Supporting Information

Acidity and basicity interplay in amide and imide self-association

Wilmer E. Vallejo Narváez, a Eddy I. Jiménez, a Eduardo Romero-Montalvo, ab Arturo Sauza-de la Vega, a Beatriz Quiroz-García, a Marcos Hernández-Rodríguez* a and Tomás Rocha-Rinza* a

aInstitute of Chemistry, National Autonomous University of Mexico, Circuito Exterior, Ciudad Universitaria, Delegación Coyoacán C.P. 04510, Mexico City, Mexico.

bPresent address: Department of Chemistry, University of British Columbia, Okanagan, 3247 University Way, Kelowna, British Columbia, Canada V1V 1V7.

*Email: marcoshr@unam.mx, tomasrocharinza@gmail.com
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3. References
1. Experimental section

Compounds A1, A2, A4-A7, I1, I2, I4, I5 and I8 are commercially available and only I3 was synthesised according to the procedure reported by Fun et al.1 2-pyrrolidone (A1) was further purified by distillation to remove water and other impurities. The dimerisation constants for the rest of systems in Table 3 and all of the molecules in Figure 7 were obtained from the literature.

1.1 General procedure for $^1$H-NMR titrations

NMR spectra were recorded in a range of 0.002 to 1.0 M at 25 °C in CDCl$_3$. Only compounds A6 and A7 were studied in a range of 8.0·10$^{-4}$ M to 0.08 M because of their low solubility in CDCl$_3$. All experiments were performed on a 300 MHz spectrometer and N-H chemical shifts are reported in ppm downfield from TMS. $^1$H-NMR spectra were processed using the MestReNova NMR software.2 The association constants were calculated from the downfield shifting of the N-H proton using the online tool supramolecular.org.3 The self-association constants of the investigated compounds are shown in Table 3. Heterodimerisation constants were calculated with the HypNMR 2008 program.4
1.2 Self-association constants of 2-pyrrolidone in different solvents

**Figure S1.** Profile of chemical shift as a function of concentration for 2-pyrrolidone, A1, in different solvents. The concentration range of A1 from 0.002 M to 1.0 M at 25 °C. The dimerisation constants are reported in Table 1 in the main body of the paper. The percentage errors are: (CDCl$_3$) ± 0.4% and (Acetonitrile-d$_3$) ± 0.6%. The values of $K_{dimer}$ in DMSO-d$_6$ could not be determined with good accuracy in virtue of its small value.
1.3 Self-association studies in CDCl₃

**Figure S2.** (a) Stacked plot of ¹H-NMR (300 MHz) spectra for the self-association study of A1 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of δN-H (dimer and monomer) in CDCl₃ at 25 °C.
Figure S3. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of A2 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S4. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of A4 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S5. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of A5 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{\text{N-H}}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S6. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of A6 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{\text{N-H}}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S7. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of A7 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S8. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I1 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S9. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I2 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S10. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I3 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S11. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I4 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S12. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I5 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{\text{N-H}}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
Figure S13. (a) Stacked plot of $^1$H-NMR (300 MHz) spectra for the self-association study of I8 at different concentrations and (b) its profile of chemical shift as a function of concentration as well as its dimerisation constant, the corresponding percentage error and values of $\delta_{N-H}$ (dimer and monomer) in CDCl$_3$ at 25 °C.
1.4 Heterodimerisation of A5 and I1 in CDCl₃

Saturation of the HB-1 signal

Saturation of the HB-2 signal

\[ K_{\text{heter}1} = 4.4 \pm 1.2 \text{ M}^{-1} \]

\[ K_{\text{heter}2} = 5.0 \pm 1.1 \text{ M}^{-1} \]

\[ K_{\text{heter}} = 4.7 \pm 1.1 \text{ M}^{-1} \ (K_{\text{heter corr}} = 2.4 \text{ M}^{-1}) \]

\[ \delta_{\text{N-H HB-1}} = 11.43 \text{ ppm} \quad \delta_{\text{N-H HB-2}} = 7.36 \text{ ppm} \]

Figure S14. Profile of chemical shift as a function of concentration for the heterodimerisation I1-A5 in CDCl₃ at 25 °C: a) imide I1 (0.1 M) upon titration with amide A5 (0-20 eq.) and b) vice versa. The heterodimerisation constants with and without statistical factor corrections are also shown.
1.5 Heterodimerisation of A1 and I2 in CDCl₃

Saturation of the HB-1 signal

Saturation of the HB-2 signal

\[ K_{\text{heter}1} = 9.7 \pm 1.1 \text{ M}^{-1} \]
\[ K_{\text{heter}2} = 8.5 \pm 1.1 \text{ M}^{-1} \]

\[ K_{\text{heter}} = 9.1 \pm 1.1 \text{ M}^{-1} \quad (K_{\text{heter corr}} = 4.5 \text{ M}^{-1}) \]

\[ \delta_{N-H} \text{ HB-1} = 12.19 \text{ ppm} \quad \delta_{N-H} \text{ HB-2} = 7.45 \text{ ppm} \]

**Figure S15.** Profile of chemical shift as a function of concentration for the heterodimerisation I2-A1 in CDCl₃ at 25 °C: a) imide I2 (0.1 M) upon titration with amide A1 (0-20 eq.) and b) vice versa. The heterodimerisation constants with and without statistical factor corrections are also shown.
1.6 ¹H-DOSY experiments

Diffusion Ordered Spectroscopy (¹H-DOSY) experiments were recorded at 25 °C, using a 2D pulse sequence (dstepgbp3s) for diffusion measurements with double stimulated echo for convection compensation. The experiment involves bipolar gradient pulses, a Longitudinal Eddy Current Delay (LED) and three spoil gradients. The standard pulse sequence dstepgbp3s, was taken from the Bruker software library. The obtained diffusion coefficients allow to estimate the size of complexes or adducts through the calculation of hydrodynamic radius by considering the tetramethylsilane (TMS) as an internal standard reference, \( r_{\text{ref}} \), from the following equation:

\[
r_H = \frac{D_{\text{ref}}}{D} r_{\text{ref}},
\]

where \( D_{\text{ref}} \) and \( D \) are the diffusion coefficients of TMS and the sample, respectively.
Concentration: 0.5 M

Diffusion coefficients

\[ (10^{-2} \text{ m}^2/\text{s}) \]

\[
\begin{array}{cc}
D & D_{\text{ref,}} \\
A1 & \text{TMS} \\
12.05 & 16.88
\end{array}
\]

Figure S16. (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide A1. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.5 M

Diffusion coefficients

\[(10^{-2} \text{ m}^2/\text{s})\]

\[
\begin{array}{cc}
D & D_{\text{ref}} \\
\text{A2} & \text{TMS} \\
11.67 & 16.72 \\
\end{array}
\]

Figure S17. (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide A2. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.6 M

Diffusion coefficients

\[ (10^{-2} \text{ m}^2/\text{s}) \]

\[ \begin{array}{cc}
D & D_{\text{ref},} \\
A4 & TMS \\
10.32 & 17.39
\end{array} \]

**Figure S18.** (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide **A4**. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.6 M

Diffusion coefficients

\[(10^{-2} \text{ m}^2/\text{s})\]

|        | \(D\)   | \(D_{\text{ref}}\) |
|--------|---------|---------------------|
| A5     | 9.48    | 15.46               |

Figure S19. (a) \(^1\)H-DOSY (500 MHz) spectrum in CDCl\(_3\) at 25 \(^\circ\)C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide A5. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.08 M

Diffusion coefficients

\( \left(10^{-2} \text{ m}^2/\text{s}\right) \)

|    |    |
|----|----|
| \(D\) | \(D_{\text{ref}}\) |
| A6  | TMS |
| 13.19 | 19.93 |

**Figure S20.** (a) \(^1\)H-DOSY (500 MHz) spectrum in CDCl\(_3\) at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide A6. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Figure S21. (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of amide A7. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.6 M

Diffusion coefficients

\[ (10^{-2} \text{ m}^2/\text{s}) \]

| \( I_1 \) | \( D_{\text{ref}} \) |
|---------|-----------------|
| 8.72    | 15.19           |

Figure S22. (a) \(^1\)H-DOSY (500 MHz) spectrum in CDCl\(_3\) at 25 \(^\circ\)C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide \( I_1 \). Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.5 M

Diffusion coefficients

$\left(10^{-2} \text{ m}^2/\text{s}\right)$

|   | $D$   | $D_{\text{ref}}$ |
|---|------|------------------|
| I2 | 6.75 | 15.04            |

Figure S23. (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide I2. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.4 M

Diffusion coefficients

\(10^{-2} \text{ m}^2/\text{s}\)

|   |   |
|---|---|
| \(D\) | \(D_{\text{ref}}\) |
| \(I_3\) | TMS | 6.75 | 15.04 |

Figure S24. (a) \(^1\text{H}-\text{DOSY}\) (500 MHz) spectrum in CDCl\(_3\) at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide I3. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Figure S25. (a) $^1$H-DOSY (500 MHz) spectrum in CDCl$_3$ at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide I4. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.4 M

Diffusion coefficients 

\( (10^2 \text{ m}^2/\text{s}) \)

|   |   |
|---|---|
| \( D \) | \( D_{\text{ref}} \) |
| I5 | TMS |
| 8.46 | 17.68 |

**Figure S26.** (a) \(^1\text{H}-\text{DOSY} \) (500 MHz) spectrum in CDCl\(_3\) at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide I5. Experimental and calculated radii are shown in Table 2 in the body of the paper.
Concentration: 0.6 M
Diffusion coefficients
\((10^{-2} \text{ m}^2/\text{s})\)

| \(D\)     | \(D_{\text{ref}}\) |
|----------|---------------------|
| I8       | TMS                 |
| 2.98     | 12.68               |

Figure S27. (a) \(^1\text{H}-\text{DOSY} (500 \text{ MHz})\) spectrum in CDCl\(_3\) at 25 °C and (b) dimer structure determined via M06-2x/6-311++G(2d,2p) calculations of imide I8. Experimental and calculated radii are shown in Table 2 in the body of the paper.
2. Computational details

All geometries of monomers, dimers and the species involved in the calculation of proton affinities were optimized using the M06-2x functional with the 6-311++G(2d,2p) basis set as implemented in the Gaussian 09 package. We chose this approximation because it yields a good description of the energetics of protonation and deprotonation processes and most importantly of intermolecular interactions such as hydrogen bonds. Each stationary structure was characterised as a minimum via the calculation of the corresponding harmonic frequencies. The inclusion of nonspecific solvent effects in the calculations was made by using the SMD method. Some earlier experimental and theoretical studies about the dimerisation of 2-pyridone, 2-pyrrolidone, δ-valerolactam and maleimide were taken as a starting point for this work. These studies conclude that the keto form is the most stable arrangement for the dimer formation. We studied the topology of the electron distribution under the formalism of the Quantum Theory of Atoms in Molecules (QTAIM) to get further insights about the chemical bonding scenario of the investigated dimers. This analysis was complemented with DFT electronic energy partitions in accordance with the Interacting Quantum Atoms (IQA) approach. In particular, we examined the steric repulsion of the carbonyl groups (spectators and those involved in the HB) with both methods with the aid of the AIMAll program. We also calculated QTAIM electron Delocalisation Indices DIs (Ω, Ω'), which are chemical bonding indicators that have been successfully used for the characterisation of non-covalent interactions like hydrogen bonds.
2.1 QTAIM molecular graphs for the examined amide and imide dimers and heterodimers

We determined the molecular graphs for the considered amide and imide homo- and heterodimers. The bond and ring critical points are displayed respectively with green and red colour. The examined electron densities were computed with the (SMD-CHCl$_3$)-M06-2x//6-311++G(2d,2p) approximation.

2.1.1 Homodimers

Table S1. QTAIM molecular graphs of the amide and imide homodimers studied in this work. The bond and ring critical points are indicated with red and green colours respectively. I11-I13 homodimers are not included because of the high computational cost of their corresponding calculations.

| Amide A1 homodimer | Amide A2 homodimer |
|--------------------|--------------------|
| ![Amide A1 homodimer](image1.png) | ![Amide A2 homodimer](image2.png) |

| Amide A3 homodimer | Amide A4 homodimer |
|--------------------|--------------------|
| ![Amide A3 homodimer](image3.png) | ![Amide A4 homodimer](image4.png) |
Amide A6 homodimer

Amide A7 homodimer

Imide I2 homodimer

Imide I3 homodimer

Imide I4 homodimer

Imide I5 homodimer
2.1.2 Heterodimers

Table S2. QTAIM molecular graphs of the amide and imide heterodimers studied in this work.

A5-I1 heterodimer  A1-I2 heterodimer
2.2 Hydrogen bond formation energies by Espinosa’s empirical formula

Figure S28. Hydrogen bond formation energies calculated with Espinosa’s empirical formula\textsuperscript{17} for HBs involved in homo- and heterodimers studied in this work a) A5 and I1 and b) A1 and I2. The Espinosa’s equation is $E_{\text{HB}} = 0.5 \cdot V(r)$ where $V(r)$ is the potential energy density at the bond critical point of the examined HB. All values are given in kcal/mol.
2.3 Use of the interacting quantum atoms approach for the study of bimolecular clusters

The Interacting Quantum Atoms (IQA) method is an electronic energy partition, $E$, in one ($E_{\text{net}}$) and two-atoms ($E_{\text{int}}$) terms\(^{18}\)

$$E = \sum_A E_{\text{net}}^A + \sum_{A>B} E_{\text{int}}^{AB}, \quad (1)$$

wherein the sums run over atomic regions which divide exhaustively the three-dimensional space. The terms $E_{\text{net}}^A$ and $E_{\text{int}}^{AB}$ are referred as (i) the IQA net energy of atom $A$ and (ii) the IQA interaction energy of the pair of atoms $A$ and $B$ respectively.\(^{19}\) The IQA interaction energy, $E_{\text{int}}^{AB}$ can be further split in classical (coulombic) and exchange-correlation contributions,

$$E_{\text{int}}^{AB} = E_{\text{cl}}^{AB} + V_{XC}^{AB}. \quad (2)$$

The components $E_{\text{cl}}^{AB}$ and $V_{XC}^{AB}$ are related to the covalency and ionicity of the interaction between atoms $A$ and $B$ respectively.

The IQA method is entirely based on the first order reduced density matrix $\rho_1(r_1,r'_1)$ and the pair density $\rho_2(r_1,r_2)$. Neither of these scalar fields are defined in conventional density functional theory. It is possible, nevertheless, to scale one and two atom terms of the Kohn-Sham exchange-correlation energy in a similar fashion to QTAIM.\(^{20}\) This procedure allows us to obtain the total DFT electronic energy in accordance with equation (1).

The IQA approach has been successfully used to study molecular clusters.\(^{21}\) Because the formalism of IQA is invariant with respect to the grouping of several QTAIM basins in functional groups or molecules, the electronic energy of a bimolecular cluster $G \cdots H$ can be written as

$$E^{G\cdots H} = E_{\text{net}}^G + E_{\text{net}}^H + E_{\text{int}}^{G,H}, \quad (3)$$
in which $E_{\text{net}}^G$ comprises the net energies of the atoms within $G$, along with their corresponding interactions

$$E_{\text{net}}^G = \sum_{A \in G} E_{\text{net}}^A + \sum_{A \in G} \sum_{B \in G, B \geq A} E_{\text{int}}^{AB}. \quad (4)$$

A similar definition holds for $E_{\text{net}}^H$ while the quantity $E_{\text{int}}^{GH}$ is defined as

$$E_{\text{int}}^{GH} = \sum_{A \in G} \sum_{B \in H} E_{\text{int}}^{AB}. \quad (5)$$

The change in energy associated with the formation of the molecular cluster $G \cdots H$, $\Delta E$, can be written as the sum of the IQA deformation energies of the monomers and its corresponding interaction defined in equation (5),

$$\Delta E = E_{\text{net}}^{G \cdot H} - (E_{\text{iso}}^G + E_{\text{iso}}^H)$$

$$= E_{\text{def}}^G + E_{\text{def}}^H + E_{\text{int}}^{GH}. \quad (6)$$

The deformation energy of monomer $I$ is defined as

$$E_{\text{def}}^I = E_{\text{net}}^I - E_{\text{iso}}^I \quad (7)$$

$E_{\text{def}}^I$ is associated with the changes of the electron density and the nuclear geometry associated with the interaction of monomer $I$ with other species. Finally, we indicate that the analysis presented in this work was performed at the DFT electron density computed with gas-phase single-point calculations at M06-2x/6-311++G(2d,2p) level of theory.
2.3.1 IQA analysis of I1-A5 and I2-A1 heterodimers as well as I1 and I2 homodimers

Table S3. Complete set of intermolecular $E_{\text{int}}$(IQA) values within the I1–I1 homodimer.† The data are reported in kcal/mol.

| $O_s$ of I1 | Atoms of I1 | $E_{\text{int}}$ | Atoms of I1 | $E_{\text{int}}$ (with all atoms of I1) |
|-------------|-------------|-----------------|-------------|----------------------------------------|
| C14         | -79.2       | C1              | -12.5       |
| C15         | -113.9      | C2              | 4.0         |
| C16         | -2.2        | C3              | -0.1        |
| C17         | -4.0        | C4              | -0.2        |
| C18         | -1.4        | C5              | -0.3        |
| H19         | -1.2        | H6              | 0.0         |
| H20         | -2.0        | H7              | 0.0         |
| H21         | -0.8        | H8              | -0.1        |
| H22         | -1.6        | H9              | -0.1        |
| H23         | -37.6       | H10             | -22.3       |
| N24         | 81.7        | N11             | 5.1         |
| O25         | 114.0       | O12             | -30.9       |
| O26         | 60.6        | O13             | 10.7        |
| C27         | -2.3        | C35             | -0.1        |
| H28         | 0.1         | H36             | 0.0         |
| H29         | 0.6         | H37             | 0.0         |
| H30         | 0.9         | H38             | 0.0         |
| C31         | -2.6        | C39             | -0.1        |
| H32         | 0.6         | H40             | 0.0         |
| H33         | 0.2         | H41             | 0.0         |
| H34         | 0.7         | H42             | 0.0         |
| **Total**   | **10.7**    | **Total**       | **-46.8**   |

†The IQA deformation energies of the interacting monomers are 16.4 and 20.0 kcal/mol, so that the IQA formation energy of the molecular cluster is $E_{\text{form}} = (16.4 + 20.0 − 46.8)$ kcal/mol = −10.4 kcal/mol.
Table S4. Complete set of intermolecular $E_{\text{int}}$(IQA) values within the I1–A5 heterodimer.\(^\dagger\) The data are reported in kcal/mol.

\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{O}_5 \text{ of I1} & \text{Atoms} & \text{Atoms} & \text{Atoms} & \text{Atoms} \\
\text{of A5} & E_{\text{int}} & \text{of I1} & (\text{with all} & \text{of A5} & (\text{with all} \\
\text{of A5} & & & \text{atoms of A5}) & \text{of A5} & \text{atoms of I1}) \\
\hline
\text{C21} & -23.2 & \text{C1} & -19.9 & \text{C21} & -3.2 \\
\text{C22} & -3.7 & \text{C2} & 0.7 & \text{C22} & -0.4 \\
\text{C23} & -3.8 & \text{C3} & -0.1 & \text{C23} & -0.2 \\
\text{C24} & -2.8 & \text{C4} & -0.2 & \text{C24} & -0.1 \\
\text{C25} & -118.4 & \text{C5} & -0.4 & \text{C25} & 6.6 \\
\text{N26} & 83.1 & \text{H6} & 0.0 & \text{N26} & 3.5 \\
\text{H27} & 1.1 & \text{H7} & -0.1 & \text{H27} & 0.1 \\
\text{H28} & -0.4 & \text{H8} & -0.1 & \text{H28} & 0.0 \\
\text{H29} & 0.2 & \text{H9} & -0.2 & \text{H29} & 0.0 \\
\text{H30} & -1.7 & \text{H10} & -32.9 & \text{H30} & 0.0 \\
\text{H31} & -35.5 & \text{N11} & 11.1 & \text{H31} & -19.7 \\
\text{O32} & 121.4 & \text{O12} & -28.6 & \text{O32} & -40.7 \\
\text{H34} & 0.4 & \text{O13} & 16.9 & \text{H34} & 0.0 \\
\text{H35} & 0.8 & \text{C14} & -0.2 & \text{H35} & 0.0 \\
\text{H36} & 0.4 & \text{H15} & 0.0 & \text{H36} & 0.0 \\
\text{H37} & -1.0 & \text{H16} & -0.1 & \text{H37} & 0.0 \\
\hline
\text{Total} & 16.9 & \text{Total} & -54.0 & \text{Total} & -54.0 \\
\hline
\end{array}
\]

\(^\dagger\)The IQA deformation energies of the amide and imide are 20.9 and 21.7 kcal/mol, so that the IQA formation energy of the molecular cluster is $E_{\text{form}} = (20.9 + 21.7 - 54.0) \text{kcal/mol} = -11.4 \text{kcal/mol}$. 

