.27526400	1.34593000
C	2.09711800	0.20546900	1.42831900
N	2.44227300	-0.47333100	0.30504600
C	1.99273600	-0.11532100	-0.97032000
N	1.14106100	0.94232700	-1.06288800
C	0.78575700	1.60294700	0.03346900
H	0.96775900	1.83179200	2.22347100
H	2.51020500	-0.16204500	2.36038400
H	3.06168600	-1.27408500	0.35753200
O	2.37729600	-0.77358800	-1.94086700
N	-0.06890800	2.63215300	-0.11527600
H	-0.49063200	3.07946000	0.68628300
H	-0.49896100	2.78422900	-1.01840900

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C-U-ftb-water-min195: Optimised twist = 215.63 deg.

O	2.53035900	1.95389000	-0.17304400
C	2.05989300	0.89935900	0.22619000
N	1.22670400	0.81452500	1.31900200
H	0.99988900	1.69216500	1.77272400
N	2.31666800	-0.31553400	-0.37235700
H	2.92299400	-0.28653700	-1.18744800
C	0.62705300	-0.35064300	1.72165600
H	-0.03496200	-0.25901500	2.57492700
C	1.74043500	-1.54988400	-0.06043400
O	2.00584700	-2.53535600	-0.73808700
C	0.84954600	-1.52027600	1.08584300
H	0.36845300	-2.43786300	1.39615100
C	-0.69265200	0.63187600	-1.56858100
C	-1.10556500	-0.65510600	-1.68195100
N	-1.97044700	-1.17280600	-0.77550600
C	-2.44744900	-0.44663000	0.32113400
N	-2.05552900	0.85207100	0.43683000
C	-1.22272800	1.37411600	-0.45795500
H	-0.00632500	1.07495300	-2.27906900
H	-0.78131200	-1.31881800	-2.47551000
H	-2.26879700	-2.13941900	-0.84115500
O	-3.19376500	-1.01198800	1.12492700
N	-0.85446000	2.65504000	-0.28836300
H	-0.20437100	3.10967700	-0.91373200
H	-1.22684000	3.18254100	0.49009900

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C-U-ftb-water-min295: Optimised twist = 294.88 deg.

O	2.62192900	-1.03953700	1.50051900
C	2.07625200	-0.65784400	0.47620300
N	1.53116200	-1.51492000	-0.45239900
H	1.51030200	-2.49475300	-0.19397000
N	1.97897900	0.67291200	0.12816500
H	2.37210300	1.33352400	0.79247000
C	0.85040300	-1.08652000	-1.56019200
H	0.42735400	-1.87297400	-2.17473700

C	1.29967700	1.21471200	-0.96397800
O	1.24153600	2.43126200	-1.10473600
C	0.71499700	0.22522700	-1.85137600
H	0.17355300	0.56312900	-2.72451700
C	-2.03365400	1.43637900	0.07730300
C	-2.65124400	0.53891200	-0.72889900
N	-2.39741200	-0.78610100	-0.58907900
C	-1.49533700	-1.29261800	0.35142100
N	-0.88100800	-0.40483700	1.17864200
C	-1.13640200	0.89533800	1.06076500
H	-2.21152900	2.49993900	-0.01107100
H	-3.35574100	0.81674900	-1.50418900
H	-2.84703800	-1.46382600	-1.19412700
O	-1.28827400	-2.51021700	0.37704400
N	-0.49791500	1.72679500	1.89990800
H	-0.65684600	2.72390100	1.88435800
H	0.10152200	1.34379200	2.61903600

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C-U-ftb-water-min55-minus: Optimised twist = 60.37 deg.

O	1.12725200	-2.61018500	0.32397500
C	1.43435100	-1.42986100	0.25547600
N	2.26864000	-0.92504100	-0.71761700
H	2.62688900	-1.59532200	-1.38816100
N	0.97255500	-0.47806700	1.13932100
H	0.37306600	-0.82062900	1.88614200
C	2.59923800	0.40125800	-0.81513400
H	3.25455800	0.65422600	-1.64024300
C	1.26956300	0.89035500	1.14732000
O	0.80977700	1.60907000	2.02398300
C	2.13188800	1.31702900	0.05915100
H	2.39250100	2.36380100	-0.01710300
C	-0.74221600	0.41914500	-1.74018800
C	-0.98752000	-0.90819400	-1.61795900
N	-1.69924400	-1.37093100	-0.55977100
C	-2.20449000	-0.53572200	0.44157900
N	-1.98072600	0.80071000	0.32044500
C	-1.27420000	1.26314800	-0.70458500
H	-0.17118600	0.81953700	-2.56776300
H	-0.63502400	-1.65047000	-2.32545400
H	-1.85340000	-2.36576300	-0.44015400
O	-2.81828900	-1.04652100	1.38355900
N	-1.06249900	2.58973900	-0.76453500
H	-0.44496100	2.99126300	-1.45566100
H	-1.34313000	3.16662000	0.01740400

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C-U-ftb-water-min55: Optimised twist = 60.37 deg.

O	1.12725200	-2.61018500	0.32397500
C	1.43435100	-1.42986100	0.25547600
N	2.26864000	-0.92504100	-0.71761700
H	2.62688900	-1.59532200	-1.38816100
N	0.97255500	-0.47806700	1.13932100
H	0.37306600	-0.82062900	1.88614200
C	2.59923800	0.40125800	-0.81513400
H	3.25455800	0.65422600	-1.64024300
C	1.26956300	0.89035500	1.14732000
O	0.80977700	1.60907000	2.02398300
C	2.13188800	1.31702900	0.05915100
H	2.39250100	2.36380100	-0.01710300



C	-0.74221600	0.41914500	-1.74018800
C	-0.98752000	-0.90819400	-1.61795900
N	-1.69924400	-1.37093100	-0.55977100
C	-2.20449000	-0.53572200	0.44157900
N	-1.98072600	0.80071000	0.32044500
C	-1.27420000	1.26314800	-0.70458500
H	-0.17118600	0.81953700	-2.56776300
H	-0.63502400	-1.65047000	-2.32545400
H	-1.85340000	-2.36576300	-0.44015400
O	-2.81828900	-1.04652100	1.38355900
N	-1.06249900	2.58973900	-0.76453500
H	-0.44496100	2.99126300	-1.45566100
H	-1.34313000	3.16662000	0.01740400

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C-U-ftb-water-min55-plus: Optimised twist = 58.47 deg.

O	2.34244800	-1.82238800	-0.18778800
C	1.94014800	-0.67701000	-0.32994400
N	1.63130000	-0.13541100	-1.55792300
H	1.76831500	-0.73942000	-2.36023500
N	1.74393000	0.18810600	0.72313400
H	1.88735900	-0.20861500	1.64881400
C	1.12770700	1.13068100	-1.71882500
H	0.90791500	1.41289800	-2.74176200
C	1.24397100	1.49318800	0.67086800
O	1.11523200	2.13810500	1.70306600
C	0.92512000	1.95432000	-0.66953100
H	0.52429900	2.95057100	-0.79651600
C	-2.03175600	-0.37610600	-1.31081200
C	-1.34445200	-1.53755200	-1.19170800
N	-0.79983000	-1.88501500	0.00277000
C	-0.91236100	-1.09214000	1.14995700
N	-1.60720900	0.07150900	1.04586400
C	-2.13520900	0.42622000	-0.12187700
H	-2.47188000	-0.06792100	-2.25002100
H	-1.18769500	-2.22832300	-2.01230500
H	-0.25344500	-2.73485400	0.09361700
O	-0.36240400	-1.47486500	2.18766000
N	-2.78551500	1.59952900	-0.17353900
H	-3.22818300	1.92734900	-1.01969900
H	-2.86663000	2.16086200	0.66368400

27

T-BrU-ftb-gas-max115: Optimised twist = 130.40 deg.

O	-1.81470400	-1.99941700	1.76358800
C	-0.77147500	-1.60226200	1.28461100
N	-0.30769200	-1.99513300	0.04272800
H	-0.92500000	-2.59573700	-0.48949000
N	0.07277100	-0.70945200	1.91644000
H	-0.20771300	-0.42401900	2.84978400
C	0.83015400	-1.49585300	-0.54329600
H	1.02767900	-1.83617600	-1.55285200
C	1.29154300	-0.18140700	1.45822100
O	1.94494400	0.55750000	2.15703500
C	1.62876500	-0.62229700	0.09808900
Br	3.16631700	0.07237400	-0.68536100
C	-2.84604000	0.00772100	-0.71256100
C	-3.12108200	0.75960600	0.37274100
N	-2.30751400	1.78653500	0.79228800
C	-1.13559800	2.14954600	0.15117000

N	-0.85543300	1.35037200	-0.94590700
C	-1.60928400	0.28558400	-1.44388100
C	-3.70168000	-1.13179300	-1.17307500
H	-3.99770300	0.58368500	0.98748900
H	-2.54391900	2.34413800	1.60276700
O	-0.42996100	3.06319700	0.51722700
O	-1.20482400	-0.35982500	-2.39934900
H	0.01351600	1.56200600	-1.42975100
H	-3.95463200	-1.02474300	-2.23176500
H	-3.18056600	-2.08879700	-1.05915000
H	-4.62313400	-1.18440200	-0.58835600

27

T-BrU-ftb-gas-max240: Optimised twist = 240.78 deg.

O	-2.66964400	-2.41477100	-1.23597100
C	-1.59208100	-1.94699000	-0.95467800
N	-0.85287300	-1.15310700	-1.82296900
H	-1.30053900	-0.95436300	-2.70895600
N	-0.95666000	-2.14661400	0.26053600
H	-1.47800600	-2.69527600	0.93799500
C	0.40675700	-0.68840800	-1.54681300
H	0.88620500	-0.10671400	-2.32770800
C	0.28781900	-1.67426700	0.68124300
O	0.68311900	-1.87645300	1.81018200
C	1.00720600	-0.93656200	-0.36561300
Br	2.73358400	-0.35123600	0.01605600
C	-1.43500100	0.99479600	1.36078000
C	-0.17791500	1.42638000	1.59188700
N	0.53660800	2.16858500	0.67583300
C	0.08287100	2.44704200	-0.59667900
N	-1.22584800	2.05154100	-0.80146200
C	-2.03878900	1.30171700	0.06010800
C	-2.24391300	0.19739800	2.33797600
H	0.34969200	1.20166000	2.51383300
H	1.51793000	2.36334700	0.83042200
O	0.76255600	2.98233800	-1.45106000
O	-3.14314300	0.94159500	-0.30257900
H	-1.61780100	2.27584500	-1.71066200
H	-3.03786900	0.80849300	2.78023200
H	-2.73752000	-0.63502600	1.82750000
H	-1.61094800	-0.19587500	3.13796700

27

T-BrU-ftb-gas-max5: Optimised twist = 33.88 deg.

O	1.53831400	-1.06434600	-1.71226600
C	0.41473400	-0.82210000	-1.31793200
N	-0.42086600	-1.79390400	-0.79163400
H	-0.03887100	-2.73018500	-0.77356400
N	-0.15894300	0.42984100	-1.34043800
H	0.42786800	1.17979500	-1.69555100
C	-1.68701900	-1.53810900	-0.32073700
H	-2.22960800	-2.39077600	0.07150700
C	-1.43489800	0.81786900	-0.90117800
O	-1.80767000	1.96102700	-1.00700400
C	-2.21393200	-0.30077900	-0.34489700
Br	-3.91895100	0.06371100	0.29908300
C	1.83827000	-0.28188700	1.50153500
C	2.77214200	-1.19110400	1.15543500
N	3.81290500	-0.90485100	0.30570900
C	3.97204100	0.31584000	-0.32484700

N	3.02681300	1.24969900	0.06276000
C	1.93951400	1.06079200	0.91991800
C	0.68791100	-0.55102500	2.42297800
H	2.75745500	-2.20727400	1.53801300
H	4.44438200	-1.62969500	-0.00803000
O	4.86411600	0.54819800	-1.11204600
O	1.15132000	1.96601200	1.12753100
H	3.12696100	2.17181200	-0.35027100
H	0.73159300	0.09834300	3.30283200
H	-0.26548300	-0.33816100	1.92587500
H	0.68839700	-1.59335300	2.75514400

27

T-BrU-ftb-gas-min205: Optimised twist = 182.03 deg.

O	-3.79321500	-1.23137900	-0.15728500
C	-2.58272300	-1.25805000	-0.20809300
N	-1.86016900	-0.92642400	-1.34055800
H	-2.40042200	-0.56404400	-2.11746400
N	-1.77861000	-1.61011300	0.86205400
H	-2.27173100	-1.83168600	1.72181400
C	-0.49185700	-0.96284200	-1.40759100
H	-0.05838900	-0.68166200	-2.36106300
C	-0.38289900	-1.59432500	0.93938700
O	0.18057200	-1.78771600	1.99728500
C	0.26303800	-1.30990400	-0.34609500
Br	2.11977900	-1.37701800	-0.42907300
C	-1.13670000	1.79921800	0.54845700
C	-0.32454400	1.48129900	1.57939300
N	1.04694000	1.48395700	1.47830800
C	1.73042400	1.87356300	0.34156800
N	0.88504900	2.14449100	-0.72306900
C	-0.50940900	2.07746000	-0.74675700
C	-2.63139500	1.87457800	0.64574000
H	-0.71026400	1.19823600	2.55420800
H	1.62495800	1.16726800	2.24697600
O	2.93759500	1.95682700	0.27754900
O	-1.11393100	2.22368300	-1.79793400
H	1.34601400	2.38264900	-1.59593700
H	-2.96743200	2.91671200	0.61569800
H	-3.11132100	1.36412100	-0.19302700
H	-2.98792400	1.42335300	1.57621200

27

T-BrU-ftb-gas-min285: Optimised twist = 288.08 deg.

O	2.85401500	-2.18992300	-0.80257900
C	1.67964200	-1.91805100	-0.67240200
N	0.94797800	-2.27372800	0.45128200
H	1.48786000	-2.68573200	1.20393000
N	0.93999800	-1.22561200	-1.61204200
H	1.46845400	-0.89004400	-2.41426600
C	-0.31646600	-1.81084300	0.69920100
H	-0.73780600	-2.08006100	1.66142600
C	-0.34631100	-0.69471800	-1.47146400
O	-0.83641100	-0.00387200	-2.33865300
C	-0.98111700	-1.05458600	-0.19653500
Br	-2.69041900	-0.40013100	0.14273200
C	0.36571500	2.26813100	-0.16657400
C	-0.32109900	2.12183600	0.98354600
N	0.10056300	1.29424300	2.00562200
C	1.22149200	0.49644200	1.92584000

N	1.95285200	0.70065600	0.77448700
C	1.61345200	1.51402800	-0.32075400
C	-0.08491800	3.10945000	-1.31981200
H	-1.25917200	2.63511500	1.16639400
H	-0.47386200	1.15310400	2.82638600
O	1.52073000	-0.32236200	2.77888800
O	2.32324000	1.52978300	-1.30794400
H	2.80548900	0.15202900	0.68014300
H	0.68899700	3.83073700	-1.59830700
H	-0.27723800	2.47330400	-2.19015100
H	-1.00275900	3.64809100	-1.07058900

27

T-BrU-ftb-gas-min85: Optimised twist = 102.41 deg.

O	-1.70355700	1.45838000	2.09832900
C	-0.66012200	1.02423900	1.64881800
N	-0.28241600	-0.30194700	1.77231100
H	-0.94610600	-0.89964400	2.24898000
N	0.25950000	1.78778900	0.96206600
H	0.01795000	2.76608900	0.83095700
C	0.84978000	-0.83209700	1.20116700
H	0.98667900	-1.90037100	1.31995400
C	1.46301300	1.37711500	0.36478300
O	2.17580000	2.17257000	-0.20048700
C	1.71429400	-0.06337800	0.51300400
Br	3.24164900	-0.76385000	-0.28387500
C	-2.84847000	-1.08949800	-0.14455900
C	-3.37709500	0.15003200	-0.19582800
N	-2.77471300	1.18609700	-0.87013800
C	-1.55798500	1.07903300	-1.51628800
N	-1.02763900	-0.19961000	-1.45792600
C	-1.54998100	-1.30780100	-0.78449700
C	-3.47544300	-2.24431000	0.57577000
H	-4.30800800	0.40423200	0.29981800
H	-3.15565500	2.12231100	-0.82364400
O	-1.00745100	2.01189500	-2.06188400
O	-0.91556600	-2.34873500	-0.72793000
H	-0.12316200	-0.32267600	-1.90634300
H	-3.67431200	-3.07099600	-0.11317900
H	-2.80549800	-2.63799500	1.34824900
H	-4.41450500	-1.94538900	1.04817600

27

T-BrU-ftb-water-max180: Optimised twist = 207.93 deg.

O	-3.07064300	-2.21283100	-0.68383700
C	-1.90437700	-1.87727600	-0.57330200
N	-1.19552800	-1.26907400	-1.58740100
H	-1.70037700	-1.10645200	-2.45214200
N	-1.17036700	-2.06203200	0.58120100
H	-1.66649900	-2.49922600	1.35387500
C	0.12014200	-0.91241700	-1.48359300
H	0.56621600	-0.47908000	-2.37164700
C	0.15081900	-1.69211600	0.82370000
O	0.65952500	-1.87755500	1.91639500
C	0.80433500	-1.08764800	-0.33388300
Br	2.61875900	-0.67904700	-0.19613100
C	-1.64600300	1.23793800	0.91085100
C	-0.52225600	1.29955800	1.65977100
N	0.65258600	1.83911900	1.19277400
C	0.79700700	2.36797300	-0.06695900

N	-0.34833600	2.27828700	-0.83303500
C	-1.58761500	1.76436800	-0.44981900
C	-2.95236600	0.70169500	1.41446400
H	-0.47966900	0.92483400	2.67711700
H	1.47600400	1.86060300	1.78352400
O	1.83308300	2.86996500	-0.47491000
O	-2.52339400	1.76817900	-1.24075500
H	-0.28377700	2.66528300	-1.77085900
H	-3.69665000	1.50217300	1.48404700
H	-3.35892900	-0.05701700	0.73840600
H	-2.82805800	0.25690500	2.40496200

27

T-BrU-ftb-water-max240-minus: Optimised twist = 257.26 deg.

O	-3.25559400	-1.80373800	-1.14034400
C	-2.08284600	-1.57899900	-0.90611300
N	-1.22385800	-1.00531500	-1.82123900
H	-1.62255300	-0.77090500	-2.72380700
N	-1.47951800	-1.88257900	0.30000300
H	-2.08287500	-2.31883700	0.99260000
C	0.10755100	-0.79721200	-1.58446600
H	0.67605300	-0.37440200	-2.40544800
C	-0.14529600	-1.71068300	0.66087600
O	0.25270300	-2.05276000	1.76123000
C	0.66303500	-1.10011300	-0.39301500
Br	2.48882600	-0.89209300	-0.07387300
C	-0.70040000	1.32649500	1.54105600
C	0.59036300	1.71007300	1.42554600
N	1.10186200	2.24796900	0.26838700
C	0.36387900	2.44176900	-0.87234000
N	-0.96113600	2.08092800	-0.73550800
C	-1.56442300	1.49029600	0.37504900
C	-1.28820500	0.73574900	2.78586000
H	1.30304200	1.60894900	2.23710900
H	2.08601300	2.48374600	0.20936200
O	0.82817500	2.89114300	-1.91008900
O	-2.73957000	1.14647900	0.31944800
H	-1.54347900	2.20955100	-1.55887300
H	-2.09869400	1.36437900	3.16874600
H	-1.71041000	-0.25466500	2.58685000
H	-0.52509700	0.63517900	3.56084000

27

T-BrU-ftb-water-max240: Optimised twist = 263.69 deg.

O	-2.78938900	-2.35980900	-1.18701000
C	-1.68349800	-1.90917800	-0.95168400
N	-0.97920600	-1.12727300	-1.84400100
H	-1.43442200	-0.94097200	-2.73087000
N	-1.00982400	-2.13591400	0.23394000
H	-1.50033300	-2.71376100	0.91180700
C	0.28470000	-0.65708800	-1.60808600
H	0.73452700	-0.08224300	-2.41017100
C	0.27041700	-1.71687100	0.58724500
O	0.75429800	-2.02609400	1.66246200
C	0.91556900	-0.90306800	-0.44170600
Br	2.66111500	-0.33259700	-0.12269000
C	-0.85288900	1.10128800	1.61649400
C	0.29297300	1.76651500	1.34928600
N	0.51885500	2.40016900	0.15005500
C	-0.38771700	2.42386900	-0.88079300

N	-1.56813000	1.77355100	-0.58694400
C	-1.87873600	1.07034700	0.57726300
C	-1.12972000	0.39443800	2.90790000
H	1.10927300	1.82982100	2.06072500
H	1.40649200	2.85790300	-0.02388500
O	-0.17634500	2.96666900	-1.95568300
O	-2.94991000	0.48199800	0.66622800
H	-2.26582400	1.76537900	-1.32638100
H	-1.99200300	0.83785600	3.41641400
H	-1.36141600	-0.66110100	2.73134400
H	-0.26297900	0.45065900	3.57032700

27

T-BrU-ftb-water-max240-plus: Optimised twist = 291.00 deg.

O	3.25972900	-1.94293700	-0.62255800
C	2.06980100	-1.74252000	-0.45145900
N	1.43720000	-1.94302200	0.75774900
H	2.01831700	-2.27272700	1.52118100
N	1.22887200	-1.28970400	-1.44696400
H	1.66695300	-1.11582200	-2.34812500
C	0.11300600	-1.68029700	0.97012100
H	-0.25495100	-1.87751900	1.97088600
C	-0.12665400	-0.98173100	-1.35200700
O	-0.74318500	-0.57912000	-2.32391700
C	-0.67146900	-1.18936000	-0.01290200
Br	-2.48766700	-0.86685000	0.25179100
C	-0.22617500	2.21057500	-0.47602400
C	-0.84018000	2.10424500	0.72292600
N	-0.22126900	1.57097200	1.82898700
C	1.06849700	1.10150100	1.82441800
N	1.69591300	1.23003900	0.60156000
C	1.15831400	1.76158500	-0.57485300
C	-0.88289000	2.75741600	-1.70576700
H	-1.86560700	2.41992100	0.88047900
H	-0.72113100	1.49410900	2.70775900
O	1.60947700	0.60007300	2.79959900
O	1.84126100	1.80196700	-1.59064500
H	2.67134800	0.94295800	0.57149900
H	-0.32787100	3.61662100	-2.09540100
H	-0.90947500	1.99382100	-2.49027700
H	-1.90601000	3.07205200	-1.48656200

27

T-BrU-ftb-water-max5: Optimised twist = 339.80 deg.

O	1.86349800	2.60617000	0.14786400
C	0.81957300	1.99091100	0.02150400
N	0.32022100	1.59153700	-1.20055400
H	0.86245100	1.85820800	-2.01578300
N	0.02906800	1.61297200	1.08807900
H	0.37641400	1.87347900	2.00797300
C	-0.86712100	0.92886200	-1.35371600
H	-1.15042100	0.69811200	-2.37425100
C	-1.19227000	0.94160700	1.05917500
O	-1.79443200	0.69878400	2.09088800
C	-1.62267800	0.58580100	-0.29052200
Br	-3.25893300	-0.28626500	-0.48821200
C	0.88605500	-1.73039500	0.09946900
C	1.35796600	-1.64085700	-1.16330100
N	2.51135400	-0.96187800	-1.47931900
C	3.28876000	-0.31216200	-0.55078000

N 2.78650200 -0.39076400 0.73226200  
C 1.64331700 -1.06819600 1.15786500  
C -0.36288100 -2.46863200 0.47555300  
H 0.85136300 -2.09825100 -2.00673200  
H 2.83951100 -0.93210900 -2.43781800  
O 4.32084800 0.27846600 -0.83006300  
O 1.33290300 -1.06107500 2.34291300  
H 3.32333500 0.09439600 1.44639500  
H -0.12576200 -3.35847400 1.06866500  
H -1.01833500 -1.84045300 1.08786300  
H -0.91276600 -2.77907200 -0.41647000  
27

T-BrU-ftb-water-max70: Optimised twist = 86.28 deg.

O -3.66274900 -1.33702400 -0.72699500  
C -2.45210100 -1.34355700 -0.59021400  
N -1.57248500 -1.20097600 -1.64396600  
H -1.98723800 -1.10540100 -2.56465000  
N -1.82978900 -1.49165500 0.63266600  
H -2.44842500 -1.60600500 1.43178400  
C -0.21347200 -1.19901000 -1.49997200  
H 0.35953400 -1.10504500 -2.41545400  
C -0.46227100 -1.48041100 0.90630900  
O -0.05472600 -1.61852400 2.04647700  
C 0.36378500 -1.29803600 -0.28441000  
Br 2.21492700 -1.35897000 -0.07434600  
C -0.12794700 2.07060600 -1.06309100  
C -1.36582000 1.92879500 -0.54385200  
N -1.58413000 1.71401400 0.79874500  
C -0.57831100 1.64539800 1.73355500  
N 0.68378200 1.76982200 1.18900400  
C 1.00822800 2.02297700 -0.14516100  
C 0.14670800 2.27865800 -2.52090900  
H -2.26301100 1.96891200 -1.15303300  
H -2.52954000 1.64243000 1.15781200  
O -0.78154400 1.48760000 2.92738100  
O 2.17638900 2.18692600 -0.47179300  
H 1.45619900 1.73115100 1.84874700  
H 0.63481000 3.24318100 -2.69335100  
H 0.82236000 1.50475800 -2.90126600  
H -0.78054800 2.24716100 -3.09769700  
27

T-BrU-ftb-water-min150: Optimised twist = 111.98 deg.

O 3.26927900 -2.02763200 -0.75274100  
C 2.08663500 -1.80428900 -0.56376800  
N 1.42684700 -2.15588500 0.59507000  
H 1.97886000 -2.63984200 1.29538200  
N 1.27740300 -1.17821300 -1.49112900  
H 1.72881100 -0.91264900 -2.36309000  
C 0.10300300 -1.89988100 0.82193100  
H -0.29375700 -2.24882300 1.76878500  
C -0.06675100 -0.83549400 -1.36144500  
O -0.64944700 -0.25244700 -2.26012700  
C -0.64879600 -1.24148100 -0.08497600  
Br -2.46821900 -0.93689000 0.17824700  
C 1.33915700 1.21400700 1.24739000  
C 1.95314200 1.51902900 0.08371700  
N 1.28971300 2.09788100 -0.97443900  
C -0.04113500 2.44203800 -0.94262200

N	-0.66675800	2.09413400	0.23783000
C	-0.08537100	1.51848300	1.36716700
C	2.02890800	0.60579200	2.43026300
H	3.00743200	1.32625800	-0.08738500
H	1.78984100	2.32804400	-1.82550400
O	-0.61511500	3.00269300	-1.86266400
O	-0.76370000	1.29771300	2.36247400
H	-1.65814200	2.31158800	0.29532300
H	2.07037900	1.31549700	3.26327900
H	1.48397600	-0.27419300	2.78697500
H	3.04894500	0.30798400	2.17477100

27

T-BrU-ftb-water-min210: Optimised twist = 223.09 deg.

O	-2.78866700	-2.30750800	-0.99057600
C	-1.65279900	-1.91100200	-0.80106100
N	-0.94598800	-1.16774000	-1.72340400
H	-1.42712500	-0.95693400	-2.59106700
N	-0.94949300	-2.16382200	0.36030200
H	-1.43992800	-2.71312600	1.06174500
C	0.33009500	-0.71997600	-1.51809600
H	0.77931800	-0.17383400	-2.34010100
C	0.32326400	-1.71646000	0.70505700
O	0.80048900	-1.97446800	1.79689300
C	0.97214900	-0.94525700	-0.35282800
Br	2.73438800	-0.40026400	-0.07752600
C	-1.66538100	0.97803200	1.14204000
C	-0.45936400	1.26039700	1.68426000
N	0.50366500	1.97882200	1.01688300
C	0.35556000	2.43192800	-0.27124400
N	-0.88432500	2.15408800	-0.81127700
C	-1.93516700	1.46148700	-0.20920000
C	-2.74550900	0.22044600	1.85346200
H	-0.18015400	0.93785300	2.68200900
H	1.40850600	2.13936600	1.44496900
O	1.23070500	3.02587000	-0.88303600
O	-2.98219400	1.28585100	-0.82053000
H	-1.04105700	2.49140500	-1.75754800
H	-3.59036000	0.87607800	2.08981700
H	-3.13285800	-0.58835500	1.22502600
H	-2.36668700	-0.20817300	2.78468000

27

T-BrU-ftb-water-min285: Optimised twist = 291.00 deg.

O	3.25970300	-1.94296900	-0.62256300
C	2.06977700	-1.74253900	-0.45146200
N	1.43717200	-1.94304500	0.75774400
H	2.01829300	-2.27273100	1.52118100
N	1.22885400	-1.28971000	-1.44696500
H	1.66693900	-1.11583300	-2.34812600
C	0.11298100	-1.68030700	0.97011500
H	-0.25498200	-1.87753100	1.97087700
C	-0.12666800	-0.98172800	-1.35201200
O	-0.74319300	-0.57911000	-2.32392200
C	-0.67148900	-1.18936000	-0.01290800
Br	-2.48768300	-0.86683100	0.25178500
C	-0.22613500	2.21060800	-0.47600700
C	-0.84014000	2.10427800	0.72294300
N	-0.22124200	1.57097500	1.82899600
C	1.06851500	1.10147500	1.82441800



N	1.69593100	1.23002000	0.60156400
C	1.15833600	1.76157100	-0.57485000
C	-0.88284100	2.75747900	-1.70574300
H	-1.86555800	2.41998000	0.88050100
H	-0.72110700	1.49410100	2.70776600
O	1.60948500	0.60002300	2.79959300
O	1.84127600	1.80192300	-1.59064700
H	2.67135800	0.94290900	0.57149300
H	-0.32779300	3.61666400	-2.09538000
H	-0.90946300	1.99388900	-2.49025700
H	-1.90594700	3.07215600	-1.48652900

27

T-BrU-ftb-water-min315: Optimised twist = 291.00 deg.