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**Table S5.** Complete $E_{\text{int}}$(IQA) values within the I2–I2 homodimer.\(^\dagger\) The data are reported in kcal/mol.

\[\begin{array}{c|c|c|c|c|c|c|c|c}
\text{O}_\text{s of I2} & \text{Atoms of I2} & E_{\text{int}} & \text{Atoms of I2} & E_{\text{int}} (\text{with all atoms of I2}) \\
\hline
N1 & 80.7 & N25 & 2.2 \\
H2 & -37.3 & H26 & -22.8 \\
C3 & -78.8 & C27 & -9.4 \\
O4 & 58.9 & O28 & 8.0 \\
C5 & -0.6 & C29 & -0.2 \\
H6 & -1.6 & H30 & -0.1 \\
H7 & -1.7 & H31 & -0.1 \\
C8 & -2.3 & C32 & -0.1 \\
C9 & -110.1 & C33 & 9.5 \\
O10 & 108.2 & O34 & -37.6 \\
C11 & -3.7 & C35 & 0.0 \\
H12 & 1.4 & H36 & 0.0 \\
H13 & 0.0 & H37 & 0.0 \\
C14 & -3.7 & C38 & 0.0 \\
H15 & 1.2 & H39 & 0.0 \\
H16 & 1.1 & H40 & 0.0 \\
C17 & -2.8 & C41 & 0.0 \\
H18 & 0.9 & H42 & 0.0 \\
H19 & 0.9 & H43 & 0.0 \\
H20 & 0.3 & H44 & 0.0 \\
C21 & -3.1 & C45 & 0.0 \\
H22 & 80.7 & H46 & 0.1 \\
H23 & -37.3 & H47 & 0.0 \\
H24 & -78.8 & H48 & 0.0 \\
\hline
\text{Total} & 8.0 & \text{Total} & -50.4
\end{array}\]

\(^\dagger\)The IQA deformation energies of the interacting monomers are 20.5 and 19.0 kcal/mol, so that the IQA formation energy of the molecular cluster is $E_{\text{form}} = (20.5 + 19.0 - 50.4)$ kcal/mol = −10.9 kcal/mol.
Table S6. Complete set of intermolecular $E_{\text{int}}$(IQA) values within the I2–A1 heterodimer.† The data are reported in kcal/mol.

| O₅ of I₂ | Atoms of A₁ | $E_{\text{int}}$ | Atoms of I₂ | $E_{\text{int}}$ (with all atoms of A₅) | Atoms of A₅ | $E_{\text{int}}$ (with all atoms of I₂) |
|---------|-------------|-----------------|-------------|-----------------------------------------|-------------|-----------------------------------------|
|         | O₁          | 114.2           | O₁₀         | -31.8                                   | O₁          | -48.7                                   |
|         | N₂          | 81.4            | N₁₁         | 8.9                                     | N₂          | 0.3                                     |
|         | C₃          | -114.9          | C₁₂         | 4.0                                     | C₃          | 13.2                                    |
|         | C₄          | -22.7           | C₁₃         | -17.0                                   | C₄          | -2.3                                    |
|         | C₅          | -3.6            | C₁₄         | -0.2                                    | C₅          | -0.2                                    |
|         | C₆          | -2.2            | C₁₅         | -0.2                                    | C₆          | 0.0                                     |
| O₁⁹     | H₇          | -35.5           | H₁₆         | -34.1                                   | H₇          | -19.3                                   |
|         | H₈          | -0.1            | H₁₇         | -0.1                                    | H₈          | 0.0                                     |
|         | H₉          | 0.3             | H₁₈         | -0.2                                    | H₉          | 0.0                                     |
|         | H₃₄         | -1.6            | O₁⁹         | 13.9                                    | H₃₄         | 0.0                                     |
|         | H₃₅         | -1.1            | C₂₀         | 0.0                                     | H₃₅         | 0.1                                     |
|         | H₃₆         | -0.5            | H₂₁         | -0.1                                    | H₃₆         | 0.0                                     |
|         | H₃₇         | 0.2             | H₂₂         | 0.1                                     | H₃₇         | 0.0                                     |

|         | Total       | 13.9            | Total       | -56.9                                   | Total       | -56.9                                   |

†The IQA deformation energies of the interacting monomers are 21.9 and 22.9 kcal/mol, so that the IQA formation energy of the molecular cluster is $E_{\text{form}} = (21.9 + 22.9 - 56.9)$ kcal/mol = −12.1 kcal/mol.
### 2.4 Data for the correlation between $|E(A)|$ vs $pK_a$ and $|E(B)|$ vs $pK_{BH^+}$

**Table S7.** Values of $|E(A)|$ computed at the (SMD-DMSO)-M06-2x/6-311++G(2d,2p) level of theory and reported experimental $pK_a$ in DMSO for the complete set of studied compounds.

| Compound | $|E(A)|$ kcal/mol | $pK_a$ in DMSO | Ref. |
|----------|------------------|----------------|------|
| 2-Pyrrolidone (A1) | 75.0 | 24.2 | 22 |
| 2-Oxazolidinone (A2) | 69.8 | 20.8 | 22 |
| 2-Piperidone (A5) | 78.8 | 26.6 | 22 |
| 1,3-Dihydroindol-2-one (A6) | 64.7 | 18.5 | 22 |
| Formamide | 72.1 | 23.5 | 23 |
| Succinimide | 60.9 | 14.7 | 24 |
| 2-Oxazolone | 59.6 | 15.0 | 24 |
| Urea | 74.7 | 26.9 | 25 |
| Thiourea | 65.7 | 21.1 | 25 |
| $N,N'$-Diphenylurea | 64.5 | 18.7 | 25 |
| $N,N'$-Diphenylthiourea | 58.2 | 13.4 | 26 |
| $N'$-Phenyl-$N$-[3-(trifluoromethyl)phenyl]thiourea | 56.3 | 12.1 | 26 |
| $N$-[3,5-Bis(trifluoromethyl)phenyl]-$N'$-phenylurea | 59.8 | 16.1 | 26 |
| $N$-[3,5-Bis(trifluoromethyl)phenyl]-$N'$-phenylthiourea | 54.6 | 10.7 | 26 |
| $N,N'$-Bis[3-(trifluoromethyl)phenyl]thiourea | 54.9 | 10.9 | 26 |
| $N,N'$-Bis[3,5-bis(trifluoromethyl)phenyl]urea | 57.9 | 13.8 | 26 |
| $N,N'$-Bis[3,5-bis(trifluoromethyl)phenyl]thiourea | 52.2 | 8.5 | 26 |
| Acetic acid | 58.9 | 12.6 | 27 |
| 3,4-Bis(phenylamino)-3-cyclobutene-1,2-dione ($N,N'$-Diphenylsquaramide) | 55.8 | 12.5 | 28 |
| $N'$-Phenyl-$N$-[3-(trifluoromethyl)phenyl]squaramide | 52.5 | 10.6 | 28 |
Figure S29. Correlation of experimental pKₐ with |E(A)| for the compounds indicated in Table S7.

Table S8. Computed values of |E(B)| at the (SMD-water)-M06-2x/6-311++G(2d,2p) level of theory and reported experimental pKₐ BH⁺ in H₂O for the set of compounds considered in this work.

| Compound                        | |E(B)|, kcal/mol | pKₐ BH⁺ in water | Ref. |
|---------------------------------|-----------------|-----------------|-----------------|-----|
| 2-Pyrrolidone (A1)              | 13.4            | -0.65           | 29              |
| 2-Piperidone (A5)               | 14.9            | -0.18           | 29              |
| ε-Caprolactam (A3)              | 14.5            | -0.46           | 29              |
| 2-Azacyclooctanone              | 14.6            | -0.38           | 29              |
| N-Methyl-2-pyrrolidone          | 12.8            | -0.75           | 29              |
| Acetamide                       | 12.5            | -0.73           | 29              |
| Propanamide                     | 12.2            | -0.86           | 30              |
| t-Butylformamide                | 12.0            | -1.11           | 30              |
| N-Methylformamide               | 9.6             | -1.49           | 30              |
| N-Methylacetamide               | 10.4            | -1.10           | 30              |
| N-Methylpropanamide             | 14.5            | -0.56           | 30              |
| 2-Cloroacetamide                | 12.4            | -0.70           | 30              |
| 4-Methylbenzamide               | 6.7             | -2.80           | 31              |
| 4-Nitrobenzamide                | 11.0            | -1.44           | 32              |
| 4-Chlorobenzamide               | 7.8             | -2.28           | 32              |
| N-(2,2,2-Trifluoroethyl)benzamide| 9.7             | -1.66           | 32              |
| 2-Fluorobenzamide               | 5.6             | -3.33           | 33              |
|                                | 8.7             | -1.98           | 34              |
Figure S30. Correlation of experimental pK_{BH+} with |E(B)| for the species indicated in Table S8.
2.5 Hydrogen bonds between A2 and a chloroform molecule

Figure S31. Hydrogen bonds between 2-oxazolidonone (A2) and a chloroform molecule. **Left:** H-bond formed with the carbonyl oxygen. **Right:** Bifurcated HBs which involve the two oxygen atoms of A2.
2.6 Correlation of experimental and that computed with the first-degree model herein

**Figure S32.** Correlation of experimental $\ln K_{\text{dimer}}$ with its computed counterpart estimated with the equation indicated in Figure 5 of the paper for all species studied in this work.
### 2.7 Acidity and basicity values of the investigated systems in CCl₄

Table S9. In $K_{dimer}$ in CCl₄ determined by infrared spectroscopy.

| Comp. | In $K_{dimer}$ | | $|E(A)|$ | $|E(B)|$ |
|-------|----------------|---|------|------|
| A1    | 5.11<sup>35</sup> | 130.0 | 35.9 |
| A3    | 4.53<sup>35</sup> | 134.7 | 38.7 |
| A5    | 4.88<sup>35</sup> | 134.0 | 39.3 |
| A8    | 3.93<sup>35</sup> | 126.5 | 30.1 |
| A9    | 4.34<sup>35</sup> | 135.2 | 40.3 |
| I14   | 2.69<sup>b,36</sup> | 112.8 | 23.5 |
| I15   | 1.98<sup>b,36</sup> | 98.9 | 9.0 |
| I16   | 0.96<sup>b,36</sup> | 107.0 | 13.0 |
| I17   | 0.10<sup>b,36</sup> | 88.9 | -3.4 |
| I18   | 4.11<sup>36</sup> | 117.0 | 32.6 |

<sup>a</sup> The $|E(B)|$ and $|E(A)|$ values were calculated with the SMD-(CCl₄)-M06-2x/6-311++G(2d,2p) method.

<sup>b</sup> Statistical factor applied.
2.8 Delocalisation indices

Figure S33. Changes in the electron delocalisation indices as a consequence of the dimerisation of the imides studied in this work. The corresponding data for I1 and I2 are reported in Figure 3 in the body of the paper. The DIs whose change is negative (in red) indicate interactions with a decreased covalent character due to the formation of the molecular cluster. A positive value for a change in a DI (in green) evidences an increased covalent bond character as a result of the formation of the HB.
### 2.9 Bond lengths

Table S10. Changes in bond lengths \((l_{dimer} - l_{monomer})\) involved in the resonance-assisted hydrogen bond within the imide homodimers examined in this study, i.e. N-H, (C=O)\(_{\text{HB}}\) and (N-C)\(_{\text{HB}}\), and the spectator chemical bonds (N-C)\(_{\text{s}}\) and (C=O,S)\(_{\text{s}}\). The data are reported in angstroms.

![Diagram](image)

| Compound \(\text{I}_1\) | \(\text{I}_2\) | \(\text{I}_3\) | \(\text{I}_4\) | \(\text{I}_5\) | \(\text{I}_6\) | \(\text{I}_7^*\) | \(\text{I}_8\) | \(\text{I}_9\) | \(\text{I}_{10}^*\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \(\text{(C=O)_{HB}}\) | 0.008           | 0.009           | 0.008           | 0.009           | 0.010           | 0.009           | 0.011           | 0.010           | 0.009           |
| \(\text{(N-C)_{HB}}\) | -0.011          | -0.012          | -0.011          | -0.012          | -0.012          | -0.008          | -0.013          | -0.013          | -0.009          |
| \(\text{N-H}\)    | 0.010           | 0.011           | 0.011           | 0.010           | 0.013           | 0.011           | 0.015           | 0.014           | 0.011           |
| \(\text{(N-C)_{s}}\) | 0.003           | 0.004           | 0.003           | 0.003           | 0.000           | 0.000           | 0.000           | 0.000           | 0.000           |
| \(\text{(C=O,S)_{s}}\) | -0.001          | -0.001          | -0.001          | -0.001          | 0.000           | 0.000           | 0.000           | 0.000           | 0.000           |

*Compounds with S.
2.10 XYZ coordinates and electronic energies

Compounds studied in chloroform

Figure S34. Structure of the compounds considered in this work. The oxygen atoms displayed in red are the most basic within the molecule and therefore, a proton is added to this atom to obtain the corresponding protonated species.
2.10.1 Compounds studied in CDCl₃

|                    | $E_e$            | $E_e + ZPV$         |
|--------------------|------------------|---------------------|
|                    | Hartree          |                    |
| A1                 | -286.613588      | -286.501756         |

XYZ coordinates

|  | X     | Y     | Z     |
|---|-------|-------|-------|
| C| -1.32088800 | -0.80804200 | 0.13764800 |
| C| 0.89035900  | -0.00002600 | -0.00773100 |
| C| -0.00870500 | 1.21439600  | 0.14718200  |
| C| -1.40379000 | 0.68867500  | -0.19928200 |
| H| 0.06160000  | 1.53332300  | 1.18958300  |
| H| 0.33803500  | 2.03122100  | -0.47994000 |
| H| -2.20300000 | 1.18636700  | 0.34303200  |
| H| -1.58648300 | 0.80660300  | -1.26667200 |
| H| 0.48498900  | -2.01724300 | -0.02466100 |
| N| 0.09127600  | -1.09058400 | -0.07646300 |
| O| 2.10882900  | -0.00692100 | -0.04464700 |
| H| -1.60234900 | -1.00175000 | 1.17536200  |
| H| -1.94421600 | -1.41908600 | -0.51119600 |
A1 (protonated)

|                | $E_e$           | $E_e + ZPV$          |
|----------------|----------------|----------------------|
|                | Hartree        |                      |
|                | -287.0332448   | -286.908137          |

XYZ coordinates

C   -1.36178500  -0.84342300  0.10484700
C   0.77592500   0.02179400  0.00196900
C   -0.08710400  1.22397400  0.13514300
C   -1.48182700  0.66113200 -0.17934500
H   0.01132800   1.57548200  1.16547100
H   0.24776800   2.01948100 -0.52558600
H   -2.26105600  1.12208100  0.41785300
H   -1.70986700  0.81759700 -1.23098600
H   0.50381000  -1.99811200 -0.05687600
N   0.08989600  -1.07206200 -0.02946500
O   2.06788500   0.11397000 -0.04454100
H   -1.65827800 -1.11148300  1.11713500
H   -1.89359500 -1.46571900 -0.60745800
H   2.51627900  -0.74751500 -0.09265900

A1 (deprotonated)

|                | $E_e$           | $E_e + ZPV$          |
|----------------|----------------|----------------------|
|                | Hartree        |                      |
|                | -286.091891    | -285.994036          |

XYZ coordinates

C   -1.28583600  -0.82130100  0.11541600
A1 homodimer

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -573.241549               | -573.016034 |

XYZ coordinates

| O  | 1.00376500 | 1.60281000 | -0.14655100 |
|----|------------|------------|-------------|
| N  | 1.71330700 | -0.57212500 | -0.04824700 |
| C  | 1.89132000 | 0.75659700 | -0.04088700 |
| C  | 2.93146300 | -1.32947700 | 0.20652900  |
| C  | 4.03243400 | -0.31219300 | -0.13065300 |
| C  | 3.36904100 | 1.03904300 | 0.14678200  |
| H  | 0.77896400 | -0.98549300 | -0.05474400 |
| H  | 2.97246200 | -2.21854600 | -0.41827800 |
| H  | 2.97726200 | -1.63934400 | 1.25296800  |
| H  | 4.28157900 | -0.38881300 | -1.18843600 |
H           4.93666300   -0.47991000   0.44809300
H           3.69184500   1.84740000  -0.50404000
H           3.50736500   1.36127000   1.18134700
O           -1.00398100   -1.60930300  -0.08425200
N           -1.70759900   0.56727000   0.01388600
C           -1.89314000  -0.75856200  -0.05770000
C           -2.93946900   1.34029000  -0.06785400
C           -4.01108000   0.30117100   0.29757500
C           -3.38324300  -1.02866100  -0.12701400
H           -0.77530600   0.97945200  -0.05402700
H           -2.91548000   2.18005700   0.62279100
H           -3.08160800   1.72789700  -1.07894100
H           -4.16677500   0.30692500   1.37563500
H           -4.96152300   0.50564800  -0.18747800
H           -3.65083100  -1.87848400   0.49535700
H           -3.61679500  -1.28136800  -1.16395300

A2

| Electronic energy (E_e) | E_e + ZPV     |
|-------------------------|---------------|
| Hartree                 |               |
| -322.531985             | -322.44332    |

XYZ coordinates

C           -1.34147900   0.73468200  -0.14961900
C           0.84874600  -0.00205000   0.01259500
C           -1.29150100  -0.76968100   0.11244600
H           0.42038300   1.98474500  -0.02959500
N           0.03299300   1.07820300   0.17885000

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### A2 (protonated)

|          | \( E_e \)       | \( E_e + ZPV \) |
|----------|-----------------|-----------------|
| \( E_e \) | -322.9364176    | -322.834595     |

### XYZ coordinates

|          | \( x \)         | \( y \)         | \( z \)         |
|----------|-----------------|-----------------|-----------------|
| C        | -1.40752600     | 0.76169600      | -0.05415000     |
| C        | 0.73348200      | -0.01780200     | -0.00043900     |
| C        | -1.37087400     | -0.77138200     | 0.05682700      |
| H        | 0.41556900      | 2.00360400      | 0.05122900      |
| N        | 0.02338200      | 1.07125000      | 0.04456100      |
| O        | 2.01743600      | -0.13320500     | -0.00046500     |
| H        | -1.88273800     | -1.27997800     | -0.75090800     |
| H        | -1.95179200     | 1.22344100      | 0.76277000      |
| H        | -1.79414100     | 1.10862800      | -1.00800600     |
| H        | -1.70515600     | -1.13775200     | 1.02143900      |
| O        | 0.05144000      | -1.11391700     | -0.05078500     |
| H        | 2.47308200      | 0.72520700      | 0.00811400      |
### A2 (deprotonated)

|                | $E_e$ (Hartree) | $E_e + ZPV$ (Hartree) |
|----------------|-----------------|-----------------------|
| Electronic energy | -322.01994      | -321.945403           |

#### XYZ coordinates

| Element | $x$ (Å) | $y$ (Å) | $z$ (Å) | $Z$ (Å) |
|---------|---------|---------|---------|---------|
| C       | 1.31296 | -0.75741 | 0.09653 | 0.00000 |
| C       | -0.82930 | -0.11247 | -0.00456 | 0.00000 |
| C       | 1.27158 | 0.75951 | -0.12153 | 0.00000 |
| N       | -0.06784 | -1.17768 | -0.08427 | 0.00000 |
| O       | -2.05899 | 0.00893 | -0.01534 | 0.00000 |
| H       | 1.91323 | 1.32469 | 0.55418 | 0.00000 |
| O       | -0.08508 | 1.09183 | 0.12441 | 0.00000 |
| H       | 1.67172 | -1.00078 | 1.10530 | 0.00000 |
| H       | 1.98704 | -1.24547 | -0.61041 | 0.00000 |
| H       | 1.52402 | 1.02149 | -1.15428 | 0.00000 |

### A2 homodimer

|                | $E_e$ (Hartree) | $E_e + ZPV$ (Hartree) |
|----------------|-----------------|-----------------------|
| Electronic energy | -645.078177     | -644.899207           |

#### XYZ coordinates

| Element | $x$ (Å) | $y$ (Å) | $z$ (Å) | $Z$ (Å) |
|---------|---------|---------|---------|---------|
| C       | -2.95896 | -1.29990 | 0.06281 | 0.00000 |
| C       | -1.86199 | 0.72380 | -0.10435 | 0.00000 |
| C       | -3.92783 | -0.13556 | 0.26882 | 0.00000 |
| H       | -4.19643 | -0.01543 | 1.31739 | 0.00000 |
| H       | -4.82209 | -0.19380 | -0.34228 | 0.00000 |
| H       | -0.78913 | -1.01691 | -0.01675 | 0.00000 |
A3

|                                  | $E_e$  | $E_e + ZPV$ |
|----------------------------------|--------|------------|
| **Electronic energy ($E_e$)**    |  -365.2280745 | -365.058037 |
| **(Hartree)**                    |        |            |
| **XYZ coordinates**              |        |            |
| C                                | -1.37783700 0.03330000 0.02834700 |
| C                                | -0.61799300 -1.14156700 0.60276500 |
| C                                |  0.58463400 -1.55759800 -0.25892200 |
| C                                |  1.84149600 -0.71977800 -0.03231300 |
| C                                |  0.63196500  1.48837800  0.41885400 |
A3 (protonated)

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -365.649532              | -365.465876 |

XYZ coordinates

C  1.26424100  -0.03231300  0.07659900
C  0.55333600  1.15641200  0.61218700
C  -0.64356100  1.55599800  -0.27195000
C  -1.88750000  0.70163900  -0.04900800
C  -0.67013800  -1.49987100  0.42699600
C  -1.72859200  -0.77649600  -0.39462200
H  0.20825200  0.92337500  1.62304900
### A3 (deprotonated)

|                | $E_e$    | $E_e + $ZPV |
|----------------|----------|-------------|
| **Electronic energy** ($E_e$) |          |             |
| **Hartree**    |          |             |
|                | -364.698904 | -364.542681 |

### XYZ coordinates

|    |       |       |       |
|----|-------|-------|-------|
| C  | 1.35488200 | -0.15332800 | 0.00837500 |
| C  | 0.62736900  | 1.04805500  | 0.63676800  |
| C  | -0.54067600 | 1.54997300  | -0.22177600 |
| C  | -1.81884100 | 0.72997100  | -0.05560600 |
| C  | -0.58627200 | -1.47549600 | 0.41380200  |
| C  | -1.67466000 | -0.75198800 | -0.39356500 |
| H  | 0.25577400  | 0.79860300  | 1.63590400  |
| H  | -0.23363600 | 1.55284300  | -1.27216100 |
### A3 homodimer

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 3.31693400   | 1.38223600   | -0.50704000  |
| C       | 3.96625300   | 1.10256800   | 0.85805300   |
| C       | 4.56625000   | -0.29606300  | 0.99249000   |
| C       | 2.83637400   | -1.48650800  | -0.47170200  |
| C       | 3.56612300   | -1.44339800  | 0.86875500   |
| H       | 3.93947600   | 0.96293900   | -1.30216800  |
| H       | 3.22942000   | 1.27209200   | 1.64781400   |
| H       | 5.33601100   | -0.41930100  | 0.22396500   |
| H       | 3.55377400   | -1.37151200  | -1.28884700  |
| H       | 3.23183000   | 2.45285100   | -0.67466000  |
| H       | 4.75982600   | 1.83526700   | 1.00851100   |
H  5.07364800  -0.37089700  1.95615500
H  2.36210700  -2.45751200  -0.59970000
H  4.09988700  -2.38775500  0.99225700
H  2.82286100  -1.38687700  1.66812200
N  1.76866600  -0.50435600  -0.60052200
O  0.94064300  1.58331100  -0.69231400
H  0.81013700  -0.85373100  -0.64251400
C  -1.91669100  -0.82628300  -0.61505600
C  -3.31684400  -1.38223200  -0.50716400
C  -3.96613800  -1.10271300  0.85797400
C  -4.56626200  0.29585800  0.99253000
C  -2.83654400  1.48655300  -0.47160900
C  -3.56622100  1.44327300  0.86887600
H  -3.93945900  -0.96295200  -1.30224400
H  -3.22925500  -1.27220200  1.64769400
H  -5.33604400  0.41909600  0.22402800
H  -3.55395500  1.37151900  -1.28873300
H  -3.23161600  -2.45282100  -0.67486700
H  -4.75963300  -1.83549800  1.00843000
H  -5.07364300  0.37057400  1.95621200
H  -2.36235400  2.45759400  -0.59958600
H  -4.10002600  2.38759000  0.99250400
H  -2.82292200  1.38670500  1.66820600
N  -1.76874000  0.50449000  -0.60054600
O  -0.94053000  -1.58310900  -0.69237200
H  -0.81025200  0.85395300  -0.64235800
A4

|                  | \( E_e \) | \( E_e + ZPV \) |
|------------------|-----------|-----------------|
|                  | Hartree   |                 |
|                  | -323.5031549 | -323.408836 |

XYZ coordinates

\[
\begin{array}{cccc}
C & 1.05070800 & -1.18165300 & 0.00021400 \\
C & 1.79522200 & -0.04954300 & 0.00017300 \\
C & 1.11009000 & 1.19584600 & -0.00006100 \\
C & -0.24681200 & 1.25714800 & -0.00017400 \\
C & -1.04968000 & 0.05742500 & -0.00002500 \\
N & -0.30610600 & -1.11468700 & 0.00009700 \\
H & 1.68403100 & 2.11363300 & -0.00010700 \\
H & 1.47245600 & -2.17567000 & 0.00035100 \\
H & 2.87157700 & -0.10442500 & 0.00032200 \\
H & -0.77879700 & 2.19693500 & -0.00035400 \\
H & -0.84406500 & -1.97157700 & 0.00011600 \\
O & -2.27745400 & 0.00857300 & -0.00022100 \\
\end{array}
\]

A4 (protonated)

|                  | \( E_e \) | \( E_e + ZPV \) |
|------------------|-----------|-----------------|
|                  | Hartree   |                 |
|                  | -323.9258062 | -323.818046 |

XYZ coordinates

\[
\begin{array}{cccc}
C & -1.06956900 & -1.20074300 & -0.00023600 \\
C & -1.83491100 & -0.07332700 & -0.00017700 \\
C & -1.19115000 & 1.17187700 & 0.00002900 \\
\end{array}
\]
### A4 (deprotonated)

|                  | Electronic energy ($E_e$) | $E_e$ + ZPV     |
|------------------|---------------------------|----------------|
|                  |                           | Hartree        |
|                  | -323.0016407              | -322.921145    |

#### XYZ coordinates

|     |                  |                  |                  |
|-----|------------------|------------------|------------------|
| C   | 0.99837500       | -1.18636800      | 0.00023400       |
| C   | 1.78042800       | -0.04349100      | 0.00016100       |
| C   | 1.09857600       | 1.18298000       | -0.00006600      |
| C   | -0.27087900      | 1.19854500       | -0.00018700      |
| C   | -1.03007200      | -0.02979500      | -0.00012200      |
| N   | -0.33356900      | -1.21523700      | 0.00011800       |
| H   | 1.65079600       | 2.11634600       | 0.00011800       |
| H   | 1.48587100       | -2.15919500      | 0.00041600       |
| H   | 2.85863700       | -0.10501700      | 0.00027700       |
| H   | -0.82431600      | 2.12855300       | -0.00034100      |
| O   | -2.28682300      | -0.02565700      | -0.00014700      |
**A4 homodimer**

|                | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------------|---------------------------|-------------|
|                |                           | Hartree     |
|                | -647.0263015              | -646.836244 |