O	3.25968100	-1.94299600	-0.62257600
C	2.06975800	-1.74255700	-0.45147100
N	1.43715600	-1.94305900	0.75773700
H	2.01827800	-2.27274200	1.52117400
N	1.22883400	-1.28972400	-1.44697100
H	1.66691500	-1.11584700	-2.34813200
C	0.11296800	-1.68030800	0.97011500
H	-0.25499200	-1.87753100	1.97087900
C	-0.12668300	-0.98172400	-1.35200800
O	-0.74320600	-0.57909000	-2.32391300
C	-0.67150100	-1.18935500	-0.01290400
Br	-2.48769000	-0.86681200	0.25179800
C	-0.22612800	2.21060100	-0.47600500
C	-0.84012000	2.10427000	0.72295100
N	-0.22120700	1.57097300	1.82900000
C	1.06854800	1.10147200	1.82440900
N	1.69595200	1.23001300	0.60154600
C	1.15834500	1.76156700	-0.57486000
C	-0.88284900	2.75746200	-1.70573700
H	-1.86553700	2.41996900	0.88052000
H	-0.72106100	1.49410800	2.70777700
O	1.60953100	0.60002700	2.79957900
O	1.84127500	1.80192300	-1.59066400
H	2.67138000	0.94290600	0.57146500
H	-0.32776600	3.61660000	-2.09542800
H	-0.90954500	1.99384500	-2.49022000
H	-1.90592900	3.07220700	-1.48649600

27

T-BrU-ftb-water-min45: Optimised twist = 58.42 deg.

O	-2.08652400	2.81378800	0.24220300
C	-1.03201400	2.21426600	0.12872700
N	-0.05746300	2.20417400	1.10410500
H	-0.25085800	2.74870000	1.93798100
N	-0.70369800	1.46948000	-0.98740900
H	-1.37532600	1.50341500	-1.75178500
C	1.11249400	1.50696700	0.99590300
H	1.78981200	1.58456600	1.83851300
C	0.46296700	0.73936900	-1.22141400
O	0.62720300	0.15635400	-2.27884600
C	1.38773100	0.75664600	-0.09224300
Br	2.98790200	-0.18419400	-0.24810000
C	-0.88340200	-1.18033200	1.43645100
C	-2.00562200	-0.43354300	1.52868800
N	-2.89530300	-0.29945300	0.48730600
C	-2.70844300	-0.87369600	-0.74591700

N	-1.57962500	-1.66167000	-0.82074000
C	-0.62771000	-1.87585600	0.17720400
C	0.10540300	-1.34339900	2.54999000
H	-2.27103900	0.11034500	2.42945600
H	-3.70090700	0.30898800	0.58114600
O	-3.46398300	-0.69906000	-1.69158100
O	0.33820100	-2.59528800	-0.04152100
H	-1.40025900	-2.09588200	-1.72224700
H	0.12200800	-2.37719400	2.91071200
H	1.11796900	-1.10758900	2.20427200
H	-0.14293100	-0.68517500	3.38625000

27

T-BrU-ftb-water-min90: Optimised twist = 111.98 deg.

O	3.26931900	-2.02757300	-0.75272100
C	2.08667000	-1.80425400	-0.56374800
N	1.42689600	-2.15583800	0.59510100
H	1.97892100	-2.63978000	1.29541500
N	1.27742100	-1.17821900	-1.49112100
H	1.72881800	-0.91267000	-2.36309200
C	0.10304600	-1.89986400	0.82196000
H	-0.29370200	-2.24879900	1.76882200
C	-0.06673900	-0.83552000	-1.36143600
O	-0.64945100	-0.25250000	-2.26012500
C	-0.64877000	-1.24149700	-0.08495600
Br	-2.46819700	-0.93693100	0.17826900
C	1.33913800	1.21405900	1.24737100
C	1.95310600	1.51905600	0.08368200
N	1.28965500	2.09786400	-0.97448500
C	-0.04119700	2.44200400	-0.94266200
N	-0.66680000	2.09412700	0.23780700
C	-0.08539300	1.51851500	1.36715400
C	2.02891300	0.60588700	2.43025200
H	3.00739700	1.32629500	-0.08742500
H	1.78977400	2.32802100	-1.82555800
O	-0.61519600	3.00262200	-1.86271400
O	-0.76371000	1.29776000	2.36247300
H	-1.65818700	2.31156800	0.29530500
H	2.07037000	1.31561000	3.26325300
H	1.48400900	-0.27410700	2.78698600
H	3.04895700	0.30810300	2.17475900

27

T-U-ftb-gas-max0: Optimised twist = 349.34 deg.

O	-0.87031700	-2.46922600	-1.00193600
C	-1.38015800	-1.44598100	-0.60121700
N	-2.20924600	-1.40898700	0.51544800
H	-2.40102500	-2.31052900	0.93241700
N	-1.20251600	-0.20969800	-1.18788400
H	-0.58932000	-0.18974300	-1.99833500
C	-2.80472800	-0.26099400	0.98241600
H	-3.44496400	-0.39015100	1.84846100
C	-1.73009700	1.02432800	-0.77338700
O	-1.45763300	2.04181500	-1.37608100
C	-2.59623700	0.93488200	0.40144900
H	-3.05596200	1.84340600	0.76547300
C	1.06459000	1.25847800	0.83087100
C	0.72710100	0.19111800	1.58075300
N	1.10921100	-1.09771400	1.26493300
C	1.92281200	-1.41645800	0.18947800

N	2.19871300	-0.32163700	-0.61125500
C	1.87691300	1.02262100	-0.37174400
C	0.66707200	2.67037000	1.13531600
H	0.12608900	0.28542100	2.48037200
H	0.88880700	-1.87475000	1.87340500
O	2.34233100	-2.53312600	-0.01962600
O	2.26179500	1.88977000	-1.13065600
H	2.80202000	-0.50495900	-1.40735300
H	1.55276600	3.29486500	1.28873900
H	0.10892900	3.09627900	0.29557000
H	0.04651600	2.71236900	2.03535400

27

T-U-ftb-gas-max120: Optimised twist = 133.97 deg.

O	-0.23092900	-1.88768800	-1.74222700
C	-0.89772500	-1.40816700	-0.84481800
N	-0.65030700	-1.65376400	0.49379700
H	0.16653600	-2.21659800	0.69967400
N	-1.96635200	-0.56016400	-1.05278500
H	-2.20484800	-0.38054700	-2.02307200
C	-1.34764900	-1.05842200	1.51925500
H	-0.98874400	-1.30211900	2.51313700
C	-2.78637600	0.05493300	-0.08700800
O	-3.71912500	0.74892500	-0.43340400
C	-2.38533200	-0.23186700	1.28829900
H	-2.94538300	0.23052900	2.08926100
C	2.25091500	-0.28672100	-0.24368600
C	1.98883600	0.49906800	-1.30797400
N	1.23512700	1.64676200	-1.21878400
C	0.67304500	2.10634000	-0.04169100
N	0.94290600	1.28159600	1.03777700
C	1.66146900	0.08558500	1.04137600
C	3.02924600	-1.56392500	-0.32423800
H	2.34379000	0.25581100	-2.30388800
H	1.04904100	2.21490500	-2.03505500
O	0.01251700	3.11967500	0.03447600
O	1.72961100	-0.58650200	2.06097500
H	0.51495100	1.56061800	1.91548800
H	3.82100400	-1.58576200	0.42987400
H	2.38414200	-2.43179900	-0.14628400
H	3.47473200	-1.68226800	-1.31481100

27

T-U-ftb-gas-max245: Optimised twist = 209.98 deg.

O	0.00746600	-2.32316600	-1.30054400
C	0.79228700	-1.44405900	-1.01444300
N	0.96341500	-0.30190600	-1.78186500
H	0.37460100	-0.24617600	-2.60363600
N	1.59966200	-1.46988000	0.10687500
H	1.46601700	-2.26893800	0.71904900
C	1.83702300	0.70916200	-1.45738400
H	1.86219000	1.54351000	-2.14916500
C	2.41714500	-0.43884100	0.59238200
O	2.89363800	-0.51528000	1.71116600
C	2.58180500	0.67221800	-0.33590700
H	3.23950700	1.48434400	-0.05886600
C	-1.79322200	-0.53311800	0.86474200
C	-0.77869500	-0.03922600	1.60130600
N	-0.17444100	1.17351400	1.32849000
C	-0.52747000	1.97879500	0.26618000

N	-1.59799500	1.48426100	-0.45361800
C	-2.27728200	0.27066700	-0.26428600
C	-2.43987800	-1.86386500	1.09457200
H	-0.35855500	-0.57310900	2.44851300
H	0.62567000	1.48331300	1.86743300
O	0.05105900	3.01105000	-0.01712900
O	-3.18615100	-0.04119500	-1.00837100
H	-1.91997000	2.06628600	-1.22058000
H	-3.51948200	-1.75095900	1.23114700
H	-2.28230600	-2.50928500	0.22469700
H	-2.02052500	-2.35256400	1.97828700

27

T-U-ftb-gas-min185: Optimised twist = 181.94 deg.

O	-3.45879900	0.73748400	0.14278200
C	-2.52661300	0.06798400	-0.24947200
N	-1.77402900	0.39745400	-1.36512000
H	-2.00331500	1.28348000	-1.79912900
N	-2.10090700	-1.09217600	0.37168700
H	-2.60561500	-1.34435000	1.21593500
C	-0.71344500	-0.35081900	-1.81054800
H	-0.22004300	0.03286900	-2.69713800
C	-0.97302800	-1.86361700	0.06093000
O	-0.61440300	-2.75290900	0.81335100
C	-0.30963000	-1.46957600	-1.17580800
H	0.53632100	-2.05300500	-1.51617900
C	0.48352000	1.21168000	1.04478300
C	0.86988900	0.04860700	1.60950300
N	1.87038500	-0.74137600	1.08867700
C	2.55608700	-0.43412300	-0.06887000
N	2.20209800	0.79602500	-0.59753300
C	1.13562000	1.60989800	-0.20581000
C	-0.59538200	2.09798800	1.58984300
H	0.40129600	-0.34388300	2.50686300
H	2.01220800	-1.68094500	1.44088900
O	3.38266300	-1.16524800	-0.57546100
O	0.80141400	2.55897600	-0.89610800
H	2.67158200	1.04905200	-1.46150200
H	-0.18384000	3.06495400	1.89719200
H	-1.35824800	2.30305300	0.83285400
H	-1.08227800	1.63471500	2.45242700

27

T-U-ftb-gas-min290: Optimised twist = 288.15 deg.

O	-2.58613900	-0.40138800	1.74820800
C	-2.14138900	-0.52291600	0.62420900
N	-2.40232200	0.39475800	-0.38207100
H	-2.90196100	1.22367800	-0.08187300
N	-1.32338600	-1.56235300	0.22986000
H	-1.04317400	-2.19527500	0.97580600
C	-1.75239300	0.38264700	-1.59038700
H	-1.98886400	1.21232200	-2.24755200
C	-0.58491400	-1.65052800	-0.95981200
O	0.22967600	-2.54051600	-1.11580200
C	-0.88370900	-0.59276800	-1.92219200
H	-0.37175100	-0.61146000	-2.87452700
C	2.22063300	-0.07320300	0.10897300
C	2.22370100	0.94380500	-0.77397100
N	1.30656500	1.97608900	-0.72792000
C	0.26470000	2.02923200	0.17343400

N	0.31484900	1.02772400	1.12013000
C	1.20161900	-0.06067900	1.16446300
C	3.15556200	-1.24136000	0.06498300
H	2.94457600	1.00566500	-1.58272800
H	1.29992600	2.69779300	-1.43622700
O	-0.61489100	2.87229700	0.12590100
O	1.07516700	-0.91455700	2.02072800
H	-0.42120100	1.03596800	1.82484100
H	3.67674800	-1.35477600	1.02005000
H	2.58865600	-2.16059200	-0.11636300
H	3.89374200	-1.11892400	-0.73190700

27

T-U-ftb-gas-min75: Optimised twist = 71.42 deg.

O	1.52678000	-1.46503800	-1.95911000
C	1.65983100	-0.84079400	-0.92225500
N	2.30524800	0.38312700	-0.86687100
H	2.67083900	0.71603500	-1.74921200
N	1.17977700	-1.26402700	0.29754200
H	0.70401700	-2.16540200	0.30527500
C	2.35807000	1.16062400	0.26734400
H	2.85363100	2.11799500	0.14958200
C	1.17513600	-0.55091100	1.51295400
O	0.64676700	-1.02795400	2.49561300
C	1.82363400	0.75510000	1.43365000
H	1.83826900	1.37022600	2.32263000
C	-1.07035000	1.39110900	-0.77512400
C	-1.06327600	0.40031900	-1.68942600
N	-1.44482900	-0.88873600	-1.39135100
C	-1.74236600	-1.30810000	-0.10771600
N	-1.84268900	-0.27237200	0.79947900
C	-1.48421100	1.06538700	0.59599400
C	-0.65620700	2.80236100	-1.05522800
H	-0.75175200	0.55767600	-2.71748800
H	-1.24882200	-1.63541500	-2.04772400
O	-1.88570900	-2.47958600	0.18533000
O	-1.51368100	1.86319600	1.51405100
H	-1.99211200	-0.55407900	1.76541200
H	-1.48047300	3.49632000	-0.86313700
H	0.16345500	3.09797400	-0.39093100
H	-0.33441200	2.91721200	-2.09422800

27

T-U-ftb-water-max0: Optimised twist = 331.88 deg.

O	0.25422000	-2.44268300	-1.10637900
C	-0.51123600	-1.78826800	-0.41650200
N	-0.48825000	-1.80692100	0.96157800
H	0.19620100	-2.42189400	1.38777200
N	-1.46849500	-0.94597900	-0.94060000
H	-1.48985700	-0.87707400	-1.95486300
C	-1.37620300	-1.10980300	1.74182600
H	-1.25302200	-1.24056700	2.81050900
C	-2.41082800	-0.18693700	-0.23993000
O	-3.20766100	0.51172600	-0.85336900
C	-2.32599500	-0.31677500	1.20414300
H	-3.02183800	0.23768300	1.81875700
C	0.42302600	1.72844400	0.40160600
C	1.13702900	1.20988400	1.42453800
N	2.12880600	0.27526500	1.24088700
C	2.47934400	-0.22614000	0.01077600

N	1.73840100	0.30253000	-1.02590100
C	0.72797000	1.26124100	-0.94719700
C	-0.65772500	2.75180300	0.57534000
H	0.96827200	1.50013500	2.45609100
H	2.64601400	-0.08349200	2.03516500
O	3.35919400	-1.05830400	-0.15248100
O	0.16096300	1.63748100	-1.96637800
H	1.94772500	-0.06693700	-1.94947200
H	-0.39334200	3.68621100	0.06927400
H	-1.60018700	2.40237700	0.14110500
H	-0.81922400	2.96284100	1.63515400

27

T-U-ftb-water-max120: Optimised twist = 112.67 deg.

O	1.47419600	0.96755800	-2.26528300
C	1.60586300	0.39184400	-1.19689400
N	2.14550900	0.98809100	-0.07840200
H	2.46208700	1.94429200	-0.19241900
N	1.21710600	-0.91590500	-0.99277800
H	0.83644600	-1.39364000	-1.80568900
C	2.30158200	0.34200100	1.12166900
H	2.73408600	0.94044200	1.91461100
C	1.35890300	-1.67442000	0.17594200
O	0.99950000	-2.84420600	0.18824300
C	1.93301200	-0.94477600	1.29132200
H	2.05207900	-1.45104000	2.23926000
C	-1.11110600	1.58598800	0.03813100
C	-1.53183100	1.05646800	-1.13146200
N	-1.93731700	-0.25180200	-1.24856400
C	-1.97527200	-1.13361000	-0.19452600
N	-1.50893300	-0.59445400	0.98719200
C	-1.09503900	0.72035400	1.21313500
C	-0.68411900	3.01317400	0.19953200
H	-1.57002400	1.63188800	-2.04991600
H	-2.27151300	-0.60519200	-2.13795300
O	-2.37845900	-2.28255900	-0.29285700
O	-0.74866200	1.06886600	2.33520900
H	-1.52069100	-1.21545900	1.79209400
H	-1.38125800	3.55788700	0.84497100
H	0.30258700	3.07458800	0.66921700
H	-0.64290900	3.51531600	-0.76990500

27

T-U-ftb-water-max190: Optimised twist = 197.99 deg.

O	0.57326000	-2.87703200	-0.29911300
C	1.06648800	-1.76367800	-0.38135800
N	1.11259300	-1.04504700	-1.55635300
H	0.70352500	-1.49255600	-2.36905300
N	1.62613200	-1.10545700	0.69364500
H	1.58484200	-1.59912900	1.58138400
C	1.64835000	0.21403200	-1.64940600
H	1.61070200	0.66012900	-2.63651000
C	2.16259100	0.18513300	0.71514400
O	2.56716900	0.65980000	1.76893200
C	2.17152300	0.84671700	-0.57806100
H	2.57839600	1.84605300	-0.64952800
C	-1.71861600	-0.43709800	0.84979000
C	-1.14978900	0.51589100	1.62008300
N	-0.70735400	1.71661900	1.11380400
C	-0.82365800	2.07280700	-0.20741100

N	-1.39516100	1.09007200	-0.98890200
C	-1.85270300	-0.16378600	-0.57865000
C	-2.20006800	-1.75674100	1.37272400
H	-0.99871300	0.38805100	2.68667200
H	-0.28282800	2.40279000	1.72738900
O	-0.45039300	3.14765100	-0.65288300
O	-2.31649200	-0.94264000	-1.40260400
H	-1.48943100	1.30921600	-1.97714600
H	-3.26784800	-1.88789100	1.17016100
H	-1.66517500	-2.57932400	0.88790100
H	-2.04000100	-1.82252900	2.45160000

27

T-U-ftb-water-max240: Optimised twist = 231.16 deg.

O	-3.13517300	0.12991500	-1.36515400
C	-2.32568600	-0.37137600	-0.60285000
N	-1.55554000	-1.46737600	-0.92986000
H	-1.68427200	-1.83950200	-1.86385800
N	-2.09625000	0.10201600	0.67295200
H	-2.65664900	0.90217400	0.95380200
C	-0.67732000	-2.05955800	-0.06041000
H	-0.15407000	-2.92545200	-0.45043700
C	-1.21346600	-0.41202900	1.62822400
O	-1.11729600	0.12847100	2.72265000
C	-0.47822400	-1.58425500	1.18761500
H	0.21809500	-2.05136700	1.87097200
C	0.81302300	1.64059700	0.05132100
C	1.63541100	1.18292000	1.02041200
N	2.41148200	0.05883500	0.86339200
C	2.42312500	-0.70219900	-0.27935000
N	1.59886600	-0.21498500	-1.27212200
C	0.75241700	0.89164000	-1.19958700
C	-0.04301000	2.86221100	0.18919000
H	1.72795200	1.67193200	1.98411500
H	2.99961500	-0.26555900	1.62250400
O	3.09580900	-1.71481000	-0.40906100
O	0.02471400	1.16753700	-2.14645400
H	1.57720200	-0.75274600	-2.13454500
H	0.27717400	3.64400000	-0.50765300
H	-1.08745600	2.63199200	-0.04451600
H	0.01045100	3.25849000	1.20582900

27

T-U-ftb-water-min160: Optimised twist = 174.99 deg.

O	3.43461900	0.85122900	-0.28786000
C	2.53215400	0.16123100	0.15808900
N	1.83248900	0.48403800	1.30124800
H	2.11707800	1.33492900	1.77328800
N	2.11213300	-1.00984400	-0.43635600
H	2.59594000	-1.26898800	-1.29201800
C	0.83161500	-0.29645800	1.81959100
H	0.37988200	0.07783100	2.73157100
C	1.08449100	-1.85682000	-0.01193600
O	0.79349300	-2.84307800	-0.67698400
C	0.44001500	-1.44139800	1.22131700
H	-0.35398800	-2.05468000	1.62677200
C	-0.55887000	1.26188300	-0.95848800
C	-0.83229500	0.10101000	-1.59268000
N	-1.77665900	-0.78867700	-1.13724300
C	-2.52290800	-0.58760500	-0.00236800

N	-2.25780500	0.61252100	0.62368100
C	-1.30323300	1.56213000	0.26139300
C	0.45797700	2.25435500	-1.43475200
H	-0.31609700	-0.20253300	-2.49772800
H	-1.92161600	-1.66860000	-1.61946700
O	-3.34442300	-1.39073400	0.41527900
O	-1.13645600	2.55832000	0.95541300
H	-2.78330900	0.79339900	1.47463000
H	-0.02308000	3.19208200	-1.73232400
H	1.17201700	2.49498500	-0.64075700
H	1.01052400	1.85944500	-2.29106500

27

T-U-ftb-water-min205: Optimised twist = 215.26 deg.

O	-3.00180500	1.25239600	-0.62548800
C	-2.25053000	0.29016200	-0.64097100
N	-1.41724600	0.00075700	-1.69972800
H	-1.44919300	0.64581000	-2.48117300
N	-2.15472000	-0.60719100	0.40172500
H	-2.74531700	-0.41456500	1.20644200
C	-0.56736600	-1.07477900	-1.71915400
H	0.02343200	-1.18121200	-2.62187700
C	-1.28976300	-1.70050900	0.50342600
O	-1.26832800	-2.36831800	1.52964700
C	-0.47450100	-1.92731600	-0.67685000
H	0.20470500	-2.76918300	-0.68775600
C	0.57427600	1.09939900	1.18106500
C	1.19207600	-0.00332800	1.65905700
N	2.13242000	-0.69919900	0.93674500
C	2.51433800	-0.35755900	-0.33712400
N	1.89641200	0.78250400	-0.80880000
C	0.93717800	1.55792300	-0.15662100
C	-0.44864900	1.88125700	1.94846400
H	0.97858500	-0.40880100	2.64220200
H	2.55460800	-1.53670600	1.32151300
O	3.32287000	-0.99713400	-0.99379800
O	0.45874700	2.53775600	-0.71541200
H	2.16050000	1.07384100	-1.74629100
H	-0.07893800	2.88579700	2.17961700
H	-1.36716600	2.00157300	1.36423900
H	-0.69350000	1.37625500	2.88615400

27

T-U-ftb-water-min285: Optimised twist = 291.79 deg.

O	-2.87726800	-0.30945800	1.57434800
C	-2.27276800	-0.41112700	0.51722900
N	-2.34150700	0.53486200	-0.48128800
H	-2.91844400	1.34620500	-0.28941400
N	-1.45318400	-1.47741600	0.21880300
H	-1.35216500	-2.17417100	0.95225600
C	-1.59251400	0.47349800	-1.62809300
H	-1.71814900	1.30822200	-2.30804500
C	-0.64113400	-1.63325000	-0.90824700
O	0.08554300	-2.61408900	-1.00503300
C	-0.75456600	-0.55553300	-1.87581000
H	-0.15581300	-0.59864100	-2.77549600
C	2.19314900	-0.20269600	0.12482200
C	2.26151500	0.81001800	-0.76694600
N	1.41803400	1.89544100	-0.72574700
C	0.42141600	2.04614100	0.20489600



N	0.36235400	1.01244000	1.11780300
C	1.18197500	-0.11778500	1.17379300
C	3.08398200	-1.40634700	0.09615000
H	2.98514600	0.82546100	-1.57465400
H	1.49433600	2.62772200	-1.42236600
O	-0.35156100	2.99355700	0.22345800
O	1.00422200	-0.95338000	2.05162500
H	-0.33190000	1.11093200	1.85533800
H	3.63963600	-1.50272500	1.03423800
H	2.48546700	-2.31403000	-0.03314600
H	3.79819900	-1.33681400	-0.72764900

27

T-U-ftb-water-min60: Optimised twist = 66.48 deg.

O	1.60905800	-2.00933100	-1.48978100
C	1.67989700	-1.13860200	-0.63678700
N	2.36303700	0.04352300	-0.81920900
H	2.82712100	0.15689800	-1.71346100
N	1.06803300	-1.24189500	0.59549100
H	0.59098800	-2.12181500	0.78003400
C	2.42219700	1.03341100	0.12630800
H	2.99438000	1.90910500	-0.15674000
C	1.06635500	-0.29506300	1.62714500
O	0.46547500	-0.53183400	2.66689300
C	1.80152300	0.91800900	1.31977900
H	1.84126200	1.70418500	2.06112500
C	-0.86933600	1.31152700	-0.99263100
C	-0.88608700	0.20108300	-1.76231600
N	-1.40622300	-0.99514300	-1.32628400
C	-1.90432000	-1.18554300	-0.06140500
N	-1.93147200	-0.03665900	0.69886800
C	-1.43932500	1.22082600	0.34943600
C	-0.31268300	2.62828700	-1.43903000
H	-0.48406500	0.18423000	-2.77011000
H	-1.33515800	-1.82190000	-1.90856200
O	-2.28115600	-2.27159900	0.35754800
O	-1.50026300	2.14599600	1.14980200
H	-2.27066700	-0.14434300	1.65105400
H	-1.09676200	3.39191100	-1.47047000
H	0.45322100	2.98033900	-0.74018700
H	0.13180700	2.54314800	-2.43344000

24

BrU-BrU-ftf-gas-max125: Optimised twist = 161.52 deg.

O	-2.22133600	4.11050800	0.58252000
C	-2.28810100	2.91625500	0.40064100
N	-3.36353900	2.30639100	-0.23068700
H	-4.10025300	2.93357000	-0.52792900
N	-1.31212500	2.01694900	0.79216500
H	-0.50285600	2.42056700	1.25708100
C	-3.45596900	0.95545900	-0.44862800
H	-4.35223600	0.61441600	-0.95442100
C	-1.29999900	0.63025200	0.63402800
O	-0.36947000	-0.03431700	1.03909800
C	-2.48727200	0.10774700	-0.05303900
Br	-2.58037600	-1.72998800	-0.32688600
C	2.37857500	-0.13486200	-0.34549800
C	2.51641600	-0.74185000	0.98593200
N	1.85160000	-1.96532500	1.10237800
C	0.99173600	-2.55560700	0.19881200

N	0.96541000	-1.91157900	-1.02844900
C	1.61845600	-0.73284800	-1.27981000
Br	3.24348800	1.48327900	-0.65933100
O	3.14664200	-0.28228600	1.91285400
H	1.86952100	-2.38970300	2.02439700
O	0.34893000	-3.55855700	0.42694100
H	1.48233100	-0.31424100	-2.27074100
H	0.32397600	-2.30489700	-1.70455900

24

BrU-BrU-ftf-gas-max355: Optimised twist = 311.61 deg.

O	-4.65492900	-0.97030400	-1.16941100
C	-3.71024000	-0.34206600	-0.74670300
N	-3.48372200	-0.11005900	0.59785200
H	-4.09217100	-0.61483300	1.23071300
N	-2.73870900	0.21870800	-1.56194600
H	-2.88777800	0.10226800	-2.56004200
C	-2.38926600	0.55827400	1.07843700
H	-2.31701100	0.63144000	2.15781400
C	-1.57736000	0.90644100	-1.18922700
O	-0.77705100	1.26327200	-2.02802900
C	-1.45729100	1.08969700	0.26099400
Br	0.02113000	2.01652400	0.90858700
C	1.83652500	-0.86638200	-0.27382200
C	1.73167200	-1.00042400	1.18478200
N	0.52187400	-1.58294900	1.59680300
C	-0.53450100	-2.00553000	0.81998900
N	-0.29314300	-1.89055300	-0.53568600
C	0.83988900	-1.30808300	-1.06126900
Br	3.35712000	-0.05374600	-0.96238300
O	2.55787600	-0.66047900	1.99968200
H	0.39381300	-1.66823600	2.60056400
O	-1.58125400	-2.42854700	1.27493300
H	0.86731900	-1.21103400	-2.14028800
H	-1.04068900	-2.20597200	-1.14154300

24

BrU-BrU-ftf-gas-min265: Optimised twist = 299.36 deg.

O	-1.90170100	-2.27342200	1.87745200
C	-0.88404100	-1.98529700	1.27398500
N	-0.76536600	-2.09678200	-0.09800700
H	-1.57034000	-2.48309500	-0.58020700
N	0.25127800	-1.49524300	1.88218400
H	0.21577100	-1.42987900	2.89529100
C	0.33029600	-1.64622500	-0.80259200
H	0.26916800	-1.73433800	-1.88183000
C	1.43856300	-1.04211900	1.28296800
O	2.35759500	-0.64611900	1.95997000
C	1.40244100	-1.11507400	-0.18581300
Br	2.86786800	-0.46869400	-1.12152400
C	-1.11871600	1.32415100	0.16448600
C	-1.08701100	1.18802700	-1.29828100
N	-2.14137300	0.40789200	-1.79567000
C	-3.09555600	-0.29441200	-1.08210600
N	-3.09389500	-0.00157800	0.26766700
C	-2.10524200	0.73895900	0.87075000
Br	0.25401900	2.27931900	0.97382700
O	-0.25986700	1.65762300	-2.04599300
H	-2.15023300	0.26173900	-2.80097700
O	-3.84806800	-1.10159600	-1.58974100

H -2.16201800 0.80468700 1.95181900  
H -3.69097900 -0.59096300 0.83816700  
24

BrU-BrU-ftf-gas-min315: Optimised twist = 299.36 deg.

O -3.84806100 -1.10160800 -1.58974000  
C -3.09555300 -0.29442000 -1.08210500  
N -3.09389300 -0.00158700 0.26766800  
H -3.69097300 -0.59097600 0.83816900  
N -2.14137600 0.40789000 -1.79567000  
H -2.15023600 0.26173800 -2.80097700  
C -2.10524300 0.73895400 0.87075100  
H -2.16201800 0.80468100 1.95181900  
C -1.08701800 1.18803000 -1.29828100  
O -0.25987800 1.65763200 -2.04599500  
C -1.11872000 1.32415100 0.16448600  
Br 0.25401300 2.27932300 0.97382600  
C 1.40244500 -1.11507300 -0.18581300  
C 1.43856500 -1.04211700 1.28296900  
N 0.25128100 -1.49524200 1.88218400  
C -0.88403700 -1.98529900 1.27398400  
N -0.76536100 -2.09678300 -0.09800800  
C 0.33030000 -1.64622500 -0.80259200  
Br 2.86787200 -0.46869300 -1.12152300  
O 2.35759600 -0.64611500 1.95997000  
H 0.21577400 -1.42987900 2.89529100  
O -1.90169700 -2.27342500 1.87745100  
H 0.26917200 -1.73433800 -1.88183000  
H -1.57033500 -2.48309700 -0.58020800  
24

BrU-BrU-ftf-gas-min50: Optimised twist = 55.71 deg.

O 3.36417600 -1.54927400 -1.56616200  
C 2.63307800 -0.61579100 -1.31244800  
N 1.50338900 -0.31970900 -2.05932300  
H 1.27250300 -0.99838400 -2.77663800  
N 2.83031100 0.24713100 -0.24974900  
H 3.61102800 0.01029100 0.35870200  
C 0.57170800 0.60897300 -1.67659200  
H -0.31843400 0.67198300 -2.29385000  
C 1.94615700 1.20833900 0.24924300  
O 2.17902300 1.79431900 1.28546500  
C 0.74860000 1.37788300 -0.58319200  
Br -0.51961500 2.62217100 -0.03369800  
C -1.39102200 -1.03205400 0.52724000  
C -0.46089700 -1.90327800 -0.19560200  
N 0.74588200 -2.10651100 0.48069300  
C 1.18130500 -1.50877500 1.65256700  
N 0.23007000 -0.68142800 2.22546100  
C -1.00727400 -0.45298400 1.68221900  
Br -3.04783900 -0.69442700 -0.24560800  
O -0.64768400 -2.39745700 -1.28975500  
H 1.42943000 -2.70320800 0.01722700  
O 2.28741200 -1.67378100 2.11793900  
H -1.64501000 0.23577000 2.22431700  
H 0.55045900 -0.14821300 3.02589700  
24

BrU-BrU-ftf-water-max0: Optimised twist = 342.04 deg.

O -4.19928100 0.41518400 -0.63438100  
C -3.04822700 0.75175800 -0.42930500

N	-2.63024600	1.36359600	0.73486500
H	-3.34471600	1.53107600	1.43516600
N	-2.02558100	0.54913500	-1.33850400
H	-2.30211800	0.11470500	-2.21600200
C	-1.35848100	1.82582800	0.93066800
H	-1.17611000	2.32574600	1.87502200
C	-0.70617000	1.00164100	-1.26671600
O	0.06161400	0.82503700	-2.19673100
C	-0.39445600	1.65654800	0.00066900
Br	1.31430800	2.36521700	0.23064200
C	0.92673100	-1.53754300	0.01004300
C	0.35761500	-1.14214000	1.29449200
N	-1.00156600	-1.44498600	1.40504900
C	-1.80381600	-2.11611200	0.50311700
N	-1.14643000	-2.48006600	-0.65305500
C	0.16887700	-2.19634100	-0.89235800
Br	2.73043900	-1.19418300	-0.31084300
O	0.94608800	-0.59364700	2.20975400
H	-1.44723800	-1.19254300	2.28392900
O	-2.98121500	-2.35178100	0.70687700
H	0.55701000	-2.52519800	-1.84941400
H	-1.69629100	-2.97389900	-1.34795400

24

BrU-BrU-ftf-water-max120-minus: Optimised twist = 127.48 deg.

O	1.41950100	3.48281400	0.46096700
C	0.58458400	2.66277900	0.12914600
N	0.68301300	1.90576300	-1.02144100
H	1.50955600	2.05815200	-1.58976100
N	-0.55883600	2.40334100	0.86023700
H	-0.66459400	2.94308300	1.71552900
C	-0.26530800	1.00587300	-1.41989700
H	-0.07159700	0.49722400	-2.35810500
C	-1.58929200	1.51548700	0.55939900
O	-2.55250400	1.40390200	1.29878700
C	-1.36649400	0.76798700	-0.67549900
Br	-2.70506200	-0.40426300	-1.24090900
C	1.50223900	-1.12171400	0.16198000
C	1.17158000	-0.36271700	1.36314900
N	-0.02421800	-0.76015700	1.95813900
C	-0.88342100	-1.76443500	1.55036300
N	-0.44727400	-2.43723400	0.42850600
C	0.69683100	-2.12390200	-0.24839700
Br	3.07056100	-0.67709000	-0.74234700
O	1.82905700	0.55077900	1.83410400
H	-0.30186500	-0.25820300	2.79864000
O	-1.91964500	-2.03192400	2.13000400
H	0.90658000	-2.72243700	-1.12735700
H	-1.05492800	-3.17316000	0.08454700

24

BrU-BrU-ftf-water-max120: Optimised twist = 126.73 deg.

O	1.42405200	3.51838500	0.50536600
C	0.59562500	2.69983400	0.15383300
N	0.71781600	1.94526500	-0.99579100
H	1.55814000	2.09494200	-1.54427400
N	-0.56461400	2.44233200	0.85856200
H	-0.68846900	2.98125300	1.71187200
C	-0.21746000	1.03936300	-1.41033200
H	-0.00089500	0.52695700	-2.34145400

C	-1.58285200	1.54683100	0.54103600
O	-2.55904000	1.43035400	1.26282900
C	-1.33184200	0.79794000	-0.68725700
Br	-2.64319800	-0.39743900	-1.26706700
C	1.47295000	-1.14662200	0.17186100
C	1.12090500	-0.37587800	1.35935200
N	-0.07744100	-0.77761100	1.94618100
C	-0.91993000	-1.79814400	1.54380000
N	-0.46073400	-2.48511800	0.44006400
C	0.68552800	-2.16610000	-0.23078500
Br	3.04512600	-0.69531200	-0.72294700
O	1.76333800	0.55093300	1.82518700
H	-0.37140600	-0.26559200	2.77497000
O	-1.96126900	-2.06730100	2.11358300
H	0.91241700	-2.77571600	-1.09775100
H	-1.05663900	-3.23192800	0.09925200

24

BrU-BrU-ftf-water-max120-plus: Optimised twist = 121.36 deg.

O	-4.11146500	-0.94749200	0.91878200
C	-3.01689600	-1.09608800	0.40466300
N	-2.61795700	-0.41650600	-0.72732100
H	-3.28571200	0.24154400	-1.11450500
N	-2.07093400	-1.97973800	0.88240900
H	-2.32635000	-2.48009400	1.72966200
C	-1.37971600	-0.54323700	-1.28742600
H	-1.19646300	0.05345300	-2.17402200
C	-0.75875700	-2.13183700	0.45039900
O	0.01915900	-2.85493500	1.05339400
C	-0.44707900	-1.35442600	-0.74489500
Br	1.24995700	-1.55409500	-1.49593000
C	0.59037900	1.72308500	0.23194100
C	0.24217200	0.78368000	1.29190400
N	1.31311700	0.00241300	1.71365300
C	2.61939900	0.04434800	1.26681300
N	2.85637900	1.04800000	0.35111000
C	1.87372400	1.84335100	-0.16774600
Br	-0.76912400	2.81515900	-0.43029700
O	-0.86667900	0.63859000	1.78298600
H	1.10606300	-0.72290800	2.39682300
O	3.48061700	-0.72423100	1.65475200
H	2.19096000	2.56264900	-0.91372700
H	3.80571500	1.12024400	0.00152800

24

BrU-BrU-ftf-water-max175: Optimised twist = 126.73 deg.

O	1.42402900	3.51838300	0.50535700
C	0.59560300	2.69982900	0.15382700
N	0.71779000	1.94526600	-0.99580100
H	1.55811400	2.09494400	-1.54428500
N	-0.56463000	2.44231900	0.85856200
H	-0.68848300	2.98123400	1.71187600
C	-0.21748300	1.03935900	-1.41033800
H	-0.00092100	0.52695900	-2.34146400
C	-1.58286700	1.54681700	0.54103800
O	-2.55905200	1.43033600	1.26283500
C	-1.33185900	0.79792800	-0.68725700
Br	-2.64321200	-0.39745700	-1.26706200
C	1.47297100	-1.14661600	0.17186600
C	1.12092200	-0.37586500	1.35935100

N	-0.07741300	-0.77760900	1.94619200
C	-0.91990900	-1.79813500	1.54380500
N	-0.46070200	-2.48512600	0.44008300
C	0.68555800	-2.16610600	-0.23076900
Br	3.04513700	-0.69529500	-0.72295500
O	1.76334600	0.55095700	1.82517600
H	-0.37138200	-0.26558500	2.77497600
O	-1.96125900	-2.06727400	2.11357500
H	0.91245300	-2.77573000	-1.09772700
H	-1.05660500	-3.23193800	0.09927400

24

BrU-BrU-ftf-water-max245: Optimised twist = 225.55 deg.

O	-2.38845500	3.14643400	0.95675100
C	-1.34655200	2.63509600	0.58764900
N	-0.19327700	2.63450800	1.34641900
H	-0.24406400	3.11249500	2.23955900
N	-1.20424900	2.00299700	-0.63074400
H	-2.04145100	1.96715800	-1.20725500
C	0.97973100	2.05911100	0.94125700
H	1.81459900	2.14856900	1.62690800
C	-0.08906800	1.33029400	-1.12355800
O	-0.13291800	0.75450800	-2.19740500
C	1.06615400	1.40147400	-0.23329900
Br	2.65843900	0.61635400	-0.80465300
C	-1.02870500	-1.28853800	0.35844300
C	-0.14996700	-2.13060600	-0.45343500
N	1.09730600	-2.34338400	0.12880500
C	1.56826100	-1.86627900	1.33528200
N	0.64936900	-1.09579000	2.01946600
C	-0.61274800	-0.83835300	1.56068400
Br	-2.76111900	-0.98332500	-0.25871000
O	-0.43202500	-2.63061800	-1.52749200
H	1.75182700	-2.91054300	-0.40405900
O	2.68413100	-2.10532500	1.75983900
H	-1.24356800	-0.25003700	2.21851800
H	0.94388700	-0.74514000	2.92470100

24

BrU-BrU-ftf-water-max290: Optimised twist = 272.77 deg.

O	1.40864100	-0.05332700	3.27640500
C	0.47067900	0.07021300	2.50780000
N	0.07823200	1.28889600	1.99246300
H	0.57901000	2.10250300	2.33471700
N	-0.29577600	-0.98862700	2.06804100
H	-0.03579100	-1.90238700	2.43111700
C	-0.94734300	1.43761000	1.09895000
H	-1.15724500	2.45304100	0.78191800
C	-1.34652400	-0.96523100	1.15044200
O	-1.93519100	-1.98882600	0.85110900
C	-1.63396800	0.37234400	0.63628300
Br	-3.03176300	0.56219100	-0.58005300
C	1.50440800	-0.47297700	-0.69053200
C	0.73656900	0.37447900	-1.60020200
N	1.03853000	1.73041300	-1.47346700
C	1.98685700	2.31862600	-0.65881900
N	2.67985300	1.41690900	0.12301800
C	2.45438600	0.06786400	0.10144000
Br	1.23864500	-2.31657200	-0.79075700
O	-0.09589300	-0.00740500	-2.40244000

H	0.52822600	2.36473500	-2.08339000
O	2.18736800	3.51930200	-0.62769900
H	3.07711100	-0.52763900	0.75961300
H	3.39217700	1.80442000	0.73283100

24

BrU-BrU-ftf-water-min150: Optimised twist = 127.49 deg.

O	1.41948800	3.48205200	0.46024800
C	0.58445400	2.66205300	0.12873200
N	0.68238100	1.90515000	-1.02193400
H	1.50855100	2.05773200	-1.59070700
N	-0.55854200	2.40239600	0.86040800
H	-0.66365200	2.94166200	1.71607000
C	-0.26616200	1.00540300	-1.42016300
H	-0.07288600	0.49692700	-2.35854700
C	-1.58900300	1.51438600	0.56007200
O	-2.55145800	1.40214200	1.30030700
C	-1.36706600	0.76752100	-0.67538300
Br	-2.70626600	-0.40399300	-1.24073500
C	1.50262100	-1.12116800	0.16183300
C	1.17221400	-0.36209900	1.36300600
N	-0.02368400	-0.75929200	1.95799700
C	-0.88293500	-1.76364200	1.55052500
N	-0.44710300	-2.43639800	0.42849900
C	0.69703000	-2.12327600	-0.24842400
Br	3.07103400	-0.67704900	-0.74267200
O	1.82989200	0.55126600	1.83396900
H	-0.30124800	-0.25724300	2.79845700
O	-1.91893500	-2.03121300	2.13052700
H	0.90668200	-2.72189800	-1.12734700
H	-1.05449900	-3.17273200	0.08495800

24

BrU-BrU-ftf-water-min210: Optimised twist = 243.49 deg.

O	-2.03738600	2.56959800	1.99481300
C	-1.05313600	2.17197900	1.39785400
N	0.06478000	1.66902900	2.03427900
H	0.04522300	1.67701900	3.04873800
N	-0.94585600	2.18610700	0.02250600
H	-1.75420800	2.54718100	-0.47808400
C	1.16591900	1.19968100	1.37289700
H	1.98748700	0.86347800	1.99597600
C	0.09717300	1.69873300	-0.76147400
O	0.04233300	1.75152400	-1.97723200
C	1.20598800	1.15680800	0.02405700
Br	2.71579300	0.56421000	-0.89517700
C	-1.20596900	-1.15676700	0.02455700
C	-0.09726400	-1.69916700	-0.76080200
N	0.94581900	-2.18618200	0.02332600
C	1.05325700	-2.17130600	1.39865400
N	-0.06452800	-1.66787400	2.03492900
C	-1.16572500	-1.19884600	1.37341600
Br	-2.71587700	-0.56465100	-0.89481200
O	-0.04255100	-1.75259600	-1.97653700
H	1.75409200	-2.54758000	-0.47716100
O	2.03753300	-2.56869700	1.99572200
H	-1.98719200	-0.86222900	1.99640500
H	-0.04484600	-1.67529900	3.04938900

24

BrU-BrU-ftf-water-min260: Optimised twist = 250.75 deg.

O	1.93298900	-2.53197800	2.23821000
C	0.99185900	-2.13912800	1.57235800
N	-0.14208300	-1.57792400	2.12496400
H	-0.17150300	-1.53159100	3.13807800
N	0.95441600	-2.21619300	0.19512600
H	1.77585600	-2.62224400	-0.24609200
C	-1.20124500	-1.12520500	1.38708200
H	-2.04260900	-0.73841500	1.95161800
C	-0.04881300	-1.77035700	-0.66218300
O	0.05583100	-1.90305800	-1.86858400
C	-1.18105900	-1.16350700	0.03788700
Br	-2.63579300	-0.60347000	-0.98408600
C	1.18000700	1.16129600	-0.03151300
C	0.03996300	1.72501500	-0.75460900
N	-0.95205900	2.22602100	0.08517300
C	-0.96956800	2.24199000	1.46506200
N	0.16987700	1.71303300	2.03790400
C	1.21794600	1.20966100	1.31701600
Br	2.62057900	0.53500800	-1.03507900
O	-0.07913600	1.78150400	-1.96563800
H	-1.77708300	2.60801000	-0.37063200
O	-1.89919700	2.68331200	2.11643600
H	2.06540600	0.85634700	1.89425800
H	0.21293300	1.73268800	3.05134800

24

BrU-BrU-ftf-water-min325: Optimised twist = 302.39 deg.

O	1.74978500	2.86625100	1.27156600
C	0.79187900	2.32796800	0.74474900
N	0.73304200	2.04567000	-0.60447600
H	1.50345400	2.38710800	-1.16995200
N	-0.33128600	1.93088600	1.44219500
H	-0.33510400	2.15700600	2.43384200
C	-0.31408700	1.38600100	-1.19339300
H	-0.21981000	1.20172200	-2.25784000
C	-1.47635400	1.30932600	0.94579600
O	-2.42912600	1.08749000	1.67112900
C	-1.37890600	0.97655100	-0.47472000
Br	-2.79299500	0.05017700	-1.25376500
C	1.06237200	-1.12480900	0.49406600
C	1.09389000	-1.37986700	-0.94428000
N	2.21446900	-0.83959800	-1.57370700
C	3.27444900	-0.16704400	-0.99558200
N	3.14783800	-0.00754400	0.36802300
C	2.08749500	-0.48117900	1.09081900
Br	-0.37264900	-1.81382100	1.46339400
O	0.24924900	-1.98171500	-1.58369500
H	2.28665300	-0.99426100	-2.57642800
O	4.22364300	0.25262700	-1.63268800
H	2.12027700	-0.29505200	2.15865400
H	3.90078700	0.48623100	0.83524300

24

BrU-BrU-ftf-water-min45: Optimised twist = 62.49 deg.

O	3.40207400	-1.85226700	-1.66531100
C	2.65672900	-0.93889900	-1.36020000
N	1.46247900	-0.69064500	-2.00545600
H	1.22031800	-1.31984600	-2.76405300
N	2.92299000	-0.05650200	-0.33125600
H	3.79654600	-0.21057300	0.16654200



C	0.60921100	0.31740400	-1.65585400
H	-0.29802200	0.39821400	-2.24534200
C	2.13938900	1.00659900	0.11302100
O	2.50742700	1.71053600	1.03754800
C	0.88622000	1.14502600	-0.62529300
Br	-0.25900200	2.53716500	-0.15456100
C	-1.52944400	-0.80715800	0.55673000
C	-0.64945800	-1.87524800	0.09783900
N	0.52224200	-1.98461300	0.84811000
C	0.89954300	-1.23765600	1.94945000
N	-0.02612500	-0.28034400	2.30776400
C	-1.20620300	-0.08147900	1.64724400
Br	-3.09453600	-0.47860700	-0.39994100
O	-0.84790600	-2.61325800	-0.85259200
H	1.15726800	-2.73587100	0.58708700
O	1.95381300	-1.40283800	2.53544600
H	-1.84070500	0.70583300	2.03603900
H	0.20812900	0.28851700	3.11480600

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C-BrU-ftf-gas-max235: Optimised twist = 308.40 deg.

H	-2.71167100	1.58632200	1.10936000
C	-1.83699800	1.51473400	0.47258600
N	-1.04442100	2.62834700	0.40590900
H	-1.25089200	3.44938800	0.95946200
C	-1.53937500	0.39833500	-0.21809400
Br	-2.59395500	-1.13354400	-0.12647600
C	0.14535600	2.68705500	-0.31268800
O	0.87283400	3.65433700	-0.28180100
C	-0.33912000	0.35946100	-1.06343900
O	0.03414400	-0.59887600	-1.70814500
N	0.38120000	1.55472800	-1.06629800
H	1.29206400	1.51947100	-1.52456300
C	0.91473800	-1.65437300	1.45332700
C	1.32793000	-2.47367700	0.45204500
N	2.25284400	-2.04962300	-0.43607000
C	2.73085100	-0.72114000	-0.46834200
N	2.37552300	0.08131100	0.58659600
C	1.50572500	-0.34586100	1.47101600
H	0.16031700	-1.96053400	2.16635500
H	0.94492800	-3.47890400	0.31370100
H	2.47702600	-2.59898800	-1.25690700
O	3.41556900	-0.35922500	-1.40770300
N	1.10083300	0.55754500	2.41679800
H	0.69570400	0.21174000	3.27513600
H	1.68407500	1.38230300	2.49827600

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C-BrU-ftf-gas-max345: Optimised twist = 355.35 deg.

H	0.91539300	-1.27630400	2.19166600
C	0.34822900	-1.34958600	1.27060200
N	-0.93633700	-1.79645700	1.38731200
H	-1.34065300	-1.99495100	2.29335000
C	0.88108700	-1.01723000	0.07693000
Br	2.64970100	-0.45455300	-0.08411600
C	-1.79635900	-1.96639900	0.30930100
O	-2.90287000	-2.43745000	0.41216600
C	0.04942600	-1.06308900	-1.12945000
O	0.38281100	-0.70634500	-2.24314500
N	-1.23152600	-1.56243600	-0.89130100

H	-1.85367900	-1.61188400	-1.69262100
C	0.50276200	2.37247200	-0.26096600
C	-0.24735400	2.22848700	-1.38112400
N	-1.51043700	1.75180900	-1.28991200
C	-2.09912400	1.32732600	-0.07541300
N	-1.33543800	1.46879600	1.05515800
C	-0.11595400	1.95448400	0.96626400
H	1.52404000	2.72663100	-0.30143100
H	0.11556800	2.46222000	-2.37562900
H	-2.07293800	1.60075600	-2.11831200
O	-3.21734800	0.84642100	-0.10608000
N	0.61119400	1.99844400	2.11798000
H	1.46211400	2.54023700	2.15158500
H	0.09141200	1.90175400	2.98039400

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C-BrU-ftf-gas-min290: Optimised twist = 299.61 deg.

H	-0.56400400	-0.39088000	-2.47378700
C	-0.21612900	-0.83256700	-1.54645100
N	1.02631900	-1.39956700	-1.57752100
H	1.60956200	-1.31620400	-2.39975400
C	-0.96075600	-0.83062300	-0.42336200
Br	-2.66137400	-0.07380100	-0.36561500
C	1.65537600	-1.94359500	-0.46173100
O	2.77984900	-2.38667900	-0.50064700
C	-0.42255000	-1.40480800	0.81720000
O	-0.98497300	-1.40524700	1.89231400
N	0.84946800	-1.95618400	0.66228300
H	1.31831600	-2.21890800	1.52632000
C	0.24685500	2.53325500	-0.55820400
C	-0.39809600	2.39017700	0.62932800
N	0.13239100	1.61084100	1.59602100
C	1.36895700	0.93528000	1.46167000
N	1.98507100	1.03197900	0.23835100
C	1.45995700	1.77994300	-0.70410200
H	-0.15931500	3.14017700	-1.35691100
H	-1.34809400	2.86363300	0.85169600
H	-0.36312400	1.42719800	2.46204500
O	1.78980500	0.29047600	2.40293000
N	2.09214800	1.76574600	-1.92104700
H	1.93487800	2.54273100	-2.54832100
H	3.04294800	1.41482700	-1.89424000

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C-BrU-ftf-gas-min80: Optimised twist = 76.16 deg.

H	-1.08761300	-1.69152500	-1.69241100
C	-0.80601200	-1.42496100	-0.68029500
N	0.36346300	-1.97486600	-0.22792800
H	1.01544700	-2.35914400	-0.90973500
C	-1.54913700	-0.59285200	0.07665300
Br	-3.13566400	0.16092700	-0.54550200
C	0.94645700	-1.59871000	0.96810300
O	2.06561500	-1.93175000	1.30344000
C	-1.07441100	-0.18849100	1.39870400
O	-1.60638400	0.60775000	2.14680300
N	0.13078500	-0.80204200	1.75236100
H	0.53136400	-0.51365600	2.63974800
C	2.21786400	1.91111100	0.67810200
C	3.34398900	1.16727900	0.54326400
N	3.44183900	0.25221800	-0.44988800

C	2.37058600	-0.05536500	-1.30776600
N	1.25854300	0.73176700	-1.21917000
C	1.17012400	1.64937200	-0.27383600
H	2.11783100	2.66163400	1.45130700
H	4.20180300	1.26376700	1.19966400
H	4.21721100	-0.39880900	-0.48519300
O	2.47121700	-1.02545200	-2.05005700
N	0.02696500	2.37202500	-0.21860300
H	-0.22100800	2.87105200	0.62403100
H	-0.73831500	2.07183700	-0.81130000

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C-BrU-ftf-water-max120-minus: Optimised twist = 132.77 deg.

H	1.29753200	-0.70888000	-2.29437600
C	0.87897300	0.03872900	-1.63240400
N	-0.28998900	0.61936200	-2.04635200
H	-0.70192100	0.35465600	-2.93435300
C	1.43728600	0.36526400	-0.45110200
Br	2.98311400	-0.47551400	0.15913700
C	-0.95799300	1.58977600	-1.33164300
O	-1.99554700	2.10488600	-1.71339500
C	0.81132700	1.36206900	0.40646300
O	1.20374600	1.71405300	1.50865300
N	-0.33675200	1.92702900	-0.14585000
H	-0.81053200	2.62777700	0.41828800
C	-3.14289700	-0.13226100	0.97668500
C	-3.39137600	-0.86718000	-0.13537900
N	-2.41941200	-1.65422300	-0.66036500
C	-1.14176500	-1.76343300	-0.09890400
N	-0.87838800	-1.02574400	1.01352500
C	-1.82075500	-0.23854900	1.52626200
H	-3.89480700	0.51162200	1.41342800
H	-4.34301400	-0.86417000	-0.65390500
H	-2.59443200	-2.20264700	-1.49492600
O	-0.31477200	-2.49688100	-0.64799900
N	-1.49105400	0.48964300	2.60779300
H	-2.11930200	1.19215100	2.97181700
H	-0.51758700	0.53706000	2.88501200

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C-BrU-ftf-water-max120: Optimised twist = 151.36 deg.

H	-1.02126100	0.07289500	-2.39801500
C	-0.61753200	-0.51059100	-1.57880900
N	0.57498900	-1.14117900	-1.82302200
H	1.01389200	-1.06034100	-2.73364400
C	-1.22470500	-0.60321200	-0.37987300
Br	-2.83915800	0.25263400	-0.02667900
C	1.21800400	-1.94187000	-0.90547500
O	2.26272000	-2.52495700	-1.13971600
C	-0.61933400	-1.39229900	0.68908800
O	-1.05594900	-1.52699500	1.82007800
N	0.56611700	-2.01814000	0.30956800
H	1.02383900	-2.58260400	1.02071900
C	2.89906600	0.54606300	0.51594300
C	2.85508500	1.19181700	-0.67473500
N	1.76530700	1.92963400	-1.00635000
C	0.65710100	2.07439700	-0.16349500
N	0.68307600	1.41633300	1.02880200
C	1.74343900	0.68776200	1.36006600
H	3.74859300	-0.05795100	0.80630300

H	3.65426600	1.15367000	-1.40615400
H	1.72605800	2.42191700	-1.89171400
O	-0.28529200	2.77261000	-0.54354700
N	1.71093200	0.05397100	2.54551800
H	2.43780700	-0.59476800	2.81270000
H	0.84582700	0.04298700	3.07119300

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C-BrU-ftf-water-max120-plus: Optimised twist = 175.59 deg.

H	0.17326300	-1.36757800	-2.29641500
C	0.69954300	-1.16089400	-1.37145600
N	2.01211700	-0.80028600	-1.49823200
H	2.43409300	-0.72883300	-2.41772300
C	0.10621000	-1.24210400	-0.16271500
Br	-1.66338400	-1.79541900	0.02427200
C	2.82753000	-0.50441800	-0.42709000
O	3.99202100	-0.16452900	-0.54758500
C	0.87912500	-0.99831300	1.05162500
O	0.47063500	-1.09153900	2.19610700
N	2.20055300	-0.63228400	0.79590400
H	2.78001100	-0.44279400	1.60982800
C	0.80491700	2.20913100	-0.43410600
C	0.06281100	2.01480700	-1.55181400
N	-1.25267300	1.70263900	-1.44701800
C	-1.92205100	1.62448800	-0.21838000
N	-1.17509000	1.76207400	0.91098600
C	0.11966800	2.04667300	0.81985500
H	1.85657600	2.46268200	-0.48496700
H	0.46489300	2.08688800	-2.55621100
H	-1.81965000	1.57537100	-2.27780400
O	-3.14039200	1.43695100	-0.22026500
N	0.80633800	2.18471300	1.96615100
H	1.80138900	2.35642300	1.97178800
H	0.34454500	1.99624900	2.84587200

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C-BrU-ftf-water-max190: Optimised twist = 202.60 deg.

H	0.70171100	-1.81032900	2.09006300
C	0.15443700	-1.65921100	1.16670400
N	-1.16687400	-2.00804400	1.19274300
H	-1.58539900	-2.35505500	2.04894600
C	0.72819800	-1.15379100	0.05474200
Br	2.54160600	-0.72676400	-0.00360900
C	-2.01595800	-1.84151800	0.11972400
O	-3.21012600	-2.08303300	0.16737900
C	-0.04565900	-1.03007100	-1.17762000
O	0.37937500	-0.66732500	-2.26072100
N	-1.38471000	-1.38240900	-1.01787400
H	-1.98360400	-1.25381500	-1.82956200
C	-1.79659100	1.29366200	1.12748100
C	-0.67157200	1.45205000	1.86873800
N	0.44786500	1.96861900	1.30508800
C	0.51179600	2.36069100	-0.03806100
N	-0.60841900	2.19593400	-0.79434500
C	-1.71094200	1.69353800	-0.25044600
H	-2.70544600	0.88742800	1.55332600
H	-0.60438900	1.18150300	2.91669100
H	1.29400600	2.08662000	1.85099100
O	1.56346600	2.84128200	-0.46654400
N	-2.78045000	1.53741800	-1.05091400

H -3.67299900 1.23165400 -0.68997700  
H -2.73596900 1.86863700 -2.00552800  
25

C-BrU-ftf-water-max240: Optimised twist = 238.65 deg.