**XYZ coordinates**

|     |                |                |                |
|-----|----------------|----------------|----------------|
| C   | -2.77370700    | -1.41105700    | -0.00021000    |
| C   | -1.86694100    | 0.82437400     | -0.00013000    |
| C   | -3.21768000    | 1.30616600     | 0.00028700     |
| C   | -4.26627700    | 0.43641400     | 0.00038500     |
| C   | -4.05688700    | -0.96384400    | 0.00020000     |
| H   | -0.76686900    | -0.91416400    | -0.00049300    |
| N   | -1.73469500    | -0.54380000    | -0.00033700    |
| C   | 2.77379500     | 1.41106900     | -0.00019900    |
| C   | 1.86689100     | -0.82425900    | -0.00010400    |
| C   | 3.21763200     | -1.30617400    | 0.00027800     |
| C   | 4.26627600     | -0.43652400    | 0.00042400     |
| C   | 4.05692700     | 0.96379600     | 0.00010900     |
| H   | 0.76691500     | 0.91428800     | -0.00015900    |
| N   | 1.73468400     | 0.54384200     | -0.00022300    |
| O   | 0.85289300     | -1.54903800    | -0.00025200    |
| H   | -4.87893800    | -1.66096200    | 0.00043600     |
| H   | -3.35966200    | 2.37649900     | 0.00052100     |
| H   | 3.35941000     | -2.37653500    | 0.00048800     |
| H   | -5.27769100    | 0.82167000     | 0.00060900     |
| H   | 2.50644400     | 2.45799800     | -0.00030500    |
| H   | 4.87902500     | 1.66086200     | 0.00009500     |
| H   | 5.27767600     | -0.82180700    | 0.00078400     |
| H   | -2.50634000    | -2.45798600    | -0.00040900    |
A5

| Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|---------------------------|-------------------------|
| Hartree                   |                         |
| -325.9236342              | -325.78234              |

XYZ coordinates

|   |      |      |      |      |
|---|------|------|------|------|
| C | 1.04235900 | -1.27720500 | 0.13433600 |
| C | -1.13153500 | -0.01409200 | -0.01818500 |
| C | -0.37156900 | 1.29250000 | -0.11167000 |
| C | 1.08790500 | 1.20052200 | 0.32042200 |
| C | 1.73554100 | -0.01128600 | -0.33700600 |
| H | 1.30754000 | -1.47582900 | 1.17641800 |
| H | 1.35808400 | -2.13528900 | -0.45756500 |
| H | -0.43446600 | 1.60033700 | -1.15917000 |
| H | -0.93078200 | 2.02598500 | 0.46630300 |
| H | 1.61216200 | 2.11769500 | 0.05417400 |
| H | 1.14745500 | 1.09766100 | 1.40704600 |
| H | 1.65041900 | 0.07221200 | -1.42336000 |
| H | 2.79488700 | -0.07833100 | -0.09119500 |
| H | -0.95868300 | -1.99704500 | 0.10586100 |
| N | -0.40877600 | -1.15498600 | 0.01528800 |
| O | -2.35767400 | -0.03564100 | -0.01411400 |
### A5 (protonated)

|                     | \(E_e\)   | \(E_e + ZPV\) |
|---------------------|-----------|---------------|
| **Electronic energy** |           |               |
| **Hartree**         |           |               |
| -326.3460087        | -326.191241|

**XYZ coordinates**

C   | 1.06418200 | -1.30050400 | 0.12405400
C   | -1.01285700| 0.01014300  | -0.00993900
C   | -0.29400900| 1.30874000  | -0.07382600
C   | 1.17605700 | 1.17988900  | 0.30766800
C   | 1.77138900 | -0.05134300 | -0.36231200
H   | 1.32485200 | -1.52994500 | 1.15685900
H   | 1.29555500 | -2.16482600 | -0.49281000
H   | -0.41054400| 1.66067800  | -1.10345700
H   | -0.83919300| 2.00936000  | 0.55814300
H   | 1.70320000 | 2.08184300  | 0.00656500
H   | 1.26767300 | 1.09172700  | 1.39150400
H   | 1.67058700 | 0.02931900  | -1.44642500
H   | 2.83058500 | -0.15049300 | -0.13384100
H   | -0.96021800| -1.97390100 | 0.13051200
N   | -0.40326300| -1.12601200 | 0.07356700
O    | -2.31602200| 0.09013700  | -0.05557900
H    | -2.76005300| -0.77432600 | -0.05126000
### A5 (deprotonated)

| XYZ coordinates | Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|-----------------|---------------------------|---------------------|
|                 | Hartree                   |                     |
|                 | -325.3954008             | -325.268562         |

### XYZ coordinates

- C: 0.99887200, -1.26832200, 0.14654300
- C: -1.10930700, -0.12791200, -0.00419100
- C: -0.39083300, 1.23395400, -0.05926100
- C: 1.09155700, 1.19769800, 0.29137900
- C: 1.70788300, -0.02224400, -0.37496500
- H: 1.31629400, -1.42361000, 1.18949100
- H: 1.36474700, -2.14401200, -0.39932700
- H: -0.52365700, 1.60857600, -1.07870400
- H: -0.94472900, 1.91315600, 0.58979200
- H: 1.58711200, 2.12275200, -0.01148600
- H: 1.21512900, 1.10756300, 1.37524200
- H: 1.57501100, 0.05010400, -1.45929000
- H: 2.78016700, -0.09294900, -0.17691700
- N: -0.45490700, -1.26154800, 0.06979900
- O: -2.37184400, -0.04872400, -0.06430400
### A5 homodimer

| XYZ coordinates | Electronic energy ($E_e$) | $E_e + ZPV$ |
|-----------------|----------------------------|-------------|
|                 | Hartree                    |             |
|                 | -651.8616575              | -651.577472 |

#### Electronic energy ($E_e$) and $E_e + ZPV$ (Hartree)

-651.8616575

#### XYZ coordinates

| Atom | X              | Y              | Z              |
|------|----------------|----------------|----------------|
| C    | -2.87015200    | -1.50642700    | -0.03056400    |
| C    | -1.91946500    | 0.80600300     | 0.00899100     |
| C    | -3.31183000    | 1.39664500     | -0.00806600    |
| C    | -4.40604600    | 0.40841700     | -0.39604700    |
| C    | -4.20229000    | -0.89465100    | 0.36523500     |
| H    | -3.48643000    | 1.77792900     | 1.00179900     |
| H    | -3.28136600    | 2.26222200     | -0.66788400    |
| H    | -5.38503000    | 0.83847200     | -0.18734600    |
| H    | -4.36223900    | 0.20914200     | -1.46980000    |
| H    | -4.21046900    | -0.69669400    | 1.43999000     |
| H    | -4.99666500    | -1.60928500    | 0.15273500     |
| H    | -0.83095800    | -0.87818700    | 0.03734600     |
| N    | -1.79069500    | -0.52539700    | 0.04147200     |
| O    | -0.93204600    | 1.55286100     | 0.02373500     |
| C    | 2.87014500     | 1.50643000     | -0.03056900    |
| C    | 1.91946400     | -0.80600500    | 0.00883800     |
| C    | 3.31183400     | -1.39664100    | -0.00809300    |
| C    | 4.40606000     | -0.40841300    | -0.39604700    |
| C    | 4.20228100     | 0.89465400     | 0.36523900     |
| H    | 3.48638900     | -1.77790400    | 1.00179100     |
| H    | 3.28140200     | -2.26223100    | -0.66789300    |
| H    | 5.38503700     | -0.83847000    | -0.18730700    |
A6

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------------------------|-------------|
| Hartree                    |             |
| -439.0350113               | -438.900058 |

XYZ coordinates

|        |        |        |        |
|--------|--------|--------|--------|
| H      | -1.44858600 | 2.47543300 | -0.00001200 |
| C      | -1.40431200 | 1.39415200 | -0.00001300 |
| C      | -2.57925800 | 0.63818600 | -0.00004900 |
| C      | -0.18830200 | 0.74231600 | 0.00002900  |
| H      | -3.53825300 | 1.13698100 | -0.00008700 |
| C      | -0.15096100 | -0.65500600 | 0.00000600  |
| C      | 1.22496700  | 1.25194100 | 0.00005600  |
| C      | -2.52243100 | -0.74988900 | -0.00007200 |
| C      | -1.30088600 | -1.42247300 | -0.00006200 |
| C      | 2.05915600  | -0.02437900 | 0.00017800  |
| H      | 1.47653300  | 1.84314200 | 0.88134300  |
A6 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$  |
|---------------------------|--------------|
| Hartree                   |              |
| -439.4427198             | -439.294569  |

XYZ coordinates

|   |   |   |   |
|---|---|---|---|
| H | -3.43963200 | -1.32312200 | -0.00007200 |
| H | -1.25500500 | -2.50268900 | -0.00009700 |
| H | 1.48684600  | -2.03961100 | -0.00011900 |
| N | 1.18171200  | -1.07796100 | 0.00001000  |
| O | 3.26771000  | -0.11707100 | -0.00002500 |
| H | 1.47659200  | 1.84307200  | -0.88126200 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | 3.23459000| -0.01777200| -0.00016700|
| H       | 1.43024400| 1.84809000 | -0.88185500|
| H       | 3.62104100| -0.91093800 | -0.00037400|

### A6 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
|                           |             |
|                           |             |
|                           | -438.5312682| -438.409747 |
|                           |             |             |

### XYZ coordinates

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -1.42157200| 2.47032000| 0.00001900|
| C       | -1.37757600| 1.38727200| -0.00002000|
| C       | -2.56203700| 0.63687200| -0.00003600|
| C       | -0.16459700| 0.73479400| 0.00000700 |
| H       | -3.52146800| 1.13601800| -0.00004300|
| C       | -0.09055000| -0.67855300| -0.00001900|
| C       | 1.25249400 | 1.21505700| 0.00004500 |
| C       | -2.49524900| -0.75187500| -0.00006200|
| C       | -1.27221600| -1.42197900| -0.00005300|
| C       | 2.03464800 | -0.11666700| 0.00003900 |
| H       | 1.51978000 | 1.80079700 | 0.88106200 |
| H       | -3.41292700| -1.32731100| -0.00008900|
| H       | -1.23263400| -2.50372500| -0.00007100|
| N       | 1.20115400 | -1.17261500| -0.00002000|
| O       | 3.27392700 | -0.14976800| 0.00007000 |
| H       | 1.51981800 | 1.80082300 | -0.88094300|
### A6 homodimer

|                  | $E_e$ | $E_e + ZPV$ |
|------------------|-------|-------------|
| **Electronic energy** |       |             |
| Hartree          |       |             |
| $-878.0847035$   | $-877.813883$ |

### XYZ coordinates

| Atom | X        | Y        | Z        | Error  |
|------|----------|----------|----------|--------|
| H    | 5.83551600 | -1.78767800 | 0.00066400 |
| C    | 5.26630200 | -0.86731700 | 0.00048400 |
| C    | 5.91875900 | 0.36728700  | 0.00055200 |
| C    | 3.88660300 | -0.89291200 | 0.00016600 |
| C    | 3.17104600 | 0.30761800  | -0.00006700 |
| C    | 2.89809600 | -2.02446200 | -0.00005000 |
| C    | 5.19003300 | 1.55072100  | 0.00031700  |
| C    | 3.79586900 | 1.54004600  | 0.00000300  |
| C    | 1.55721800 | -1.30525200 | -0.00037900 |
| H    | 2.96248300 | -2.66394400 | 0.88104700  |
| H    | 5.71051300 | 2.49872000  | 0.00037900  |
| H    | 3.22433900 | 2.45782500  | -0.00017600 |
| H    | 1.05085900 | 0.72977000  | -0.00059900 |
| N    | 1.79812300 | 0.03023500  | -0.00036100 |
| O    | 0.44994800 | -1.82694600 | -0.00065000 |
| H    | 2.96291300 | -2.66406500 | -0.88093800 |
| H    | -5.83550000 | 1.78770400  | 0.00040400  |
| C    | -5.26629600 | 0.86733700  | 0.00030200  |
| C    | -5.91876600 | -0.36726000 | 0.00035500  |
| C    | -3.88659700 | 0.89291700  | 0.00010100  |
| C    | -3.17105300 | -0.30762000 | -0.00002800 |
| C    | -2.89807900 | 2.02445800  | -0.00005800 |
| C    | -5.19005300 | -1.55070200 | 0.00014000  |
### A7

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -478.3427623              | -478.17983  |

#### XYZ coordinates

|     | X          | Y          | Z          |
|-----|------------|------------|------------|
| H   | 1.23416700 | 2.42761600 | -0.46474300|
| C   | 1.36721000 | 1.36979700 | -0.27678600|
| C   | 2.64635700 | 0.83966100 | -0.09043800|
| C   | 0.27753700 | 0.52540000 | -0.21912900|
| C   | 0.46744600 | -0.83644800| 0.02844700 |
| C   | -1.19726800| 0.78985500 | -0.37006300|
| C   | 2.81569800 | -0.51810300| 0.15008600 |
| C   | 1.72317300 | -1.38295400| 0.21483600 |
| C   | -1.80797500| -0.59662900| -0.15351200|
| H   | -1.43966700| 1.08818000 | -1.39325100|
H  3.81127600 -0.91619600  0.29179600
H  1.85479400 -2.43899200  0.40584000
H  -0.92454600 -2.45531500  0.23939600
N  -0.77744900 -1.47509500  0.05191400
O  -2.98686200 -0.88031300  -0.15057700
H  3.50910000  1.48950400  -0.13288100
C  -1.78077400  1.80777200  0.60766300
H  -1.35120400  2.79261100  -0.42912000
H  -2.86070200  1.87043200  0.48253600
H  -1.56459400  1.52023500  1.63678400

**A7 (protonated)**

|                | $E_e$ | $E_e + ZPV$ |
|----------------|------|-------------|
| **Electronic energy ($E_e$)** |      |             |
| **Hartree**     |      |             |
|                | -478.7508526 | -478.57474  |

**XYZ coordinates**

H  -3.23970800 -1.67494200  -0.02540800
H  1.33682400  2.42116700  -0.47415700
C  1.44056800  1.36191400  -0.28217500
C  2.69886600  0.78980000  -0.09891500
C  0.33349300  0.53923100  -0.21580700
C  0.50671000 -0.81586300  0.03451200
C  -1.13836200  0.82819200  -0.36107800
C  2.84214700 -0.57232000  0.14665900
C  1.73354700 -1.41251000  0.22083400
C  -1.71296100 -0.53708900  -0.14999800
H  -1.38788000  1.12336500  -1.38541300
A7 (deprotonated)

| XYZ coordinates |
|------------------|
| H                |
| C                |
| C                |
| C                |
| C                |
| C                |
| C                |
| C                |
| C                |
| H                |
| H                |

Electronic energy ($E_e$)  | $E_e + ZPV$  |
---------------------------|--------------|
Hartree                    |              |
-477.8387278               | -477.689254  |
A7 homodimer

|                | \( E_e \) | \( E_e + ZPV \) |
|----------------|-----------|------------------|
|                | Hartree   |                  |
|                | -956.7002347 | -956.372892      |

XYZ coordinates

|    |     |     |     |
|----|-----|-----|-----|
| H  | 5.96666700 | 1.29439400 | -0.15584100 |
| C  | 5.32792600 | 0.42034200 | -0.15139300 |
| C  | 5.88287800 | -0.86161400 | -0.14691400 |
| C  | 3.95478700 | 0.55298900 | -0.15148600 |
| C  | 3.14627900 | -0.58634000 | -0.13952500 |
| C  | 3.06878800 | 1.77005800 | -0.14793900 |
| C  | 5.06251900 | -1.98357100 | -0.14077000 |
| C  | 3.67311100 | -1.86399700 | -0.13607700 |
| C  | 1.67324100 | 1.15294500 | -0.11789400 |
| H  | 3.15313400 | 2.32265300 | -1.08727700 |
| H  | 5.50605300 | -2.96991600 | -0.13724200 |
| H  | 3.03232900 | -2.73496500 | -0.12764100 |
| H  | 0.99597300 | -0.82950400 | -0.10082000 |
N  1.80004900 -0.19782500 -0.12681400
O  0.61610500  1.76883900 -0.08203600
H -5.96666400 -1.29441100 -0.15564400
C -5.32792800 -0.42035600 -0.15122800
C -5.88288600  0.86159800 -0.14678000
C -3.95478800 -0.55299600 -0.15133600
C -3.14628500  0.58633800 -0.13942300
C -3.06878400 -1.77006200 -0.14776900
C -5.06253300  1.98355900 -0.14068200
C -3.67312400  1.86399200 -0.13600700
C -1.67324000 -1.15294200 -0.11776300
H -3.15314600 -2.32268700 -1.08708700
H -5.50607200  2.96990100 -0.13717700
H -3.03234600  2.73496300 -0.12760900
H -0.99597600  0.82950700 -0.10072500
N -1.80005300  0.19782800 -0.12673600
O -0.61609800 -1.76882700 -0.08188900
H -6.95695300  0.98292000 -0.14806100
H  6.95694400 -0.98294200 -0.14820700
C -3.27848100 -2.72662900  1.02474100
H -4.27087200 -3.17208400  0.97346200
H -2.53689700 -3.52358800  0.99426000
H -3.18546300 -2.19791400  1.97351300
C  3.27850800  2.72666100  1.02453600
H  4.27089900  3.17211400  0.97322600
H  2.53692400  3.52362100  0.99404100
H  3.18550500  2.19797700  1.97332700
|   | Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|---|--------------------------|---------------------|
|   | Hartree                  |                     |
|   | -478.5844151             | -478.406679         |

XYZ coordinates

C     0.99896900  1.23963300  -0.12011000
C     0.99803900  -1.24009500 -0.12045900
C     -0.46359800 -1.23662900 -0.48304300
C     -1.21852500  0.00034200  0.01359400
C     -0.46304400  1.23758300 -0.48151300
H     -0.51027700 -1.28433200 -1.57583400
H     -0.89625100 -2.15777800 -0.09494200
H     2.58986100  -0.00081900  0.23392200
N     1.60559300  -0.00049500 -0.00892500
O     1.64615800 -2.24805300  0.05034800
O     1.64807300  2.24702000  0.05017500
H     -0.89470600  2.15834600 -0.09135900
H     -0.51049700  1.28747800 -1.57416100
C     -2.62945900  0.00092400 -0.56775900
H     -3.18009800 -0.88244100 -0.24016700
H     -3.17993400  0.88392600  0.23890600
H     -2.60418800  0.00169800 -1.65873300
C     -1.29552700 -0.00049100  1.54281200
H     -1.83080000  0.88236300  1.89522300
H     -1.83003700 -0.88410400  1.89439600
H     -0.30720600 -0.00020700  2.00772800
**I1 (protonated)**

| Electronic energy \( (E_e) \) | \( E_e + \text{ZPV} \) |
|-------------------------------|-------------------------|
| Hartree                       |                         |
| -478.9830873                 | -478.792182             |

**XYZ coordinates**

C  -1.11930000  -1.00201800  -0.09826000
C  -0.74584600  1.41077000  -0.14980000
C   0.66404500  1.15512500  -0.57444300
C   1.24117200  -0.13773900   0.01720900
C   0.30712900  -1.29375600  -0.36459900
H   0.64880600   1.09298500  -1.66807900
H   1.25290000   2.02704600  -0.29630200
H  -2.54643600   0.40599300   0.20834600
N  -1.56600400   0.22489600  -0.00548500
O  -1.27472200   2.45834400   0.05364200
O  -1.90623300  -2.01664300   0.02531000
H   0.55822900  -2.21862000   0.15607300
H   0.36481200  -1.50548900  -1.43935200
C   2.61790000  -0.39847800  -0.58486800
H   3.30038100   0.41035100  -0.32385100
H   3.03125200  -1.33039300  -0.19732200
H   2.56623500  -0.46894500  -1.67203800
C   1.35280000  -0.02490400   1.53934200
H   1.79075600  -0.93318000  -1.95334200
H   1.99554300   0.81462900   1.80419200
H   0.38505200   0.13067600   2.02307600
H  -2.84499200  -1.78692900   0.15120700
**I1 (deprotonated)**

|                | Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|----------------|---------------------------|---------------------|
|                | Hartree                   |                     |
|                | -478.079397972           | -477.915378         |

**XYZ coordinates**

|    |          |          |          |
|----|----------|----------|----------|
| C  | -1.06669600 | -1.17470000 | -0.09559200 |
| C  | -1.06627500 | 1.17495200  | -0.09576600 |
| C  | 0.41566400  | 1.21932800  | -0.46574900 |
| C  | 1.20173300  | -0.00017200 | 0.00490300  |
| C  | 0.41535900  | -1.21972600 | -0.46508200 |
| H  | 0.46679500  | 1.28630400  | -1.55784000 |
| H  | 0.83012800  | 2.14517300  | -0.06501800 |
| N  | -1.71509500 | 0.00025000  | 0.06168200  |
| O  | -1.64976800 | 2.25774600  | 0.02883300  |
| O  | -1.65066000 | -2.25727200 | 0.02885800  |
| H  | 0.82941600  | -2.14543500 | -0.06361600 |
| H  | 0.46674100  | -1.28753100 | -1.55711300 |
| C  | 2.60159000  | -0.00048000 | -0.60369800 |
| H  | 3.16282600  | 0.88314400  | -0.29044200 |
| H  | 3.16260100  | -0.88413300 | -0.29012200 |
| H  | 2.55351800  | -0.00066500 | -1.69454500 |
| C  | 1.31444200  | 0.00023000  | 1.53192600  |
| H  | 1.85536700  | -0.88347500 | 1.87708500  |
| H  | 1.85547000  | 0.88405400  | 1.87662000  |
| H  | 0.33131600  | 0.00041800  | 2.00564500  |
**I1 homodimer**

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|--------------------------|-------------|
| Hartree                  |             |
| -957.1793819             | -956.822554 |

XYZ coordinates

|        |          |          |          |          |
|--------|----------|----------|----------|----------|
| C      | 2.85405400 | -1.56820100 | -0.27129100 |
| C      | 1.97300600 | 0.72829200  | -0.41707600 |
| C      | 3.37473600 | 1.27412500  | -0.43281100 |
| C      | 4.38691300 | 0.38216800  | 0.29181600  |
| C      | 4.26031300 | -1.02858000 | -0.29038400 |
| H      | 3.65423900 | 1.37186600  | -1.48709100 |
| H      | 3.33941800 | 2.27631500  | -0.00799100 |
| H      | 4.57427400 | -1.02498600 | -1.33939700 |
| H      | 4.89054400 | -1.74244700 | 0.23832200  |
| H      | 0.87227600 | -0.99690300 | -0.38592000 |
| N      | 1.83075100 | -0.63766400 | -0.37763900 |
| O      | 0.98821800 | 1.44513400  | -0.45922200 |
| O      | 2.59005000 | -2.74634300 | -0.19449800 |
| C      | -2.85404800| 1.56818700  | -0.27141200 |
| C      | -1.97299700| -0.72831300 | -0.41706600 |
| C      | -3.37472700| -1.27414700 | -0.43279700 |
| C      | -4.38691900| -0.38215300 | 0.29176300  |
| C      | -4.26030600| 1.02856600  | -0.29050500 |
| H      | -3.65421000| -1.37194500 | -1.48707700 |
| H      | -3.33941600| -2.27631500 | -0.00792300 |
| H      | -4.57424500| 1.02491600  | -1.33952500 |
| H      | -4.89054900| 1.74246000  | 0.23815000  |
| H      | -0.87226800| 0.99688300  | -0.38598000 |
I2

| XYZ coordinates |
|-----------------|
| O               |
| N               |

Electronic energy ($E_e$) $E_e + ZPV$

| Hartree     |         |
|-------------|---------|
| -517.8863724| -517.680422 |