H -0.20430300 -0.37540800 -2.36678900  
C 0.06617000 -0.82947100 -1.42066200  
N 1.34411300 -1.30891400 -1.33210100  
H 1.98096900 -1.20844600 -2.11493600  
C -0.79006500 -0.91907900 -0.38184200  
Br -2.55109300 -0.31629500 -0.51083100  
C 1.85104900 -1.92831600 -0.20942100  
O 2.99631000 -2.33902100 -0.13442200  
C -0.38543200 -1.60603400 0.84281000  
O -1.09205800 -1.81605900 1.81346600  
N 0.93558700 -2.04866600 0.81523100  
H 1.26939600 -2.52226300 1.65049100  
C 1.51406400 2.09496500 -1.10210200  
C 0.24496600 2.57302900 -1.08350600  
N -0.51400000 2.43970900 0.03149800  
C -0.06050500 1.80130800 1.19091400  
N 1.20808900 1.30409200 1.18040200  
C 1.96764100 1.44951100 0.09990600  
H 2.14553700 2.18972000 -1.97594400  
H -0.21859400 3.07239700 -1.92662200  
H -1.46867500 2.78080800 0.04977900  
O -0.82152200 1.72093900 2.15800200  
N 3.21671900 0.95436000 0.15208100  
H 3.82346400 0.95717300 -0.65526400  
H 3.51773300 0.44993700 0.97564900  
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C-BrU-ftf-water-max355: Optimised twist = 5.41 deg.

H -0.52419800 -1.00984900 -2.32203700  
C 0.00895900 -1.14267100 -1.38750800  
N 1.35090600 -1.37008200 -1.49103400  
H 1.79143300 -1.40598500 -2.40349900  
C -0.60437800 -1.08185400 -0.18626700  
Br -2.45375100 -0.87209000 -0.04188600  
C 2.17280300 -1.60376000 -0.40776500  
O 3.35422100 -1.87919200 -0.51139000  
C 0.16591400 -1.26851200 1.03812200  
O -0.27043800 -1.22734500 2.17724200  
N 1.51921100 -1.50917800 0.80551300  
H 2.09723600 -1.65933400 1.62842600  
C -0.93573400 2.20963500 0.67787200  
C -0.04130400 1.97732200 1.66835300  
N 1.25151600 1.69854800 1.36137200  
C 1.72576400 1.64023700 0.04582900  
N 0.83831700 1.87522400 -0.95685700  
C -0.43513200 2.12362400 -0.66642500  
H -1.97555100 2.42235300 0.88775700  
H -0.29580000 1.99095300 2.72166100  
H 1.92780100 1.51435700 2.09389700  
O 2.91504200 1.36447900 -0.14117100  
N -1.28441800 2.27614600 -1.69556600  
H -2.26468000 2.47117200 -1.55189700  
H -0.93561600 2.21721800 -2.64301400  
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C-BrU-ftf-water-max65-minus: Optimised twist = 62.59 deg.

H	0.39410100	-0.27766100	-2.32350500
C	0.86399800	-0.50748100	-1.37412600
N	2.15737600	-0.08918300	-1.23121200
H	2.59530700	0.45282300	-1.96827100
C	0.21890500	-1.14804300	-0.37724400
Br	-1.53191500	-1.75701900	-0.57173700
C	2.89585200	-0.27429800	-0.08393900
O	4.03954600	0.12673600	0.04799400
C	0.90763100	-1.43588800	0.87692200
O	0.43979800	-2.02716400	1.83511300
N	2.21444200	-0.95116200	0.90908300
H	2.73815800	-1.12319500	1.76363700
C	-1.26832200	1.26347600	1.67984600
C	0.04927300	1.57431900	1.72708500
N	0.67123900	2.06309300	0.62166100
C	0.01301500	2.24867000	-0.60014500
N	-1.31687500	1.97032500	-0.64954600
C	-1.94031900	1.51829700	0.43400400
H	-1.78981200	0.86690600	2.54112100
H	0.66314600	1.45064000	2.61246200
H	1.64770700	2.33538600	0.65605400
O	0.67098200	2.63820800	-1.56989300
N	-3.26623300	1.31893300	0.34861800
H	-3.77662600	0.86271700	1.09130300
H	-3.71741800	1.40745800	-0.55236700

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C-BrU-ftf-water-max65: Optimised twist = 37.78 deg.

H	-0.10133500	-0.12156400	-2.24587100
C	0.31014100	-0.64389300	-1.39001300
N	1.67059500	-0.77800900	-1.36866300
H	2.23617200	-0.31436600	-2.07211800
C	-0.45882800	-1.12946200	-0.39338900
Br	-2.31725100	-0.98486700	-0.43033900
C	2.35911800	-1.37724000	-0.33756000
O	3.57566400	-1.44257800	-0.29506700
C	0.15201500	-1.82732200	0.73250000
O	-0.43896900	-2.31238000	1.68306600
N	1.54125100	-1.89693000	0.64721600
H	2.01776300	-2.36554300	1.41366700
C	-0.79086000	1.68263100	1.48576800
C	0.42393400	1.23285000	1.87994400
N	1.50142600	1.38246800	1.06325700
C	1.42982300	2.01568400	-0.18297400
N	0.21160100	2.45601100	-0.59652700
C	-0.85051100	2.30671200	0.19077500
H	-1.66899500	1.57309000	2.10845800
H	0.60234500	0.74018400	2.82935400
H	2.42433900	1.09498600	1.37116100
O	2.46258800	2.11925400	-0.85166700
N	-2.02405200	2.77399000	-0.26160700
H	-2.88185700	2.64129000	0.25462800
H	-2.07365600	3.18542800	-1.18412000

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C-BrU-ftf-water-max65-plus: Optimised twist = 31.20 deg.

H	-0.19076700	-0.03437500	-2.21633800
C	0.17880200	-0.62332700	-1.38496200
N	1.51698800	-0.90357400	-1.39896600
H	2.11404200	-0.49648200	-2.11124600

C	-0.61849600	-1.05472700	-0.38562100
Br	-2.45261900	-0.71841500	-0.38150800
C	2.15513000	-1.61835900	-0.40920500
O	3.35433600	-1.83595700	-0.40798700
C	-0.06337600	-1.84438200	0.70787600
O	-0.68292700	-2.28517100	1.66195800
N	1.30658400	-2.06722600	0.58446100
H	1.74375100	-2.61235200	1.32318400
C	-0.63095200	1.79799200	1.41633400
C	0.47770400	1.19250000	1.90373900
N	1.62305300	1.17972400	1.16978500
C	1.73664000	1.80997100	-0.07468400
N	0.62154700	2.39593200	-0.58696800
C	-0.51083500	2.39243100	0.11155100
H	-1.55963100	1.81834400	1.97125900
H	0.51561800	0.69478500	2.86626200
H	2.47025000	0.76775700	1.54613300
O	2.82569600	1.77932700	-0.65514000
N	-1.58079700	2.97767800	-0.44774100
H	-2.48497300	2.97344800	0.00214400
H	-1.50280000	3.37746800	-1.37342600

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C-BrU-ftf-water-min155: Optimised twist = 175.59 deg.

H	0.17332200	-1.36772100	-2.29637700
C	0.69958600	-1.16097000	-1.37142600
N	2.01215900	-0.80036000	-1.49820400
H	2.43414400	-0.72893400	-2.41769400
C	0.10623800	-1.24211100	-0.16268700
Br	-1.66334600	-1.79545400	0.02431700
C	2.82754800	-0.50439400	-0.42707100
O	3.99203200	-0.16448500	-0.54757300
C	0.87913400	-0.99823300	1.05164900
O	0.47062900	-1.09139800	2.19613100
N	2.20055800	-0.63219800	0.79592400
H	2.78000000	-0.44263200	1.60984100
C	0.80488300	2.20914400	-0.43411400
C	0.06281900	2.01476400	-1.55184200
N	-1.25266300	1.70258200	-1.44708200
C	-1.92208100	1.62445300	-0.21846200
N	-1.17516100	1.76208500	0.91092400
C	0.11959300	2.04670600	0.81982700
H	1.85653300	2.46273500	-0.48494500
H	0.46493800	2.08681200	-2.55622600
H	-1.81959700	1.57522800	-2.27788300
O	-3.14041700	1.43689400	-0.22038600
N	0.80622300	2.18479800	1.96614200
H	1.80128000	2.35647200	1.97180200
H	0.34441000	1.99633600	2.84585200

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C-BrU-ftf-water-min205: Optimised twist = 232.11 deg.

H	-0.07962700	-0.84010600	-2.38747700
C	0.31128500	-1.03418300	-1.39544700
N	1.66677400	-1.19894200	-1.30866600
H	2.24199000	-1.12923200	-2.14092500
C	-0.47718500	-1.10911500	-0.30347800
Br	-2.33521300	-0.97384000	-0.42684800
C	2.32732900	-1.48215800	-0.13193000
O	3.53294800	-1.64725300	-0.06685500

C	0.10493600	-1.42520700	0.99909400
O	-0.50840300	-1.57496700	2.04141400
N	1.49157700	-1.56533700	0.96272100
H	1.94437200	-1.78195300	1.84674800
C	1.04505100	2.14306500	-1.22471600
C	-0.27974100	2.37315700	-1.40006500
N	-1.12862300	2.28186600	-0.34731400
C	-0.70942700	1.95221800	0.94631400
N	0.61585400	1.69770700	1.13118000
C	1.45575400	1.78530400	0.10524200
H	1.74915700	2.20554400	-2.04418100
H	-0.72093100	2.63479900	-2.35499900
H	-2.12203500	2.44151100	-0.47058300
O	-1.54931600	1.91202600	1.84858200
N	2.74761300	1.49348300	0.33876700
H	3.45034800	1.57590000	-0.38196700
H	3.04698200	1.27958500	1.28105900

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C-BrU-ftf-water-min285: Optimised twist = 290.69 deg.

H	-0.33240700	-0.16196000	-2.43829000
C	-0.06232100	-0.69353200	-1.53266100
N	1.17709700	-1.26557400	-1.52143000
H	1.80523700	-1.12759700	-2.30535300
C	-0.88744400	-0.78784300	-0.46811200
Br	-2.59456800	-0.03940600	-0.48666000
C	1.69629500	-1.93469100	-0.43312500
O	2.82783500	-2.38760700	-0.40720600
C	-0.48432700	-1.55201700	0.70848100
O	-1.16351200	-1.74753500	1.70301100
N	0.80308100	-2.07107600	0.60936200
H	1.15615800	-2.55288100	1.43174300
C	0.40162400	2.51666400	-0.64590100
C	-0.44010300	2.47590900	0.41676600
N	-0.12554100	1.72323400	1.49974600
C	1.06260900	0.98955800	1.60153000
N	1.90521800	1.00579300	0.53145700
C	1.60240600	1.73638100	-0.53632200
H	0.17731600	3.10179600	-1.52810800
H	-1.38049400	3.01308900	0.45720100
H	-0.74441000	1.68929800	2.30242400
O	1.28262000	0.35818900	2.63729300
N	2.45607100	1.68936300	-1.57728300
H	2.35650600	2.32095900	-2.35973900
H	3.35254000	1.23736800	-1.44844800

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C-BrU-ftf-water-min35: Optimised twist = 31.20 deg.

H	-0.19075400	-0.03436600	-2.21633200
C	0.17883000	-0.62331800	-1.38496300
N	1.51702400	-0.90352900	-1.39897000
H	2.11406300	-0.49642100	-2.11125300
C	-0.61845600	-1.05474700	-0.38562500
Br	-2.45258700	-0.71848000	-0.38150800
C	2.15518600	-1.61829900	-0.40921300
O	3.35440200	-1.83584700	-0.40798700
C	-0.06331400	-1.84438800	0.70787000
O	-0.68284600	-2.28518400	1.66195900
N	1.30665100	-2.06721200	0.58444000
H	1.74383500	-2.61232000	1.32316500



C	-0.63103100	1.79796400	1.41632400
C	0.47763500	1.19249700	1.90373700
N	1.62299300	1.17976300	1.16979600
C	1.73657700	1.81002600	-0.07466400
N	0.62146900	2.39594600	-0.58696400
C	-0.51091900	2.39241100	0.11154400
H	-1.55971900	1.81828500	1.97123700
H	0.51555000	0.69477300	2.86625400
H	2.47019700	0.76781000	1.54614300
O	2.82564500	1.77943200	-0.65509900
N	-1.58089500	2.97762200	-0.44775800
H	-2.48506900	2.97338600	0.00213100
H	-1.50289700	3.37744200	-1.37343000

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C-BrU-ftf-water-min90: Optimised twist = 92.51 deg.

H	-0.24872700	-1.59413400	2.14038500
C	-0.59459800	-1.40909200	1.13068600
N	-1.95005600	-1.33656700	0.96608400
H	-2.56486700	-1.44125700	1.76570200
C	0.24746600	-1.23818800	0.08990800
Br	2.09551500	-1.39369600	0.28707900
C	-2.56002100	-1.11185300	-0.24913400
O	-3.76904400	-1.03027800	-0.38488800
C	-0.27933400	-1.02570100	-1.25375300
O	0.38025700	-0.89334000	-2.27098500
N	-1.67246800	-0.98090500	-1.29802300
H	-2.09001900	-0.82838900	-2.21257800
C	-0.12878400	2.32756500	-1.29003800
C	-1.35152700	2.16213400	-0.73295300
N	-1.45836200	1.81196800	0.57657600
C	-0.34773800	1.64534200	1.41236200
N	0.88296700	1.84621600	0.87357300
C	0.99992600	2.14412600	-0.41641900
H	-0.00847400	2.58503400	-2.33399200
H	-2.28105500	2.27929600	-1.27887600
H	-2.36934400	1.71507700	1.01194300
O	-0.54050900	1.31070300	2.58568600
N	2.24091100	2.29412300	-0.90705100
H	2.40595200	2.45732100	-1.88989500
H	3.03456900	2.09986600	-0.31100000

26

C-C-ftf-gas-min210: Optimised twist = 152.03 deg.

O	-2.74336500	-1.30154800	-0.31563100
C	-2.17607300	-0.23885100	-0.08728400
N	-2.18958700	0.25349800	1.23475200
H	-2.72417700	-0.29690400	1.89487500
N	-1.49868100	0.49602700	-1.01410800
C	-0.71533700	1.48515600	-0.62450200
C	-0.60248800	1.91400100	0.74850400
C	-1.38659200	1.26855800	1.64402400
H	-1.41873300	1.51897100	2.69928500
H	0.05491900	2.72432000	1.03625600
N	0.00596300	2.13739200	-1.56864700
H	0.89754600	2.52143200	-1.26877000
H	0.06853700	1.63710200	-2.44803200
C	1.38836700	-1.27070100	1.64209200
C	0.60351100	-1.91516900	0.74652300
C	0.71486500	-1.48450200	-0.62603400

N	2.19069300	-0.25490300	1.23334300
C	2.17575900	0.23913600	-0.08804400
N	1.49761000	-0.49469800	-1.01513000
H	1.42163500	-1.52248500	2.69699200
H	-0.05339000	-2.72603400	1.03389200
N	-0.00724400	-2.13560600	-1.57033400
O	2.74258700	1.30225200	-0.31560900
H	2.72583700	0.29474900	1.89364300
H	-0.89834800	-2.52046200	-1.27010600
H	-0.07095400	-1.63406500	-2.44892800

26

C-C-ftf-water-max10: Optimised twist = 339.32 deg.

O	0.24858200	-2.40684800	-0.93859000
C	0.89334200	-1.36810300	-0.77051900
N	0.62291700	-0.27071000	-1.59586400
H	-0.11697400	-0.39112400	-2.27858300
N	1.85676800	-1.21924800	0.17907500
C	2.50905500	-0.06609300	0.28209300
C	2.27650500	1.05480900	-0.58586300
C	1.30317000	0.90044500	-1.51608000
H	1.01641400	1.67451900	-2.21836800
H	2.83394200	1.97731000	-0.49031000
N	3.41779000	0.04431400	1.26735600
H	4.00025800	0.86396300	1.35936000
H	3.62716000	-0.76158900	1.84110000
C	-0.68614600	-0.04633200	1.78686900
C	-0.59875100	1.20882300	1.28181700
C	-1.43387900	1.49527400	0.14945600
N	-1.55255000	-0.93678400	1.24442700
C	-2.38480700	-0.62935700	0.16356800
N	-2.28767200	0.61926000	-0.36987100
H	-0.08769400	-0.39844500	2.61924000
H	0.08697700	1.94051000	1.68866500
N	-1.34037300	2.69640900	-0.44919000
O	-3.16308200	-1.49338700	-0.25096300
H	-1.59948900	-1.88752100	1.59202400
H	-0.76541500	3.43340200	-0.06690100
H	-1.96825300	2.92136600	-1.20938600

26

C-C-ftf-water-max120: Optimised twist = 157.70 deg.

O	-2.24467600	-2.18752000	0.05730700
C	-1.89588700	-1.03090300	0.31981900
N	-1.15468900	-0.80601600	1.48300900
H	-0.93983100	-1.62180700	2.04491300
N	-2.17818700	0.04234500	-0.46548500
C	-1.74817500	1.25018900	-0.11303100
C	-1.00323400	1.50380300	1.09061900
C	-0.72191300	0.42524400	1.85926600
H	-0.15425500	0.47696500	2.78140900
H	-0.66461600	2.49665500	1.35568200
N	-2.04449800	2.27542000	-0.92877300
H	-1.69784000	3.20775300	-0.75550000
H	-2.52616900	2.09453200	-1.79915500
C	2.50667700	-1.00441200	0.83463400
C	1.72468000	-1.73930700	0.00728100
C	1.00393800	-1.00949400	-0.99930200
N	2.58669700	0.34143900	0.67346400
C	1.90765900	1.03016900	-0.33608400

N	1.10741400	0.30215300	-1.16297700
H	3.08927500	-1.42865900	1.64410700
H	1.63277500	-2.81247900	0.11145300
N	0.19403600	-1.67955300	-1.85179700
O	2.05616200	2.25188300	-0.42533200
H	3.17210200	0.89881200	1.28524800
H	-0.14245500	-2.59381800	-1.57633100
H	-0.47875000	-1.11511500	-2.35891900

26

C-C-fff-water-max245: Optimised twist = 213.53 deg.

O	2.24604500	0.34639700	2.14515500
C	1.95142300	0.30915900	0.94673200
N	2.33308700	-0.80780700	0.19735200
H	2.84010500	-1.53214800	0.69300100
N	1.26702100	1.29488000	0.30373600
C	0.97306500	1.16376400	-0.98353700
C	1.35469700	0.02312800	-1.76848800
C	2.03959500	-0.94953100	-1.12039700
H	2.37544700	-1.86440400	-1.59471200
H	1.09096900	-0.06396800	-2.81420600
N	0.30809100	2.18018400	-1.57462900
H	-0.14307300	2.02048100	-2.46535100
H	-0.13772200	2.85434000	-0.96377100
C	-0.89417500	-1.10065600	1.71337300
C	-1.44277700	0.13679900	1.72336500
C	-1.93253200	0.62362900	0.46350500
N	-0.85394800	-1.81414500	0.55770900
C	-1.40752900	-1.35552300	-0.64157100
N	-1.92900100	-0.09795500	-0.65129300
H	-0.46043300	-1.57239200	2.58758400
H	-1.46957000	0.74149200	2.62018000
N	-2.39850200	1.88516600	0.38080100
O	-1.39314300	-2.10210000	-1.62457200
H	-0.45729400	-2.74683700	0.54292900
H	-2.54966800	2.44065100	1.21097700
H	-2.84981100	2.18154500	-0.47492000

26

C-C-fff-water-max45: Optimised twist = 40.65 deg.

O	-2.82439700	0.31155600	1.68818900
C	-2.22797800	0.15231600	0.61841000
N	-1.98712500	1.26955600	-0.18684500
H	-2.31325800	2.16081300	0.16896300
N	-1.80036900	-1.05649000	0.16346600
C	-1.14086700	-1.13279400	-0.98543700
C	-0.88097400	0.00387700	-1.82470700
C	-1.33332900	1.19873500	-1.37219900
H	-1.19803800	2.13166500	-1.90692100
H	-0.34834100	-0.08654500	-2.76216600
N	-0.72721600	-2.35245700	-1.38369000
H	-0.11050800	-2.45885200	-2.17640400
H	-0.80821500	-3.12831600	-0.73991400
C	2.57992700	-0.51239800	-0.76987300
C	2.31901700	0.81504100	-0.83615900
C	1.46445400	1.34563500	0.19106400
N	2.06228200	-1.25470800	0.24142400
C	1.28048600	-0.71023200	1.26586500
N	0.97316300	0.61426100	1.18451700
H	3.19153800	-1.04035800	-1.49231700

H	2.70912900	1.43526000	-1.63233600
N	1.11366500	2.64372700	0.14610700
O	0.91572000	-1.44723200	2.18539000
H	2.26101200	-2.24650400	0.30531500
H	1.51485800	3.27623700	-0.53125200
H	0.56601700	3.03369900	0.90177000

26

C-C-ftf-water-min205: Optimised twist = 188.43 deg.

O	3.27894400	-0.47729700	1.22168200
C	2.46058800	-0.34469900	0.30639000
N	1.96436900	-1.49211200	-0.32012000
H	2.31516300	-2.37979700	0.02132500
N	2.00695200	0.86060200	-0.13341900
C	1.10362600	0.91121400	-1.10630800
C	0.56547600	-0.25769100	-1.74629200
C	1.03769100	-1.45058500	-1.31061600
H	0.71305900	-2.40479900	-1.70988500
H	-0.17734300	-0.18936700	-2.53081600
N	0.69935700	2.12823600	-1.51453000
H	-0.10867100	2.22832800	-2.11289800
H	0.99367200	2.93742300	-0.98339600
C	-1.03769100	-1.45057700	1.31062700
C	-0.56547900	-0.25767900	1.74629600
C	-1.10362900	0.91122100	1.10630400
N	-1.96436600	-1.49211200	0.32013000
C	-2.46058500	-0.34470400	-0.30639000
N	-2.00695200	0.86060100	0.13341100
H	-0.71305900	-2.40478800	1.70990400
H	0.17733800	-0.18934900	2.53082200
N	-0.69936300	2.12824600	1.51451900
O	-3.27893700	-0.47731000	-1.22168500
H	-2.31515800	-2.37980000	-0.02131000
H	0.10865800	2.22834400	2.11289300
H	-0.99368100	2.93743000	0.98338200

26

C-C-ftf-water-min315: Optimised twist = 308.54 deg.

O	1.72310700	-2.35785400	0.52229800
C	1.67862200	-1.23610100	0.00419900
N	1.01082200	-1.09050400	-1.21431200
H	0.54700900	-1.91965700	-1.57298700
N	2.22665500	-0.12497700	0.56355400
C	2.06854300	1.05680300	-0.02560000
C	1.34776900	1.23469900	-1.25604100
C	0.82460400	0.11451600	-1.81100500
H	0.24684300	0.11414200	-2.72814900
H	1.21614700	2.20940100	-1.70720400
N	2.60109900	2.12795100	0.58595200
H	2.56232900	3.04884300	0.17366100
H	3.13827000	2.00072500	1.43316300
C	-0.82459800	0.11450900	1.81100900
C	-1.34766100	1.23474600	1.25605700
C	-2.06845100	1.05693000	0.02561500
N	-1.01092400	-1.09048700	1.21430200
C	-1.67872800	-1.23600800	-0.00421600
N	-2.22666500	-0.12482900	-0.56355600
H	-0.24683900	0.11407200	2.72815400
H	-1.21595100	2.20943100	1.70723200
N	-2.60091700	2.12813100	-0.58592300

O -1.72330100 -2.35774700 -0.52233700  
H -0.54717900 -1.91968400 1.57296300  
H -2.56206800 3.04901500 -0.17362000  
H -3.13809800 2.00096300 -1.43313600  
26

C-C-ftf-water-min40: Optimised twist = 18.56 deg.

O -1.85143900 2.40251400 -0.25375700  
C -1.73331700 1.19504500 -0.02548800  
N -2.12788900 0.28537500 -1.01151500  
H -2.47384100 0.68226500 -1.87749900  
N -1.24767100 0.68815600 1.14106500  
C -1.19002700 -0.62754000 1.31567100  
C -1.62529700 -1.57647800 0.32708000  
C -2.08521200 -1.05943100 -0.83760200  
H -2.42762500 -1.66551100 -1.66840200  
H -1.56967400 -2.64408900 0.49524300  
N -0.70049400 -1.07496300 2.48507000  
H -0.59632300 -2.06087500 2.67581800  
H -0.36483400 -0.41149600 3.17034400  
C 2.08522000 -1.05941000 0.83761600  
C 1.62530800 -1.57647500 -0.32705800  
C 1.19003100 -0.62755300 -1.31566200  
N 2.12788800 0.28540000 1.01151100  
C 1.73330900 1.19505400 0.02547200  
N 1.24766600 0.68814500 -1.14107400  
H 2.42763800 -1.66547600 1.66842400  
H 1.56969200 -2.64408900 -0.49520700  
N 0.70049900 -1.07499500 -2.48505500  
O 1.85142200 2.40252600 0.25372500  
H 2.47383600 0.68230300 1.87749000  
H 0.59634000 -2.06091100 -2.67579200  
H 0.36483800 -0.41153900 -3.17033900  
26

C-C-ftf-water-min80-minus: Optimised twist = 109.54 deg.

O 1.36553900 2.53288100 -0.78975300  
C 1.48133400 1.48787000 -0.13503900  
N 0.82697100 1.40007700 1.09562900  
H 0.30948300 2.22006800 1.39151300  
N 2.22097500 0.42217200 -0.53611600  
C 2.18492600 -0.70255100 0.16687900  
C 1.40912900 -0.85706300 1.36773200  
C 0.75461900 0.24538100 1.80593400  
H 0.15978400 0.27061400 2.71194400  
H 1.37198700 -1.79444200 1.90734900  
N 2.95232100 -1.72671800 -0.25543700  
H 2.83089800 -2.65064200 0.13469500  
H 3.37660200 -1.66198500 -1.17149400  
C -2.75766800 -0.94063300 0.81414200  
C -2.73271000 0.39266000 0.56693100  
C -1.78068000 0.83963500 -0.41167700  
N -1.92335400 -1.77138000 0.14184600  
C -1.01866300 -1.32155900 -0.82705600  
N -0.97936000 0.01564100 -1.07619000  
H -3.41825200 -1.40242700 1.53886900  
H -3.38253500 1.08052700 1.09152700  
N -1.67579600 2.15693300 -0.68816200  
O -0.30674600 -2.14968200 -1.40142400  
H -1.93510100 -2.76894500 0.32099100

H -2.14977800 2.82984300 -0.10101400  
H -0.82744900 2.47228200 -1.15302100  
26

C-C-ftf-water-min80: Optimised twist = 85.53 deg.

O -2.06574800 -1.33964600 -1.62268200  
C -1.83201500 -0.49893300 -0.74943000  
N -2.02629400 -0.85282400 0.59051000  
H -2.35638500 -1.79546700 0.76450500  
N -1.38728500 0.76067700 -1.00808200  
C -1.12410700 1.58789300 -0.00506000  
C -1.35739500 1.25749500 1.37349800  
C -1.80884500 0.00389100 1.62021900  
H -2.00258800 -0.37813500 2.61585700  
H -1.15567200 1.95861100 2.17273600  
N -0.63327100 2.80582800 -0.31948500  
H -0.25355600 3.39859800 0.40578800  
H -0.26052800 2.93211800 -1.25268800  
C 1.80888900 -0.00390900 1.62019200  
C 1.35743500 -1.25751100 1.37346900  
C 1.12410800 -1.58789300 -0.00508600  
N 2.02630600 0.85281800 0.59048700  
C 1.83199300 0.49894200 -0.74945300  
N 1.38725600 -0.76066500 -1.00810600  
H 2.00265800 0.37810600 2.61582900  
H 1.15573700 -1.95863700 2.17270500  
N 0.63326700 -2.80582500 -0.31951100  
O 2.06570100 1.33966500 -1.62270100  
H 2.35640200 1.79545900 0.76448300  
H 0.25357800 -3.39861000 0.40576400  
H 0.26050800 -2.93211100 -1.25270800  
26

C-C-ftf-water-min80-plus: Optimised twist = 109.54 deg.

O -0.30685000 -2.14971900 -1.40138400  
C -1.01872300 -1.32155100 -0.82703000  
N -1.92345300 -1.77131400 0.14186300  
H -1.93527300 -2.76888000 0.32099800  
N -0.97933800 0.01564600 -1.07616900  
C -1.78063700 0.83968500 -0.41168800  
C -2.73271300 0.39276900 0.56690200  
C -2.75774500 -0.94052000 0.81412700  
H -3.41837100 -1.40227300 1.53884200  
H -3.38251600 1.08067400 1.09147500  
N -1.67568600 2.15697600 -0.68818700  
H -2.14966400 2.82991300 -0.10106800  
H -0.82731100 2.47228500 -1.15302000  
C 0.75462800 0.24536700 1.80592500  
C 1.40908900 -0.85710500 1.36771700  
C 2.18490500 -0.70261800 0.16687600  
N 0.82703900 1.40006500 1.09563300  
C 1.48140600 1.48783200 -0.13503800  
N 2.22100500 0.42210900 -0.53611500  
H 0.15979100 0.27061800 2.71193300  
H 1.37189200 -1.79449000 1.90732100  
N 2.95226100 -1.72681200 -0.25544000  
O 1.36565000 2.53285000 -0.78974700  
H 0.30958800 2.22007700 1.39151800  
H 2.83081300 -2.65073000 0.13469300  
H 3.37658000 -1.66208100 -1.17147900

28

C-T-ftf-gas-max240: Optimised twist = 275.13 deg.

H	0.22701800	0.19035600	-2.67458700
C	0.72395900	0.32182900	-1.71784700
N	0.64008200	1.58725900	-1.18414100
H	0.00558200	2.26684000	-1.58292300
C	1.38998000	-0.67871600	-1.10920800
C	1.52474400	-2.06286100	-1.66412500
C	1.08758500	1.90557800	0.08899200
O	0.86631200	2.98283500	0.60537000
C	2.03996900	-0.39451100	0.17859900
O	2.71467400	-1.19732200	0.79312300
N	1.82922600	0.89842300	0.67070200
H	2.12526700	1.06475800	1.62801700
C	-2.54626700	-0.55212300	-0.82551800
C	-2.11915200	-1.78054800	-0.43480800
N	-1.30844100	-1.90678600	0.63912400
C	-0.86611900	-0.80518400	1.41517100
N	-1.29147200	0.43448900	1.00685100
C	-2.07238300	0.55646000	-0.03821800
H	-3.18901800	-0.41882900	-1.68614900
H	-2.39360700	-2.69586400	-0.94907500
H	-0.97000100	-2.81042400	0.94809900
O	-0.14695200	-1.01435200	2.37069800
N	-2.38156000	1.83108900	-0.42903300
H	-3.22251400	1.98618000	-0.96731200
H	-2.14014200	2.55197000	0.24401000
H	2.57508900	-2.30797300	-1.85065800
H	1.15432500	-2.80217300	-0.94587800
H	0.96696400	-2.16499900	-2.59981800

28

H	0.22701800	0.19035600	-2.67458700
C	0.72395900	0.32182900	-1.71784700
N	0.64008200	1.58725900	-1.18414100
H	0.00558200	2.26684000	-1.58292300
C	1.38998000	-0.67871600	-1.10920800
C	1.52474400	-2.06286100	-1.66412500
C	1.08758500	1.90557800	0.08899200
O	0.86631200	2.98283500	0.60537000
C	2.03996900	-0.39451100	0.17859900
O	2.71467400	-1.19732200	0.79312300
N	1.82922600	0.89842300	0.67070200
H	2.12526700	1.06475800	1.62801700
C	-2.54626700	-0.55212300	-0.82551800
C	-2.11915200	-1.78054800	-0.43480800
N	-1.30844100	-1.90678600	0.63912400
C	-0.86611900	-0.80518400	1.41517100
N	-1.29147200	0.43448900	1.00685100
C	-2.07238300	0.55646000	-0.03821800
H	-3.18901800	-0.41882900	-1.68614900
H	-2.39360700	-2.69586400	-0.94907500
H	-0.97000100	-2.81042400	0.94809900
O	-0.14695200	-1.01435200	2.37069800
N	-2.38156000	1.83108900	-0.42903300
H	-3.22251400	1.98618000	-0.96731200
H	-2.14014200	2.55197000	0.24401000
H	2.57508900	-2.30797300	-1.85065800

H 1.15432500 -2.80217300 -0.94587800  
H 0.96696400 -2.16499900 -2.59981800  
28

C-T-*ftf-gas-max345-minus*: Optimised twist = 76.83 deg.

H 3.05829900 0.35916400 2.51212900  
C 2.85701900 0.25697600 1.45095900  
N 3.52166300 -0.77598300 0.82681400  
H 4.12764900 -1.39681000 1.34637800  
C 2.00526400 1.07133400 0.79983000  
C 1.20914500 2.15588000 1.45371100  
C 3.36098100 -1.09436400 -0.50557500  
O 3.92872800 -2.02007000 -1.04856400  
C 1.77000500 0.81205900 -0.61715700  
O 1.00453400 1.45845100 -1.32861000  
N 2.50102600 -0.23216800 -1.16347900  
H 2.32860300 -0.44752800 -2.14021100  
C -4.03255300 0.43566500 -0.71263100  
C -2.90328400 1.05753900 -1.13831600  
N -1.69551100 0.67067600 -0.67598000  
C -1.53005000 -0.38449500 0.24505400  
N -2.66349600 -1.01762900 0.67704900  
C -3.83922800 -0.63254900 0.23019500  
H -5.01449800 0.73246600 -1.05734600  
H -2.90778500 1.87653700 -1.85017000  
H -0.83021800 1.11333200 -0.99607700  
O -0.39554500 -0.67042400 0.60481200  
N -4.92886600 -1.27864500 0.72517400  
H -5.82562100 -1.19080000 0.27272000  
H -4.75522300 -2.11094200 1.27224900  
H 1.32374100 3.10354000 0.91925700  
H 0.14618600 1.89008200 1.44395800  
H 1.51963100 2.29529000 2.49253800

28

H 3.05829900 0.35916400 2.51212900  
C 2.85701900 0.25697600 1.45095900  
N 3.52166300 -0.77598300 0.82681400  
H 4.12764900 -1.39681000 1.34637800  
C 2.00526400 1.07133400 0.79983000  
C 1.20914500 2.15588000 1.45371100  
C 3.36098100 -1.09436400 -0.50557500  
O 3.92872800 -2.02007000 -1.04856400  
C 1.77000500 0.81205900 -0.61715700  
O 1.00453400 1.45845100 -1.32861000  
N 2.50102600 -0.23216800 -1.16347900  
H 2.32860300 -0.44752800 -2.14021100  
C -4.03255300 0.43566500 -0.71263100  
C -2.90328400 1.05753900 -1.13831600  
N -1.69551100 0.67067600 -0.67598000  
C -1.53005000 -0.38449500 0.24505400  
N -2.66349600 -1.01762900 0.67704900  
C -3.83922800 -0.63254900 0.23019500  
H -5.01449800 0.73246600 -1.05734600  
H -2.90778500 1.87653700 -1.85017000  
H -0.83021800 1.11333200 -0.99607700  
O -0.39554500 -0.67042400 0.60481200  
N -4.92886600 -1.27864500 0.72517400  
H -5.82562100 -1.19080000 0.27272000



H	-4.75522300	-2.11094200	1.27224900
H	1.32374100	3.10354000	0.91925700
H	0.14618600	1.89008200	1.44395800
H	1.51963100	2.29529000	2.49253800

28

C-T-ftf-gas-max345: Optimised twist = 34.38 deg.

H	0.92034900	-0.77739600	2.54252200
C	1.30897500	-0.28109100	1.65927200
N	2.37977700	-0.90361300	1.06702100
H	2.65138400	-1.83473300	1.35486600
C	0.76589600	0.86089400	1.18713500
C	-0.39656400	1.56291200	1.82069300
C	2.93073100	-0.48819300	-0.12824700
O	3.83083900	-1.07043000	-0.69532000
C	1.29495800	1.40025300	-0.06390000
O	0.84971900	2.37450300	-0.65380100
N	2.36816400	0.68764000	-0.60179400
H	2.76884400	1.04510100	-1.46313100
C	-2.92747800	0.62295900	-0.81402200
C	-1.85828700	0.73390500	-1.64065500
N	-0.85694700	-0.17301500	-1.57050500
C	-0.81617500	-1.21627200	-0.61922300
N	-1.89046200	-1.32253500	0.22212300
C	-2.88380600	-0.46411900	0.12825800
H	-3.74245100	1.33448900	-0.83732500
H	-1.74336200	1.52850900	-2.36938100
H	-0.03397100	-0.08722000	-2.15531100
O	0.16561800	-1.94145200	-0.59649900
N	-3.90251600	-0.60109800	1.01616800
H	-4.77385800	-0.11282600	0.87783400
H	-3.91481100	-1.44306400	1.57564800
H	-0.10887900	2.55764800	2.17699600
H	-1.20192900	1.70540700	1.09287100
H	-0.78633900	0.98398400	2.66242400

28

C-T-ftf-gas-max345-plus: Optimised twist = 67.61 deg.

H	-0.27235600	0.00832000	-2.49098800
C	-0.83195300	0.23150200	-1.58795300
N	-1.64053300	-0.79715800	-1.14589200
H	-1.47989200	-1.72569400	-1.52728300
C	-0.71607800	1.40678800	-0.93776800
C	0.18452400	2.52149400	-1.37233500
C	-2.25251100	-0.77430100	0.08634500
O	-2.75099300	-1.75666200	0.60977900
C	-1.46331100	1.58062900	0.30945700
O	-1.44207700	2.57731900	1.00886900
N	-2.22881400	0.46905700	0.68903900
H	-2.71005700	0.53608800	1.58038300
C	1.70360700	0.22816600	1.57981700
C	0.74596700	-0.70828600	1.78890900
N	0.50729500	-1.65642000	0.85013300
C	1.15391700	-1.67148800	-0.40510400
N	2.16353700	-0.77201800	-0.59207300
C	2.42331500	0.12522200	0.33745900
H	1.90457400	1.00804000	2.30268000
H	0.13542000	-0.74889400	2.68500500
H	-0.24349400	-2.33075200	0.96985000
O	0.75651900	-2.46144500	-1.25164600

N	3.41241700	1.01282400	0.07698900
H	3.75694800	1.64065000	0.78633100
H	3.96449600	0.87234800	-0.75782600
H	-0.38577700	3.43623600	-1.56194300
H	0.90951200	2.75157800	-0.58439000
H	0.73085900	2.24603100	-2.27815900

28

H	-0.27235600	0.00832000	-2.49098800
C	-0.83195300	0.23150200	-1.58795300
N	-1.64053300	-0.79715800	-1.14589200
H	-1.47989200	-1.72569400	-1.52728300
C	-0.71607800	1.40678800	-0.93776800
C	0.18452400	2.52149400	-1.37233500
C	-2.25251100	-0.77430100	0.08634500
O	-2.75099300	-1.75666200	0.60977900
C	-1.46331100	1.58062900	0.30945700
O	-1.44207700	2.57731900	1.00886900
N	-2.22881400	0.46905700	0.68903900
H	-2.71005700	0.53608800	1.58038300
C	1.70360700	0.22816600	1.57981700
C	0.74596700	-0.70828600	1.78890900
N	0.50729500	-1.65642000	0.85013300
C	1.15391700	-1.67148800	-0.40510400
N	2.16353700	-0.77201800	-0.59207300
C	2.42331500	0.12522200	0.33745900
H	1.90457400	1.00804000	2.30268000
H	0.13542000	-0.74889400	2.68500500
H	-0.24349400	-2.33075200	0.96985000
O	0.75651900	-2.46144500	-1.25164600
N	3.41241700	1.01282400	0.07698900
H	3.75694800	1.64065000	0.78633100
H	3.96449600	0.87234800	-0.75782600
H	-0.38577700	3.43623600	-1.56194300
H	0.90951200	2.75157800	-0.58439000
H	0.73085900	2.24603100	-2.27815900

28

H	0.92034900	-0.77739600	2.54252200
C	1.30897500	-0.28109100	1.65927200
N	2.37977700	-0.90361300	1.06702100
H	2.65138400	-1.83473300	1.35486600
C	0.76589600	0.86089400	1.18713500
C	-0.39656400	1.56291200	1.82069300
C	2.93073100	-0.48819300	-0.12824700
O	3.83083900	-1.07043000	-0.69532000
C	1.29495800	1.40025300	-0.06390000
O	0.84971900	2.37450300	-0.65380100
N	2.36816400	0.68764000	-0.60179400
H	2.76884400	1.04510100	-1.46313100
C	-2.92747800	0.62295900	-0.81402200
C	-1.85828700	0.73390500	-1.64065500
N	-0.85694700	-0.17301500	-1.57050500
C	-0.81617500	-1.21627200	-0.61922300
N	-1.89046200	-1.32253500	0.22212300
C	-2.88380600	-0.46411900	0.12825800
H	-3.74245100	1.33448900	-0.83732500
H	-1.74336200	1.52850900	-2.36938100

H	-0.03397100	-0.08722000	-2.15531100
O	0.16561800	-1.94145200	-0.59649900
N	-3.90251600	-0.60109800	1.01616800
H	-4.77385800	-0.11282600	0.87783400
H	-3.91481100	-1.44306400	1.57564800
H	-0.10887900	2.55764800	2.17699600
H	-1.20192900	1.70540700	1.09287100
H	-0.78633900	0.98398400	2.66242400

28

C-T-ftf-gas-min290-minus: Optimised twist = 318.13 deg.

H	1.68619400	2.37928800	1.25146200
C	1.59467100	1.53835000	0.57122900
N	2.25082000	0.39616600	0.95976900
H	2.75906100	0.35411700	1.83242700
C	0.88438600	1.61169700	-0.57189800
C	0.15570800	2.83538000	-1.03587600
C	2.24702000	-0.78340300	0.22897900
O	2.83032800	-1.78026500	0.59422400
C	0.78280200	0.40000500	-1.39264400
O	0.07996100	0.30939400	-2.38822300
N	1.54647700	-0.68203500	-0.95940800
H	1.37729300	-1.56841500	-1.43140000
C	-2.34296900	0.81007800	0.78823000
C	-2.76077400	0.28865600	-0.39392700
N	-2.25495900	-0.88291500	-0.83421900
C	-1.22007600	-1.57652000	-0.17016200
N	-0.80608800	-1.05758500	1.03168300
C	-1.33258100	0.05868100	1.48058700
H	-2.72830900	1.74782100	1.16722500
H	-3.49970700	0.76777100	-1.02738700
H	-2.46019900	-1.22459900	-1.76584300
O	-0.74787400	-2.56725000	-0.69842800
N	-0.83459100	0.54485500	2.65758100
H	-1.39518700	1.19586500	3.18871800
H	-0.29036700	-0.11770000	3.19668500
H	0.52622400	3.16228900	-2.01270900
H	-0.91261600	2.62644400	-1.15278700
H	0.27755800	3.65514200	-0.32192400

28

H	1.68619400	2.37928800	1.25146200
C	1.59467100	1.53835000	0.57122900
N	2.25082000	0.39616600	0.95976900
H	2.75906100	0.35411700	1.83242700
C	0.88438600	1.61169700	-0.57189800
C	0.15570800	2.83538000	-1.03587600
C	2.24702000	-0.78340300	0.22897900
O	2.83032800	-1.78026500	0.59422400
C	0.78280200	0.40000500	-1.39264400
O	0.07996100	0.30939400	-2.38822300
N	1.54647700	-0.68203500	-0.95940800
H	1.37729300	-1.56841500	-1.43140000
C	-2.34296900	0.81007800	0.78823000
C	-2.76077400	0.28865600	-0.39392700
N	-2.25495900	-0.88291500	-0.83421900
C	-1.22007600	-1.57652000	-0.17016200
N	-0.80608800	-1.05758500	1.03168300
C	-1.33258100	0.05868100	1.48058700

H	-2.72830900	1.74782100	1.16722500
H	-3.49970700	0.76777100	-1.02738700
H	-2.46019900	-1.22459900	-1.76584300
O	-0.74787400	-2.56725000	-0.69842800
N	-0.83459100	0.54485500	2.65758100
H	-1.39518700	1.19586500	3.18871800
H	-0.29036700	-0.11770000	3.19668500
H	0.52622400	3.16228900	-2.01270900
H	-0.91261600	2.62644400	-1.15278700
H	0.27755800	3.65514200	-0.32192400

28

C-T-ftf-gas-min290: Optimised twist = 309.68 deg.

H	-0.98741600	0.26354800	-2.80386100
C	-1.17473300	0.35432500	-1.73837600
N	-1.90078200	-0.66951300	-1.18290200
H	-2.17907000	-1.47002200	-1.73364600
C	-0.72616500	1.40010700	-1.01480100
C	0.05898800	2.54287500	-1.57979800
C	-2.20322100	-0.75614000	0.16834700
O	-2.81614400	-1.68650800	0.64404500
C	-0.99582400	1.40403000	0.42768100
O	-0.57781900	2.25534200	1.19687600
N	-1.76768000	0.34011600	0.89114100
H	-1.83518600	0.24371100	1.90194600
C	2.44048300	-0.25144000	-0.90032200
C	2.63461400	0.60552200	0.13503800
N	1.96125600	0.43241400	1.29247900
C	1.02922300	-0.60950000	1.50297400
N	0.80893000	-1.45439100	0.44310900
C	1.46646200	-1.28499700	-0.67996700
H	2.96000800	-0.13567300	-1.84268500
H	3.31477200	1.44977700	0.08975100
H	2.01196800	1.11342800	2.04182700
O	0.46664300	-0.68166900	2.57934800
N	1.14355200	-2.12273400	-1.71374900
H	1.81522800	-2.24926600	-2.45795400
H	0.62864900	-2.95146200	-1.44010100
H	-0.47204400	3.48943700	-1.43688200
H	1.02202900	2.63978600	-1.06741000
H	0.24373000	2.39948800	-2.64833600

28

C-T-ftf-gas-min290-plus: Optimised twist = 318.13 deg.

H	1.68641400	2.37922300	1.25144000
C	1.59480800	1.53828800	0.57121500
N	2.25088900	0.39605700	0.95974200
H	2.75917900	0.35398900	1.83237000
C	0.88449000	1.61167700	-0.57188800
C	0.15588900	2.83541000	-1.03585400
C	2.24700000	-0.78350600	0.22894800
O	2.83026200	-1.78040400	0.59416800
C	0.78279500	0.39998600	-1.39262500
O	0.07990900	0.30941900	-2.38817600
N	1.54641900	-0.68209800	-0.95941500
H	1.37716800	-1.56847100	-1.43139900
C	-2.34294600	0.81017000	0.78825200
C	-2.76078700	0.28877300	-0.39390500
N	-2.25502300	-0.88281200	-0.83421400
C	-1.22017500	-1.57647800	-0.17016200

N	-0.80613700	-1.05755700	1.03166900
C	-1.33257600	0.05873000	1.48058800
H	-2.72824500	1.74792400	1.16725900
H	-3.49970600	0.76792600	-1.02735100
H	-2.46029700	-1.22448900	-1.76583200
O	-0.74804900	-2.56724600	-0.69842500
N	-0.83454600	0.54487400	2.65757700
H	-1.39510600	1.19590100	3.18873100
H	-0.29033500	-0.11770600	3.19666400
H	0.52643000	3.16231100	-2.01268000
H	-0.91244700	2.62654100	-1.15277800
H	0.27778400	3.65515600	-0.32189100

28

H	1.68641400	2.37922300	1.25144000
C	1.59480800	1.53828800	0.57121500
N	2.25088900	0.39605700	0.95974200
H	2.75917900	0.35398900	1.83237000
C	0.88449000	1.61167700	-0.57188800
C	0.15588900	2.83541000	-1.03585400
C	2.24700000	-0.78350600	0.22894800
O	2.83026200	-1.78040400	0.59416800
C	0.78279500	0.39998600	-1.39262500
O	0.07990900	0.30941900	-2.38817600
N	1.54641900	-0.68209800	-0.95941500
H	1.37716800	-1.56847100	-1.43139900
C	-2.34294600	0.81017000	0.78825200
C	-2.76078700	0.28877300	-0.39390500
N	-2.25502300	-0.88281200	-0.83421400
C	-1.22017500	-1.57647800	-0.17016200
N	-0.80613700	-1.05755700	1.03166900
C	-1.33257600	0.05873000	1.48058800
H	-2.72824500	1.74792400	1.16725900
H	-3.49970600	0.76792600	-1.02735100
H	-2.46029700	-1.22448900	-1.76583200
O	-0.74804900	-2.56724600	-0.69842500
N	-0.83454600	0.54487400	2.65757700
H	-1.39510600	1.19590100	3.18873100
H	-0.29033500	-0.11770600	3.19666400
H	0.52643000	3.16231100	-2.01268000
H	-0.91244700	2.62654100	-1.15277800
H	0.27778400	3.65515600	-0.32189100

28

H	-0.98741600	0.26354800	-2.80386100
C	-1.17473300	0.35432500	-1.73837600
N	-1.90078200	-0.66951300	-1.18290200
H	-2.17907000	-1.47002200	-1.73364600
C	-0.72616500	1.40010700	-1.01480100
C	0.05898800	2.54287500	-1.57979800
C	-2.20322100	-0.75614000	0.16834700
O	-2.81614400	-1.68650800	0.64404500
C	-0.99582400	1.40403000	0.42768100
O	-0.57781900	2.25534200	1.19687600
N	-1.76768000	0.34011600	0.89114100
H	-1.83518600	0.24371100	1.90194600
C	2.44048300	-0.25144000	-0.90032200
C	2.63461400	0.60552200	0.13503800

N	1.96125600	0.43241400	1.29247900
C	1.02922300	-0.60950000	1.50297400
N	0.80893000	-1.45439100	0.44310900
C	1.46646200	-1.28499700	-0.67996700
H	2.96000800	-0.13567300	-1.84268500
H	3.31477200	1.44977700	0.08975100
H	2.01196800	1.11342800	2.04182700
O	0.46664300	-0.68166900	2.57934800
N	1.14355200	-2.12273400	-1.71374900
H	1.81522800	-2.24926600	-2.45795400
H	0.62864900	-2.95146200	-1.44010100
H	-0.47204400	3.48943700	-1.43688200
H	1.02202900	2.63978600	-1.06741000
H	0.24373000	2.39948800	-2.64833600

28

C-T-ftf-gas-min90: Optimised twist = 82.88 deg.

H	-1.88212800	-2.25950100	-1.27217400
C	-1.71406500	-1.53126100	-0.48536800
N	-0.65939800	-1.82161200	0.34754600
H	0.05172400	-2.47541400	0.02496100
C	-2.48804700	-0.43382600	-0.34870500
C	-3.65309900	-0.10678100	-1.23321400
C	-0.21148500	-0.93759500	1.30470700
O	0.82401200	-1.08661500	1.92881800
C	-2.12442300	0.53113800	0.68668600
O	-2.66839800	1.61106700	0.86175900
N	-1.05037700	0.14620600	1.49288700
H	-0.74501500	0.81696000	2.19085600
C	2.15913200	1.81060800	0.16734000
C	3.11902400	0.88663200	0.42200300
N	3.03549100	-0.34920200	-0.12103900
C	1.92395000	-0.77729300	-0.86803500
N	0.98366400	0.16293100	-1.17796500
C	1.07812300	1.37958800	-0.67644700
H	2.20915700	2.81225200	0.57376600
H	3.98096900	1.08388400	1.04986800
H	3.67787600	-1.08442300	0.14785900
O	1.84330600	-1.96158400	-1.17464000
N	0.09477800	2.25657500	-0.99725600
H	-0.05157500	3.08310500	-0.43593100
H	-0.72431300	1.87211100	-1.45173000
H	-4.57265800	-0.01067400	-0.64735200
H	-3.50202900	0.85098500	-1.74223600
H	-3.79712200	-0.88377400	-1.98840400

28

H	-1.88212800	-2.25950100	-1.27217400
C	-1.71406500	-1.53126100	-0.48536800
N	-0.65939800	-1.82161200	0.34754600
H	0.05172400	-2.47541400	0.02496100
C	-2.48804700	-0.43382600	-0.34870500
C	-3.65309900	-0.10678100	-1.23321400
C	-0.21148500	-0.93759500	1.30470700
O	0.82401200	-1.08661500	1.92881800
C	-2.12442300	0.53113800	0.68668600
O	-2.66839800	1.61106700	0.86175900
N	-1.05037700	0.14620600	1.49288700
H	-0.74501500	0.81696000	2.19085600

C	2.15913200	1.81060800	0.16734000
C	3.11902400	0.88663200	0.42200300
N	3.03549100	-0.34920200	-0.12103900
C	1.92395000	-0.77729300	-0.86803500
N	0.98366400	0.16293100	-1.17796500
C	1.07812300	1.37958800	-0.67644700
H	2.20915700	2.81225200	0.57376600
H	3.98096900	1.08388400	1.04986800
H	3.67787600	-1.08442300	0.14785900
O	1.84330600	-1.96158400	-1.17464000
N	0.09477800	2.25657500	-0.99725600
H	-0.05157500	3.08310500	-0.43593100
H	-0.72431300	1.87211100	-1.45173000
H	-4.57265800	-0.01067400	-0.64735200
H	-3.50202900	0.85098500	-1.74223600
H	-3.79712200	-0.88377400	-1.98840400

28

C-T-ftf-water-max120: Optimised twist = 148.27 deg.

H	-1.43640600	1.21510100	-2.31031100
C	-1.37724100	0.44933200	-1.54451300
N	-0.63395400	-0.65954000	-1.88913600
H	-0.21751200	-0.72781000	-2.81039100
C	-1.96144700	0.58370800	-0.33637600
C	-2.72069300	1.79974600	0.09227600
C	-0.46549000	-1.74624100	-1.06885000
O	0.15414900	-2.74993700	-1.39356600
C	-1.77150800	-0.48988900	0.63314200
O	-2.18116900	-0.47711100	1.78926800
N	-1.06533000	-1.59718900	0.16394900
H	-0.93290800	-2.36432900	0.81705500
C	2.36036800	-0.76822200	0.53337900
C	2.70762900	-0.11533600	-0.60286400
N	2.13881000	1.08006800	-0.89890300
C	1.19422500	1.70056700	-0.07353300
N	0.82593900	1.04576200	1.06204400
C	1.37307300	-0.12779700	1.35785100
H	2.78774600	-1.72788000	0.79266800
H	3.42798000	-0.49773700	-1.31672000
H	2.39358000	1.57712600	-1.74470200
O	0.73894600	2.79461800	-0.41586700
N	0.96490400	-0.72898300	2.49249300
H	1.23787700	-1.68009500	2.69755300
H	0.13735600	-0.36975000	2.95413400
H	-3.73603500	1.53930800	0.40777100
H	-2.22174400	2.27647900	0.94234800
H	-2.78142100	2.52298700	-0.72428100

28

C-T-ftf-water-max240-minus: Optimised twist = 229.35 deg.

H	0.35880800	0.35938200	2.64250600
C	0.77461300	0.51999200	1.65356600
N	1.78135500	-0.35125900	1.30031500
H	2.07869300	-1.07518500	1.94423900
C	0.33723000	1.49875700	0.83311200
C	-0.74900900	2.46746100	1.19153200
C	2.43055000	-0.31118800	0.09193900
O	3.32709800	-1.08336500	-0.21826000
C	0.97499900	1.62376700	-0.47599400
O	0.69989800	2.47567100	-1.31160800

N	1.97474200	0.68708200	-0.74160900
H	2.42980800	0.75038700	-1.64795100
C	-1.05942400	-2.06560300	0.76649500
C	-2.08414600	-1.31423100	1.23754100
N	-2.58627000	-0.30419000	0.48374000
C	-2.10757600	0.00373100	-0.79396800
N	-1.06713200	-0.73255400	-1.27162900
C	-0.55748200	-1.71269400	-0.53372300
H	-0.63202300	-2.87491700	1.34398700
H	-2.54366900	-1.46831500	2.20709700
H	-3.35649500	0.25991400	0.82448100
O	-2.64375400	0.92267700	-1.41973700
N	0.48061600	-2.39619700	-1.04685000
H	0.97113900	-3.09802000	-0.51122800
H	0.87167400	-2.11164600	-1.93533800
H	-0.36356800	3.49205100	1.22103900
H	-1.55144400	2.44055200	0.44660800
H	-1.17057200	2.22580700	2.17060900

28

C-T-fff-water-max240: Optimised twist = 232.71 deg.

H	0.14038500	0.24559600	2.54510700
C	0.69839200	0.32456700	1.61807100
N	1.42663700	-0.79524500	1.28346000
H	1.40844500	-1.61374200	1.88095300
C	0.67714800	1.43413500	0.84913700
C	-0.11855900	2.66157600	1.17278900
C	2.18911400	-0.89339000	0.14676900
O	2.82324600	-1.89521300	-0.15539100
C	1.47935700	1.43119500	-0.37261400
O	1.57957300	2.37412100	-1.14804200
N	2.17772600	0.24999200	-0.62174900
H	2.73658300	0.21970100	-1.46977700
C	-1.76748900	-1.76190500	0.73812000
C	-2.51948600	-0.68971500	1.08715900
N	-2.55236900	0.40489100	0.28647200
C	-1.83873400	0.49155500	-0.91367200
N	-1.06582600	-0.57312100	-1.26699000
C	-1.02986100	-1.64971000	-0.49072700
H	-1.71919700	-2.64973200	1.35481700
H	-3.11510300	-0.64570500	1.99166300
H	-3.11876900	1.20826300	0.53424500
O	-1.93965000	1.52009500	-1.58721800
N	-0.26507000	-2.68128700	-0.89482500
H	-0.07925200	-3.46280000	-0.28199000
H	0.34288500	-2.55682800	-1.69409000
H	0.53450400	3.53363400	1.28086000
H	-0.82706700	2.87830600	0.36564400
H	-0.67573600	2.52482500	2.10301200

28

C-T-fff-water-max240-plus: Optimised twist = 248.47 deg.