XYZ coordinates

| O   | N   |
|-----|-----|
| 0.81405700 | 2.07512500 |
| 2.27557000 | 0.36606400 |
| -0.65797000| -0.56758300 |
I2 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
|                           | Hartree    |
|                           | -518.2826477 | -518.064321 |

XYZ coordinates

O    0.76070200  2.25757600 -0.55139800
N    2.04518700  0.34571000 -0.55434900
C    0.95972800  1.01907900 -0.28163300
C    1.94270500 -1.02680600 -0.11332000
C    0.57243100 -1.17962700  0.48815000
C   -0.08843100  0.21273600  0.41925600
H    2.87705600  0.71321600 -1.01219500
H    0.67622400 -1.55490100  1.50510300
H    0.03238600 -1.92909900 -0.09084200
O    2.83115700 -1.79863500 -0.25580500
C   -1.37279000  0.23436200 -0.43655500
H   -1.66781800  1.27287400 -0.60062100
H   -1.14292900 -0.19867700 -1.41456700
C   -2.53027500 -0.53151000  0.19747400
H   -2.19970500 -1.53223000  0.48639800
H   -2.84830300 -0.02606000  1.11014900
C   -3.70925500 -0.63763300 -0.76306400
H   -4.54753800 -1.15374200 -0.29677600
H   -4.05305200  0.35127600 -1.06971800
H   -3.43328600 -1.18962400 -1.66259700
C   -0.30304400  0.83171400  1.80954900
H   -0.76457100  1.81471400  1.72703100
H   -0.95692900  0.18256400  2.38718800

S86
I2 (deprotonated)

|                  | $E_e$     | $E_e + ZPV$ |
|------------------|----------|------------|
| **Electronic energy (E_e)** |          |            |
| **Hartree**      |          |            |
|                  | -517.390075609 | -517.196955 |

**XYZ coordinates**

|      | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | 0.78907700 | 2.26127800 | -0.68977100 |
| N    | 2.14809400 | 0.40661100 | -0.64047200 |
| C    | 1.00678000 | 1.09094700 | -0.38134200 |
| C    | 2.02815100 | -0.85162600 | -0.15376400 |
| C    | 0.65994200 | -1.09839900 | 0.48419500  |
| C    | -0.04296200 | 0.25355000 | 0.38495200  |
| H    | 0.79453000 | -1.45424400 | 1.50622700  |
| H    | 0.15390300 | -1.88888300 | -0.07306000 |
| O    | 2.89281700 | -1.72579700 | -0.20396000 |
| C    | -1.33808200 | 0.20919500 | -0.43529600 |
| H    | -1.64378100 | 1.23597800 | -0.65327500 |
| H    | -1.11868400 | -0.26265300 | -1.39920600 |
| C    | -2.49291700 | -0.53415900 | 0.23144100  |
| H    | -2.15659500 | -1.52273100 | 0.55700700  |
| H    | -2.80242500 | 0.00128600 | 1.13119300  |
| C    | -3.69044900 | -0.68373700 | -0.70121400 |
| H    | -4.52190800 | -1.19079800 | -0.21003000 |
| H    | -4.04526000 | 0.29239200 | -1.03749400 |
| H    | -3.42390800 | -1.26075200 | -1.58858400 |

S87
I2 homodimer

|                   | \( E_e \)       | \( E_e + ZPV \) |
|-------------------|-----------------|-----------------|
|                   | Hartree         |                 |
|                   | -1035.784487    | -1035.371707    |

XYZ coordinates

|   |   |   |   |
|---|---|---|---|
| O | 1.44298600 | 1.10682400 | -0.27626700 |
| N | 1.45858200 | -1.18118500 | -0.29209900 |
| C | 2.04839800 | 0.05390100 | -0.30483900 |
| C | 2.36690400 | -2.22515000 | -0.31981200 |
| C | 3.75730200 | -1.62946500 | -0.30839600 |
| C | 3.56230900 | -0.10472500 | -0.38479100 |
| H | 0.44287700 | -1.30375700 | -0.27445500 |
| H | 4.32571700 | -2.03865800 | -1.14234200 |
| H | 4.24662400 | -1.94525100 | 0.61382200  |
| O | -1.44334200 | -1.10744300 | -0.27585600 |
| N | -1.45843400 | 1.18057400 | -0.29216700 |
| C | -2.04850500 | -0.05439400 | -0.30484700 |
| C | -2.36652500 | 2.22471300 | -0.32059800 |
| C | -3.75706500 | 1.62934200 | -0.30971200 |
| C | -3.56237500 | 0.10451700 | -0.38513200 |
| H | -0.44267700 | 1.30293700 | -0.27431900 |
| H | -4.24698700 | 1.94580300 | 0.61195300  |
Electronic energy \((E_e)\) \(E_e + ZPV\)

|       |                |                |                |
|-------|----------------|----------------|----------------|
|       | 5.07057500     | 0.28594100     | -1.88881800    |
|       | 3.46677100     | -0.01892800    | -2.55421300    |

I3

XYZ coordinates

|       |                |                |                |
|-------|----------------|----------------|----------------|
| H     | -0.68300200    | 1.83910200     | -0.00003400    |
| C     | -0.35898100    | 0.80683100     | -0.00004400    |
| C     | -1.28745100    | -0.24738300    | -0.00005700    |
| C     | 0.98174500     | 0.50252900     | -0.00001600    |
| C     | 1.43877600     | -0.80832300    | 0.00005200     |
| C     | 2.16916200     | 1.40790900     | -0.00006000    |
| C     | -0.80950400    | -1.56118800    | 0.00002200     |
| C     | 0.55431300     | -1.86260200    | 0.00005900     |
| H     | -1.51013200    | -2.38242900    | 0.00007300     |
| H     | 0.89932800     | -2.88748200    | 0.00011700     |
| O     | 3.70405300     | -1.70452700    | -0.00001900    |
| O     | 2.20464200     | 2.61116000     | 0.00015500     |
| C     | 2.92860200     | -0.78373500    | 0.00009700     |
| N     | 3.27458900     | 0.56483900     | -0.00019300    |
| H     | 4.22874100     | 0.89616500     | -0.00043800    |
| C     | -2.78039000    | 0.08230400     | -0.00001800    |
| C     | -3.11281700    | 0.90861400     | -1.25226800    |
| H     | -4.17659600    | 1.15202100     | -1.26099700    |
I3 (protonated)

| Electronic energy ($E_e$) | $E_e$ + ZPV          |
|---------------------------|----------------------|
| Hartree                   |                      |
| -670.6910814              | -670.448315          |

XYZ coordinates

|        | 0.75902400 | 1.85580300 | 0.00027100 |
|--------|------------|------------|------------|
| H      | 0.41515700 | 0.83085700 | 0.00011700 |
| C      | 1.32512000 | -0.24750400| -0.00008400|
| C      | -0.92409800| 0.55042900 | 0.00009300 |
| C      | -1.40329900| -0.76058500| -0.00010500|
| C      | -2.09066400| 1.46654100 | 0.00022700 |
| C      | 0.82571500 | -1.55251100| -0.00029200|
| C      | -0.54179000| -1.83587800| -0.00030300|
| H      | 1.51304000 | -2.38450200| -0.00044500|
| H      | -0.90061800| -2.85523400| -0.00045500|
| O      | -3.62183100| -1.70714600| -0.00014600|
O       -2.18322800  2.64859000  0.00052300
C       -2.85290800 -0.67923300 -0.00002400
N       -3.24076200  0.58245600  0.00024600
H       -4.19829700  0.91956500  0.00040500
C       2.81854200  0.06012800 -0.00007300
C       3.15532700  0.88446200  1.25349300
H       4.22253600  1.10895100  1.26147700
H       2.61445700  1.83061600  1.27216900
H       2.91518900  0.33184800  2.16269200
C       3.15526400  0.88484600 -1.25340500
H       4.22247100  1.10934400 -1.26136900
H       2.91508900  0.33250600 -2.16276100
H       2.61438700  1.83100200 -1.27176800
C       3.67112500 -1.20795500 -0.00029000
H       3.48756900 -1.81637600 -0.88622500
H       3.48753100 -1.81609800 -0.88698700
H       4.72438700 -0.92839200 -0.00026900
H      -4.57190100 -1.48935000  0.00004200

**I3 (deprotonated)**

|                  | Electronic energy ($E_e$) | $E_e + ZPV$ |
|------------------|---------------------------|-------------|
|                  | Hartree                   |             |
|                  | -669.8039591              | -669.586987 |

**XYZ coordinates**

H      0.65337800  1.83759800  0.00009100
C      0.32433300  0.80602000  0.00007200
C      1.25263800 -0.25094200 -0.00007000
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -1.01814800 | 0.50924700 | 0.00000000 |
| C       | -1.48057600 | -0.79341300 | -0.00006800 |
| C       | -2.25193100 | 1.38822600 | -0.00032300 |
| C       | 0.76994100 | -1.56120300 | -0.00027300 |
| C       | -0.60057600 | -1.85119000 | -0.00028000 |
| H       | 1.46634100 | -2.38682700 | -0.00037800 |
| H       | -0.94872300 | -2.87618900 | -0.00030800 |
| O       | -3.73130300 | -1.67597000 | -0.00033000 |
| O       | -2.20637500 | 2.61363700 | 0.00084200 |
| C       | -2.99144100 | -0.69847900 | 0.00039800 |
| N       | -3.36989700 | 0.61196000 | 0.00025400 |
| C       | 2.74822900 | 0.07576500 | -0.00066000 |
| C       | 3.08767700 | 0.90098200 | 1.25103300 |
| H       | 4.15163000 | 1.14682100 | 1.25898500 |
| H       | 2.52663200 | 1.83510200 | 1.27850100 |
| H       | 2.85847500 | 0.34198200 | 2.15964100 |
| C       | 3.08759000 | 0.90142000 | -1.25089900 |
| H       | 4.15154100 | 1.14726500 | -1.25883900 |
| H       | 2.85832800 | 0.34273900 | -2.15968800 |
| H       | 2.52654100 | 1.83554900 | -1.27800200 |
| C       | 3.62032400 | -1.18081400 | -0.00031500 |
| H       | 3.44307000 | -1.79347800 | 0.88484700 |
| H       | 3.44301000 | -1.79316600 | -0.88568000 |
| H       | 4.67211200 | -0.89081600 | -0.00030000 |
I3 homodimer

|                     | \( E_e \) | \( E_e + ZPV \) |
|---------------------|-----------|-----------------|
| **Electronic energy** (Hartree) |           |                 |
| -1340.606438        | -1340.145607 |

**XYZ coordinates**

|  | C                  | 3.64612700 | -1.73908200 | 0.05810200 |
|---|--------------------|------------|-------------|------------|
|  | C                  | 2.28277900 | -2.34167300 | 0.07385900 |
|  | C                  | 3.50780200 | -0.35884100 | 0.01063900 |
|  | C                  | 2.05035700 | -0.04784300 | -0.00069700 |
|  | H                  | 0.38207500 | -1.34750100 | 0.02450600 |
|  | N                  | 1.39833300 | -1.26279100 | 0.03769400 |
|  | O                  | 1.51740700 | 1.04010800  | -0.03569700 |
|  | C                  | -3.64648800| 1.73934400  | 0.05816800 |
|  | C                  | -2.28330600| 2.34229900  | 0.07397400 |
|  | C                  | -3.50779400| 0.35913300  | 0.01082600 |
|  | C                  | -2.05027400| 0.04850800  | -0.00019300 |
|  | H                  | -0.38237700| 1.34867600  | 0.02480600 |
|  | N                  | -1.39857400| 1.26362700  | 0.03815400 |
|  | O                  | -1.51703000| -1.03931100 | -0.03492900 |
|  | O                  | -1.96768500| 3.50253500  | 0.10851600 |
|  | C                  | -4.89317100| 2.32087000  | 0.07800400 |
|  | C                  | -6.00192100| 1.47172300  | 0.04576200 |
|  | H                  | -6.98389600| 1.91987000  | 0.06142600 |
|  | C                  | -5.88084600| 0.07995400  | -0.00697900 |
|  | C                  | -4.59375100| -0.48338500 | -0.02157000 |
|  | H                  | -5.01491100| 3.39466800  | 0.11613000 |
|  | H                  | -4.44889500| -1.55483700 | -0.05865400 |
|  | O                  | 1.96687400 | -3.50184600 | 0.10858300 |
I4

|          |       |       |       |
|----------|-------|-------|-------|
| C        | 7.04775600 | 1.80317700 | 1.14627500 |
| H        | 7.91238000 | 2.46842600 | 1.12171500 |
| H        | 6.15012100 | 2.42142300 | 1.13757700 |
| H        | 7.07020200 | 1.24811300 | 2.08538100 |

Electronic energy \((E_e)\)  \(E_e + ZPV\) Hartree

|          |       |       |
|----------|-------|-------|
|          | -359.4207477 | -359.352346 |

XYZ coordinates

|          |       |       |       |
|----------|-------|-------|-------|
| C        | 1.14192100 | -0.15770600 | 0.00007500 |
| C        | -1.14191300 | -0.15809800 | -0.00006000 |
| C        | 0.66330800 | 1.26467300 | 0.00013900 |
| H        | 0.00014800 | -1.95119500 | -0.00011400 |
| N        | 0.00002400 | -0.94218600 | -0.00003400 |
| O        | -2.27636900 | -0.55777800 | -0.00025500 |
| H        | 1.34901900 | 2.09661000 | 0.00027100 |
| C        | -0.66315500 | 1.26450700 | -0.00005700 |
| H        | -1.34918700 | 2.09621700 | -0.00013700 |
| O        | 2.27622900 | -0.55804500 | 0.00021000 |
**I4 (protonated)**

|                      | \( E_e \)       | \( E_e + \text{ZPV} \) |
|----------------------|-----------------|--------------------------|
| **Electronic energy**|                 |                          |
| **Hartree**          |                 |                          |
| -359.8087917         | -359.727835     |

**XYZ coordinates**

|     |       |       |       |
|-----|-------|-------|-------|
| C   | 1.02385300 | -0.13163400 | 0.00011200 |
| C   | -1.21182300 | -0.14869800 | -0.00028200 |
| C   | 0.58762400  | 1.27836000  | 0.00007300  |
| H   | 0.02517100  | -1.95383500 | 0.00009800  |
| N   | -0.00746900 | -0.93925500 | 0.00006200  |
| O   | -2.30386100 | -0.60287700 | -0.00024500 |
| H   | 1.27911000  | 2.10635100  | 0.00010700  |
| C   | -0.74056700 | 1.27555800  | 0.00010800  |
| H   | -1.42653500 | 2.10730100  | 0.00021200  |
| O   | 2.22033600  | -0.57938800 | 0.00011700  |
| H   | 2.88821400  | 0.13156900  | 0.00010000  |

**I4 (deprotonated)**

|                      | \( E_e \)       | \( E_e + \text{ZPV} \) |
|----------------------|-----------------|--------------------------|
| **Electronic energy**|                 |                          |
| **Hartree**          |                 |                          |
| -358.92754           | -358.871828     |

**XYZ coordinates**

|     |       |       |       |
|-----|-------|-------|-------|
| C   | 1.09033500 | -0.22361300 | 0.00063800 |
| C   | -1.09037500 | -0.22393400 | -0.00012300 |
| C   | 0.66132300  | 1.23829100  | -0.00015000 |
| N   | -0.00006000 | -1.03406900 | -0.00011800 |
O          -2.26803100  -0.56633500  -0.00001600
H           1.35851600   2.06295900  -0.00049300
C          -0.66111500   1.23849100  0.00010300
H          -1.35826800   2.06322500  0.00013500
O           2.26792600  -0.56655400  -0.00018800

**I4 homodimer**

|                        | $E_e$          | $E_e + ZPV$ |
|------------------------|---------------|-------------|
| **Electronic energy**  | **Hartree**   |             |
|                        | -718.8519154  | -718.71311  |

**XYZ coordinates**

|         |            |             |             |             |
|---------|------------|-------------|-------------|
| C       | 3.17895700 | -0.75466000 | -0.00014200 |
| C       | 1.77223400 | 1.02865000  | -0.00008900 |
| C       | 4.00219700 | 0.50154300  | 0.00044200  |
| H       | 1.04064800 | -0.95916200 | -0.00051800 |
| N       | 1.85239200 | -0.34384500 | -0.00064100 |
| O       | 0.75399800 | 1.68369400  | -0.00006600 |
| C       | -3.17898600| 0.75464300  | -0.00006200 |
| C       | -1.77221100| -1.02862600 | -0.00006400 |
| C       | -4.00219000| -0.50158300 | 0.00052200  |
| H       | -1.04068700| 0.95921000  | -0.00044200 |
| N       | -1.85240800| 0.34386700  | -0.00061000 |
| O       | -0.75395700| -1.68364200 | -0.00004300 |
| H       | 5.07992200 | 0.47833500  | 0.00074700  |
| H       | -5.07991500| -0.47840600 | 0.00084600  |
| C       | -3.18026600| -1.54229100 | 0.00050600  |
| C       | 3.18030300 | 1.54227500  | 0.00045900  |

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H  -3.40432200  -2.59681200  0.00081200
H  3.40438900  2.59679000  0.00077900
O  3.56708900  -1.89182400  -0.00019100
O  -3.56714800  1.89179400  -0.00006300

**I5**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -650.6657051              | -650.402994 |

**XYZ coordinates**

|   |        |        |        |        |
|---|--------|--------|--------|--------|
| O | 4.40654100 | -0.48560700 | 0.05197100 |
| N | 0.40004100 | 0.09087900  | -0.02967900 |
| N | 2.59882400 | 0.86456300  | 0.04529500  |
| C | 1.23531700 | 1.14834100  | -0.13963100 |
| C | 3.20095500 | -0.37055400 | 0.01197000  |
| C | 0.90122700 | -1.16669900 | 0.51970600  |
| C | 2.23946600 | -1.52057800 | -0.10238400 |
| H | 0.17658800 | -1.94737300 | 0.30533900  |
| H | 2.11728900 | -1.73219700 | -1.16779700 |
| H | 3.20376500 | 1.67422800  | 0.00156900  |
| O | 0.90063700 | 2.29646100  | -0.38126200 |
| H | 2.68363400 | -2.39241000 | 0.37129300  |
| H | 0.99942700 | -1.09012500 | 1.60641500  |
| C | -1.05005800 | 0.31490100  | -0.09715600 |
| C | -1.69704500 | -0.53188000 | -1.19263500 |
| C | -1.71783400 | 0.08005500  | 1.25854900  |
| H | -1.17098600 | 1.36430500  | -0.36138800 |
**I5 (protonated in the oxygen of the carbonyl in position 2)**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|--------------------------|-------------|
| Hartree                  |             |
| -651.0749587             | -650.799463 |

**XYZ coordinates**

|       |         |         |         |
|-------|---------|---------|---------|
| O     | -4.37356200 | -0.56787000 | 0.05080600 |
| N     | -0.39204800 | 0.12237600 | -0.14645600 |
| N     | -2.60347900 | 0.82127500 | -0.11018500 |
| C     | -1.27766100 | 1.07275700 | -0.04358500 |
| C     | -3.18234800 | -0.44793200 | 0.06165000 |
| C     | -0.88361100 | -1.23986000 | -0.45116300 |
| C     | -2.17312100 | -1.53086600 | 0.29194900 |
| H     | -0.11612900 | -1.94261800 | -0.14917700 |
|   |   |   |   |
|---|---|---|---|
| H | -1.99265000 | -1.57725300 | 1.36917800 |
| H | -3.22288600 | 1.62488200 | -0.12230300 |
| O | -1.01428800 | 2.34235100 | 0.12765500 |
| H | -2.59682400 | -2.47929200 | -0.02655100 |
| H | -1.02173800 | -1.31555900 | -1.53002200 |
| C | 1.07527100 | 0.33778300 | -0.04741500 |
| C | 1.62481600 | -0.26055100 | 1.24604900 |
| C | 1.78803300 | -0.20272900 | -1.28603900 |
| H | 1.26090400 | 1.41260800 | -0.01937800 |
| C | 3.12930500 | -0.00018600 | 1.33828500 |
| H | 1.44302000 | -1.33810300 | 1.25603900 |
| H | 1.10445900 | 0.17274800 | 2.10119700 |
| C | 3.28912900 | 0.06958700 | -1.17339900 |
| H | 1.62878000 | -1.28027200 | -1.36371400 |
| H | 1.37194400 | 0.26120400 | -2.18141000 |
| C | 3.86261100 | -0.53125800 | 0.10832800 |
| H | 3.51874200 | -0.45926500 | 2.24648600 |
| H | 3.30327100 | 1.07619300 | 1.42633600 |
| H | 3.79357800 | -0.33853500 | -2.04868100 |
| H | 3.46365200 | 1.14934000 | -1.17845900 |
| H | 4.92700100 | -0.30855400 | 0.18270600 |
| H | 3.76505000 | -1.62020800 | 0.07091300 |
| H | -0.07323100 | 2.56081000 | 0.06767800 |
I5 (protonated in the oxygen of the carbonyl in position 4)

|             | Electronic energy ($E_e$) | $E_e + ZPV$ |
|-------------|---------------------------|-------------|
|             | Hartree                   |             |
|             | -651.0675076              | -650.791884 |

XYZ coordinates

|     | x          | y          | z          |
|-----|------------|------------|------------|
| O   | -4.35400300| -0.59627300| 0.05127000 |
| N   | -0.34960900| 0.13036200 | -0.07286900|
| N   | -2.59087000| 0.84352800 | -0.06554900|
| C   | -1.17108200| 1.17038800 | 0.06478200 |
| C   | -3.08577900| -0.35685200| 0.02553100 |
| C   | -0.84875100| -1.15938600| -0.55207700|
| C   | -2.16444400| -1.50810800| 0.12091700 |
| H   | -0.11392600| -1.92133900| -0.31500500|
| H   | -2.02688100| -1.70946500| 1.18838600 |
| H   | -3.19017900| 1.66682300 | -0.07754400|
| O   | -0.91420200| 2.32558700 | 0.29762400 |
| H   | -2.63627900| -2.37734800| -0.33144800|
| H   | -0.97312200| -1.13146200| -1.63593300|
| C   | 1.10900800 | 0.34547500 | 0.03444000 |
| C   | 1.68879900 | -0.43755500| 1.21050500 |
| C   | 1.81365000 | 0.00516900 | -1.27740800|
| H   | 1.23352100 | 1.40924700 | 0.23082600 |
| C   | 3.19214900 | -0.18158400| 1.32495200 |
| H   | 1.51908100 | -1.50794400| 1.06116700 |
| H   | 1.17589100 | -0.14591100| 2.12820700 |
| C   | 3.31500200 | 0.26561600 | -1.14913600|
| H   | 1.65449300 | -1.05018100| -1.51711700|
| H   | 1.38470700 | 0.59777400 | -2.08747400|
I5 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -650.1572283              | -649.908293 |

XYZ coordinates

|       |       |       |       |
|-------|-------|-------|-------|
| O     | 4.40116800 | -0.43579900 | 0.28254800 |
| N     | 0.43895300 | 0.06008300 | -0.15753800 |
| N     | 2.64309700 | 0.97551100 | 0.04013500 |
| C     | 1.30565600 | 1.14975100 | -0.19550400 |
| C     | 3.19557100 | -0.24578500 | 0.06359900 |
| C     | 0.93541500 | -1.20429000 | 0.35464200 |
| C     | 2.31279600 | -1.45245600 | -0.21842700 |
| H     | 0.24669400 | -1.99837200 | 0.06896300 |
| H     | 2.24514100 | -1.58522700 | -1.30174000 |
| O     | 0.84640400 | 2.27425200 | -0.43775900 |
| H     | 2.77370400 | -2.33955000 | 0.21034100 |
| H     | 0.98995600 | -1.19171700 | 1.45092000 |
| C     | -1.00339900 | 0.28909300 | -0.13583500 |
C  -1.73379100  -0.54344000  -1.19220400
C  -1.60964000   0.05457800   1.25188000
H   -1.13371000   1.33974000  -0.38818600
C  -3.23230300  -0.23674700  -1.18815700
H  -1.59019200  -1.60973000  -0.99117200
H  -1.29963400  -0.33667900  -2.17177400
C  -3.10739300   0.36180500   1.25408000
H  -1.46008800  -0.98973300   1.54446900
H  -1.08746100   0.67445900   1.98361300
C  -3.83989900  -0.46242700   0.19604200
H  -3.74289800  -0.85023200  -1.93257000
H  -3.38422200   0.80741200  -1.47823700
H  -3.52845600   0.17263700   2.24316200
H  -3.25458000   1.42553200   1.04374000
H  -4.90240300  -0.21134600   0.18880000
H  -3.76484200  -1.52448500   0.45249600