H	-0.17046900	-0.26325300	2.50102700
C	-0.69240200	0.09728400	1.62081400
N	-0.40627900	1.39661800	1.26658400
H	0.28278500	1.92759800	1.78656600
C	-1.55217100	-0.67208900	0.91995800
C	-1.85194000	-2.10225000	1.24618900
C	-0.88184100	1.98397000	0.12166400
O	-0.51841800	3.08777100	-0.26739800



C	-2.22175400	-0.07349600	-0.23352600
O	-3.08242900	-0.62503300	-0.90799900
N	-1.82434800	1.22757500	-0.53683900
H	-2.21933500	1.64322000	-1.37556800
C	2.74623000	-0.30255200	0.69126700
C	2.37592400	-1.60699000	0.67357300
N	1.44503000	-2.03669700	-0.21353700
C	0.82808600	-1.18815400	-1.14015600
N	1.18146300	0.12700100	-1.12286900
C	2.09018600	0.55730300	-0.25459500
H	3.48457100	0.06998300	1.38902900
H	2.78591600	-2.35365700	1.34373000
H	1.16540700	-3.01087100	-0.23602100
O	-0.00330500	-1.66546900	-1.91607500
N	2.38948900	1.87055500	-0.27400000
H	2.97124500	2.27649700	0.44567100
H	1.78493100	2.49639500	-0.79479100
H	-2.91780100	-2.24487300	1.45051900
H	-1.59339600	-2.74453200	0.39673200
H	-1.28001900	-2.42817700	2.11836900

28

C-T-ftf-water-max315-minus: Optimised twist = 298.36 deg.

H	-0.35833100	-0.39887700	-2.72392000
C	-0.81490100	-0.16636600	-1.76735300
N	-1.41552000	-1.22855400	-1.13735100
H	-1.36593100	-2.15488300	-1.54470800
C	-0.79026200	1.07576600	-1.23580900
C	-0.14414200	2.25297000	-1.89800300
C	-1.98643200	-1.14442200	0.10865500
O	-2.46438000	-2.10475900	0.69668800
C	-1.43184900	1.27553100	0.05979500
O	-1.49334800	2.34771600	0.65226300
N	-1.99885100	0.13436100	0.62186300
H	-2.37207300	0.23003600	1.56195600
C	2.50610500	-0.18608800	-0.73949900
C	2.48766000	0.98994600	-0.06613600
N	1.73178600	1.11763100	1.05349000
C	0.98908300	0.06293900	1.59707900
N	0.98032000	-1.11573700	0.91552300
C	1.69667400	-1.24164800	-0.19601100
H	3.09136700	-0.31894400	-1.63986700
H	3.04844500	1.86524700	-0.37375800
H	1.71254200	1.99179700	1.56683300
O	0.37372300	0.25106500	2.64935200
N	1.61705200	-2.41523400	-0.85137400
H	2.23055700	-2.62233900	-1.62693000
H	1.14203400	-3.18945100	-0.40522100
H	-0.88478200	3.02216900	-2.14069800
H	0.59330300	2.71460600	-1.23258400
H	0.35979500	1.94943300	-2.81887900

28

C-T-ftf-water-max315: Optimised twist = 327.91 deg.

H	1.96240900	1.57497600	1.82728400
C	1.75788500	0.95196700	0.96328700
N	1.98336700	-0.39017100	1.14985300
H	2.30658900	-0.73357400	2.04659100
C	1.31101800	1.45889000	-0.20645100
C	1.05441900	2.91579400	-0.44289300

C	1.77375800	-1.33860800	0.17909400
O	1.98119400	-2.53159100	0.34824000
C	1.05421300	0.52513300	-1.29852700
O	0.62795700	0.84234100	-2.40419900
N	1.33235700	-0.81167200	-1.01676400
H	1.12126800	-1.48921100	-1.74473900
C	-1.97422000	1.26599500	0.62695200
C	-2.32965200	0.96798300	-0.64594200
N	-2.14006600	-0.28694100	-1.12629600
C	-1.57057300	-1.31458800	-0.37071200
N	-1.19892200	-1.02583800	0.90683300
C	-1.38738900	0.19812900	1.38980200
H	-2.10595000	2.25788500	1.03913700
H	-2.76670900	1.68609500	-1.33012300
H	-2.38080800	-0.51220500	-2.08464800
O	-1.41886600	-2.42139300	-0.89672600
N	-0.97976500	0.43473600	2.64805300
H	-1.13031500	1.32700800	3.09640000
H	-0.60067100	-0.32449200	3.19834500
H	1.69311700	3.30018000	-1.24487900
H	0.01487400	3.08012400	-0.74549700
H	1.24836300	3.49338000	0.46420000

28

C-T-fff-water-max315-plus: Optimised twist = 333.19 deg.

H	-2.43048600	-0.74805600	1.84403300
C	-2.00289200	-0.26618100	0.97138800
N	-1.71017300	1.06666200	1.13053700
H	-1.88814600	1.52653500	2.01551300
C	-1.77222200	-0.92859300	-0.18311400
C	-2.07557100	-2.38086300	-0.39008800
C	-1.16118500	1.84825100	0.14387600
O	-0.92009400	3.03831600	0.28373900
C	-1.17708100	-0.18368600	-1.28817100
O	-0.89668400	-0.66098700	-2.38259900
N	-0.92913700	1.16460300	-1.03210500
H	-0.49502600	1.70346000	-1.77690000
C	1.37194600	-1.85098000	0.52562900
C	1.81710400	-1.62355300	-0.73350200
N	2.10751300	-0.35878600	-1.13105500
C	1.96613800	0.75400100	-0.29770600
N	1.50465800	0.54135500	0.96548800
C	1.21794000	-0.69362600	1.36491500
H	1.12588800	-2.84596800	0.87312200
H	1.95744000	-2.40611400	-1.47008400
H	2.42454400	-0.17672500	-2.07643900
O	2.24981600	1.86828600	-0.74675700
N	0.74482100	-0.84414700	2.61307400
H	0.51965800	-1.75274600	2.99165000
H	0.64552400	-0.03311300	3.20901900
H	-2.80129400	-2.51730000	-1.19844200
H	-1.16869800	-2.92762300	-0.66962200
H	-2.48253800	-2.82370900	0.52215800

28

C-T-fff-water-max355: Optimised twist = 13.25 deg.

H	0.12975900	0.45915300	-2.40250000
C	-0.54949100	0.48198000	-1.55674200
N	-1.36947300	-0.61535500	-1.44359300
H	-1.28015000	-1.38810600	-2.09313900

C	-0.58372100	1.51291900	-0.68422300
C	0.27338600	2.73632700	-0.80514900
C	-2.29609500	-0.77090700	-0.44315100
O	-3.04503100	-1.73277100	-0.35616600
C	-1.51270600	1.42116000	0.43678000
O	-1.62708200	2.25930100	1.32477800
N	-2.30812200	0.27524900	0.45742400
H	-2.97744500	0.19715600	1.21814100
C	2.29298700	0.57881500	0.96321000
C	1.33190400	0.17774900	1.82919300
N	0.60060900	-0.93508000	1.56249800
C	0.82025700	-1.73908500	0.43762300
N	1.76418900	-1.33101800	-0.45326700
C	2.45705000	-0.22074300	-0.21993400
H	2.88635000	1.46580900	1.14243700
H	1.09441100	0.70389600	2.74680800
H	-0.10685200	-1.25494800	2.21471000
O	0.14341400	-2.76173400	0.30232700
N	3.33686100	0.16701000	-1.15901100
H	3.94205300	0.96382000	-1.02231800
H	3.49292600	-0.42281700	-1.96562900
H	-0.33840600	3.62347700	-1.00137600
H	0.82487800	2.91672200	0.12220700
H	0.99220300	2.62254200	-1.62086000

28

C-T-ftf-water-max75: Optimised twist = 70.64 deg.

H	-1.74433200	-1.72855100	-1.97408300
C	-1.55762100	-1.33839600	-0.97952100
N	-0.51619600	-1.93619600	-0.31114000
H	0.09330500	-2.58481500	-0.79778400
C	-2.29996300	-0.34677600	-0.44099700
C	-3.45439800	0.30802100	-1.13639000
C	-0.08604600	-1.53048300	0.92601800
O	0.88225300	-2.01397600	1.49746300
C	-1.94286800	0.12280000	0.89258000
O	-2.52086500	1.01471000	1.50406400
N	-0.85155300	-0.52241100	1.47377300
H	-0.56735500	-0.20140900	2.39520100
C	1.54078600	1.90616600	0.70027300
C	2.58114100	1.07801000	0.96546500
N	2.84522000	0.03277200	0.14291200
C	2.05279700	-0.28025000	-0.96378300
N	1.02884700	0.56334500	-1.26432000
C	0.77336200	1.60290500	-0.47612700
H	1.30613000	2.74938000	1.33642400
H	3.23959000	1.20000900	1.81752100
H	3.58561900	-0.62249800	0.36627800
O	2.30825000	-1.30323700	-1.60854900
N	-0.26706600	2.38549100	-0.80881400
H	-0.52462300	3.19401800	-0.26155600
H	-0.79780900	2.17511700	-1.64361400
H	-4.38260100	0.16271900	-0.57413800
H	-3.29611200	1.38843800	-1.22112100
H	-3.58680400	-0.10537400	-2.13892500

28

C-T-ftf-water-min155: Optimised twist = 164.32 deg.

H	-0.35016700	1.12991700	-2.56728500
C	-0.80785600	0.91866600	-1.60668300

N	-1.73871000	-0.09547900	-1.61774700
H	-1.94162400	-0.59383000	-2.47647600
C	-0.48526500	1.59861300	-0.48557700
C	0.52174700	2.70602100	-0.43648900
C	-2.40385700	-0.52519100	-0.49720300
O	-3.20639900	-1.44853200	-0.50110900
C	-1.16816300	1.23459300	0.75293300
O	-0.98842700	1.77299400	1.83824400
N	-2.08395500	0.18733000	0.63926900
H	-2.56927500	-0.09034000	1.48796300
C	0.46116900	-1.99186100	0.26657300
C	0.99727700	-1.90820800	-0.97562400
N	1.94995200	-0.98037600	-1.24056300
C	2.43369000	-0.08679600	-0.27698300
N	1.90100400	-0.15839200	0.97326800
C	0.95668200	-1.05545100	1.23791000
H	-0.30449100	-2.71757300	0.50985500
H	0.70293300	-2.54904200	-1.79898400
H	2.35910000	-0.91056800	-2.16544000
O	3.31135800	0.71594100	-0.60542700
N	0.46146700	-1.08299500	2.48823900
H	-0.33411800	-1.66028300	2.72116800
H	0.70047800	-0.33126200	3.12169500
H	0.05476600	3.64115900	-0.11043100
H	1.31842500	2.46348400	0.27421000
H	0.97086300	2.86217100	-1.42034100

28

C-T-ftf-water-min280: Optimised twist = 298.36 deg.

H	-0.35832000	-0.39888900	-2.72390200
C	-0.81489600	-0.16636300	-1.76734000
N	-1.41553700	-1.22853700	-1.13733500
H	-1.36596200	-2.15486900	-1.54468700
C	-0.79024300	1.07577200	-1.23580500
C	-0.14410700	2.25296500	-1.89800500
C	-1.98646600	-1.14438700	0.10866100
O	-2.46444200	-2.10471100	0.69669200
C	-1.43183500	1.27555500	0.05979400
O	-1.49332500	2.34774500	0.65225400
N	-1.99886200	0.13439800	0.62186500
H	-2.37209700	0.23008700	1.56195200
C	2.50608500	-0.18610100	-0.73951800
C	2.48767000	0.98992000	-0.06613000
N	1.73181800	1.11759400	1.05351000
C	0.98910800	0.06290200	1.59709100
N	0.98031800	-1.11576000	0.91551300
C	1.69665300	-1.24166100	-0.19603300
H	3.09132900	-0.31894800	-1.63989800
H	3.04846100	1.86521800	-0.37374800
H	1.71260500	1.99174700	1.56687700
O	0.37376800	0.25102000	2.64937700
N	1.61700400	-2.41523500	-0.85142000
H	2.23051500	-2.62233900	-1.62697100
H	1.14200600	-3.18945900	-0.40525800
H	-0.88474300	3.02215800	-2.14073400
H	0.59331700	2.71461600	-1.23257400
H	0.35985500	1.94941200	-2.81886100

28

C-T-ftf-water-min325: Optimised twist = 333.19 deg.

H	-2.43046600	-0.74817300	1.84402900
C	-2.00289200	-0.26627300	0.97138800
N	-1.71023600	1.06658400	1.13054900
H	-1.88823900	1.52644100	2.01552600
C	-1.77218500	-0.92866400	-0.18311800
C	-2.07545000	-2.38095100	-0.39009800
C	-1.16128200	1.84820600	0.14389700
O	-0.92024200	3.03828000	0.28376800
C	-1.17707300	-0.18372200	-1.28816700
O	-0.89664500	-0.66100400	-2.38259500
N	-0.92920300	1.16457900	-1.03209100
H	-0.49510400	1.70346100	-1.77687600
C	1.37203200	-1.85093300	0.52557700
C	1.81716600	-1.62345000	-0.73355200
N	2.10752000	-0.35865900	-1.13107100
C	1.96610500	0.75409700	-0.29768900
N	1.50466100	0.54139400	0.96550900
C	1.21798900	-0.69361000	1.36490000
H	1.12601600	-2.84594100	0.87304300
H	1.95752600	-2.40598400	-1.47016000
H	2.42452000	-0.17655500	-2.07645700
O	2.24972000	1.86841000	-0.74671300
N	0.74486400	-0.84418500	2.61305100
H	0.51984900	-1.75281600	2.99163800
H	0.64562600	-0.03318400	3.20905000
H	-2.80111100	-2.51743200	-1.19849900
H	-1.16853000	-2.92766800	-0.66956400
H	-2.48245500	-2.82380900	0.52212500

28

C-T-ftf-water-min35: Optimised twist = 54.30 deg.

H	-0.17888600	-0.10749100	-2.44747000
C	-0.75260800	0.17348900	-1.57048900
N	-1.68895200	-0.75182900	-1.17078200
H	-1.72374800	-1.65874300	-1.62341500
C	-0.55192200	1.33817200	-0.91725100
C	0.46796000	2.35688700	-1.32407300
C	-2.45308200	-0.61062400	-0.04129800
O	-3.22552200	-1.46902700	0.36337200
C	-1.36457200	1.60488300	0.26526800
O	-1.29705000	2.61834900	0.95073200
N	-2.26536100	0.59431000	0.60406900
H	-2.82904300	0.74395400	1.43644700
C	1.85125000	0.40865800	1.41534900
C	0.80279500	-0.34394300	1.82712400
N	0.40827700	-1.41682800	1.09310000
C	1.03876300	-1.79696300	-0.09719600
N	2.10599500	-1.06260200	-0.50959100
C	2.49937000	-0.01033600	0.20166900
H	2.18512300	1.27377600	1.97333000
H	0.23517700	-0.13936100	2.72820500
H	-0.35432200	-2.00667300	1.40888700
O	0.58846700	-2.76498600	-0.71820900
N	3.55338500	0.68580400	-0.25349000
H	3.90923800	1.49410500	0.23612100
H	4.01244600	0.39534200	-1.10634100
H	-0.01038300	3.29893600	-1.61176200
H	1.14559100	2.57581600	-0.49190300
H	1.06051600	1.99234100	-2.16700400

28

C-T-ftf-water-min90: Optimised twist = 57.09 deg.

H	-1.99413000	-1.56096100	-2.06694400
C	-1.62585800	-1.31086000	-1.07795700
N	-0.55914700	-2.06523800	-0.65084000
H	-0.15543200	-2.76976800	-1.25681200
C	-2.17822300	-0.33496500	-0.32489900
C	-3.35776900	0.48519900	-0.75034400
C	0.04148700	-1.90585700	0.57189100
O	0.97524900	-2.59222700	0.96349100
C	-1.58830600	-0.07066700	0.98232000
O	-1.96889200	0.79287500	1.76511600
N	-0.51021200	-0.88893500	1.32291800
H	-0.09163300	-0.73470800	2.23610300
C	1.13372500	2.01864500	0.83162800
C	2.13585100	1.18568500	1.20374700
N	2.54656800	0.19995200	0.36651500
C	1.99403800	-0.00161300	-0.90293000
N	0.97349400	0.81523200	-1.27939700
C	0.55701300	1.77772700	-0.46262300
H	0.77899600	2.80954100	1.47904100
H	2.64580200	1.25178800	2.15791600
H	3.28268800	-0.43918900	0.64458800
O	2.44684000	-0.90522200	-1.61160500
N	-0.45794300	2.54915000	-0.88649300
H	-0.85059800	3.27835300	-0.30873900
H	-0.87241200	2.37042600	-1.79149200
H	-4.20660100	0.32496700	-0.07726800
H	-3.11814300	1.55291600	-0.72100800
H	-3.66518200	0.22234100	-1.76532200

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C-U-ftf-gas-max235: Optimised twist = 225.26 deg.

H	-3.18779700	-1.54123500	1.77932400
C	-2.61164600	-1.16020200	0.94334700
N	-2.70630300	0.19637600	0.73394600
H	-3.25130900	0.78829800	1.34699000
C	-1.85473000	-1.94615300	0.15724500
H	-1.77256000	-3.01292600	0.31373600
C	-2.02476800	0.86151100	-0.26988500
O	-2.06083500	2.07621000	-0.37952300
C	-1.11710300	-1.35709900	-0.96055500
O	-0.39347700	-1.95352700	-1.72626400
N	-1.32342700	0.03019100	-1.10854300
H	-0.77552800	0.48494900	-1.83474000
C	0.64654200	0.97790200	1.26912100
C	1.03326300	-0.22822600	1.75232900
N	1.98962700	-0.93954200	1.11116900
C	2.67483200	-0.46701000	-0.04051500
N	2.23518800	0.72362900	-0.56087900
C	1.28746600	1.40149800	0.04534000
H	-0.09283600	1.59151900	1.76824600
H	0.61664700	-0.67086300	2.65162700
H	2.30260800	-1.83923700	1.45360600
O	3.58060100	-1.14045300	-0.48845500
N	0.90132400	2.57896300	-0.51244100
H	-0.03065000	2.93200200	-0.32882400
H	1.30311300	2.78901200	-1.41734800

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C-U-ftf-gas-max345-minus: Optimised twist = 16.81 deg.

H	0.44717500	-1.58409300	2.13370400
C	0.96586400	-0.83793700	1.54220900
N	2.02764700	-1.30168100	0.81686400
H	2.20171900	-2.29486000	0.73114000
C	0.58808100	0.45795200	1.51957400
H	-0.25338000	0.82210200	2.09325500
C	2.74576800	-0.51255100	-0.06923700
O	3.65619800	-0.93302400	-0.74683500
C	1.26587400	1.38084000	0.62220400
O	0.95356400	2.54498900	0.42026600
N	2.33859400	0.81242300	-0.07043600
H	2.84178900	1.41808200	-0.71098500
C	-2.77987700	0.96453300	0.01959200
C	-1.81502800	1.51317800	-0.76007800
N	-0.90239500	0.71490900	-1.36114700
C	-0.80251500	-0.67000000	-1.10410900
N	-1.81663500	-1.23522000	-0.37692700
C	-2.74436000	-0.46777300	0.15177100
H	-3.52368900	1.57191700	0.51846600
H	-1.71594300	2.57889300	-0.93298000
H	-0.13298000	1.11527400	-1.88522100
O	0.16859100	-1.27260600	-1.53265900
N	-3.69641200	-1.08012000	0.90804500
H	-4.55271800	-0.59470500	1.12929900
H	-3.73723000	-2.08910600	0.85079500

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C-U-ftf-gas-max345: Optimised twist = 33.59 deg.

H	0.49390700	-1.48155500	2.12827800
C	1.00223700	-0.73356000	1.53015000
N	2.10943300	-1.17704300	0.85867200
H	2.31242600	-2.16738200	0.80558900
C	0.56780400	0.54124900	1.44336900
H	-0.30801900	0.88745400	1.97534800
C	2.81723500	-0.39426400	-0.03792000
O	3.76295800	-0.79975600	-0.67764400
C	1.22743400	1.45654000	0.52500100
O	0.87374000	2.59513800	0.26343600
N	2.34358600	0.90587700	-0.11800200
H	2.84678100	1.51326600	-0.75705500
C	-2.64686500	1.06747100	-0.28167500
C	-1.61475600	1.28344100	-1.13395500
N	-0.80215200	0.25653100	-1.47956300
C	-0.89816300	-1.03124000	-0.90607300
N	-1.97302200	-1.26411200	-0.09206000
C	-2.79413800	-0.27884800	0.20270500
H	-3.30720100	1.86765200	0.02570500
H	-1.38143400	2.25405700	-1.55678800
H	0.00028200	0.40344200	-2.08058500
O	-0.02373800	-1.84565900	-1.15777300
N	-3.81433100	-0.56091100	1.05565100
H	-4.59185500	0.07482200	1.14821400
H	-3.97790000	-1.53666900	1.26464400

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C-U-ftf-gas-max345-plus: Optimised twist = 180.13 deg.

H	2.38322000	-2.65320800	-0.00206900
C	2.71878000	-1.62193100	-0.00124900
N	1.71006300	-0.69404400	-0.00018500

H	0.71269900	-0.98412200	0.00009800
C	4.02329500	-1.27747900	-0.00128700
H	4.81580300	-2.01276000	-0.00215800
C	1.95103300	0.65280500	0.00086500
O	1.05508100	1.49673900	0.00173700
C	4.39072300	0.13175600	-0.00010700
O	5.51668100	0.58888300	0.00008100
N	3.28004800	0.99851500	0.00087500
H	3.48323600	1.99307400	0.00165600
C	-4.00753900	1.22272000	-0.00165900
C	-2.71504300	1.63801200	-0.00131200
N	-1.70656700	0.73923600	-0.00028900
C	-1.93352900	-0.64136700	0.00039400
N	-3.21912000	-1.07728600	0.00097400
C	-4.20554900	-0.19941100	-0.00051600
H	-4.83319800	1.92231700	-0.00433000
H	-2.42412000	2.68309300	-0.00202000
H	-0.72542000	1.04895000	0.00026900
O	-0.95874300	-1.40177600	0.00118400
N	-5.46327700	-0.69518300	-0.00677500
H	-6.27467500	-0.09945600	0.03102100
H	-5.58274400	-1.69795800	0.02054600

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C-U-ftf-gas-min290: Optimised twist = 319.96 deg.

H	-1.72564800	2.49426200	1.38232300
C	-1.62744600	1.44850200	1.11298400
N	-2.31953800	1.06021200	-0.00318300
H	-2.86609900	1.71791900	-0.54232000
C	-0.87544600	0.58060300	1.81651400
H	-0.31333300	0.87807300	2.69082300
C	-2.30370100	-0.23680600	-0.50868100
O	-2.91583100	-0.54851300	-1.50555000
C	-0.75214600	-0.79777100	1.35229200
O	-0.00900100	-1.63502900	1.83844500
N	-1.56100300	-1.11457300	0.25776500
H	-1.38466100	-2.01650300	-0.18139600
C	2.40307800	1.14469700	0.36703600
C	2.82080300	-0.12562200	0.60380700
N	2.27839300	-1.15557000	-0.07947100
C	1.19976900	-1.00446200	-0.97659600
N	0.78378700	0.27995500	-1.22621600
C	1.35101800	1.28599300	-0.60035600
H	2.81976000	1.99133800	0.89670600
H	3.58964600	-0.37344900	1.32752200
H	2.48709000	-2.11549000	0.16876800
O	0.69432900	-2.00318900	-1.45787600
N	0.85205300	2.53223600	-0.86185300
H	1.42971400	3.33621100	-0.66127100
H	0.27612900	2.59487100	-1.69260700

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C-U-ftf-gas-min80: Optimised twist = 82.06 deg.

H	-1.91687300	-2.25273300	-1.69413900
C	-1.86665300	-1.53927300	-0.87936500
N	-0.94205700	-1.83483600	0.08740700
H	-0.18553400	-2.48026200	-0.13410800
C	-2.65646100	-0.44667500	-0.82164300
H	-3.39525300	-0.22865500	-1.58039900
C	-0.64547800	-0.95915600	1.11490900



O	0.29102100	-1.11585700	1.87604500
C	-2.46532300	0.51356200	0.25444500
O	-3.02807500	1.58993000	0.36938500
N	-1.51036700	0.11616400	1.19980100
H	-1.30909200	0.77725700	1.94329400
C	1.87296200	1.82436700	0.34564700
C	2.79724100	0.90633000	0.72298100
N	2.79077900	-0.33107600	0.17651100
C	1.78948000	-0.76483800	-0.70955600
N	0.89093900	0.16901500	-1.13827500
C	0.91156200	1.38682400	-0.62971800
H	1.86476800	2.82647400	0.75396300
H	3.57054500	1.10953100	1.45562700
H	3.40007400	-1.06141000	0.52411200
O	1.75769300	-1.94923800	-1.02593100
N	-0.02865700	2.25568300	-1.07304300
H	-0.24225100	3.08961200	-0.54554200
H	-0.77994000	1.87000100	-1.63179700

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C-U-fff-water-max120: Optimised twist = 152.57 deg.

H	0.61750900	-1.48440900	-2.65362600
C	0.99148900	-1.01023100	-1.75383100
N	1.06447900	0.36058700	-1.80253200
H	0.80373900	0.85842000	-2.64611700
C	1.34743700	-1.70149700	-0.65257500
H	1.26426600	-2.77838800	-0.60389700
C	1.54680900	1.13243000	-0.76941200
O	1.65739400	2.34696300	-0.83563200
C	1.79510800	-0.98028100	0.52549200
O	2.08355300	-1.47481100	1.60854900
N	1.88967700	0.40319700	0.34944600
H	2.21343600	0.94349700	1.14702100
C	-1.34772500	1.63611200	0.71354800
C	-1.95389900	1.49018900	-0.48972900
N	-2.23878500	0.24964700	-0.96054500
C	-1.94141900	-0.92036200	-0.25311500
N	-1.31984300	-0.78656500	0.95069300
C	-1.03256200	0.42316300	1.41783000
H	-1.09641000	2.61083300	1.11052100
H	-2.23057900	2.32357500	-1.12517900
H	-2.69697800	0.13141500	-1.85709800
O	-2.24643500	-2.00666200	-0.75207800
N	-0.41353700	0.49319000	2.61033800
H	-0.07443000	1.37306900	2.97270000
H	-0.06200600	-0.35946500	3.02790100

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C-U-fff-water-max240-minus: Optimised twist = 227.33 deg.

H	0.42884400	-0.29459200	2.75229100
C	0.83938300	0.09474600	1.82775200
N	1.74915300	-0.72192700	1.20368400
H	1.99483900	-1.61882100	1.60650500
C	0.49005300	1.29286200	1.31542400
H	-0.22690200	1.93697400	1.80653800
C	2.37189800	-0.39869200	0.01880500
O	3.18529100	-1.12716200	-0.52852800
C	1.08860200	1.73506400	0.06684300
O	0.87354100	2.80078600	-0.49531400
N	1.99283500	0.82496800	-0.48914700

H	2.43113200	1.09414700	-1.36560500
C	-1.27632300	-1.93946600	0.31218600
C	-2.22620600	-1.30374200	1.04020000
N	-2.66622700	-0.07892100	0.65864000
C	-2.19250900	0.58063700	-0.48075700
N	-1.23492200	-0.04522000	-1.21876500
C	-0.78666200	-1.23831900	-0.84366700
H	-0.89977900	-2.91453600	0.59275300
H	-2.67066500	-1.71935800	1.93720800
H	-3.37767300	0.40358000	1.19576700
O	-2.66156700	1.68728300	-0.76015800
N	0.18206400	-1.79667900	-1.58968100
H	0.59122900	-2.68914300	-1.35315000
H	0.54112300	-1.29959400	-2.39412800

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C-U-ftf-water-max240: Optimised twist = 231.65 deg.

H	0.09564100	-0.02736400	2.64617200
C	0.69788100	0.13024700	1.75866800
N	1.23930900	-1.00538100	1.21074600
H	1.06574200	-1.91162700	1.63069800
C	0.90644100	1.34856500	1.21837500
H	0.47356700	2.24337300	1.64461800
C	2.02772300	-1.00131300	0.08168700
O	2.50209700	-2.01683200	-0.40505500
C	1.73048800	1.46848300	0.02722800
O	2.00955700	2.51040700	-0.55215800
N	2.23697500	0.25454100	-0.44378700
H	2.81592300	0.29338200	-1.27797100
C	-2.07808700	-1.46436600	0.47995500
C	-2.68880700	-0.37779400	1.01238900
N	-2.50060400	0.84582600	0.45835500
C	-1.68517900	1.05953200	-0.65834000
N	-1.05795700	-0.02304400	-1.19712000
C	-1.24534100	-1.22660600	-0.66768300
H	-2.20838800	-2.45432300	0.89714700
H	-3.33824600	-0.42096000	1.87905300
H	-2.95219400	1.66419000	0.85047500
O	-1.57202300	2.20698300	-1.09592900
N	-0.61806700	-2.26457100	-1.25003300
H	-0.61030100	-3.17859000	-0.82014300
H	0.05290400	-2.08461800	-1.98570900

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C-U-ftf-water-max240-plus: Optimised twist = 253.82 deg.

H	-0.22036200	0.20704800	2.73906200
C	-0.79771500	0.17639800	1.82226200
N	-0.83784600	1.35094700	1.11556400
H	-0.31142800	2.15844000	1.42935100
C	-1.44141700	-0.93029900	1.39532600
H	-1.41290400	-1.85655700	1.95274800
C	-1.44706800	1.46806900	-0.11351900
O	-1.37620400	2.48245100	-0.79456600
C	-2.22005400	-0.87587700	0.16893800
O	-2.90177300	-1.78398600	-0.28860000
N	-2.16032900	0.35386000	-0.49082600
H	-2.63275800	0.41492800	-1.38826200
C	2.70846900	0.34658000	0.62431900
C	2.69905700	-0.99602500	0.81573300
N	1.86793300	-1.78093200	0.08689100

C	0.99292300	-1.27161300	-0.87958700
N	0.98624000	0.07561400	-1.07377700
C	1.79644600	0.85298800	-0.36315300
H	3.35919500	0.99867600	1.19167000
H	3.33081100	-1.50123800	1.53706500
H	1.85345300	-2.78496300	0.22579600
O	0.27358500	-2.05722900	-1.50137400
N	1.73167200	2.17825400	-0.59028700
H	2.24266200	2.83017800	-0.01185700
H	0.96894300	2.53807300	-1.15413100

25

C-U-ftf-water-max355: Optimised twist = 26.67 deg.

H	-0.97076000	1.57317100	-2.23901800
C	-1.29466400	0.84921700	-1.50063800
N	-0.64338500	-0.35684200	-1.54026900
H	0.08832500	-0.52221500	-2.22259800
C	-2.26065200	1.10587700	-0.59405500
H	-2.76866700	2.05966900	-0.55672200
C	-0.93118400	-1.40448500	-0.69289000
O	-0.36140600	-2.48291800	-0.74780000
C	-2.61866800	0.08414900	0.37296900
O	-3.45223700	0.19707500	1.26333400
N	-1.91935700	-1.11764200	0.22504600
H	-2.15084900	-1.86512000	0.87376500
C	0.63737000	1.19748800	1.30563000
C	0.77914400	-0.05559900	1.80280700
N	1.62481900	-0.93115900	1.20433200
C	2.38509700	-0.60701800	0.07525600
N	2.24555800	0.64584900	-0.43880600
C	1.41132300	1.50694900	0.13459900
H	-0.03280700	1.91792300	1.75643100
H	0.24110100	-0.41901500	2.67112500
H	1.71789400	-1.87825800	1.55314400
O	3.13661800	-1.46347000	-0.39838100
N	1.27789900	2.71466300	-0.43943300
H	0.69697200	3.43337800	-0.03216100
H	1.84966200	2.95141500	-1.23934700

25

C-U-ftf-water-min165: Optimised twist = 168.40 deg.

H	-0.49031300	-2.19507100	-1.94160900
C	-0.88958100	-1.31003300	-1.45996400
N	-1.77434600	-1.54808100	-0.43922900
H	-2.00693900	-2.49737300	-0.17066200
C	-0.54642000	-0.05774900	-1.82708500
H	0.15816600	0.12921600	-2.62620900
C	-2.35718900	-0.54758500	0.30600100
O	-3.11689100	-0.76470500	1.23759900
C	-1.13060200	1.07560300	-1.13127600
O	-0.91944700	2.25676700	-1.37280900
N	-2.00645000	0.72263000	-0.09934400
H	-2.42827300	1.48597700	0.42259000
C	0.61844000	-0.32444100	1.76439600
C	1.14642500	-1.47186400	1.27233900
N	2.03289800	-1.42467400	0.24712000
C	2.44509500	-0.22739500	-0.34959200
N	1.93224300	0.93202700	0.14321200
C	1.05316800	0.89499700	1.13901700
H	-0.09556600	-0.32826700	2.57827100

H	0.89646800	-2.45623200	1.65159100
H	2.42925300	-2.27722800	-0.13196000
O	3.24666900	-0.28104700	-1.28666600
N	0.56210800	2.06779700	1.57544000
H	-0.17272000	2.10466600	2.26751100
H	0.76609300	2.90910600	1.05208000

25

C-U-ftf-water-min280: Optimised twist = 316.01 deg.

H	-1.48552100	2.32163500	1.69134300
C	-1.47974300	1.31877200	1.28101500
N	-2.11040500	1.17734400	0.07409800
H	-2.52397000	1.97918900	-0.38735500
C	-0.89145800	0.27369800	1.90134200
H	-0.38235100	0.38523500	2.84883400
C	-2.17876300	-0.01701400	-0.61013000
O	-2.70383400	-0.12518600	-1.70781400
C	-0.91892700	-1.03344800	1.27008500
O	-0.38368300	-2.04937900	1.70180300
N	-1.63340200	-1.08155900	0.07263200
H	-1.56814400	-1.94797600	-0.45583000
C	2.40728800	1.05441500	0.52205000
C	2.79982500	-0.23949800	0.61604700
N	2.21177500	-1.18529400	-0.15802600
C	1.18360300	-0.89933700	-1.05919500
N	0.78088400	0.39662000	-1.16572700
C	1.35798500	1.33256300	-0.41840200
H	2.85527100	1.83189700	1.12645600
H	3.57748700	-0.58132300	1.28894000
H	2.48070400	-2.15914900	-0.07575200
O	0.68143800	-1.82763700	-1.70141100
N	0.89985800	2.59070400	-0.54422800
H	1.35069800	3.36445700	-0.07699900
H	0.22463200	2.79804900	-1.26837700

25

C-U-ftf-water-min45: Optimised twist = 51.89 deg.

H	0.28636900	-0.33116800	-2.70370400
C	0.84946200	-0.25858400	-1.78066400
N	0.94781600	1.00511400	-1.25576000
H	0.43817300	1.77703300	-1.67578700
C	1.41514100	-1.32604300	-1.17886500
H	1.33740800	-2.32160300	-1.59363800
C	1.58378900	1.28276300	-0.06734100
O	1.62101500	2.40114000	0.42369800
C	2.12827400	-1.14279400	0.07234100
O	2.67147300	-2.02350500	0.72713900
N	2.16177200	0.18048000	0.52493200
H	2.64353700	0.35190700	1.40335000
C	-1.29556800	-1.19014800	1.32703900
C	-0.92087000	-0.00260200	1.86078800
N	-1.15148100	1.15046700	1.18074200
C	-1.73358600	1.17734200	-0.08994800
N	-2.14509000	-0.00277700	-0.62322100
C	-1.93441000	-1.13638200	0.04005100
H	-1.12127500	-2.12678800	1.84002400
H	-0.43000200	0.09407000	2.82259000
H	-0.82834400	2.03950300	1.54745800
O	-1.82104700	2.26275300	-0.67523800
N	-2.33060500	-2.27784500	-0.54385600

H -2.23003900 -3.17184400 -0.08518600  
H -2.79762300 -2.24360900 -1.44016600  
27

T-BrU-ftf-gas-max10: Optimised twist = 37.57 deg.

H 0.98921400 -0.88334300 -2.01620200  
C 0.89499800 -0.02340600 -1.36339100  
N -0.25993200 0.70994400 -1.49597200  
H -0.98109000 0.42297300 -2.14662600  
C 1.83681900 0.30061500 -0.45752400  
Br 3.39798100 -0.68785600 -0.25523500  
C -0.58837100 1.77493900 -0.67712100  
O -1.65566000 2.35266400 -0.73316200  
C 1.63343200 1.44902600 0.43289300  
O 2.39018200 1.83167200 1.29723600  
N 0.41705900 2.10903200 0.20735700  
H 0.22608500 2.90357000 0.81005400  
C -1.33765000 -0.80331300 1.29907900  
C -2.23978100 0.15881700 1.59038900  
N -3.37611500 0.37635100 0.84724500  
C -3.68466400 -0.32904000 -0.29848800  
N -2.74803400 -1.30852500 -0.59427400  
C -1.56417800 -1.60180600 0.09145800  
C -0.12728100 -1.10444300 2.13326200  
H -2.12068800 0.81506000 2.44718600  
H -3.95682200 1.18759900 1.01710400  
O -4.66806100 -0.12068800 -0.97576500  
O -0.79930700 -2.44493200 -0.34662200  
H -2.95565900 -1.87979500 -1.40783100  
H -0.26142500 -2.04037900 2.68623000  
H 0.75832900 -1.23469800 1.50514400  
H 0.06469800 -0.30170700 2.85083400  
27

T-BrU-ftf-gas-max130: Optimised twist = 82.65 deg.

H -1.74202000 -2.32373700 -0.46452500  
C -1.31918300 -1.54719400 0.16332600  
N -0.16011900 -1.88032300 0.82266100  
H 0.34419800 -2.72211600 0.56085000  
C -1.89623100 -0.33779800 0.29796800  
Br -3.47224300 0.11375200 -0.57735100  
C 0.56352100 -0.97596200 1.57621700  
O 1.65597400 -1.22952500 2.04822300  
C -1.27907100 0.67545500 1.16722400  
O -1.71680100 1.77404800 1.41358200  
N -0.06919700 0.24028600 1.73191600  
H 0.41871600 0.91826300 2.30974100  
C 2.70110600 1.39263300 -0.28061600  
C 3.55576800 0.39131400 0.00752900  
N 3.35656000 -0.90960600 -0.40807800  
C 2.20382900 -1.32722400 -1.03134600  
N 1.37160800 -0.28866400 -1.39223000  
C 1.49022800 1.06519100 -1.03833800  
C 2.88303100 2.81697100 0.14662200  
H 4.46048000 0.55188900 0.58440200  
H 3.91673300 -1.65632100 -0.01683000  
O 1.93440600 -2.50043700 -1.23531400  
O 0.61844500 1.85350700 -1.34698100  
H 0.52387400 -0.54618800 -1.88944400  
H 2.94346800 3.47737800 -0.72394500

H	2.02479500	3.15302800	0.73747800
H	3.79210300	2.93356400	0.74209700

27

T-BrU-ftf-gas-max240: Optimised twist = 267.33 deg.

H	1.59831000	1.26259100	2.04077400
C	1.73683800	0.81249600	1.06395600
N	2.76689100	-0.07860600	0.95318500
H	3.28900300	-0.37315300	1.76830700
C	0.94522300	1.11857600	0.01696100
Br	-0.46611400	2.32552200	0.15494900
C	3.05546300	-0.77759700	-0.21043200
O	3.93950500	-1.59963700	-0.28540000
C	1.17311100	0.47640200	-1.28343400
O	0.51458000	0.64833100	-2.28715500
N	2.26003200	-0.39996400	-1.27799400
H	2.45320000	-0.87822300	-2.15270100
C	-1.44660700	-1.05857300	1.51097200
C	-2.62024600	-0.53953200	1.09716100
N	-3.02986300	-0.57951300	-0.21390700
C	-2.28868900	-1.15243100	-1.23397900
N	-1.08213900	-1.67108600	-0.79255400
C	-0.56814300	-1.65675200	0.50350100
C	-0.96513000	-1.02615400	2.92837800
H	-3.30945500	-0.05423500	1.78110800
H	-3.90776400	-0.16816100	-0.50203600
O	-2.66782000	-1.20707100	-2.38224600
O	0.54360300	-2.10828800	0.73464500
H	-0.49109000	-2.06470000	-1.51890300
H	-0.76466400	-2.03724400	3.29579700
H	-0.02498500	-0.46889200	3.00483300
H	-1.70287800	-0.55236400	3.58122600

27

T-BrU-ftf-gas-min155: Optimised twist = 145.28 deg.

H	2.27505100	-2.03022600	0.04571400
C	2.03142900	-0.98018300	-0.07142000
N	0.70962600	-0.69801600	-0.29355200
H	0.00346100	-1.43910900	-0.34170600
C	2.97009800	-0.01518000	-0.00380800
Br	4.76650200	-0.39561000	0.29500800
C	0.22985100	0.58300000	-0.46300900
O	-0.94649900	0.83479400	-0.66206000
C	2.58313800	1.39018400	-0.16868400
O	3.32138100	2.34921300	-0.13083200
N	1.20764200	1.55377200	-0.38763800
H	0.88792000	2.51072300	-0.50292100
C	-4.67682900	0.51213500	-0.08534000
C	-4.23930100	0.06533700	-1.27727200
N	-3.28065500	-0.92083200	-1.39749300
C	-2.61579700	-1.45073600	-0.32457300
N	-3.10540000	-1.04361500	0.88838000
C	-4.08185200	-0.06274200	1.12498900
C	-5.71933200	1.57221300	0.09278300
H	-4.62274200	0.44819600	-2.21716000
H	-2.87834400	-1.13875900	-2.29942000
O	-1.68344900	-2.24292700	-0.44218400
O	-4.37796800	0.24204200	2.26318000
H	-2.64823300	-1.42871600	1.70880000
H	-6.56373400	1.18849400	0.67345100

H -5.30946500 2.42166700 0.64748100  
H -6.08614100 1.92575800 -0.87423400  
27

T-BrU-ftf-gas-min320: Optimised twist = 312.25 deg.

H -1.06065300 -0.58115500 -2.37949700  
C -0.49091300 -0.96475400 -1.54044400  
N 0.78767500 -1.36733300 -1.82007200  
H 1.19807900 -1.15190800 -2.72138400  
C -0.99516900 -1.02966200 -0.29243900  
Br -2.72338400 -0.46793300 0.10765800  
C 1.68526800 -1.78519500 -0.85039000  
O 2.85425800 -2.00210800 -1.08628600  
C -0.15447900 -1.50294300 0.81457400  
O -0.47328700 -1.53039400 1.98532900  
N 1.11571500 -1.91761200 0.40375200  
H 1.77136200 -2.14329300 1.14949900  
C -0.08738300 2.21526800 -0.14404000  
C -0.13337800 1.99907300 1.18631900  
N 0.87619200 1.36142400 1.87232200  
C 2.00018800 0.83985600 1.26611500  
N 2.05073300 1.09369400 -0.09512300  
C 1.06002400 1.68666200 -0.88411700  
C -1.18656100 2.85997100 -0.92969900  
H -0.97993300 2.30318500 1.79324500  
H 0.74848000 1.08851900 2.83938200  
O 2.84711500 0.20317000 1.85992400  
O 1.17149200 1.70405900 -2.10006700  
H 2.85569800 0.70208000 -0.58034400  
H -0.81002200 3.71219800 -1.50328300  
H -1.61040000 2.14945800 -1.64870000  
H -1.98856800 3.19988300 -0.26958300  
27

T-BrU-ftf-gas-min50: Optimised twist = 63.26 deg.

H 0.70057300 -0.65038600 -2.36186600  
C 1.01455800 -0.83477600 -1.34036000  
N 2.31785300 -0.50828600 -1.05196400  
H 2.84174000 0.05834100 -1.71105700  
C 0.17781400 -1.32871900 -0.40751200  
Br -1.59822500 -1.72858100 -0.77981400  
C 2.83426200 -0.55051900 0.22807500  
O 3.91273800 -0.07977000 0.52990300  
C 0.65157700 -1.52946200 0.96747400  
O -0.00102900 -1.94352600 1.89997000  
N 1.99464300 -1.16779800 1.13795700  
H 2.36286300 -1.25806500 2.08031300  
C -1.13245800 1.45981500 1.28701400  
C 0.19640100 1.60220700 1.45249600  
N 1.04718100 1.95018100 0.41733700  
C 0.62623700 2.11072100 -0.88511400  
N -0.74198800 2.04042300 -1.02867000  
C -1.69542300 1.73727400 -0.04152400  
C -2.07405600 1.01299500 2.36128600  
H 0.68319300 1.42988000 2.40749300  
H 2.04722000 2.02684700 0.56815900  
O 1.39554100 2.27620000 -1.81822100  
O -2.87674800 1.71613200 -0.31937000  
H -1.09893300 2.18773100 -1.96790700  
H -2.88494300 1.73570400 2.49014800

H -2.52643000 0.05452700 2.08553900  
H -1.54872200 0.88461300 3.31078600  
27

T-BrU-ftf-water-max120-minus: Optimised twist = 113.84 deg.

H -0.15892400 -0.72927100 -2.43793600  
C 0.47316100 -0.82128700 -1.56151700  
N 1.78471400 -0.47068100 -1.72717900  
H 2.11349300 -0.14241900 -2.62910300  
C 0.00880100 -1.24674100 -0.36768500  
Br -1.76037700 -1.78969300 -0.13759400  
C 2.73588100 -0.56900600 -0.73203300  
O 3.90247400 -0.25820300 -0.89278200  
C 0.92651600 -1.41452700 0.75815400  
O 0.63079800 -1.82514500 1.86696900  
N 2.23899100 -1.05406100 0.46086200  
H 2.91650500 -1.15292600 1.21286000  
C 0.47569600 1.76534900 1.11145400  
C 0.88474600 2.17153200 -0.11073500  
N 0.02896100 2.26107100 -1.18430800  
C -1.30857800 1.94967500 -1.11833100  
N -1.72705300 1.59246700 0.14486300  
C -0.93997800 1.44078600 1.28576800  
C 1.38246700 1.63094500 2.29604800  
H 1.91382500 2.44674500 -0.32008500  
H 0.37412700 2.55920700 -2.08961700  
O -2.05738000 1.98931600 -2.08371800  
O -1.44870000 1.06845700 2.33513300  
H -2.70785900 1.33983800 0.23096200  
H 1.07940000 2.31180800 3.09802200  
H 1.33802800 0.61351400 2.70062500  
H 2.41549300 1.85543600 2.01882600  
27

T-BrU-ftf-water-max120: Optimised twist = 103.96 deg.

H -0.60267700 -2.07062000 1.79057500  
C -0.97569300 -1.54276400 0.92027000  
N -2.27093800 -1.11218300 0.98869100  
H -2.82308900 -1.29006900 1.82124000  
C -0.21434800 -1.30746700 -0.16963400  
Br 1.52609600 -1.96686400 -0.30962900  
C -2.91123100 -0.45072600 -0.03995200  
O -4.06631100 -0.07128100 0.02919300  
C -0.78826000 -0.64058000 -1.33600400  
O -0.21344700 -0.41578100 -2.38702100  
N -2.11638100 -0.25831500 -1.15281800  
H -2.55968000 0.21978400 -1.93343800  
C 0.26856000 2.28563600 -0.48586800  
C -0.67797200 2.21601500 0.47492700  
N -0.46822300 1.58285100 1.67913100  
C 0.70939700 0.95645000 2.00912200  
N 1.69319000 1.10064400 1.05623400  
C 1.56979100 1.68278400 -0.20645900  
C 0.04688100 2.91232500 -1.82751100  
H -1.66736300 2.64384000 0.34883800  
H -1.20977700 1.53610500 2.36901100  
O 0.87035100 0.33081200 3.04787200  
O 2.51812800 1.66852100 -0.98079700  
H 2.57414600 0.63523600 1.25780500  
H 0.77883600 3.70393500 -2.01595000



H 0.15648300 2.16179500 -2.61744500  
H -0.95628900 3.34106400 -1.88959100  
27

T-BrU-ftf-water-max120-plus: Optimised twist = 105.05 deg.

H -2.64680800 0.44040400 1.35038300  
C -1.96945500 0.79311100 0.58181900  
N -1.70258400 2.13271800 0.58557400  
H -2.13573500 2.73588300 1.27680200  
C -1.39829200 -0.03303600 -0.32032500  
Br -1.78811600 -1.85728500 -0.35575200  
C -0.87145200 2.74848100 -0.32857400  
O -0.63395900 3.94310400 -0.31448600  
C -0.51887400 0.50225600 -1.35428600  
O 0.02909700 -0.13968600 -2.23439500  
N -0.33179200 1.88066600 -1.25661900  
H 0.28119700 2.30223200 -1.95019400  
C 2.55293600 0.03733000 -0.18078300  
C 2.16155100 1.08453300 0.57498300  
N 1.25482600 0.95835800 1.60681500  
C 0.69478000 -0.23913300 1.98059800  
N 1.13573300 -1.30776200 1.23214800  
C 2.00846500 -1.27960000 0.14323000  
C 3.48478800 0.14924200 -1.34742700  
H 2.51940200 2.09439100 0.40305200  
H 1.00719600 1.76306600 2.17195900  
O -0.12670900 -0.34660800 2.88052600  
O 2.27032400 -2.31520100 -0.45460200  
H 0.72525300 -2.20860700 1.46358100  
H 4.35242100 -0.50531000 -1.21870300  
H 2.97583000 -0.15423000 -2.26831300  
H 3.83529700 1.17731900 -1.46441400  
27

T-BrU-ftf-water-max185: Optimised twist = 206.17 deg.

H -0.52403500 -1.47416700 -2.28624500  
C -0.12976700 -1.49270900 -1.27673800  
N 1.16626500 -1.90732200 -1.14883400  
H 1.70166700 -2.16715800 -1.97022200  
C -0.86078800 -1.12641500 -0.20264600  
Br -2.65220800 -0.63396900 -0.35584200  
C 1.82242100 -1.98961700 0.06134300  
O 2.98482900 -2.33960100 0.16847900  
C -0.28618300 -1.20426500 1.13712900  
O -0.85323900 -0.92259200 2.17941400  
N 1.03880100 -1.63300700 1.13996900  
H 1.50324900 -1.65657000 2.04453700  
C 1.80336900 1.39177500 -0.74287700  
C 0.76600400 1.75338400 -1.53079600  
N -0.44657300 2.15816600 -1.02545300  
C -0.72117400 2.23263100 0.31900500  
N 0.33144200 1.82462600 1.11358300  
C 1.60525600 1.43176800 0.70282900  
C 3.14482200 0.97678600 -1.26828500  
H 0.82937300 1.74753000 -2.61377500  
H -1.19477700 2.43327100 -1.65130400  
O -1.78666200 2.61933300 0.77343100  
O 2.45186100 1.13223000 1.53691900  
H 0.15819800 1.84043400 2.11541500  
H 3.91902800 1.68450800 -0.95392100

H 3.43295800 -0.00747000 -0.88449000  
H 3.13398600 0.93629300 -2.36010200  
27

T-BrU-ftf-water-max240: Optimised twist = 217.95 deg.

H -0.43035900 -1.30458300 -2.33541800  
C -0.10531500 -1.39458100 -1.30519600  
N 1.16394500 -1.86494400 -1.11815600  
H 1.73861700 -2.10826700 -1.91783300  
C -0.89426100 -1.06219700 -0.26159800  
Br -2.65882500 -0.50761900 -0.50585700  
C 1.73401000 -2.04898800 0.12512800  
O 2.86960200 -2.45968100 0.28214600  
C -0.41796900 -1.25272900 1.10583300  
O -1.05016900 -1.02640300 2.12367300  
N 0.89116900 -1.72577300 1.17026600  
H 1.28510700 -1.83747800 2.10114300  
C 1.77427800 1.43672000 -0.83138500  
C 0.65682400 1.91208000 -1.42485500  
N -0.46420700 2.27278700 -0.71553700  
C -0.56727600 2.16453600 0.65027800  
N 0.56725000 1.64694200 1.24360000  
C 1.76434800 1.29288400 0.62108800  
C 3.01906700 1.04734500 -1.56938600  
H 0.57854400 2.04171700 -2.49905900  
H -1.28179800 2.62774300 -1.19818800  
O -1.55833100 2.49423400 1.28350500  
O 2.70329900 0.87839200 1.29072200  
H 0.52810100 1.54542800 2.25470100  
H 3.85310500 1.70338100 -1.29920200  
H 3.31875900 0.02540900 -1.31309900  
H 2.86425100 1.10747700 -2.64907700  
27

T-BrU-ftf-water-max5: Optimised twist = 24.35 deg.

H -0.74479800 -1.73991800 -2.10685200  
C -0.30597900 -1.63812900 -1.12107200  
N 0.97281700 -2.10313400 -0.98415000  
H 1.44317900 -2.53705300 -1.77123000  
C -0.96895800 -1.08169300 -0.08539000  
Br -2.74749300 -0.54241800 -0.24050600  
C 1.66100000 -2.09892500 0.21200000  
O 2.77065500 -2.57961600 0.34979500  
C -0.34029800 -1.00271600 1.23024100  
O -0.84982100 -0.56568900 2.24761500  
N 0.96765300 -1.48871700 1.24073200  
H 1.44392400 -1.47393700 2.13942200  
C 0.07789500 2.23204300 0.44426400  
C 1.15663300 2.02499000 1.23103000  
N 2.30823300 1.42601500 0.77508000  
C 2.46293800 0.96511900 -0.50898200  
N 1.35300400 1.16932900 -1.30178100  
C 0.15495600 1.79513000 -0.94660100  
C -1.18316100 2.88376300 0.92424600  
H 1.17890400 2.31871800 2.27482900  
H 3.09420800 1.28660000 1.39948200  
O 3.47728900 0.41607000 -0.91346300  
O -0.73067400 1.93167000 -1.78068700  
H 1.43565500 0.85591200 -2.26542700  
H -1.40593500 3.77951400 0.33564200

H -2.03445100 2.20329800 0.82366700  
H -1.09011400 3.17008600 1.97450200  
27

T-BrU-ftf-water-max70-minus: Optimised twist = 176.32 deg.

H -0.26638000 -1.56199800 -2.26222800  
C 0.25473300 -1.47742000 -1.31538800  
N 1.61912400 -1.52882300 -1.37733900  
H 2.08381900 -1.65611700 -2.27004600  
C -0.38943000 -1.31926400 -0.14073400  
Br -2.25057200 -1.31899700 -0.03716500  
C 2.43512200 -1.47292300 -0.26690200  
O 3.64930500 -1.55401900 -0.32576800  
C 0.36509000 -1.24460100 1.10663600  
O -0.10705100 -1.13912300 2.22518700  
N 1.74544000 -1.30539500 0.91752000  
H 2.31647800 -1.26402700 1.75824700  
C 1.31165600 1.79353600 -0.36418200  
C 0.55547900 1.75117400 -1.48290300  
N -0.81784100 1.81355100 -1.45423600  
C -1.54569200 1.97847500 -0.29927400  
N -0.77004200 1.94863400 0.84176300  
C 0.62277100 1.90172500 0.91922200  
C 2.81080100 1.78852200 -0.36919600  
H 0.98900700 1.66741000 -2.47407100  
H -1.34624100 1.81483900 -2.31950800  
O -2.75724900 2.12915500 -0.28121600  
O 1.17793800 1.94521100 2.00998200  
H -1.27154600 2.04772200 1.72053800  
H 3.20124100 2.76961600 -0.07778500  
H 3.20618100 1.06136500 0.34616900  
H 3.19397800 1.54517000 -1.36365500  
27

T-BrU-ftf-water-max70: Optimised twist = 148.80 deg.

H -0.90831200 -0.79282700 -2.34620100  
C -0.34756800 -1.09281800 -1.46813100  
N 0.93920800 -1.49769500 -1.68773300  
H 1.32179200 -1.49381700 -2.62715500  
C -0.87121500 -1.06784400 -0.22444100  
Br -2.64503200 -0.58313800 0.08731200  
C 1.78804200 -1.92206900 -0.68551200  
O 2.94236700 -2.25474400 -0.88692800  
C -0.08954100 -1.54873200 0.91232500  
O -0.47715900 -1.62936400 2.06457000  
N 1.20364700 -1.93877300 0.56537400  
H 1.78745600 -2.28756900 1.32146100  
C 1.96481400 1.29190000 0.24521700  
C 1.70164400 1.51937600 -1.06012600  
N 0.48049100 1.97312200 -1.49978600  
C -0.56818400 2.27153000 -0.66062500  
N -0.28827000 2.04473600 0.67088200  
C 0.90749900 1.57178700 1.21462700  
C 3.29304000 0.82549200 0.75852200  
H 2.43780800 1.35389300 -1.84009200  
H 0.32546900 2.14946600 -2.48592400  
O -1.64112400 2.70065300 -1.05622200  
O 1.01725400 1.42777100 2.42536700  
H -1.04159000 2.24673900 1.32290900  
H 3.74232700 1.58184600 1.41032200

H 3.18669700 -0.08887400 1.35139600  
H 3.97705900 0.62499700 -0.06923200  
27

T-BrU-ftf-water-max70-plus: Optimised twist = 113.84 deg.

H -0.15890500 -0.72935100 -2.43792800  
C 0.47317600 -0.82133300 -1.56150300  
N 1.78472800 -0.47072700 -1.72717000  
H 2.11351100 -0.14249400 -2.62910300  
C 0.00881100 -1.24674700 -0.36765900  
Br -1.76036700 -1.78969900 -0.13755800  
C 2.73589000 -0.56901200 -0.73201400  
O 3.90248200 -0.25821200 -0.89276800  
C 0.92652000 -1.41449000 0.75819100  
O 0.63079800 -1.82507200 1.86701900  
N 2.23899400 -1.05402400 0.46089600  
H 2.91650500 -1.15286300 1.21290000  
C 0.47568400 1.76538100 1.11141400  
C 0.88473300 2.17151500 -0.11079100  
N 0.02894700 2.26101700 -1.18436700  
C -1.30859100 1.94962100 -1.11837800  
N -1.72706600 1.59246100 0.14483000  
C -0.93999000 1.44082300 1.28574100  
C 1.38245800 1.63101700 2.29601000  
H 1.91381300 2.44671600 -0.32015400  
H 0.37411700 2.55910100 -2.08969100  
O -2.05739300 1.98922500 -2.08376600  
O -1.44871200 1.06853300 2.33511900  
H -2.70787100 1.33983300 0.23093800  
H 1.07939600 2.31190900 3.09796000  
H 1.33801900 0.61359900 2.70062200  
H 2.41548300 1.85549600 2.01877500  
27

T-BrU-ftf-water-min155: Optimised twist = 113.84 deg.