**I5 homodimer**

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|------------|
| Hartree                   |            |
| -1301.344274              | -1300.816632 |

**XYZ coordinates**

|   | 0.55485500 | 3.68775100 | -0.84010800 |
|---|------------|------------|-------------|
| O | 3.32999700 | 0.84535900 | -0.09385000 |
| N | 1.12171100 | 1.56253300 | -0.33497200 |
| C | 2.02806900 | 0.51118300 | -0.20199400 |
| C | 1.42469200 | 2.86408800 | -0.65484500 |
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 3.692885 | 2.241158 | 0.139971 |
| C    | 2.896546 | 3.149247 | -0.777333 |
| H    | 4.756084 | 2.354529 | -0.052168 |
| H    | 3.175124 | 2.971249 | -1.819189 |
| H    | 0.136725 | 1.282028 | -0.333433 |
| O    | -0.554587 | -3.687474 | -0.840050 |
| N    | -3.330025 | -0.845322 | -0.094006 |
| N    | -1.121622 | -1.562362 | -0.334631 |
| C    | -2.028064 | -0.511087 | -0.201703 |
| C    | -1.424496 | -2.863914 | -0.654657 |
| C    | -3.692966 | -2.241640 | 0.139500 |
| C    | -2.896290 | -3.149060 | -0.777655 |
| H    | -3.510453 | -2.505620 | 1.185016 |
| H    | -3.067340 | -4.197999 | -0.550076 |
| H    | -0.136632 | -1.281799 | -0.333170 |
| O    | -1.604154 | 0.642890 | -0.186036 |
| O    | 1.604129 | -0.642794 | -0.186959 |
| H    | -3.174536 | -2.970986 | -1.819585 |
| H    | -4.756092 | -2.354340 | -0.053056 |
| H    | 3.067559 | 4.198115 | -0.549560 |
| H    | 3.509987 | 2.505453 | 1.185461 |
| C    | -4.328726 | 0.204767 | 0.144124 |
| C    | -5.441909 | 0.170496 | -0.903126 |
| C    | -4.894353 | 0.125640 | 1.562762 |
| H    | -3.793904 | 1.147069 | 0.040114 |
| C    | -6.444556 | 1.297899 | -0.652999 |
| H    | -5.966877 | -0.788324 | -0.858484 |
| H    | -5.002885 | 0.258565 | -1.898100 |
| C    | -5.899213 | 1.252136 | 1.803708 |

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| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | -5.39560200 | -0.83706000 | 1.70259700 |
| H     | -4.07607000 | 0.17731400  | 2.28368200 |
| C     | -7.01660700 | 1.22508200  | 0.76195800 |
| H     | -7.24519000 | 1.25015400  | -1.39237000|
| H     | -5.94190600 | 2.26010500  | -0.78769700|
| H     | -6.31248300 | 1.16943700  | 2.80968700 |
| H     | -5.37995900 | 2.21344700  | 1.74889100 |
| H     | -7.71172200 | 2.04848500  | 0.93123600 |
| H     | -7.58719400 | 0.29724700  | 0.87127600 |
| C     | 4.32863200  | -0.20481900 | 0.14416600 |
| C     | 5.44186300  | -0.17046400 | -0.90305300|
| C     | 4.89422000  | -0.12594600 | 1.56282100 |
| H     | 3.79375600  | -1.14707500 | 0.03997900 |
| C     | 6.44447200  | -1.29792500 | -0.65302700|
| H     | 5.96682600  | 0.78835100  | -0.85825500|
| H     | 5.00288200  | -0.25840400 | -1.89805600|
| C     | 5.89905300  | -1.25248100 | 1.80365200 |
| H     | 5.39549000  | 0.83671900  | 1.70281900 |
| H     | 4.07591600  | -0.17770600 | 2.28370900 |
| C     | 7.01649300  | -1.22529900 | 0.76195200 |
| H     | 7.24511000  | -1.25012700 | -1.39238900|
| H     | 5.94178000  | -2.26009400 | -0.78783500|
| H     | 6.31227300  | -1.16991900 | 2.80966300 |
| H     | 5.37981100  | -2.21378900 | 1.74867600 |
| H     | 7.71160000  | -2.04872500 | 0.93114400 |
| H     | 7.58708600  | -0.29748100 | 0.87140600 |
Electronic energy ($E_e$) $E_e +$ ZPV

| Hartree          |                    |
|------------------|--------------------|
|                  | -3223.020819       |
|                  | -3222.791119       |

XYZ coordinates

|    |     |     |              |
|----|-----|-----|--------------|
| O  | -0.95237900 | 2.97875500 | 0.00018600  |
| N  | 1.18846600  | 2.23784000 | -0.00122800 |
| N  | -0.57028900 | 0.71930900 | -0.00014300 |
| C  | -0.17643900 | 2.04584200 | -0.00005100 |
| C  | 0.35375300  | -0.28700100|  0.00037800 |
| C  | 1.68037200  | -0.07354900|  0.00025600 |
| C  | 2.19933400  | 1.28431900 |  0.00013200 |
| H  | 1.48633400  | 3.20602600 | -0.00089300 |
| O  | 3.36599800  | 1.61089900 |  0.00052200 |
| H  | -0.05159400 | -1.28848200|  0.00049000 |
| C  | -2.01527900 | 0.39523300 | -0.00010200 |
| C  | -2.41145100 | -0.36336700| -1.26421100 |
| C  | -2.41154400 | -0.36280200|  1.26427200 |
| H  | -2.51488200 | 1.36149100 | -0.00024500 |
| C  | -3.91495600 | -0.64158300| -1.25911900 |
| H  | -1.87053400 | -1.31376600| -1.30572200 |
| H  | -2.12634600 | 0.21701300 | -2.14287500 |
| C  | -3.91517500 | -0.64085400|  1.25907100 |
| H  | -1.87083500 | -1.31331900|  1.30597300 |
| H  | -2.12649200 | 0.21772800 |  2.14285100 |
| C  | -4.33187100 | -1.39967200|  0.00017100 |
| H  | -4.18587400 | -1.20459500| -2.15265900 |
| H  | -4.45431000 | 0.30907500 | -1.30358200 |
| H  | -4.18657300 | -1.20305200|  2.15297000 |
I6 (protonated)

|                  | $E_e$          | $E_e + ZPV$ |
|------------------|---------------|-------------|
|                  | Hartree       |             |
|                  | -3223.4215700 | -3223.179139|

XYZ coordinates

|     |         |         |         |
|-----|---------|---------|---------|
| O   | 0.92166400 | 2.98019800 | -0.00018800 |
| N   | -1.20895700 | 2.20349400 | -0.00010400 |
| N   | 0.58564200 | 0.70591900 | -0.00030800 |
| C   | 0.18208900 | 2.03695300 | -0.00053900 |
| C   | -0.30295900 | -0.29680000 | -0.00022200 |
| C   | -1.65601000 | -0.10368400 | -0.00010800 |
| C   | -2.11253500 | 1.21776600 | 0.00004100 |
| H   | -1.51352300 | 3.17551400 | 0.00018800 |
| O   | -3.38726400 | 1.46575000 | 0.00041400 |
| H   | 0.10967300 | -1.29702400 | -0.00024900 |
| C   | 2.05174100 | 0.40764400 | -0.00019000 |
| C   | 2.44328200 | -0.34575100 | 1.26655100 |
| C   | 2.44330200 | -0.34646700 | -1.26648200 |
| H   | 2.52849400 | 1.38474300 | -0.00045100 |
| C   | 3.94898600 | -0.61369700 | 1.25895900 |
| H   | 1.91024300 | -1.30062800 | 1.30259700 |
| H   | 2.15458600 | 0.23258100 | 2.14504300 |
### I6 (deprotonated)

|          | $E_e$       | $E_e + ZPV$   |
|----------|-------------|--------------|
|          | Hartree     |              |
|          | -3222.525863| -3222.309948 |

### XYZ coordinates

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| O       | 0.98389300   | 2.95589000   | -0.00007300  |
| N       | -1.20141100  | 2.32659600   | -0.00016000  |
| N       | 0.55389500   | 0.72228100   | -0.00031000  |
| C       | 0.11829600   | 2.07229700   | -0.00019800  |
| C       | -0.36205500  | -0.28218600  | 0.00001900   |
| C       | -1.67852000  | -0.02612100  | 0.00005200   |
| C       | -2.15756000  | 1.36133900   | 0.00020500   |
| O       | -3.36418700  | 1.62253500   | -0.00002300  |
| H       | 0.02789500   | -1.29007600  | 0.00000600   |
\begin{tabular}{ccc}
\textbf{C} & 1.98633500 & 0.39848000 -0.00003000 \\
\textbf{C} & 2.39577900 & -0.35982600 1.26267900 \\
\textbf{C} & 2.39572000 & -0.36001500 -1.26264400 \\
\textbf{H} & 2.48598000 & 1.36478300 -0.00010500 \\
\textbf{C} & 3.89984500 & -0.63419100 1.25922900 \\
\textbf{H} & 1.85729900 & -1.31184200 1.31083100 \\
\textbf{H} & 2.10917400 & 0.22126700 2.14069900 \\
\textbf{C} & 3.89978300 & -0.63440300 -1.25922600 \\
\textbf{H} & 1.85721500 & -1.31202700 -1.31061600 \\
\textbf{H} & 2.10908000 & 0.22094600 -2.14073900 \\
\textbf{C} & 4.31977000 & -1.39161900 0.00005500 \\
\textbf{H} & 4.17695400 & -1.19562700 2.15274400 \\
\textbf{H} & 4.43643200 & 0.31850500 1.30090800 \\
\textbf{H} & 4.17683700 & -1.19599500 -2.15266000 \\
\textbf{H} & 4.43637900 & 0.31828000 -1.30109800 \\
\textbf{H} & 5.39854600 & -1.55600400 0.00004300 \\
\textbf{H} & 3.84631900 & -2.37883700 0.00014900 \\
\textbf{Br} & -2.92135700 & -1.45815600 0.00003000 \\
\end{tabular}

**I6 homodimer**

| Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|--------------------------|---------------------|
| Hartree                  | -6446.054275        |
|                          | -6445.593736        |

**XYZ coordinates**

\begin{tabular}{ccc}
\textbf{O} & 3.00961800 & -2.27878200 -0.04587400 \\
\textbf{O} & 0.67750500 & 1.59395100 -0.31272200 \\
\textbf{N} & 4.20681700 & -0.32651900 0.02197600 \\
\end{tabular}

S110
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| N       | 1.88640800 | -0.31666400| -0.17817600|
| C       | 3.03682000 | -1.06679900| -0.06610400|
| C       | 1.77038100 | 1.05540700 | -0.21857100|
| C       | 3.04161800 | 1.74549200 | -0.13950600|
| C       | 4.17817200 | 1.03567500 | -0.02184800|
| H       | 1.00920000 | -0.84631600| -0.23903800|
| H       | 5.13887500 | 1.52562100 | 0.04598400 |
| O       | -3.00967400| 2.27882700 | -0.04609100|
| N       | -1.88641000| 0.31672100 | -0.17816200|
| N       | -4.20683200| 0.32654200 | 0.02188500 |
| C       | -3.03685800| 1.06684400 | -0.06633200|
| C       | -4.17815900| -1.03565200| -0.02185100|
| C       | -3.04159600| -1.74545300| -0.13947500|
| C       | -1.77036600| -1.05535300| -0.21848800|
| H       | -1.00920200| 0.84638400 | -0.23899200|
| C       | 5.49880900 | -1.03579600| 0.16404100 |
| C       | 6.39800700 | -0.79737800| -1.04630700|
| C       | 6.19046800 | -0.66354100| 1.47268100 |
| H       | 5.23196100 | -2.08972200| 0.19792700 |
| C       | 7.70463300 | -1.57659100| -0.88992500|
| H       | 6.62346400 | 0.27016600 | -1.13191600|
| H       | 5.87217200 | -1.09625900| -1.95418000|
| C       | 7.49609100 | -1.44626500| 1.61656100 |
| H       | 6.41379900 | 0.40747800 | 1.47990100 |
| H       | 5.51996400 | -0.86646500| 2.30896700 |
| C       | 8.41144200 | -1.21543800| 0.41535100 |
| H       | 8.35282400 | -1.37850700| -1.74388000|
| H       | 7.48441200 | -2.64804500| -0.89621000|
| H       | 7.99671000 | -1.15792300| 2.54113500 |
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| H | 7.26673100 | -2.51280400| 1.69564700 |
| H | 9.32652000 | -1.79947600| 0.52103400 |
| H | 8.70683900 | -0.16188300| 0.38555200 |
| O | -0.67748400| -1.59389900| -0.31254500|
| H | -5.13885400| -1.52561200| 0.04597200 |
| C | -5.49884900| 1.03578400 | 0.16388500 |
| C | -6.39819000| 0.79682600 | -1.04624400|
| C | -6.19030700| 0.66398000 | 1.47276600 |
| H | -5.23207000| 2.08974200 | 0.19734200 |
| C | -7.70485700| 1.57599900 | -0.88998800|
| H | -6.62356700| -0.27077400| -1.13140300|
| H | -5.87250600| 1.09539500 | -1.95430800|
| C | -7.49596400| 1.44666300 | 1.61652400 |
| H | -6.41356900| -0.40705000| 1.48044900 |
| H | -5.51970000| 0.86728300 | 2.30887700 |
| C | -8.41146200| 1.21531400 | 0.41552900 |
| H | -8.35315300| 1.37752100 | -1.74377100|
| H | -7.48472100| 2.64746800 | -0.89673900|
| H | -7.99643600| 1.15862900 | 2.54127500 |
| H | -7.26666800| 2.51324600 | 1.69518400 |
| H | -9.32656300| 1.79933500 | 0.52111400 |
| H | -8.70679700| 0.16172900 | 0.38618500 |
| Br| -3.05097400| -3.62347900| -0.19900300|
| Br| 3.05102300 | 3.62351300 | -0.19908700|
### I7

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -972.4112848              | -972.174424 |

XYZ coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| S    | -4.49211000 | -0.43457600 | -0.00003400 |
| O    | -0.47627100 | 2.36492100 | 0.00027000 |
| C    | -2.83266400 | -0.29551500 | -0.00006300 |
| C    | -0.87920500 | 1.22051800 | 0.00016200 |
| N    | -0.05670900 | 0.10953800 | 0.00004400 |
| N    | -2.23196600 | 0.93496400 | 0.00016700 |
| H    | -2.83079700 | 1.75179800 | 0.00020300 |
| C    | -0.59030300 | -1.14564000 | -0.00019700 |
| H    | 0.12996600  | -1.95093000 | -0.00032500 |
| C    | -1.91784200 | -1.39081200 | -0.00025900 |
| H    | -2.29479000 | -2.39894900 | -0.00046000 |
| C    | 1.41051900  | 0.30054100  | 0.00008900  |
| C    | 2.04200300  | -0.27536000 | 1.26547400  |
| C    | 2.04204000  | -0.27469800 | -1.26556700 |
| H    | 1.55218500  | 1.37912300  | 0.00037000  |
| C    | 3.54931000  | -0.01789200 | 1.25947900  |
| H    | 1.85963300  | -1.35344700 | 1.31168500  |
| H    | 1.57494100  | 0.17493900  | 2.14258100  |
| C    | 3.54934600  | -0.01719200 | -1.25941000 |
| H    | 1.85974100  | -1.35277300 | -1.31233900 |
| H    | 1.57498100  | 0.17600700  | -2.14246900 |
| C    | 4.20278300  | -0.58446900 | -0.00011100 |
| H    | 3.99844000  | -0.45214800 | 2.15304700  |
### I7 (protonated)

|            | Electronic energy ($E_e$) | $E_e + ZPV$ |
|------------|---------------------------|-------------|
|            | Hartree                   |             |
|            | -972.8092863              | -972.559616 |

### XYZ coordinates

|     |        |        |        |
|-----|--------|--------|--------|
| S   | 4.46668200 | -0.47531600 | -0.00002900 |
| O   | 0.42266600  | 2.33839700  | -0.00039600 |
| C   | 2.83397800  | -0.34937200  | 0.00005500  |
| C   | 0.90579500  | 1.12702000  | -0.00017300 |
| N   | 0.05637400  | 0.11253700  | 0.00003600  |
| H   | 2.22122700  | 0.90833900  | -0.00016000 |
| H   | 2.84289200  | 1.71236500  | -0.00032500 |
| C   | 0.57222600  | -1.17529300  | 0.00032500  |
| H   | -0.16986100  | -1.95838700  | 0.00053400  |
| C   | 1.89011400  | -1.42735100  | 0.00035000  |
| H   | 2.25458800  | -2.44140400  | 0.00058100  |
| C   | -1.42958800  | 0.30983200  | -0.00039000 |
| C   | -2.03899900  | -0.27684300  | -1.26995600 |
| C   | -2.03907000  | -0.27629800  | 1.27009300  |
| H   | -1.58674000  | 1.38487800  | -0.00027900 |
| C   | -3.55059400  | -0.04096600  | -1.25944500 |
I7 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -971.9153671              | -971.691789 |

XYZ coordinates

| S          | -4.56596800 | -0.08407200 | 0.00000600 |
| O          | 0.01394500  | -1.92933100 | -0.00021300 |
| C          | -2.85428000 | 0.05546800  | -0.00000500 |
| C          | -0.71580900 | -0.93702200 | -0.00011700 |
| N          | -0.11944600 | 0.34054600  | 0.00000300  |
| N          | -2.07269900 | -1.02387100 | -0.00014000 |
| C          | -0.90975300 | 1.44899700  | 0.00015100  |
| H          | -0.38902300 | 2.39702000  | 0.00026700  |
**I7 homodimer**

|                  | Electronic energy ($E_e$) | $E_e + ZPV$ |
|------------------|---------------------------|-------------|
|                  |   Hartree                  |             |
|                  | -1944.835237              | -1944.35918 |

**XYZ coordinates**

|      |                  |                 |               |
|------|------------------|-----------------|---------------|
| S    | -0.17134600      | 4.11863700      | 0.17889600    |
| O    | -1.58462800      | -0.56091900     | -0.14897400   |
| C    | -1.37943400      | 2.97509200      | 0.09588900    |
**Electronic energy ($E_e$) $E_e + ZPV$**

|                |           |           |
|----------------|-----------|-----------|
|                | Hartree   |           |
| $E_e + ZPV$    | -1368.983715 | -1368.640198 |

**XYZ coordinates**

- **C**
- **H**
- **C**
- **H**
- **C**
- **H**
- **C**
- **H**
- **C**
- **H**
- **C**
- **H**
- **C**
- **O**
- **O**
- **C**
- **H**
- **H**
- **H**
- **O**
- **O**
- **O**
- **C**
- **C**
- **O**
- **C**
- **O**
- **C**
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -1.19239700 | 4.81482100 | 1.02093500 |
| H | -2.68736100 | 3.90718200 | 1.23653100 |
| H | -2.47722800 | 4.91614100 | -0.21600800 |
| O | -2.43081100 | 0.41756900 | 0.17119200 |
| C | -3.02323100 | 0.24153400 | -1.03678800 |
| O | -2.45284600 | -0.21761000 | -1.98548000 |
| C | -4.44437000 | 0.70310000 | -0.99874700 |
| H | -4.90814100 | 0.54093200 | -1.96596100 |
| H | -4.46917900 | 1.76342200 | -0.74642100 |
| H | -4.98279100 | 0.15867400 | -0.22380000 |
| N | 2.35151800  | 0.47871500 | 0.41478400  |
| C | 2.40778900  | -0.41607600 | -0.64579700 |
| N | 3.67103300  | -0.65482400 | -1.12663100 |
| H | 3.72403000  | -1.29872700 | -1.90656200 |
| C | 4.87526900  | -0.12827600 | -0.66222300 |
| C | 4.72266900  | 0.77558900  | 0.46004400  |
| H | 5.60179800  | 1.22554600  | 0.88958900  |
| C | 3.49818300  | 1.02824600  | 0.94217500  |
| H | 3.33902700  | 1.69233900  | 1.77992000  |
| O | 1.41795700  | -0.93403500 | -1.11491100 |
| O | 5.92302600  | -0.43925500 | -1.19267800 |
### I8 (protonated)

|                | $E_e$       | $E_e + ZPV$   |
|----------------|-------------|---------------|
| Electronic     | Hartree     |
| energy ($E_e$) | -1369.388555 | -1369.032396   |

**XYZ coordinates**

|    | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| C  | 0.97513500 | 0.79762700 | 1.08730900 |
| H  | 1.13892800 | 1.64110300 | 1.75780600 |
| C  | -0.15738300 | 1.15864100 | 0.10565400 |
| H  | 0.16892200 | 1.29631300 | -0.92046400 |
| C  | -1.13702700 | -0.01058500 | 0.28533600 |
| H  | -0.88756000 | -0.78765600 | -0.42851000 |
| C  | -0.84108400 | -0.46907400 | 1.70735400 |
| H  | -1.31598000 | 0.20991900 | 2.42337000 |
| C  | -1.24455200 | -1.87997600 | 2.05761300 |
| H  | -0.76564100 | -2.17147100 | 2.98984900 |
| H  | -2.32490100 | -1.92847200 | 2.17239200 |
| O  | -0.80767400 | -2.81792100 | 1.07481900 |
| C  | -1.68965800 | -3.13598400 | 0.10393500 |
| C  | -1.09472900 | -4.09931400 | -0.87248200 |
| H  | -1.85915700 | -4.44009700 | -1.56253300 |
| H  | -0.64912400 | -4.94077600 | -0.34512600 |
| H  | -0.30266400 | -3.58961400 | -1.42259600 |
| O  | -2.79817900 | -2.67243400 | 0.04750800 |
| O  | 0.58354000  | -0.34452800 | 1.79381900 |
| O  | -0.72799000 | 2.36081400  | 0.61246500 |
| C  | -1.50007900 | 3.07392700  | -0.24447900 |
| O  | -1.61166500 | 2.78997100  | -1.40484400 |
| C  | -2.16874000 | 4.21189500  | 0.45520500 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -1.46532500 | 4.72620800 | 1.10656500 |
| H       | -2.96831300 | 3.80734900 | 1.07789800 |
| H       | -2.58711800 | 4.89481800 | -0.27687200 |
| O       | -2.48738700 | 0.37031800 | 0.16267800 |
| C       | -3.04946800 | 0.18686500 | -1.06309600 |
| O       | -2.43638000 | -0.23540200 | -2.00144000 |
| C       | -4.48592900 | 0.59485500 | -1.05104300 |
| H       | -4.92913000 | 0.40193800 | -2.02205100 |
| H       | -4.55153900 | 1.65795700 | -0.81741000 |
| H       | -5.01591500 | 0.04524100 | -0.27423600 |
| N       | 2.28502500  | 0.53232200 | 0.46884100  |
| C       | 2.34955400  | -0.39966700 | -0.56214500 |
| N       | 3.63950400  | -0.59753500 | -1.06390000 |
| H       | 3.69431600  | -1.27163200 | -1.82479400 |
| C       | 4.74140200  | 0.01116400 | -0.61023800 |
| C       | 4.63508400  | 0.92613300 | 0.43850000 |
| H       | 5.50896700  | 1.42534800 | 0.82009800 |
| C       | 3.39093600  | 1.14698100 | 0.94117500 |
| H       | 3.22924000  | 1.84211000 | 1.75322900 |
| O       | 1.40242200  | -0.98148000 | -1.00790800 |
| O       | 5.90647800  | -0.24063600 | -1.13234900 |
| H       | 5.88419500  | -0.87263000 | -1.87074500 |
|          |          |          |          |
|----------|----------|----------|----------|
|          | 1.09933300 | 0.75975200 | 0.99589300 |
|          | 1.24955200 | 1.59623600 | 1.68001700 |
|          | -0.06534200 | 1.13664100 | 0.05626700 |
|          | 0.23181200 | 1.28565700 | -0.97427000 |
|          | -1.05658600 | -0.01184300 | 0.25823200 |
|          | -0.82096900 | -0.79423400 | -0.45391700 |
|          | -0.74437900 | -0.45380100 | 1.68156900 |
|          | -1.19854000 | 0.25349800 | 2.38798900 |
|          | -1.20291100 | -1.84130400 | 2.06635600 |
|          | -0.70670000 | -2.14267000 | 2.98653400 |
|          | -2.28039000 | -1.84574000 | 2.21413900 |
|          | -0.83777100 | -2.81152600 | 1.08508600 |
|          | -1.74871100 | -3.09852300 | 0.13824900 |
|          | -1.18498700 | -4.02636400 | -0.88972700 |
|          | -1.97260800 | -4.35349300 | -1.56011200 |
|          | -0.70794600 | -4.87741800 | -0.40691300 |
|          | -0.41823000 | -3.49227500 | -1.45248100 |
|          | -2.86445200 | -2.64273900 | 0.13418300 |
|          | 0.66969700 | -0.37606500 | 1.74189500 |
|          | -0.61910500 | 2.34706800 | 0.59937800 |
|          | -1.41877800 | 3.07427700 | -0.19943500 |
|          | -1.63431800 | 2.80402900 | -1.35143600 |
|          | -1.99381600 | 4.24385300 | 0.53963100 |
I8 homodimer

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| -2737.980679 Hartree      | -2737.292   |

XYZ coordinates

C  -5.16912300 -1.96192600 -0.26629400
H  -5.41186000 -3.00833300 -0.08081700
C  -5.82510200 -1.11692400  0.84465300
H  -5.11999800 -0.67780100  1.54108400
C  -6.63482200 -0.08688800  0.05133000
H  -6.00251000  0.77171200 -0.14147900
C  -6.93791000 -0.83886100 -1.23776900
H  -7.75703900 -1.54741900 -1.06793500
C  -7.30114900  0.01154700 -2.43076200
H  -7.27418000 -0.59484900 -3.33334600
H  -8.30073200  0.41851700 -2.29467000
O  -6.36114900  1.06647000 -2.63238200
C  -6.64766100  2.25828000 -2.07348300
C  -5.53328800  3.23345000 -2.27882700
H  -5.84592800  4.21958700 -1.95227500
H  -5.23399400  3.24915200 -3.32524700
H  -4.67512100  2.90492400 -1.69064100
O  -7.66955500  2.47644000 -1.47475100
O  -5.72486700 -1.54099100 -1.49472600
O  -6.71208900 -2.00786200  1.52758000
C  -7.13858200 -1.62724600  2.75111200
O  -6.74113500 -0.63935700  3.30653200
C  -8.14652800 -2.59161500  3.29141100
H  -7.76408400 -3.60873000  3.22503300
H  -9.05011000 -2.53450600  2.68352300
H  -8.37796300 -2.33933000  4.32098700
O  -7.83645700  0.29994000  0.68356700
C  -7.78077000  1.43474900  1.42529400
O  -6.77462300  2.06667700  1.58018300
C  -9.12576900  1.76529900  1.98822500

S125
| At   | x     | y     | z     |
|------|-------|-------|-------|
| H    | -9.03421900 | 2.58178100 | 2.69660600 |
| H    | -9.55335200 | 0.88843900 | 2.47213000 |
| H    | -9.78563900 | 2.05612800 | 1.17027200 |
| N    | -3.72022500 | -1.89892900 | -0.35157100 |
| C    | -3.10105300 | -0.65414100 | -0.40554900 |
| N    | -1.73956800 | -0.69177500 | -0.57264700 |
| H    | -1.26580700 | 0.21930500 | -0.61916000 |
| C    | -0.94607700 | -1.81663500 | -0.68950900 |
| C    | -1.66120000 | -3.07052400 | -0.64707700 |
| H    | -1.11262000 | -3.99211200 | -0.74458300 |
| C    | -2.99348300 | -3.05650900 | -0.49215800 |
| H    | -3.57545300 | -3.96670600 | -0.46527700 |
| O    | -3.71907300 | 0.38230100 | -0.30134700 |
| O    | 0.26784200 | -1.70603500 | -0.82064000 |
| C    | 5.17024300 | 1.97494000 | -0.13857500 |
| H    | 5.40846100 | 3.00517800 | 0.12570300 |
| C    | 5.81393100 | 1.05222900 | 0.91666800 |
| H    | 5.10230000 | 0.56214400 | 1.57165600 |
| C    | 6.63631000 | 0.08341000 | 0.06161100 |
| H    | 6.01036400 | -0.76173400 | -0.19899600 |
| C    | 6.95279700 | 0.92573200 | -1.16700300 |
| H    | 7.77045100 | 1.61899100 | -0.93694300 |
| C    | 7.33013200 | 0.16298700 | -2.41386800 |
| H    | 7.31589800 | 0.83340900 | -3.27019600 |
| H    | 8.32704100 | -0.25541700 | -2.29436100 |
| O    | 6.39178500 | -0.87251000 | -2.70397900 |
| C    | 6.66603400 | -2.09985500 | -2.22107200 |
| C    | 5.55400400 | -3.05551500 | -2.51227200 |
| H    | 5.85048800 | -4.05968000 | -2.22823000 |
H  5.29027400 -3.01500000 -3.56768500
H  4.67834900 -2.75178000 -1.93663200
O  7.67678700 -2.36003600 -1.62004500
O  5.74325000  1.64591800 -1.38695900
O  6.69120900  1.89294200  1.67185200
C  7.10968900  1.42283400  2.86657800
O  6.70551400  0.39849700  3.34626900
C  8.11803600  2.34136300  3.48099800
H  7.73534300  3.36041000  3.49665100
H  9.02075700  2.33320700  2.86919100
H  8.35050400  2.00774300  4.48680000
O  7.83298400 -0.34454000  0.67698700
C  7.77174200 -1.52719100  1.33990600
O  6.76315800 -2.16474600  1.44806200
C  9.11120100 -1.89238700  1.89460100
H  9.03758800 -2.82809800  2.43834400
H  9.45927300 -1.09983100  2.55675000
H  9.82572200 -1.98761200  1.07734500
N  3.72265600  1.91662600 -0.24644200
C  3.10508300  0.67831700 -0.39016400
N  1.74302200  0.72606800 -0.55055400
H  1.26933900 -0.18036700 -0.65181200
C  0.94861900  1.85526600 -0.59049600
C  1.66315600  3.10413300 -0.46630600
H  1.11325500  4.02940600 -0.50090000
C  2.99512100  3.08053800 -0.30928700
H  3.57568900  3.98755300 -0.21755500
O  3.72429400 -0.36232200 -0.36367600
O -0.26577300  1.75229400 -0.72456500
|                | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------------|---------------------------|-------------|
|                | Hartree                   |             |
|                | -1219.723739              | -1219.36625 |

XYZ coordinates

|     | X            | Y            | Z            |
|-----|--------------|--------------|--------------|
| N   | 1.62407700   | -0.78728600  | -0.42866100  |
| H   | 4.49705400   | -1.55408100  | -1.68614900  |
| C   | 2.51903200   | -1.32495200  | -1.34210900  |
| N   | 3.83865000   | -1.16340800  | -1.02432800  |
| C   | 4.36667400   | -0.54638500  | 0.09891800   |
| C   | 3.37852600   | -0.03405500  | 1.03146500   |
| C   | 2.05939200   | -0.18171600  | 0.75610000   |
| O   | 2.17722000   | -1.90867400  | -2.35456300  |
| C   | 3.89077900   | 0.64735900   | 2.26937900   |
| H   | 4.96633700   | 0.77847200   | 2.18445200   |
| H   | 3.43546700   | 1.62769800   | 2.40550100   |
| H   | 3.69544700   | 0.05929800   | 3.16794000   |
| C   | 0.21674500   | -0.88840100  | -0.81014900  |
| H   | 0.22585700   | -1.16250800  | -1.86024800  |
| C   | -0.63490900  | -1.89825400  | -0.01763800  |
| H   | -0.87827800  | -2.75182100  | -0.64616000  |
| H   | -0.12137400  | -2.26359000  | 0.86724300   |
| C   | -1.90675200  | -1.12153300  | 0.32733600   |
| H   | -1.97429600  | -0.89191800  | 1.38857200   |
| C   | -1.78534900  | 0.16677100   | -0.50488900  |
| H   | -2.24347000  | -0.00840000  | -1.48561000  |
| C   | -2.39117100  | 1.38913100   | 0.14339700   |
| H   | -3.46745600  | 1.27056700   | 0.23425800   |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -1.955585 | 1.557858  | 1.126445  |
| O       | -0.392123 | 0.377847  | -0.655519 |
| O       | -2.173946 | 2.527513  | -0.694850 |
| C       | -1.162098 | 3.356914  | -0.382714 |
| O       | -0.480800 | 3.240753  | 0.602296  |
| C       | -1.024312 | 4.440132  | -1.406835 |
| H       | -0.862861 | 3.994238  | -2.387549 |
| H       | -1.947896 | 5.016479  | -1.451142 |
| H       | -0.192702 | 5.086017  | -1.145901 |
| O       | -3.052816 | -1.885952 | -0.052210 |
| C       | -4.209375 | -1.629513 | 0.587724  |
| O       | -4.316347 | -0.782850 | 1.436785  |
| C       | -5.307037 | -2.521822 | 0.101465  |
| H       | -5.018165 | -3.563444 | 0.235314  |
| H       | -6.218619 | -2.310045 | 0.650164  |
| H       | -5.463675 | -2.353794 | -0.963736 |
| C       | 1.032828  | 0.324729  | 1.724998  |
| H       | 0.686909  | 1.315905  | 1.429908  |
| H       | 0.165756  | -0.324165 | 1.785697  |
| H       | 1.473121  | 0.386092  | 2.715094  |
| O       | 5.576498  | -0.484191 | 0.236578  |
**I9 (protonated)**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -1220.13633              | -1219.765936 |

**XYZ coordinates**

|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| N | 1.56068800  | -0.88053200 | -0.39044400 |
| H | 4.46801200  | -1.64024200 | -1.59278600 |
| C | 2.47242900  | -1.45551900 | -1.27207300 |
| N | 3.80013200  | -1.22977500 | -0.94535900 |
| C | 4.21419800  | -0.54454000 | 0.12963300  |
| C | 3.29176200  | -0.01308500 | 1.02544500  |
| C | 1.95279800  | -0.22293400 | 0.74322600  |
| O | 2.17241600  | -2.10222800 | -2.24243400 |
| C | 3.75549000  | 0.76242100  | 2.22600400  |
| H | 4.81840000  | 0.97242000  | 2.15554500  |
| H | 3.22622000  | 1.71136700  | 2.29442500  |
| H | 3.58142300  | 0.20757500  | 3.14820000  |
| C | 0.14479500  | -0.96435800 | -0.83113700 |
| H | 0.19950700  | -1.25910600 | -1.87420700 |
| C | -0.74519200 | -1.93704300 | -0.04179900 |
| H | -1.03182900 | -2.77229800 | -0.67567200 |
| H | -0.24498300 | -2.33350100 | 0.83744200  |
| C | -1.97903200 | -1.10395400 | 0.31900100  |
| H | -2.02802000 | -0.88440600 | 1.38353500  |
| C | -1.81129600 | 0.18640500  | -0.50186700 |
| H | -2.31358300 | 0.05451800  | -1.46589000 |
| C | -2.30974400 | 1.43793600  | 0.18126500  |
| H | -3.38215200 | 1.37091600  | 0.34030500  |
|   |        |        |        |
|---|--------|--------|--------|
| H | -1.80765400 | 1.58456800 | 1.13613500 |
| O | -0.40851100 | 0.31829000 | -0.71329000 |
| O | -2.09379700 | 2.56476800 | -0.67205200 |
| C | -1.01885000 | 3.33846600 | -0.44563800 |
| O | -0.25147500 | 3.16755400 | 0.46698200 |
| C | -0.91945700 | 4.42880900 | -1.46552300 |
| H | -0.79070700 | 3.98520600 | -2.45269300 |
| H | -1.84356600 | 5.00464600 | -1.47905000 |
| H | -0.07765700 | 5.07203300 | -1.23237300 |
| O | -3.15484700 | -1.81782100 | -0.05548600 |
| C | -4.29797900 | -1.50251700 | 0.59097400 |
| O | -4.35619600 | -0.63658700 | 1.42361800 |
| C | -5.43492100 | -2.35673600 | 0.13228800 |
| H | -5.19328400 | -3.40576500 | 0.29931100 |
| H | -6.33355600 | -2.08695300 | 0.67673800 |
| H | -5.58679000 | -2.21497800 | -0.93731900 |
| C | 0.93185600 | 0.28938300 | 1.69929000 |
| H | 0.64193100 | 1.30315200 | 1.41188800 |
| H | 0.04052500 | -0.32463900 | 1.72213200 |
| H | 1.35896500 | 0.31633700 | 2.69718700 |
| O | 5.49694600 | -0.38993500 | 0.33964900 |
| H | 6.05563400 | -0.77742400 | -0.35266700 |
### I9 (deprotonated)

|         | $E_e$ | $E_e + ZPV$ |
|---------|-------|------------|
|         | Hartree |           |
|         | -1219.222145 | -1218.878925 |

**XYZ coordinates**

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| N       | 1.64909400 | -0.75436500 | -0.43658500 |
| C       | 2.57022900 | -1.33733100 | -1.35392900 |
| N       | 3.88026300 | -1.24623800 | -1.11162500 |
| C       | 4.36630300 | -0.63437200 | -0.00240500 |
| C       | 3.42487700 | -0.07996400 | 0.98332900  |
| C       | 2.09801800 | -0.17384800 | 0.74437300  |
| O       | 2.10091700 | -1.92089400 | -2.34320200 |
| C       | 3.98607500 | 0.58420200  | 2.21133100  |
| H       | 5.05316700 | 0.73368000  | 2.06806300  |
| H       | 3.52485000 | 1.55397600  | 2.40144700  |
| H       | 3.85676300 | -0.02469000 | 3.11025600  |
| C       | 0.25123100 | -0.84721100 | -0.78622800 |
| H       | 0.23435400 | -1.11276700 | -1.83774000 |
| C       | -0.59750300 | -1.86162200 | 0.01095000  |
| H       | -0.81969300 | -2.72813400 | -0.60830200 |
| H       | -0.08462100 | -2.20548700 | 0.90490600  |
| C       | -1.88243800 | -1.10213100 | 0.33686600  |
| H       | -1.96199400 | -0.85946000 | 1.39445900  |
| C       | -1.76788900 | 0.17775500  | -0.50863200 |
| H       | -2.19337300 | -0.02361600 | -1.50046100 |
| C       | -2.42425400 | 1.39444500  | 0.10151600  |
| H       | -3.50378600 | 1.27431600  | 0.12769600  |
| H       | -2.04797500 | 1.56923700  | 1.10740800  |
**I9 homodimer**

| XYZ coordinates | Electronic energy ($E_e$) | $E_e + ZPV$ |
|-----------------|--------------------------|-------------|
|                 |                          | Hartree     |
| O               | -0.38181300 0.41967000 -0.61415900 | -2439.460967 |
| O               | -2.15376100 2.52806900 -0.72927600 | -2438.745335 |
| C               | -1.16424300 3.35789900 -0.35295300 |               |
| O               | -0.61233300 3.30235000 0.71453900  |
| C               | -0.85407200 4.34592000 -1.43411500 |
| H               | -0.35443200 3.81797000 -2.24730700 |
| H               | -1.77179300 4.77793200 -1.82863900 |
| H               | -0.19948900 5.11993800 -1.04737000 |
| O               | -3.02036000 -1.88573000 -0.04112600 |
| C               | -4.18370100 -1.63408000 0.57921900  |
| O               | -4.31725000 -0.77390400 1.41255200 |
| C               | -5.26442900 -2.55146200 0.09763400 |
| H               | -4.95895700 -3.58640900 0.24509900 |
| H               | -6.18339300 -2.34892700 0.63760500 |
| H               | -5.41713200 -2.39884100 -0.97047200 |
| C               | 1.09753000 0.36097900 1.73313600 |
| H               | 0.77423400 1.36541200 1.45814800 |
| H               | 0.20810400 -0.25796100 1.80168500 |
| H               | 1.55082500 0.39737300 2.71959600 |
| O               | 5.59140600 -0.55136000 0.19327800 |

**Electronic energy ($E_e$)**

| XYZ coordinates | Electronic energy ($E_e$) | $E_e + ZPV$ |
|-----------------|--------------------------|-------------|
|                 |                          | Hartree     |
| I9 homodimer    | -2439.460967             | -2438.745335 |

**XYZ coordinates**

| XYZ coordinates | Electronic energy ($E_e$) | $E_e + ZPV$ |
|-----------------|--------------------------|-------------|
|                 |                          | Hartree     |
| O               | -0.38181300 0.41967000 -0.61415900 | -2439.460967 |
| O               | -2.15376100 2.52806900 -0.72927600 | -2438.745335 |
| C               | -1.16424300 3.35789900 -0.35295300 |               |
| O               | -0.61233300 3.30235000 0.71453900  |
| C               | -0.85407200 4.34592000 -1.43411500 |
| H               | -0.35443200 3.81797000 -2.24730700 |
| H               | -1.77179300 4.77793200 -1.82863900 |
| H               | -0.19948900 5.11993800 -1.04737000 |
| O               | -3.02036000 -1.88573000 -0.04112600 |
| C               | -4.18370100 -1.63408000 0.57921900  |
| O               | -4.31725000 -0.77390400 1.41255200 |
| C               | -5.26442900 -2.55146200 0.09763400 |
| H               | -4.95895700 -3.58640900 0.24509900 |
| H               | -6.18339300 -2.34892700 0.63760500 |
| H               | -5.41713200 -2.39884100 -0.97047200 |
| C               | 1.09753000 0.36097900 1.73313600 |
| H               | 0.77423400 1.36541200 1.45814800 |
| H               | 0.20810400 -0.25796100 1.80168500 |
| H               | 1.55082500 0.39737300 2.71959600 |
| O               | 5.59140600 -0.55136000 0.19327800 |

S133
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | -1.03912100 | -0.72653300 | -0.77000700 |
| C       | -3.07481700 | -0.58290600 | -0.85774000 |
| N       | -1.88622300 | -0.68288400 | -0.19090200 |
| C       | -1.71337100 | -0.75762200 | 1.17174000 |
| H       | -0.57714700 | -0.83909100 | 1.63565200 |
| C       | -1.74004500 | -0.70602900 | 3.72633400 |
| H       | -3.37036100 | -0.07108000 | 3.95840100 |
| C       | -3.10592600 | -1.81060100 | 3.83928500 |
| H       | -5.17919900  | 0.00268600  | -1.75584000 |
| C       | -6.39482100 | -1.55449400 | -0.87439100 |
| H       | -6.39550800 | -1.92751700 | 1.89586400 |
| H       | -6.08784100 | -2.36328700 | -0.21725300 |
| C       | -7.77577200 | -1.00331400 | -0.51468000 |
| H       | -8.13085900 | -1.37122200 | 0.44574700 |
| C       | -7.55961000 | 0.51951000  | -0.47109600 |
| H       | -7.73103200 | 0.92402400  | -1.47591000 |
| C       | -8.41278500 | 1.25202700  | 0.53751100 |
| H       | -9.46040300 | 1.19579000  | 0.25529100 |
| H       | -8.27773000 | 0.83481800  | 1.53351900 |
| O       | -6.19824500 | 0.68571000  | -0.11229200 |
| O       | -8.05854300 | 2.63793500  | 0.52762200 |
| C       | -7.23237800 | 3.08512500  | 1.48977100 |
| O       | -6.86362100 | 2.41629400  | 2.41993600 |
| C       | -6.84388200 | 4.50937800  | 1.24221400 |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| H | -6.17014000 | 4.53947700 | 0.38504300 |
| H | -7.72222000 | 5.10402100 | 0.99874400 |
| H | -6.34046800 | 4.90932200 | 2.11610900 |
| O | -8.71484200 | -1.37444500 | -1.52577500 |
| C | -10.01547500 | -1.41227400 | -1.18122700 |
| O | -10.41241800 | -1.11855000 | -0.08344500 |
| C | -10.86508200 | -1.87173800 | -2.32349200 |
| H | -10.61662100 | -2.90716600 | -2.55714400 |
| H | -11.91296500 | -1.79537000 | -2.05346100 |
| H | -10.65369500 | -1.27201500 | -3.20732500 |
| C | -5.39038800 | -0.70468000 | 2.13858100 |
| H | -5.72191000 | 0.30815600 | 2.37119200 |
| H | -6.19985200 | -1.20300400 | 1.61679200 |
| H | -5.20968800 | -1.23821400 | 3.06679600 |
| N | 4.20441800 | -0.53708500 | 0.05204300 |
| H | 1.03677900 | -0.72357600 | 0.77091700 |
| C | 3.07242700 | -0.57892000 | 0.85857200 |
| N | 1.88388100 | -0.67998600 | 0.19180700 |
| C | 1.71122300 | -0.75701800 | -1.17074300 |
| C | 2.92235100 | -0.75309200 | -1.96217400 |
| C | 4.12220000 | -0.67054500 | -1.33396700 |
| O | 3.12140200 | -0.53892400 | 2.07399100 |
| O | 0.57509800 | -0.83955500 | -1.63469800 |
| C | 2.78225100 | -0.84329200 | -3.45549200 |
| H | 1.73864000 | -0.70585600 | -3.72555400 |
| H | 3.37129300 | -0.07722700 | -3.95832100 |
| H | 3.10048100 | -1.81559900 | -3.83616200 |
| C | 5.46228400 | -0.32834100 | 0.76441400 |
| H | 5.17653000 | 0.01069500 | 1.75525900 |
C    6.39035800  -1.55178900   0.88041400
H    6.39046000  -1.92056700   1.90343500
H    6.08181400  -2.36265700   0.22652200
C    7.77202200  -1.00439800   0.51806200
H    8.12611500  -1.37673700  -0.44094100
C    7.55854900   0.51834100   0.46872800
H    7.73116200   0.92647800   1.47185700
C    8.41436500   1.24362900  -0.54252000
H    9.46215600   1.18089900  -0.26168200
H    8.27539900   0.82515800  -1.53745400
O    6.19754900   0.68612900   0.10971200
O    8.06917800   2.63176700  -0.53496300
C    7.24271100   3.08161400  -1.49579800
O    6.86775300   2.41289500  -2.42348200
C    6.86238100   4.50831400  -1.24979600
H    6.18915500   4.54295100  -0.39236900
H    7.74395100   5.09850000   2.70213400
H    10.52463600  -2.81631500   2.70213400
H    11.90030100  -1.90439100   2.02226300
H    10.75490100  -1.12870800   3.14676800
C    5.38852900  -0.70867500  -2.13690600
H    5.72166000   0.30302400  -2.37214900
H    6.19695700  -1.20694100  -1.61336700
H    5.20739200  -1.24448200  -3.06373300
### Electronic energy \( (E_e) \) vs \( E_e + ZPV \) in Hartree

|           | \( E_e \)      | \( E_e + ZPV \)  |
|-----------|----------------|------------------|
| \( -1542.676711 \) | \( -1542.321616 \) |