H -0.15892100 -0.72929900 -2.43793300  
C 0.47316100 -0.82130700 -1.56151100  
N 1.78471600 -0.47071000 -1.72717200  
H 2.11350000 -0.14245700 -2.62909800  
C 0.00879500 -1.24674600 -0.36767600  
Br -1.76038800 -1.78968400 -0.13758300  
C 2.73588000 -0.56902800 -0.73202100  
O 3.90247400 -0.25823300 -0.89277000  
C 0.92650400 -1.41452000 0.75816900  
O 0.63078000 -1.82511800 1.86699100  
N 2.23898200 -1.05406500 0.46087700  
H 2.91649200 -1.15292100 1.21288000  
C 0.47570000 1.76535500 1.11144700  
C 0.88476400 2.17151400 -0.11074500  
N 0.02898900 2.26104700 -1.18432700  
C -1.30855300 1.94966500 -1.11835700  
N -1.72704300 1.59247800 0.14483800  
C -0.93998000 1.44080900 1.28575300  
C 1.38246100 1.63095900 2.29604900  
H 1.91384800 2.44671100 -0.32009200  
H 0.37416800 2.55915700 -2.08964000  
O -2.05734700 1.98930200 -2.08375100  
O -1.44871600 1.06850200 2.33511900  
H -2.70785200 1.33985700 0.23093100  
H 1.07938800 2.31182800 3.09801500

H 1.33802000 0.61353000 2.70063300  
H 2.41548900 1.85544800 2.01883300  
27

T-BrU-ftf-water-min210: Optimised twist = 224.39 deg.

H 1.11309600 -2.31503600 1.64925800  
C 0.62611900 -1.95450000 0.75062300  
N -0.60275800 -2.48844500 0.48053600  
H -1.00213300 -3.18398300 1.10165000  
C 1.17899000 -1.02550600 -0.05635400  
Br 2.85533900 -0.28659500 0.28739200  
C -1.36317100 -2.14093600 -0.61599500  
O -2.46310800 -2.61319500 -0.84155100  
C 0.48860000 -0.60529100 -1.27158600  
O 0.90795600 0.19330800 -2.09213300  
N -0.75860100 -1.20561400 -1.43342500  
H -1.28771300 -0.93603200 -2.25965400  
C -1.80407400 0.66444300 1.20028500  
C -0.60327500 1.04293300 1.69111500  
N 0.23126400 1.91130100 1.02724000  
C -0.06905500 2.47410100 -0.19004600  
N -1.28931300 2.06795400 -0.69156200  
C -2.20856000 1.20455300 -0.09545000  
C -2.74780700 -0.25512000 1.91609100  
H -0.22548800 0.68467600 2.64354700  
H 1.12410700 2.17004300 1.43144100  
O 0.66724600 3.25644800 -0.77032900  
O -3.25929100 0.93991000 -0.66741600  
H -1.54124300 2.44725100 -1.60027800  
H -3.66113800 0.27524800 2.20572400  
H -3.04938000 -1.08784000 1.27225300  
H -2.28015700 -0.65968800 2.81716000  
27

T-BrU-ftf-water-min285: Optimised twist = 292.34 deg.

H -0.45136000 0.07190200 -2.36992300  
C 0.05233000 -0.51963700 -1.61339700  
N 1.39918300 -0.67974000 -1.77831200  
H 1.87465200 -0.22043300 -2.54791300  
C -0.59642900 -1.06610600 -0.56287200  
Br -2.43675200 -0.87693100 -0.34502000  
C 2.19382400 -1.39457700 -0.90700100  
O 3.40045200 -1.50131200 -1.03958100  
C 0.12831300 -1.89166200 0.39961300  
O -0.35560900 -2.46492300 1.36039600  
N 1.49325500 -1.97492400 0.13144700  
H 2.04938800 -2.50965600 0.79399400  
C -0.40692300 2.39815000 -0.03528300  
C -1.02565700 1.87818200 1.04734000  
N -0.38104100 1.06198300 1.94689500  
C 0.95168200 0.73998500 1.86403300  
N 1.57543000 1.27138300 0.75213300  
C 1.00495000 2.08586100 -0.22913200  
C -1.08822000 3.26756200 -1.04811300  
H -2.07335900 2.05707400 1.26252900  
H -0.87951000 0.68981000 2.74743400  
O 1.53017000 0.03800700 2.67923300  
O 1.68542300 2.46616800 -1.17452700  
H 2.57199400 1.08452300 0.67014100  
H -0.59874100 4.24427000 -1.11545100

H -1.04474600 2.81425400 -2.04422900  
H -2.13650000 3.41986200 -0.78131900  
27

T-BrU-ftf-water-min320: Optimised twist = 292.34 deg.

H -0.45137000 0.07191900 -2.36991800  
C 0.05230800 -0.51963600 -1.61339600  
N 1.39915600 -0.67977300 -1.77831600  
H 1.87463500 -0.22047300 -2.54791500  
C -0.59646200 -1.06609200 -0.56287200  
Br -2.43678100 -0.87687100 -0.34501900  
C 2.19378100 -1.39463200 -0.90701000  
O 3.40040600 -1.50140100 -1.03959300  
C 0.12826200 -1.89166500 0.39961200  
O -0.35567300 -2.46491500 1.36039600  
N 1.49320100 -1.97495900 0.13144300  
H 2.04932400 -2.50970100 0.79399000  
C -0.40686100 2.39816900 -0.03526400  
C -1.02560000 1.87819600 1.04735400  
N -0.38099500 1.06196800 1.94689200  
C 0.95172000 0.73994400 1.86401700  
N 1.57547300 1.27134800 0.75212300  
C 1.00500300 2.08584800 -0.22912900  
C -1.08813900 3.26761900 -1.04807300  
H -2.07329700 2.05710800 1.26255500  
H -0.87946700 0.68979700 2.74743000  
O 1.53020000 0.03794100 2.67920200  
O 1.68547600 2.46615000 -1.17452600  
H 2.57203200 1.08446300 0.67012100  
H -0.59862800 4.24431300 -1.11539500  
H -1.04468600 2.81433000 -2.04419800  
H -2.13641300 3.41994800 -0.78126800  
27

T-BrU-ftf-water-min40: Optimised twist = 62.65 deg.

H 0.94019100 -0.38214900 -2.38655800  
C 1.25238900 -0.52318200 -1.35769100  
N 2.48308300 -0.02209800 -1.03311900  
H 3.03628300 0.45893400 -1.73429700  
C 0.47920200 -1.13661400 -0.43779400  
Br -1.18171900 -1.86276400 -0.86902800  
C 3.03649500 -0.11481500 0.22555800  
O 4.13037300 0.33981400 0.51015300  
C 0.96995300 -1.32643800 0.92504200  
O 0.38184900 -1.89820400 1.82619400  
N 2.22808900 -0.76474300 1.13847800  
H 2.61704000 -0.87109400 2.07215900  
C -1.49257200 1.07439700 1.31942200  
C -0.22876400 1.50602700 1.51482300  
N 0.52157400 2.08236900 0.51200600  
C 0.06807600 2.24398100 -0.77468200  
N -1.23325200 1.82755000 -0.95583700  
C -2.09128000 1.28571300 0.00277800  
C -2.31325100 0.38938400 2.36769900  
H 0.28072500 1.40775500 2.46808500  
H 1.45162100 2.43627900 0.70614600  
O 0.75564700 2.70121500 -1.67682400  
O -3.24928200 1.02171400 -0.29144600  
H -1.61262000 1.95480000 -1.89031400  
H -3.24035700 0.93790200 2.56097900

H -2.58758100 -0.61709100 2.03281500  
H -1.75176700 0.30284600 3.30069900  
27

T-BrU-ftf-water-min95: Optimised twist = 105.05 deg.

H -2.64666500 0.44099800 1.35042200  
C -1.96924600 0.79355900 0.58184900  
N -1.70206900 2.13310500 0.58561500  
H -2.13506500 2.73636000 1.27686000  
C -1.39829000 -0.03270800 -0.32031600  
Br -1.78854700 -1.85686500 -0.35576000  
C -0.87081500 2.74868800 -0.32854200  
O -0.63305100 3.94325700 -0.31444800  
C -0.51877800 0.50239600 -1.35429300  
O 0.02901100 -0.13966000 -2.23443300  
N -0.33137100 1.88076000 -1.25660700  
H 0.28169200 2.30219700 -1.95019400  
C 2.55293900 0.03676600 -0.18078400  
C 2.16179800 1.08402800 0.57502800  
N 1.25505000 0.95801800 1.60685900  
C 0.69473000 -0.23936000 1.98059400  
N 1.13543600 -1.30805900 1.23209900  
C 2.00817700 -1.28005400 0.14318500  
C 3.48482300 0.14851300 -1.34741800  
H 2.51987700 2.09381100 0.40313700  
H 1.00761500 1.76275800 2.17204200  
O -0.12677900 -0.34668500 2.88052100  
O 2.26980600 -2.31569400 -0.45468200  
H 0.72476200 -2.20882200 1.46350700  
H 4.35232700 -0.50621100 -1.21869600  
H 2.97581700 -0.15484200 -2.26831500  
H 3.83553600 1.17652400 -1.46438500  
27

T-U-ftf-gas-max0: Optimised twist = 47.40 deg.

H -1.22752300 0.93131900 -2.60046400  
C -1.53693000 0.34033100 -1.74627100  
N -0.68697100 -0.68686800 -1.40446900  
H 0.16718500 -0.85279600 -1.92219700  
C -2.66166300 0.59316100 -1.05099900  
H -3.32835400 1.40298700 -1.31255400  
C -0.87235000 -1.49374900 -0.29575000  
O -0.07665400 -2.35144900 0.03853500  
C -2.98388900 -0.21606300 0.11940300  
O -3.94963000 -0.08172900 0.84342000  
N -2.03618500 -1.22082200 0.39013200  
H -2.21833500 -1.80394200 1.20089500  
C 0.70102600 1.03400600 1.07284100  
C 1.24716600 -0.05875200 1.64668200  
N 2.30116100 -0.75034100 1.09633400  
C 2.86329800 -0.43747100 -0.12372600  
N 2.29474700 0.68559500 -0.70619100  
C 1.22493500 1.45211300 -0.22957000  
C -0.42518700 1.82613900 1.66638200  
H 0.88253900 -0.45601200 2.58870500  
H 2.58492200 -1.64262700 1.48034600  
O 3.75970200 -1.07252100 -0.63807900  
O 0.78333600 2.36796600 -0.90310400  
H 2.70678500 0.97760600 -1.58714200  
H -0.09036100 2.83137400 1.94271200

H -1.23537700 1.95017700 0.94178800  
H -0.82322300 1.33254000 2.55714200  
27

T-U-ftf-gas-max130: Optimised twist = 166.34 deg.

H -1.92924500 1.41124100 -2.28440400  
C -1.85276500 0.63122000 -1.53505800  
N -0.97123500 -0.38497800 -1.82626800  
H -0.44131500 -0.39271400 -2.68754700  
C -2.54973300 0.65453300 -0.38537500  
H -3.21355200 1.46906800 -0.13154400  
C -0.73248400 -1.46037500 -0.98215400  
O 0.07323100 -2.33072100 -1.24768300  
C -2.34170000 -0.40254100 0.60097200  
O -2.82142300 -0.43218300 1.71740500  
N -1.48667300 -1.42999500 0.17053600  
H -1.23979100 -2.12689800 0.86966600  
C 2.23087600 -0.30716800 0.12284600  
C 2.37810800 0.73765400 -0.71368800  
N 1.57582300 1.86137200 -0.65373300  
C 0.55756300 2.03043200 0.26608000  
N 0.42177500 0.95506000 1.12318300  
C 1.18048200 -0.22410200 1.14536600  
C 3.04113100 -1.56432200 0.06504900  
H 3.13281200 0.75224000 -1.49363300  
H 1.73355300 2.64951700 -1.26741100  
O -0.14572900 3.02058200 0.30076000  
O 0.93205800 -1.09654500 1.95589100  
H -0.31418500 1.03349200 1.82232800  
H 3.51741100 -1.76035000 1.03019200  
H 2.38873700 -2.41297900 -0.16369200  
H 3.81377900 -1.49388200 -0.70519700  
27

T-U-ftf-gas-max240: Optimised twist = 271.10 deg.

H -3.36412500 -2.12637300 0.81533100  
C -2.73237600 -1.46297400 0.23471400  
N -3.17708100 -0.16901800 0.13268200  
H -4.04565900 0.12664200 0.55880300  
C -1.58749900 -1.87085400 -0.34614000  
H -1.23338900 -2.88966900 -0.27040300  
C -2.51355400 0.81795500 -0.58943900  
O -2.94243100 1.94242100 -0.70779400  
C -0.78438900 -0.91491500 -1.10382000  
O 0.27644100 -1.15618300 -1.65125400  
N -1.33476800 0.37082700 -1.15894300  
H -0.80246200 1.07587100 -1.66085500  
C 0.90772000 -0.14209400 1.50307000  
C 1.73163000 -1.13772900 1.11689600  
N 2.67867500 -0.98256200 0.13464000  
C 2.82943800 0.17657800 -0.60500900  
N 1.99688600 1.19835500 -0.18153800  
C 1.01223900 1.14380900 0.80743300  
C -0.13414300 -0.26670700 2.57178900  
H 1.69455400 -2.12431800 1.56871400  
H 3.20334300 -1.77526700 -0.21048000  
O 3.63003400 0.29257700 -1.50779600  
O 0.30602900 2.11161500 1.03169500  
H 2.09239900 2.07642700 -0.68205800  
H 0.06631300 0.42506000 3.39610700



H -1.12232900 -0.00698800 2.17557300  
H -0.16961100 -1.28646600 2.96561300  
27

T-U-ftf-gas-min170: Optimised twist = 173.74 deg.

H -2.46224600 0.27014700 -2.46436700  
C -2.14312500 -0.08685100 -1.49134300  
N -1.43659400 -1.26711500 -1.49948800  
H -1.22930500 -1.75238200 -2.36214300  
C -2.41061500 0.57376700 -0.34993400  
H -2.93777500 1.51762800 -0.33717700  
C -0.91669600 -1.85680700 -0.35595400  
O -0.24529300 -2.86831900 -0.39119300  
C -1.92633400 0.03732800 0.91927400  
O -2.05099800 0.56770800 2.00604200  
N -1.24046700 -1.18236200 0.80262200  
H -0.80453000 -1.53314300 1.65375600  
C 2.06791100 -0.32578400 -0.15596100  
C 1.92912800 0.37269300 -1.29966000  
N 1.19757300 1.54071900 -1.37661300  
C 0.53797400 2.10707700 -0.30003100  
N 0.71187600 1.39767900 0.87237600  
C 1.40163800 0.19223000 1.04580500  
C 2.83093900 -1.60878500 -0.03155800  
H 2.38548600 0.05260700 -2.23117200  
H 1.11812600 2.05290900 -2.24478000  
O -0.12694200 3.11923500 -0.39083300  
O 1.40188700 -0.36573600 2.12816200  
H 0.18209500 1.73258300 1.67542200  
H 3.59786800 -1.52443700 0.74419500  
H 2.15792300 -2.42385200 0.25190000  
H 3.31148500 -1.86681600 -0.97914800  
27

T-U-ftf-gas-min315: Optimised twist = 309.35 deg.

H -2.87559800 1.98008500 -0.35206700  
C -2.38705800 1.03315800 -0.15012100  
N -1.95796800 0.34884300 -1.25871400  
H -1.98434400 0.77059200 -2.17930700  
C -2.20647200 0.55610200 1.09721200  
H -2.53771500 1.09420100 1.97463300  
C -1.31160000 -0.87509400 -1.19932500  
O -0.90924400 -1.45721900 -2.18406300  
C -1.48553100 -0.69783100 1.28678100  
O -1.15137700 -1.17271300 2.35827100  
N -1.15559000 -1.35103700 0.09115400  
H -0.65231100 -2.23356400 0.16919300  
C 1.11778500 1.53320100 0.47052400  
C 1.34401600 0.67726800 1.48798600  
N 1.72122900 -0.63053700 1.28795700  
C 1.80774300 -1.21037800 0.03677200  
N 1.66169900 -0.30587900 -0.99881800  
C 1.23259900 1.02118500 -0.89862100  
C 0.69047200 2.95696000 0.64691300  
H 1.22978700 0.96660200 2.52784800  
H 1.70539400 -1.28479600 2.06138400  
O 1.97963100 -2.40211400 -0.12928400  
O 0.96341000 1.66326100 -1.90008700  
H 1.62833200 -0.71883600 -1.92832800  
H 1.40545000 3.64027400 0.17829600

H -0.27716200 3.12935900 0.16292100  
H 0.60149800 3.20920100 1.70695900  
27

T-U-ftf-gas-min65: Optimised twist = 67.04 deg.

H 0.19308400 -0.70584300 2.68296600  
C 0.80553100 -0.62471100 1.79149000  
N 0.60522900 -1.61469500 0.85560900  
H -0.13219900 -2.30278400 0.97941000  
C 1.69265000 0.37042900 1.60211900  
H 1.83964000 1.15696800 2.32928500  
C 1.24198100 -1.63238200 -0.37121100  
O 0.96309300 -2.43015300 -1.24932300  
C 2.47209400 0.41391600 0.36842200  
O 3.28708700 1.26020000 0.06243900  
N 2.20092900 -0.65299000 -0.50871500  
H 2.69908300 -0.64454400 -1.39348600  
C -0.80259600 1.38819600 -0.94347700  
C -0.88916200 0.22614700 -1.62053200  
N -1.60920600 -0.86181100 -1.16199700  
C -2.16589400 -0.90267200 0.09598000  
N -2.18716900 0.32461400 0.72646000  
C -1.50993500 1.49131300 0.33839900  
C -0.00297000 2.57269600 -1.39225700  
H -0.38764100 0.06804100 -2.57032300  
H -1.45900500 -1.76806600 -1.59344700  
O -2.57666800 -1.92755300 0.61479000  
O -1.52907000 2.47508300 1.05152800  
H -2.63803400 0.34721000 1.63602700  
H -0.63928300 3.45838900 -1.48064200  
H 0.77770200 2.80778600 -0.66110100  
H 0.47244000 2.37881600 -2.35726100  
27

T-U-ftf-water-max120: Optimised twist = 140.00 deg.

H 0.33313600 -2.93476800 0.37251800  
C 0.82307200 -1.97410100 0.48439900  
N 1.66071000 -1.62055400 -0.54138700  
H 1.78759400 -2.23521100 -1.33754100  
C 0.62395600 -1.16856600 1.54896100  
H -0.04411900 -1.44282900 2.35429900  
C 2.36588700 -0.43578600 -0.57179000  
O 3.08590400 -0.11306300 -1.50322300  
C 1.34121100 0.09240900 1.63466100  
O 1.26594200 0.90030700 2.55070700  
N 2.18533600 0.34645700 0.54858200  
H 2.71239900 1.21515200 0.57072600  
C -0.66135200 1.16811300 -1.04366100  
C -0.79554900 -0.00599100 -1.69782300  
N -1.61916300 -1.01255100 -1.25040700  
C -2.37759100 -0.92196800 -0.10758300  
N -2.26400700 0.29331100 0.53261400  
C -1.45880600 1.37156600 0.16443400  
C 0.21874400 2.28779400 -1.50862900  
H -0.25810000 -0.22695700 -2.61438700  
H -1.69097700 -1.88187000 -1.76696500  
O -3.08698700 -1.82933000 0.30162000  
O -1.46160800 2.39599600 0.83467800  
H -2.81661300 0.40248200 1.37856500  
H -0.37769000 3.16655800 -1.77493400

H 0.90824700 2.59463000 -0.71533100  
H 0.80254700 1.98407300 -2.38084000  
27

T-U-ftf-water-max240: Optimised twist = 255.96 deg.

H 2.97828300 -1.81447200 1.42780200  
C 2.51316500 -1.12331400 0.73479500  
N 1.76595500 -1.70365300 -0.25548800  
H 1.68266800 -2.71228800 -0.31204700  
C 2.64941700 0.21660700 0.83254400  
H 3.23815500 0.67382700 1.61577700  
C 1.08936400 -0.98355200 -1.21627100  
O 0.40585800 -1.50392000 -2.08276100  
C 2.00163100 1.07255300 -0.14476900  
O 2.05217900 2.29531100 -0.17566300  
N 1.25430400 0.38249600 -1.10526100  
H 0.80122100 0.94155000 -1.82396900  
C -1.25876700 -0.91372800 0.97396200  
C -0.65574900 0.10677000 1.62244900  
N -0.74344400 1.41202500 1.19482900  
C -1.42607000 1.79574900 0.06651900  
N -2.04099100 0.74733000 -0.58713900  
C -2.05983400 -0.59541900 -0.20630900  
C -1.18184100 -2.34482400 1.41056500  
H -0.06507600 -0.04115000 2.52027600  
H -0.26594300 2.15035500 1.69968200  
O -1.48614000 2.95176600 -0.32572600  
O -2.71779600 -1.40507000 -0.84581800  
H -2.58425900 0.99651000 -1.40927700  
H -2.16665700 -2.71545700 1.71309900  
H -0.83709200 -2.97988400 0.58748500  
H -0.49276900 -2.45613400 2.25142400  
27

T-U-ftf-water-max320: Optimised twist = 316.40 deg.

H -2.89282900 1.76955700 -0.92718600  
C -2.39958200 0.90462200 -0.49918600  
N -1.88715800 0.01568600 -1.40990900  
H -1.97339200 0.19226500 -2.40450700  
C -2.28237000 0.70785100 0.83051300  
H -2.67518700 1.41432500 1.54885700  
C -1.24775000 -1.15068900 -1.05678500  
O -0.80762600 -1.94734500 -1.87062600  
C -1.58900500 -0.47134400 1.31717500  
O -1.37845800 -0.75185500 2.49006100  
N -1.12973800 -1.32509000 0.30725100  
H -0.67783100 -2.18707500 0.60451700  
C 1.02888900 1.60170700 0.32246700  
C 1.27095100 0.87671500 1.43677800  
N 1.70392600 -0.42733100 1.39212500  
C 1.89836000 -1.12121000 0.22376900  
N 1.68831400 -0.36313500 -0.90825200  
C 1.24594500 0.95871500 -0.97053900  
C 0.54781400 3.01984900 0.33588900  
H 1.12950500 1.27729800 2.43477700  
H 1.83240600 -0.95066100 2.25073100  
O 2.21705900 -2.30153300 0.18630400  
O 1.06041900 1.49080000 -2.05863000  
H 1.79408900 -0.85276800 -1.79312400  
H 1.27203700 3.68220000 -0.14917300

H -0.39630900 3.11248700 -0.21148100  
H 0.38944400 3.36363100 1.36073000  
27

T-U-ftf-water-max355: Optimised twist = 19.40 deg.

H 1.15854200 0.45349900 2.78670700  
C 1.37199900 0.01587300 1.81861000  
N 0.62708900 -1.09171000 1.49916800  
H -0.04617400 -1.46505600 2.15913300  
C 2.29518100 0.51796100 0.97298600  
H 2.87732300 1.39504900 1.22031200  
C 0.78793200 -1.80429200 0.32992000  
O 0.14593200 -2.80914000 0.06898300  
C 2.50082700 -0.11709000 -0.31680600  
O 3.26608500 0.26617400 -1.19222100  
N 1.73051900 -1.26678500 -0.52049800  
H 1.85978600 -1.75497100 -1.40282100  
C -0.54847500 1.54939900 -0.68822600  
C -0.67431600 0.56523600 -1.60505300  
N -1.51991900 -0.50635300 -1.43369800  
C -2.33486600 -0.66387600 -0.33893600  
N -2.18913300 0.33812700 0.59891000  
C -1.34199000 1.44490200 0.53316000  
C 0.34210000 2.74237200 -0.85968300  
H -0.11229100 0.56008000 -2.53321800  
H -1.57787300 -1.23035000 -2.14084400  
O -3.11210200 -1.59661600 -0.20347900  
O -1.30396500 2.24138000 1.46360600  
H -2.76595400 0.25225900 1.43142000  
H -0.24866700 3.66330400 -0.90675600  
H 1.02957200 2.83840400 -0.01380700  
H 0.92790400 2.65754100 -1.77824100  
27

T-U-ftf-water-min160: Optimised twist = 169.18 deg.

H 2.15947400 -1.37108900 -2.23053000  
C 1.97883800 -0.85047000 -1.29728600  
N 1.85967400 0.51118700 -1.40178500  
H 1.94951800 0.96750800 -2.30239700  
C 1.87287600 -1.48611100 -0.11115200  
H 1.95826000 -2.56098000 -0.03066700  
C 1.63283100 1.33877800 -0.32330700  
O 1.53937200 2.55141700 -0.42016900  
C 1.61237500 -0.71323600 1.09022800  
O 1.46564600 -1.16570500 2.21837900  
N 1.51239900 0.66533900 0.87528900  
H 1.31814700 1.24186000 1.69052100  
C -1.60806900 1.12157300 -0.23824200  
C -1.54289200 0.49088000 -1.43083200  
N -1.40590500 -0.87443500 -1.54230300  
C -1.33695100 -1.72207400 -0.46408600  
N -1.38961000 -1.06787900 0.74950900  
C -1.50947100 0.30443800 0.96830300  
C -1.75468800 2.60400400 -0.07860000  
H -1.59195100 1.02305900 -2.37489600  
H -1.37067800 -1.31029200 -2.45648400  
O -1.22864800 -2.93516900 -0.56350200  
O -1.50892800 0.74235400 2.11241600  
H -1.29559400 -1.65444000 1.57485300  
H -2.67107600 2.84623800 0.46918100

H -0.91046900 3.01569700 0.48320700  
H -1.79017100 3.09309200 -1.05490300  
27

T-U-ftf-water-min280: Optimised twist = 296.48 deg.

H 3.05871600 1.82023100 -0.37067500  
C 2.49422600 0.93462500 -0.10290900  
N 1.77925400 1.02727700 1.06380300  
H 1.80998300 1.87394500 1.62104400  
C 2.47627800 -0.18202000 -0.86066900  
H 3.03000500 -0.25213100 -1.78678300  
C 1.04369900 -0.01280400 1.58940700  
O 0.44581700 0.05899000 2.65050500  
C 1.68751800 -1.32255600 -0.43009300  
O 1.55486500 -2.37751200 -1.03739300  
N 1.03067200 -1.13938900 0.79192700  
H 0.51397700 -1.93556000 1.15914900  
C -0.81507200 1.17903000 -1.14093400  
C -0.81860100 -0.01681100 -1.77046800  
N -1.38541300 -1.14186500 -1.22057000  
C -1.94891600 -1.16883700 0.03118900  
N -1.98544600 0.06452900 0.64541300  
C -1.44985000 1.26213500 0.17118800  
C -0.19600300 2.41728500 -1.71092400  
H -0.36635200 -0.16186800 -2.74616800  
H -1.30430600 -2.03479100 -1.69405800  
O -2.37254600 -2.18873300 0.55726900  
O -1.52442300 2.27846000 0.85114300  
H -2.37555900 0.08085600 1.58393500  
H -0.95144400 3.19252500 -1.87542400  
H 0.54577200 2.83295400 -1.02020400  
H 0.29635500 2.20006000 -2.66174400  
27

T-U-ftf-water-min330: Optimised twist = 332.72 deg.

H 1.06289300 -2.90645600 -1.30706800  
C 1.20222200 -2.07817000 -0.62249800  
N 1.84750600 -0.98774000 -1.14764800  
H 2.15229400 -0.98881400 -2.11450100  
C 0.77077100 -2.10100500 0.65593500  
H 0.25450200 -2.95689400 1.06906200  
C 2.11180200 0.15705900 -0.43083800  
O 2.68852900 1.12358700 -0.90324200  
C 0.97569600 -0.93670400 1.49929800  
O 0.60777500 -0.81448000 2.66048200  
N 1.64724100 0.11685400 0.86877700  
H 1.83343300 0.94458200 1.43006400  
C -1.99998000 -0.42842800 -0.06768100  
C -1.95409600 0.31978400 1.05576000  
N -1.27035400 1.51144000 1.12349500  
C -0.57870300 2.05301000 0.06886300  
N -0.62571900 1.28010200 -1.07382300  
C -1.28033700 0.05779500 -1.24124400  
C -2.72382300 -1.73524600 -0.17575200  
H -2.44615000 0.02209100 1.97520600  
H -1.24894000 2.03839000 1.98898900  
O 0.03051400 3.11067700 0.13467200  
O -1.21358900 -0.52876000 -2.31475500  
H -0.12237600 1.64727000 -1.87764800  
H -3.50773000 -1.68502000 -0.93829300

H -2.03379500 -2.53366600 -0.46888800  
H -3.18199000 -2.00284500 0.77915500  
27

T-U-ftf-water-min40: Optimised twist = 57.78 deg.

H 0.27644900 -0.09568800 2.72672900  
C 0.84837000 -0.28929800 1.82620500  
N 0.44716300 -1.38395700 1.10152500  
H -0.30013000 -1.98045200 1.44035700  
C 1.87636800 0.48846500 1.42784900  
H 2.18432200 1.35792800 1.99245800  
C 1.05580200 -1.78209800 -0.06951900  
O 0.68110800 -2.74555400 -0.71940700  
C 2.59545400 0.15370800 0.21042600  
O 3.54408200 0.77083200 -0.25575900  
N 2.11392400 -0.98320900 -0.44561600  
H 2.58374700 -1.24892100 -1.30709000  
C -0.55341800 1.27242400 -0.96461600  
C -0.83373500 0.11086000 -1.59391800  
N -1.77795200 -0.77641300 -1.13060300  
C -2.49641400 -0.58319200 0.02223300  
N -2.21584900 0.61276400 0.65119800  
C -1.29904600 1.58621600 0.25179000  
C 0.47105600 2.25597400 -1.44150600  
H -0.32440900 -0.19632600 -2.50163400  
H -1.91955800 -1.66104000 -1.60533900  
O -3.30217600 -1.39246100 0.45912300  
O -1.16328500 2.60718300 0.91396100  
H -2.74148300 0.80022100 1.50085500  
H -0.00049900 3.19921300 -1.73639500  
H 1.18604700 2.48576700 -0.64448300  
H 1.02005700 1.85664000 -2.29799300