**XYZ coordinates**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| N       | -1.34404400 | -0.81990200 | 0.40088900 |
| H       | -4.21123800 | -1.62860600 | 1.62798600 |
| C       | -2.23857800 | -1.40234500 | 1.28497700 |
| N       | -3.55861900 | -1.18918200 | 0.99078700 |
| C       | -4.07582100 | -0.46788600 | -0.04972600 |
| C       | -3.10797400 | 0.11264500  | -0.93529300 |
| C       | -1.77918100 | -0.12337600 | -0.72170500 |
| O       | -1.90226000 | -2.06619000 | 2.24679800 |
| C       | -3.59024100 | 0.94025100  | -2.09238200 |
| H       | -4.48623400 | 1.48218500  | -1.79998000 |
| H       | -2.84389200 | 1.66437000  | -2.40629300 |
| H       | -3.85632100 | 0.31838600  | -2.95021300 |
| C       | 0.06491400  | -0.92634500 | 0.79364900 |
| H       | 0.04399400  | -1.21928200 | 1.83876500 |
| C       | 0.92785400  | -1.91796100 | -0.00822000 |
| H       | 1.18052700  | -2.77465200 | 0.61219400 |
| H       | 0.41958300  | -2.28003900 | -0.89748800 |
| C       | 2.19087000  | -1.12132100 | -0.34328400 |
| H       | 2.25120200  | -0.87272600 | -1.40065600 |
| C       | 2.05853100  | 0.15143100  | 0.51014100 |
| H       | 2.51892400  | -0.34332200 | 1.48757000 |
| C       | 2.64953300  | 1.39106700  | -0.11896100 |
| H       | 3.72715500  | 1.28629000  | -0.21074100 |
H  2.21292100  1.56943800  -1.09989300
O  0.66224000  0.34567600  0.66626100
O  2.41885600  2.51397100  0.73619200
C  1.39984900  3.33851800  0.43432600
O  0.71805200  3.22685300  -0.55095400
C  1.25498900  4.10152000  1.46934900
H  1.09661500  3.95367700  2.44567300
H  2.17491700  4.99190600  1.51897900
H  0.41906300  5.05303900  1.21485500
O  3.34550400  -1.87983900  0.01878700
C  4.49723500  -1.59779600  -0.62053400
O  4.59046200  -0.73315500  -1.45261000
C  5.60686300  -2.48641400  -0.15603500
H  5.33098200  -3.52855600  -0.31163200
H  6.51395100  -2.25132300  -0.70266400
H  5.76435900  -2.33902900  0.91211600
C  -0.75428700  0.34445700  -1.71183000
H  -0.40001000  1.34445700  -1.45833100
H  0.10487800  -0.31473000  -1.74800400
H  -1.19606700  0.36422900  -2.70314000
S  -5.73355200  -0.36563100  -0.21459100
|               | I10 (protonated) |               |
|---------------|------------------|---------------|
|               | $E_e$            | $E_e + ZPV$   |
| Electronic    | Hartree          | Hartree       |
| energy $E_e$  | -1543.075065     | -1542.707704  |

**XYZ coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| N | 1.30443000 | -0.96387500 | -0.30062500 |
| H | 4.19553600 | -1.87385300 | -1.37341900 |
| C | 2.22467600 | -1.58209800 | -1.02947600 |
| N | 3.51269400 | -1.36188600 | -0.81987500 |
| C | 4.02417800 | -0.44426000 | 0.09992600  |
| C | 3.02540900 | 0.18444500  | 0.92281000  |
| C | 1.71165800 | -0.13339900 | 0.76714600  |
| O | 1.81944200 | -2.42517200 | -1.94217100 |
| C | 3.48478900 | 1.14533200  | 1.97584200  |
| H | 4.29416900 | 1.75366500  | 1.57828300  |
| H | 2.68442000 | 1.80465300  | 2.29502200  |
| H | 3.87785000 | 0.61312100  | 2.84494900  |
| C | -0.11740500| -1.04633600 | -0.75897000 |
| H | -0.06582500| -1.38627700 | -1.78868000 |
| C | -1.03444500| -1.95684000 | 0.06933600  |
| H | -1.33334400| -2.81732100 | -0.52409500 |
| H | -0.55053700| -2.31800500 | 0.97221500  |
| C | -2.25285100| -1.07750800 | 0.37133100  |
| H | -2.31792000| -0.81397800 | 1.42449300  |
| C | -2.03802700| 0.17366200  | -0.49700900 |
| H | -2.53640500| 0.02185200  | -1.45953900 |
| C | -2.50570800| 1.46198800  | 0.13583100  |
| H | -3.57843700| 1.41816900  | 0.30258400  |
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | -1.201051 | 3.331549 | -0.549734 |
| O     | 0.438092  | 3.180971 | 0.369313 |
| C     | -0.251228 | 5.039904 | -1.377097 |
| O     | 4.585282  | -1.415150 | 0.614936 |
| O     | 4.634252  | -0.533061 | 1.430168 |
| C     | -5.736543 | -2.243797 | 0.145660 |
| H     | -5.522667 | -3.298022 | 0.316824 |
| H     | -6.634931 | -1.950727 | 0.678255 |
| H     | -5.872064 | -2.099556 | -0.925918 |
| C     | 0.671606  | 0.341074  | 1.730043 |
| H     | 0.308903  | 1.330745  | 1.450522 |
| H     | -0.171345 | -0.337324 | 1.780382 |
| H     | 1.113161  | 0.390930  | 2.721931 |
| S     | 5.651852  | -0.239549 | 0.187254 |
| H     | 2.541642  | -2.769220 | -2.493974 |
I10 (deprotonated)

|                         | Electronic energy ($E_e$) | $E_e +$ ZPV |
|-------------------------|---------------------------|-------------|
|                         |                           | Hartree     |
|                         | -1542.181632              | -1541.840559|

XYZ coordinates

N  1.36966700  -0.79116200  -0.40387000
C  2.28222900  -1.41226000  -1.28792700
N  3.60160000  -1.26213100  -1.06664900
C  4.06850200  -0.54866700  -0.04092100
C  3.15312700  0.08216800   0.89409800
C  1.81771100  -0.10320200  0.71035300
O  1.82997500  -2.08384600  -2.22135400
C  3.67787300  0.90579800   2.03736200
H  4.55560500  1.45760200   1.71025900
H  2.93998100  1.61959000   2.39617900
H  3.99522700  0.28440200   2.87891400
C  -0.03184000 -0.89117200  -0.76679100
H  -0.03611800 -1.18091700  -1.81237900
C  -0.88857500 -1.88493900  0.04464800
H  -1.11746700 -2.75939600  -0.56051300
H  -0.38066600 -2.21765700  0.94557100
C  -2.16755400 -1.10678300  0.35491100
H  -2.24453800 -0.84435700  1.40796100
C  -2.04217700  0.15654400  -0.51338300
H  -2.47283900 -0.05619600  -1.50014300
C  -2.67951500  1.39224900  0.07876400
H  -3.76006000  1.28449100  0.11483000
H  -2.29396400  1.58001600  1.07879500
I10 homodimer

| Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|---------------------------|--------------------|
| Hartree                   |                    |
| -3085.366567              | -3084.654225       |

XYZ coordinates

N  -3.30546900  -0.94027000  -0.51289700
H   -0.10554800   -1.36663300   -0.55057300
C   -1.96706700   -0.60092100   -0.52730500
N   -1.09113800   -1.64317000   -0.53405900
C   -1.40049000   -2.97541700   -0.51853000
C   -2.80236100   -3.28569000   -0.51808700
C   -3.71234700   -2.26921200   -0.56825800
O   -1.57989300    0.56081900   -0.54455800
C   -3.23481000   -4.72409900   -0.49797400
H   -2.50215600   -5.31536400    0.04447500
H   -4.19898500   -4.84501000   -0.01126800
H   -3.30021800   -5.13789500   -1.50698400
C   -4.23332600    0.18357200   -0.34574100
H   -3.61719600    1.01355300   -0.01380500
C   -5.03855100    0.59761800   -1.58988400
H   -4.66636500    1.54477600   -1.97265700
H   -4.97318400   -0.13982200   -2.38482000
C   -6.46804900    0.76490800   -1.06891300
H   -7.14357500    0.00574900   -1.45892500
C   -6.32262100    0.63852500    0.45913700
H   -6.16260600    1.63903000    0.87726500
C   -7.48033400   -0.04011000    1.15399400
H   -8.37891100    0.56409500    1.07283200
H   -7.65913900   -1.02525000    0.72763700
O   -5.16336300   -0.15564500    0.65856100
O   -7.18126400   -0.15102400    2.54870100
C   -6.75469700   -1.33869500    3.01250700
O   -6.72022200   -2.34321400    2.34973300
C   -6.33785900   -1.23474900    4.44619900
H   -5.41392900   -0.65759100    4.49698500
|   |   |   |   |
|---|---|---|---|
|  H | 4.66709800 | -1.54223300 | -1.97530200 |
|  H | 4.97442600 | 0.14285000 | -2.38525500 |
|  C | 6.46838800 | -0.76371500 | -1.06961000 |
|  H | 7.14426300 | -0.00429300 | -1.45851400 |
|  C | 6.32219100 | -0.63892700 | 0.45848700  |
|  H | 6.16189700 | -1.63986000 | 0.87547900  |
|  C | 7.47966400 | 0.03883300  | 1.15456700  |
|  H | 8.37829800 | -0.56522000 | 1.07276700  |
|  H | 7.65849900 | 1.02454300  | 0.72953700  |
|  O | 5.16285900 | 0.15510000  | 0.65820100  |
|  O | 7.18035000 | 0.14787800  | 2.54936000  |
|  C | 6.75400800 | 1.33501300  | 3.01480700  |
|  O | 6.71926400 | 2.34033500  | 2.35329500  |
|  C | 6.33816200 | 1.22928600  | 4.44866400  |
|  H | 5.41584800 | 0.64961900  | 4.49992000  |
|  H | 7.09773500 | 0.70153400  | 5.02222700  |
|  H | 6.17104000 | 2.22062300  | 4.85654900  |
|  O | 6.95668600 | -2.05193700 | -1.44884000 |
|  C | 8.29120700 | -2.22433800 | -1.47737900 |
|  O | 9.07010200 | -1.35667300 | -1.17818800 |
|  C | 8.64958100 | -3.60666800 | -1.92170900 |
|  H | 8.22399300 | -3.79406200 | -2.90680000 |
|  H | 9.72870300 | -3.71238500 | -1.95101500 |
|  H | 8.22024600 | -4.33160800 | -1.23072600 |
|  C | 5.17651900 | 2.56514800  | -0.70286900 |
|  H | 5.63617100 | 2.69096300  | 0.27852100  |
|  H | 5.70599900 | 1.77342000  | -1.21876800 |
|  H | 5.30364000 | 3.48010500  | -1.27375800 |
|  S | 0.15893500 | 4.09257800  | -0.54261500 |
|          | Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|----------|---------------------------|-------------------|
|          | Hartree                   |                   |
|          | -1981.201943              | -1980.699161      |

| XYZ coordinates          |
|--------------------------|
| N 1.23875900 2.66065100 0.38140600 |
| C 0.97365800 3.94663300 0.81090900 |
| N 1.49349300 4.92724400 -0.02639500 |
| C 2.42336200 4.71055900 -1.02437200 |
| C 2.61935600 3.25003400 -1.35678000 |
| O 0.41497800 4.20842600 1.84866200 |
| C 0.48477900 1.53934800 0.90168000 |
| H 0.16093200 1.83388400 1.89640400 |
| C -0.70830500 1.16772200 0.01289700 |
| H -1.06247000 2.01129000 -0.56850100 |
| C -0.16307100 0.02044200 -0.86022100 |
| H 0.13854600 0.41738100 -1.82843600 |
| C 1.02326200 -0.53273200 -0.06304400 |
| H 0.73612300 -1.47543000 0.40546100 |
| C 2.23516700 -0.74609100 -0.93470500 |
| H 1.98656100 -1.41364100 -1.76160800 |
| H 2.59427800 0.20146000 -1.33627300 |
| O 1.30549300 0.40421300 0.97664300 |
| O 3.24707400 -1.34269400 -0.12192100 |
| C 4.41455900 -1.58176300 -0.72977100 |
| O 4.61170500 -1.32851700 -1.89250800 |
| O -1.08953500 -1.04341200 -1.03972000 |
| C -2.27711600 -0.71247200 -1.57836400 |
| O -2.50291200 0.38129200 -2.03042800 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| O       | 1.45199800 | 2.53020000 | -0.99955000 |
| O       | 3.01833000 | 5.61034100 | -1.56083600 |
| C       | -3.26904100 | -1.81550900 | -1.50344800 |
| C       | -2.92201600 | -3.09090400 | -1.06398000 |
| C       | -4.59265500 | -1.51488300 | -1.81597100 |
| C       | -3.90261900 | -4.06494000 | -0.94225300 |
| H       | -1.89486300 | -3.31664900 | -0.81573100 |
| C       | -5.57062900 | -2.48798700 | -1.68126300 |
| H       | -4.84383500 | -0.51472100 | -2.14104200 |
| C       | -5.22567200 | -3.76241800 | -1.24419300 |
| H       | -3.63561100 | -5.05739700 | -0.60644100 |
| H       | -6.00828000 | -2.25242900 | -1.91024800 |
| H       | -5.98931900 | -4.52122700 | -1.13714400 |
| C       | 5.42299100  | -2.18996600 | 0.17983800  |
| C       | 6.64869900  | -2.56868900 | -0.36188600 |
| C       | 5.16521000  | -2.38269700 | 1.53535500  |
| C       | 7.61425600  | -3.14360600 | 0.44980900  |
| H       | 6.83066100  | -2.40998400 | -1.41569800 |
| C       | 6.13594600  | -2.95519600 | 2.34458600  |
| H       | 4.21431800  | -2.08252900 | 1.95107900  |
| C       | 7.35780600  | -3.33643800 | 1.80303400  |
| H       | 8.56501200  | -3.44181300 | 0.03011900  |
| H       | 5.93909200  | -3.10356100 | 3.39728700  |
| H       | 8.11167700  | -3.78376300 | 2.43682100  |
| O       | -1.75777400 | 0.64308800  | 0.80978400  |
| C       | -2.91460700 | 1.34637200  | 0.84630500  |
| O       | -2.99483700 | 2.49478800  | 0.50617600  |
| C       | -4.05342300 | 0.51801200  | 1.32046200  |
| C       | -3.89402200 | -0.82426500 | 1.66168500  |
I11 (protonated)

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -1981.598212              | -1981.081481|

XYZ coordinates

N  1.10256700  1.72021200  0.81441900
H  2.25376900  4.22911200  2.42172500
C  1.16480900  2.67104000  1.71830500
N  2.26410300  3.42733800  1.79605300
C  3.50933500  2.99954600  1.27261700
C  3.38367200  1.74248000  0.44520700
O  0.21657500  2.91921900  2.57176900
C  0.22071300  0.54130800  0.77707000
H  -0.41181500  0.59971400  1.66507300

S148
C  -0.61041500  0.49460700  -0.51069000
H  -0.14040600  1.07453600  -1.30358500
C  -0.57930500  -0.99931000  -0.86422900
H  -0.73106700  -1.18614300  -1.92395500
C  0.79650600  -1.40448800  -0.36183300
H  0.81158000  -2.43976300  -0.02960200
C  1.86738700  -1.16407100  -1.40470600
H  1.74960200  -1.87888500  -2.21996000
H  1.82365700  -0.15733300  -1.81711700
O  1.01452000  -0.59329700  0.81242200
O  3.12113400  -1.36837900  -0.75716800
C  4.20661800  -1.02732800  -1.47125700
O  4.13511000  -0.55382100  -2.57659600
O  -1.54291500  -1.69329500  -0.08108400
C  -2.79988000  -1.72895200  -0.58199300
O  -3.08948400  -1.22966500  -1.63706900
O  2.08292200  1.73046800  -0.15073000
O  4.51191200  3.59332700  1.51371000
C  -3.75006200  -2.44001300  0.30767600
C  -3.32531800  -3.13632100  1.43774100
C  -5.10275500  -2.39252100  -0.02475900
C  -4.25785200  -3.79087300  2.22901600
H  -2.27506900  -3.17287500  1.68876700
C  -6.03041000  -3.04144300  0.77445200
H  -5.41063900  -1.84516000  -0.90514700
C  -5.60748000  -3.74198300  1.89903900
H  -3.93396400  -4.34165300  3.10112300
H  -7.08069000  -3.00516100  0.52055000
H  -6.33171700  -4.25293300  2.51894800

S149
I11 (deprotonated)

|                | $E_e$   | $E_e + ZPV$ |
|----------------|---------|-------------|
| Electronic energy (hartree) |         |             |
|                | -1980.710316 | -1980.220563 |

XYZ coordinates

N                  1.25646000    2.72227000    0.47831600
C                  0.84114400    4.04500700    0.83134100
N                  1.26773200    5.07582600    0.07198600
C                  2.14349500    4.86308700    -0.92860100
C                  2.49118400    3.43231600    -1.30470500
O                  0.18260700    4.16911400    1.85917700
C                  0.48287000    1.60891500    0.96071800
H                  0.14151500    1.88144200    1.95321000
C                  -0.69713000    1.23686200    0.05234200
H                  -1.06955300    2.08740000    -0.50713000
C                  -0.12603700    0.12150400    -0.84622400
H                  0.16527800    0.54278200    -1.80642100
C                  1.06875900    -0.42770100    -0.05608400
H                  0.80948700    -1.41052700    0.34321300
C                  2.30205300    -0.55763100    -0.91638200
H                  2.08260600    -1.17313300    -1.79043500
H                  2.65671800    0.41979200    -1.24057100
O                  1.28543100    0.44480100    1.04485800
O                  3.30759500    -1.19766500    -0.12355800
C                  4.45179600    -1.47983900    -0.74941700
O                  4.64220600    -1.24457800    -1.91752500
O                  -1.02623800    -0.96697200    -1.04835200
C                  -2.21490500    -0.66925700    -1.59362400
\begin{tabular}{cccc}
\hline
& & & \\
C & -3.79824900 & -0.92754400 & 1.66034300 \\
C & -5.32866800 & 0.90904400 & 1.31827900 \\
C & -4.86205800 & -1.74268100 & 2.02072700 \\
H & -2.79172500 & -1.31966100 & 1.63814400 \\
C & -6.38862200 & 0.09219200 & 1.68080000 \\
H & -5.49180300 & 1.93913800 & 1.03373500 \\
C & -6.15587700 & -1.23380400 & 2.02959600 \\
H & -4.68169100 & -2.77498900 & 2.28802500 \\
H & -7.39528600 & 0.48654000 & 1.68772000 \\
H & -6.98476700 & -1.87137300 & 2.30683300 \\
H & 2.57809200 & 3.34732000 & -2.38506100 \\
H & 3.43393600 & 3.14039300 & -0.83005600 \\
\hline
\end{tabular}

I12

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -1554.338102              | -1553.859145 |

XYZ coordinates

\begin{tabular}{cccc}
\hline
& & & \\
N & 2.66372700 & -0.74599200 & 0.33756600 \\
H & 4.79858000 & -2.23219100 & -1.57605400 \\
C & 3.65541600 & -0.85684000 & -0.62067400 \\
N & 4.08638800 & -2.13856400 & -0.86223500 \\
C & 3.69894900 & -3.30204400 & -0.19910500 \\
C & 2.73017600 & -3.07458700 & 0.85107500 \\
C & 2.27440500 & -1.83080800 & 1.07860500 \\
O & 4.09983000 & 0.11067500 & -1.20539300 \\
O & 4.17783900 & -4.37452000 & -0.51606400 \\
\hline
\end{tabular}
I12 (protonated)

| Electronic energy ($E_e$) | $E_e +$ ZPV | Hartree |
|---------------------------|-------------|---------|
| -1554.745128              | -1554.25349 |         |

**XYZ coordinates**

|     |          |          |          |
|-----|----------|----------|----------|
| N   | 2.71707000 | -0.68337100 | 0.36178200 |
| H   | 5.08062800 | -1.99962600 | -1.41982900 |
C  3.78175400  -0.70290400  -0.52791100
N  4.30823000  -1.97539700  -0.75762400
C  3.87679700  -3.09790700  -0.16553800
C  2.83082000  -3.02594900   0.75079700
C  2.29719900  -1.79208200   0.99180700
O  4.22062500   0.27977200  -1.05912300
O  4.43015300  -4.24786100  -0.43611300
C  2.18094000   0.68943400   0.68146700
H  3.04057900   1.25952600   1.03154700
H  2.94485000   1.36160500  -0.55496800
H  1.69117200   0.77194600  -1.45528600
H  0.06226800  1.55593600  -0.16925800
H  0.63338600  1.16643000  -0.90979400
C -0.10492000   0.82642200  1.15845800
H -0.62476300  1.44766500  1.88542400
C -0.84745800  -0.48972200   0.99025000
H -0.37302100  -1.07653200  0.18885900
H -0.78235400  -1.06521700  1.91860100
O  1.22433400   0.58725300  1.67101000
O -0.10246700  2.95489300  -0.10194000
O -2.18224600  -0.17763000  0.68873700
H  2.48610300  -3.91078200  1.25772600
O  2.03241000  2.65389300  -0.77601000
C  1.16868300  3.59469300  -0.13366500
C  1.07836700  4.82432700  -1.00334900
H  0.37307900  5.53197400  -0.57050000
H  2.05484800  5.30142100  -1.07510700
H  0.74103200  4.54325000  -1.99914800
C  1.64745600  3.90638100  1.27373400
H  2.65463500  4.31986900  1.23839400
H  0.98114900  4.63881300  1.72762100
H  1.65064900  3.01560000  1.90171500
Si -3.16138500 -1.19744500 -0.20791600
C  -4.85322800 -0.38078400 -0.17517200
C  -3.16095900 -2.88882100  0.58302700
H  -3.76034300 -3.59052500  0.00142000
H  -2.14754500 -3.29370400  0.63597900
H  -3.56239600 -2.86008400  1.59718300
C  -2.46492500 -1.31815600 -1.93873600
H  -3.12314000 -1.91092000 -2.57757400
H  -2.35096600 -0.33498500 -2.39779000
H  -1.49111500 -1.81247400 -1.94119300
C  -5.26112000 -0.09521800  1.27554100
H  -4.56234500  0.58793800  1.76046000
H  -6.25270000  0.36724300  1.29873600
H  -5.31221700 -1.00874900  1.87245400
C  -5.88589100 -1.31550900 -0.81687100
H  -6.86843000 -0.83408900 -0.82649300
H  -5.63234500 -1.55909500 -1.85142000
H  -5.98360300 -2.25132900 -0.26243500
C  -4.80324900  0.93729600 -0.95819300
H  -4.58877700  0.76861100 -2.01545000
H  -5.77043300  1.44539400 -0.89502900
H  -4.04638900  1.61773600 -0.56153300
H  1.51427900 -1.64489900  1.72119200
H  5.17545300 -4.19162900 -1.05675800
I12 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -1553.841104             | -1553.375546 |

XYZ coordinates

N  2.53739700  -0.91576400  0.33662700
C  3.44726800  -1.19881200  -0.71455500
N  3.72708500  -2.47511600  -1.01411100
C  3.25082400  -3.50934500  -0.26836600
C  2.45531200  -3.19638100   0.91883200
C  2.13677000  -1.91742200   1.17363300
O  3.91993300  -0.21804400  -1.30420900
O  3.49120500  -4.69149500  -0.56501600
C  2.28213800   0.50466000   0.62448900
H  3.23073900   0.98462200   0.86141000
C  1.60766000   1.22851000  -0.56178900
H  1.60897500   0.60443200  -1.44790300
C  0.20280700   1.60559800  -0.05114800
H  -0.60063100  1.31805900  -0.72638800
C  0.07829300   0.89934900   1.28971300
H  -0.38773500  1.54713700  2.03168500
C  -0.72305600  -0.39057900  1.17181300
H  -0.28783700  -1.02322200  0.38856000
H  -0.67117000  -0.94049500  2.11462500
O  1.41785000   0.63820200  1.72622700
O  0.22074700   3.01958000   0.04629500
O  -2.06321800  -0.04833400  0.88279000
H  2.13422600  -3.99358200  1.57074800

S158
O      2.20450300  2.46340100  -0.88341100
C      1.54389400  3.49996500  -0.17504800
C      1.48043100  4.71908900  -1.06630100
H      0.93577700  5.51878700  -0.56599700
H      2.48831700  5.06725300  -1.28913300
H      0.97483100  4.46537700  -1.99616800
C      2.23141800  3.79102500  1.15028300
H      3.26447400  4.08812800  0.97191000
H      1.71379300  4.60285400  1.66130700
H      2.22062600  2.91446700  1.79640000
Si     -2.97145100 -0.96672600  -0.17449800
C     -4.65872900 -0.12876800  -0.20458800
C     -3.06373400 -2.72379400  0.45337700
H     -3.60259300 -3.36227200  -0.24913600
H     -2.06004200 -3.14133400  0.56436300
H     -3.56119000 -2.78745000  1.42234600
C     -2.16339300 -0.96173600  -1.85998900
H     -2.73912900 -1.57322400  -2.55819600
H     -2.08535000  0.04238200  -2.27900200
H     -1.15824200 -1.38766200  -1.81738800
C     -5.19702900  0.01115200  1.22395700
H     -4.53979600  0.62486000  1.84178400
H     -6.18229200  0.48855400  1.20622400
H     -5.31203300 -0.95885400  1.71291100
C     -5.63535300 -0.97192600  -1.03342200
H     -6.60749600 -0.47191300  -1.09211900
H     -5.28150800 -1.11869700  -2.05672200
H     -5.79785500 -1.95600100  -0.58831800
C     -4.52897400  1.26468900  -0.83265500
I13

|                | $E_e$          | $E_e + ZPV$ |
|----------------|----------------|-------------|
|                | Hartree        |             |
|                | -1782.194815   | -1781.673788|

XYZ coordinates

|    |         |         |         |
|----|---------|---------|---------|
| N  | 2.15617400 | -0.72673100 | -0.55277400 |
| H  | 2.49260100 | -2.43395100 | -3.27851800 |
| C  | 2.44543300 | -0.95518000 | -1.88953800 |
| N  | 2.32833900 | -2.26629100 | -2.29294100 |
| C  | 2.07290500 | -3.37465700 | -1.49432300 |
| C  | 2.02362800 | -3.06410500 | -0.07534100 |
| C  | 2.10759200 | -1.78732000 | 0.32974900  |
| O  | 2.75166900 | -0.06651800 | -2.65464400 |
| O  | 1.96105500 | -4.48032300 | -1.98202000 |
| C  | 2.00959400 | 0.69063900  | -0.09897500 |
| H  | 3.00274000 | 1.12848100  | -0.02606700 |
| C  | 1.09823700 | 1.53065700  | -1.03358800 |
| H  | 0.82915000 | 0.99839500  | -1.93723500 |
| C  | -0.11330300 | 1.90246700 | -0.16274200 |
| H  | -1.06771100 | 1.78141400 | -0.67248700 |
| C  | -0.00343300 | 0.98620500 | 1.03798600  |
| H  | -0.31377500 | 1.47912100 | 1.95705300  |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -0.79643400  | -0.29901900  | 0.84131200   |
| H       | -0.50609800  | -0.76342200  | -0.11017900  |
| H       | -0.55737800  | -1.00004500  | 1.64402500   |
| O       | 1.40247100   | 0.70527700   | 1.16038600   |
| O       | 0.08306800   | 3.26756700   | 0.15114900   |
| O       | -2.16763900  | 0.02962800   | 0.85581800   |
| H       | 1.99919700   | -3.87476700  | 0.63514200   |
| O       | 1.67413700   | 2.75916600   | -1.38629900  |
| C       | 1.29494800   | 3.74602800   | -0.42919900  |
| C       | 1.01961400   | 5.03544400   | -1.16708400  |
| H       | 0.66088200   | 5.79026600   | -0.46881300  |
| H       | 1.93263300   | 5.39790800   | -1.63782100  |
| H       | 0.26399700   | 4.86604400   | -1.93235700  |
| C       | 2.35443000   | 3.90621100   | 0.64759800   |
| H       | 3.30532500   | 4.18545700   | 0.19517900   |
| H       | 2.05056300   | 4.69006800   | 1.34076100   |
| H       | 2.47877700   | 2.98211200   | 1.21056300   |
| Si      | -3.25623500  | -0.80504600  | -0.09939800  |
| C       | -4.92259800  | -0.00633000  | 0.26220900   |
| C       | -3.20883800  | -2.61389200  | 0.35870500   |
| H       | -3.86591200  | -3.20422800  | -0.28239200  |
| H       | -2.19752600  | -3.01139500  | 0.24116300   |
| H       | -3.50914900  | -2.77432000  | 1.39518800   |
| C       | -2.76674900  | -0.60322300  | -1.89455200  |
| H       | -3.49109800  | -1.09699600  | -2.54561800  |
| H       | -2.71846900  | 0.44702300   | -2.18718100  |
| H       | -1.79496200  | -1.05924800  | -2.09764500  |
| C       | -5.19822600  | -0.04010400  | 1.76994400   |
| H       | -4.43732800  | 0.50610000   | 2.32939000   |
I13 (protonated)

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -1782.596338              | -1782.061465|

XYZ coordinates

N  2.36112700  -0.52208400  -0.41866700
H  3.41987100  -1.94009400  -3.13717300
C  2.89360200  -0.58807100  -1.70092000
N  3.09461100  -1.89110700  -2.17385800
I13 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -1781.703663              | -1781.196068 |

XYZ coordinates

|   |                  |                  |                  |
|---|------------------|------------------|------------------|
| N | 2.09603600       | -0.83701600      | -0.60249600      |
| C | 2.31324600       | -1.11648700      | -1.98117500      |
| N | 1.98951300       | -2.33040000      | -2.45354000      |
| C | 1.61252000       | -3.34120400      | -1.63008800      |
| C | 1.74162900       | -3.12904200      | -0.18085300      |
| C | 1.98783900       | -1.89097800      | 0.27155600       |
| O | 2.76317900       | -0.19325800      | -2.66572700      |
| O | 1.21336500       | -4.43271200      | -2.05897100      |
| C | 2.08453600       | 0.56319600       | -0.14272200      |
| H | 3.10289300       | 0.94343700       | -0.08060300      |
| C | 1.21171000       | 1.47394000       | -1.04367400      |
| H | 0.92625500       | 0.97591500       | -1.96045300      |
| C | 0.01938600       | 1.87931000       | -0.16088900      |
| H | -0.94372700      | 1.79120200       | -0.66059100      |
| C | 0.11472800       | 0.96019100       | 1.04031100       |
| H | -0.16607600      | 1.47105900       | 1.96023900       |
| C | -0.74153500      | -0.28848100      | 0.86834200       |
| H | -0.50424200      | -0.77370500      | -0.08567300      |
| H | -0.51511600      | -0.99784000      | 1.66724200       |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| O       | 1.5054300  | 0.6289600  | 1.1431400  |
| O       | 0.2547400  | 3.2405900  | 0.1572900  |
| O       | -2.1014800 | 0.10036100 | 0.9227660  |
| H       | 1.68166300 | -3.96665800| 0.4966700  |
| O       | 1.83541600 | 2.69226900 | -1.37349400|
| C       | 1.49099000 | 3.67331900 | -0.40562200|
| C       | 1.27435900 | 4.98858800 | -1.11984800|
| H       | 0.94908700 | 5.74734900 | -0.40911000|
| H       | 2.20265600 | 5.31827100 | -1.58497800|
| H       | 0.51269000 | 4.86523300 | -1.88789400|
| C       | 2.54933500 | 3.77337000 | 0.68113800 |
| H       | 3.51032600 | 4.03583500 | 0.23972100 |
| H       | 2.26626100 | 4.54596900 | 1.39588700 |
| H       | 2.64425200 | 2.82870000 | 1.21421200 |
| Si      | -3.21594700| -0.63751600| -0.07775000|
| C       | -4.86093800| 0.17813000 | 0.35196700 |
| C       | -3.22081100| -2.47505900| 0.25176300 |
| H       | -3.90157400| -2.99602000| -0.42378500|
| H       | -2.22265600| -2.88964300| 0.08931000 |
| H       | -3.51243600| -2.70415900| 1.27793000 |
| C       | -2.74444300| -0.33185700| -1.86125900|
| H       | -3.48118000| -0.77740100| -2.53313600|
| H       | -2.68224500| 0.73249900 | -2.09263800|
| H       | -1.78099200| -0.78771400| -2.10151300|
| C       | -5.11173700| 0.08518700 | 1.86149200 |
| H       | -4.33260300| 0.59639500 | 2.42888400 |
| H       | -6.07050900| 0.55136200 | 2.11172100 |
| H       | -5.15199300| -0.95114800| 2.20415900 |
| C       | -5.99562900| -0.53310200| -0.39541900|
### 2.10.2 Heterodimers of I1-A5 and I2-A1

**I1-A5 heterodimer**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| **Hartree**               |             |
| -804.5205426              | -804.2000390|

**XYZ coordinates**

| C | -2.05627600 | 1.48504500 | -0.27579000 |
| C | -1.22581600 | -0.82166400 | -0.45785300 |
| C | -2.63979400 | -1.33731700 | -0.49512000 |
| C | -3.63838000 | -0.43776600 | 0.23772000  |
| C | -3.47507800 | 0.97737600  | -0.32304600 |
| X         | Y         | Z         |
|-----------|-----------|-----------|
| -2.914324 | -1.410918 | -1.552655 |
| -2.628891 | -2.347468 | -0.087936 |
| -3.775915 | 0.994753  | -1.375737 |
| -4.095829 | 1.697996  | 0.207729  |
| -0.076229 | 0.878981  | -0.349640 |
| -1.049960 | 0.537661  | -0.383571 |
| -0.259900 | -1.564434 | -0.510464 |
| -1.773813 | 2.657466  | -0.172938 |
| -3.358814 | -0.448807 | 1.743290  |
| -4.066076 | 0.197348  | 2.265132  |
| -3.463035 | -1.458599 | 2.142873  |
| -2.351354 | -0.098368 | 1.977199  |
| -5.058253 | -0.932623 | -0.021515 |
| -5.187107 | -1.946895 | 0.360406  |
| -5.785401 | -0.289700 | 0.477352  |
| 3.641853  | -1.625201 | 0.000221  |
| 5.004608  | -0.968717 | -0.129793 |
| 5.044694  | 0.299768  | 0.712726  |
| 4.005126  | 1.287211  | 0.192564  |
| 2.649915  | 0.673235  | -0.071928 |
| 2.564970  | -0.657438 | -0.194685 |
| 4.829580  | 0.049674  | 1.754754  |
| 3.518640  | -2.414881 | -0.739628 |
| 5.768059  | -1.678773 | 0.186427  |
| 3.847262  | 2.121564  | 0.873797  |
| 1.626148  | -1.017161 | -0.347360 |
| 1.654738  | 1.397692  | -0.199774 |
| -5.284202 | -0.938913 | -1.089042 |
| 3.541724  | -2.079561 | 0.989432  |
I2-A1 heterodimer

|                | $E_e$          | $E_e + ZPV$     |
|----------------|----------------|----------------|
|                | Hartree        |                |
|                | -804.513376166 | -804.194751    |

XYZ coordinates

| ch   | $X$    | $Y$    | $Z$    |
|------|--------|--------|--------|
| O    | -2.63978900 | 1.36473500 | -0.29686400 |
| N    | -2.90249600 | -0.87325600 | 0.10734900 |
| C    | -3.34136600 | 0.35928300 | -0.18293700 |
| C    | -3.96605700 | -1.85312100 | 0.28651200 |
| C    | -5.15202300 | -1.18821500 | -0.42990200 |
| C    | -4.84895700 | 0.30868600 | -0.32129600 |
| H    | -1.93116700 | -1.03742000 | 0.35738000 |
| H    | -6.10452100 | -1.46973400 | 0.01006700 |
| H    | -5.15444600 | -1.48798600 | -1.47706800 |
| O    | 0.00881100  | -1.00627900 | 0.70539700 |
| N    | 0.15121600  | 1.16740200  | 0.00462500 |
| C    | 0.67027000  | -0.02266100 | 0.43743200 |
| C    | 1.11518400  | 2.12956500  | -0.23049400 |
| C    | 2.46943500  | 1.51629500  | 0.05338800 |
| C    | 2.18846300  | 0.08354100  | 0.53862700 |
| H    | -0.86293800 | 1.31701700  | -0.12187500 |
| H    | 3.05190100  | 1.54598000  | -0.86748700 |
| H    | 2.98542700  | 2.12959300  | 0.79110500 |
|  | X     | Y     | Z     |
|---|-------|-------|-------|
| O | 0.88447700 | 3.25274000 | -0.60341200 |
| C | 2.80133600 | -0.99174200 | -0.37272000 |
| H | 2.38662400 | -1.96128000 | -0.08661800 |
| H | 2.47826800 | -0.79890000 | -1.40102400 |
| C | 4.32483700 | -1.05864900 | -0.32883700 |
| H | 4.74730300 | -0.06557000 | -0.50463500 |
| H | 4.65006700 | -1.36549200 | 0.66657900 |
| C | 4.87209300 | -2.03728100 | -1.36220700 |
| H | 5.95929200 | -2.09932100 | -1.31447800 |
| H | 4.47144100 | -3.03918500 | -1.19831900 |
| H | 4.59739100 | -1.73189300 | -2.37310800 |
| C | 2.57471100 | -0.11741800 | 2.00682700 |
| H | 2.33800900 | -1.13115400 | 2.32983800 |
| H | 3.64144000 | 0.05480700 | 2.14444200 |
| H | 2.03574700 | 0.58341400 | 2.64649700 |
| H | -5.17613300 | 0.90245500 | -1.17070900 |
| H | -5.27085100 | 0.75049500 | 0.58414100 |
| H | -3.69000100 | -2.80811700 | -0.15428700 |
| H | -4.16914300 | -2.00599800 | 1.34840500 |
2.10.3 A2···CHCl₃ complexes

Cx-1

| Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|---------------------------|--------------------|
|                           | Hartree            |
| -1741.829204             | -1741.719637       |

XYZ coordinates

|   |      |      |      |      |
|---|------|------|------|------|
| C | 3.33613300 | -0.72711800 | 0.87797700 |
| C | 1.89560900 | 0.23621200 | -0.65918500 |
| C | 4.05476000 | 0.33593900 | 0.04746400 |
| H | 1.18360900 | -0.98814900 | 0.80499500 |
| N | 1.95975600 | -0.40336000 | 0.53840500 |
| O | 0.92035400 | 0.45737200 | -1.33646400 |
| H | 4.98670800 | -0.00786400 | -0.38858700 |
| H | 3.52954800 | -0.61162100 | 1.94068500 |
| H | 3.59935200 | -1.73820500 | 0.56495900 |
| H | 4.21972100 | 1.24910100 | 0.61766800 |
| O | 3.13557300 | 0.63505200 | -1.01868000 |
| H | -1.28063400 | 0.48831100 | -1.05753900 |
| C | -1.82868300 | 0.11834600 | -0.20392400 |
| Cl | -1.50090700 | -1.62048900 | -0.06533000 |
| Cl | -1.24362000 | 0.97437900 | 1.23080300 |
| Cl | -3.55846900 | 0.40565600 | -0.44687600 |
**Cx-2**

| Electronic energy \((E_e)\) | \(E_e + ZPV\) |
|----------------------------|---------------|
| Hartree                    |               |
| -1741.831369              | -1741.721785  |

**XYZ coordinates**

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| C     | -3.36561400| 0.45329500 | -0.49154800|
| C     | -1.78020300| -0.80089200| 0.64246300 |
| C     | -2.18648800| 1.32712800 | -0.05926300|
| H     | -3.32025300| -1.71382900| -0.33194300|
| N     | -2.78775100| -0.86141300| -0.26363200|
| O     | -1.20785400| -1.70673800| 1.19852500 |
| H     | -2.48069700| 2.23024900 | 0.46488300 |
| H     | -3.62124400| 0.60724100 | -1.53611500|
| H     | -4.24698600| 0.61826600 | 0.12937400 |
| H     | -1.53919600| 1.57492100 | -0.89995400|
| O     | -1.44461400| 0.49532600 | 0.84981400 |
| H     | 0.84834800 | -0.45737000| 0.93045900 |
| C     | 1.45887300 | -0.05882900| 0.13084400 |
| Cl    | 3.07932600 | -0.76302600| 0.25220800 |
| Cl    | 0.70024200 | -0.50861300| -1.40784800|
| Cl    | 1.53423300 | 1.70325600 | 0.29487800 |
## 2.10.4 Compounds studied in CCl₄

### A1

|                        |           |          |
|------------------------|-----------|----------|
| **Electronic energy (Eₑ)** | **Eₑ + ZPV** |
| **Hartree**         |           |
| -286.6105564          | -286.49861|

**XYZ coordinates**

|             |          |          |          |
|-------------|----------|----------|----------|
| C           | -1.33056700 | -0.83686600 | 0.00023600 |
| C           | 0.90111800  | -0.00389100 | -0.00000100 |
| C           | 0.01538600  | 1.22994800  | 0.00023900  |
| C           | -1.43056700 | 0.71036300  | -0.00031900 |
| H           | 0.26104600  | 1.82617600  | 0.87720300  |
| H           | 0.26147400  | 1.82690400  | 0.87652600  |
| H           | -1.97543900 | 1.05317800  | 0.87503800  |
| H           | -1.97445100 | 1.05258100  | -0.87652600 |
| H           | 0.49212800  | -2.01825600 | -0.0009300  |
| N           | 0.09682100  | -1.09217800 | -0.00014000 |
| O           | 2.11584700  | -0.01874200 | -0.00007200 |
| H           | -1.80103600 | -1.27169800 | -0.88144200 |
| H           | -1.80046900 | -1.27102900 | 0.88255200  |
### A1 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -287.0051477             | -286.879757|

XYZ coordinates

|      | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.36661700 | -0.84004100 | 0.10543500 |
| C    | 0.77672900   | 0.01821200   | 0.00286500  |
| C    | -0.08349800  | 1.22277800  | 0.13744400  |
| C    | -1.47942300  | 0.66471300  | -0.18227300 |
| H    | 0.01335000   | 1.57256800  | 1.16884300  |
| H    | 0.25536100   | 2.02109800  | -0.51850500 |
| H    | -2.25975600  | 1.13032400  | 0.40969700  |
| H    | -1.70369100  | 0.82093100  | -1.23475000 |
| H    | 0.49330800   | -2.00329000 | -0.05604300 |
| N    | 0.08701900   | -1.07472000 | -0.02851500 |
| O    | 2.06817500   | 0.11197300  | -0.04527000 |
| H    | -1.66339000  | -1.10561500 | 1.11839300  |
| H    | -1.90041600  | -1.46217600 | -0.60561300 |
| H    | 2.52755700   | -0.74055600 | -0.10108400 |

### A1 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -286.0651134             | -285.96761 |

XYZ coordinates

|      | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.28368600 | -0.82029700 | 0.11680800 |
C    0.86342500 -0.11227300 -0.00648800
C    0.00863400  1.16966500  0.15989100
C   -1.38983400  0.68852300 -0.20009200
H    0.07880600  1.49351300  1.20273600
H    0.39670400  1.97215500 -0.46533700
H   -2.19808500  1.18651900  0.33835700
H   -1.56381100  0.82260300 -1.26982000
N    0.11023000 -1.19457400 -0.05183800
O    2.11026900 -0.03045700 -0.06034800
H   -1.62180100 -1.00815900  1.14891200
H   -1.93681300 -1.41465300 -0.52991100

A1 homodimer

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -573.239106               | -573.013622 |

XYZ coordinates

O    0.99254300  1.60181100 -0.03256400
N    1.70954600 -0.57363300 -0.03217900
C    1.88237900  0.75700800  0.00780300
C    2.93856300 -1.33322300  0.13667600
C    4.02182800 -0.29990300 -0.21360200
C    3.36820800  1.03858300  0.13833400
H    0.77606600 -0.98979700 -0.00320000
H    2.95456100 -2.19820700 -0.52261500
H    3.03619800 -1.68396600  1.16687200
H    4.22508500 -0.33985100 -1.28307100
|          |          |          |          |
|----------|----------|----------|----------|
| H        | 4.95151100 | -0.48374600 | 0.31808800 |
| H        | 3.65887800 | 1.87027400  | -0.49759100 |
| H        | 3.55315800 | 1.32673700  | 1.17555400 |
| O        | -0.99254500| -1.60181700 | 0.03242800 |
| N        | -1.70954100| 0.57362900  | 0.03214000 |
| C        | -1.88238100| -0.75701000 | -0.00786300 |
| C        | -2.93856700| 1.33323000  | -0.13659900 |
| C        | -4.02181300| 0.29990000  | 0.21371000 |
| C        | -3.36821900| -1.03857700 | -0.13831000 |
| H        | -0.77606200| 0.98979200  | 0.00311500 |
| H        | -2.95451700| 2.19818600  | 0.52273000 |
| H        | -3.03627000| 1.68401800  | -1.16677300 |
| H        | -4.22500800| 0.33981300  | 1.28319200 |
| H        | -4.95152600| 0.48376200  | -0.31792000 |
| H        | -3.65885200| -1.87028700 | 0.49760700 |
| H        | -3.55323500| -1.32669700 | -1.17552700 |

**A3**

|                     |          |          |
|---------------------|----------|----------|
| Electronic energy ($E_e$) |          |          |
| $E_e + ZPV$          |          |          |
| **Hartree**          |          |          |
| -365.2250446         | -365.054783 |

**XYZ coordinates**

|          |          |          |          |
|----------|----------|----------|----------|
| C        | -1.38219300 | 0.03188400 | 0.02701700 |
| C        | -0.61949100 | -1.14458800 | 0.59900700 |
| C        | 0.58559100  | -1.55766900 | -0.25976300 |
| C        | 1.84212100  | -0.71980900 | -0.02954900 |
| C        | 0.63172500  | 1.48947000  | 0.41778800  |
A3 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -365.6244961              | -365.440382|

XYZ coordinates

|   |      |      |      |
|---|------|------|------|
| C | 1.26349800 | -0.03560900 | 0.07988100 |
| C | 0.55703400 | 1.15310100 | 0.62072200 |
| C | -0.63627900 | 1.55935600 | -0.26753400 |
| C | -1.88327500 | 0.70669100 | -0.05419000 |
| C | -0.67800200 | -1.50113100 | 0.42805200 |
| C | -1.72648200 | -0.77144600 | -0.40143900 |
| H | 0.20802300 | 0.91761000 | 1.62970000 |
A3 (deprotonated)

|                | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------------|---------------------------|-------------|
|                | Hartree                   |             |
|                | -364.672207               | -364.516189 |

XYZ coordinates

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.35756600| -0.15839600| 0.00674600|
| C       | 0.62685500| 1.04383000| 0.64458200|
| C       | -0.53523400| 1.55104900| -0.21773600|
| C       | -1.81646900| 0.73282600| -0.06121200|
| C       | -0.58497600| -1.47374500| 0.41661200|
| C       | -1.67251400| -0.75013900| -0.39639800|
| H       | 0.24959100| 0.79308000| 1.64183900|
| H       | -0.22108100| 1.55255800| -1.26588600|
A3 homodimer

|               | Electronic energy ($E_e$) | $E_e + ZPV$          |
|---------------|---------------------------|----------------------|
|               | Hartree                   |                      |
|               | -730.4681104              | -730.124847          |

XYZ coordinates

|     |               |                 |                |
|-----|----------------|-----------------|----------------|
| C   | 1.90426000    | 0.83427600      | -0.59194900    |
| C   | 3.30516600    | 1.39518200      | -0.49640800    |
| C   | 3.97667500    | 1.10077000      | 0.85436200     |
| C   | 4.58492900    | -0.29664700     | 0.96284400     |
| C   | 2.83738100    | -1.47606500     | -0.49050000    |
| C   | 3.58897400    | -1.44769500     | 0.83885300     |
| H   | 3.91881600    | 0.99230700      | -1.30697500    |
| H   | 3.25125300    | 1.25707800      | 1.65702800     |
| H   | 5.34522000    | -0.40675600     | 0.18282300     |
| H   | 3.54222600    | -1.34912300     | -1.31724600    |
| H   | 3.20953400    | 2.46720200      | -0.64766300    |
| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| H     | 4.76938600 | 1.83464900 | 1.00395900 |
| H     | 5.10664900 | -0.38107700| 1.91795700 |
| H     | 2.36661200 | -2.44814600| -0.62346500|
| H     | 4.12998600 | -2.39039900| 0.94281400 |
| H     | 2.85769400 | -1.40598100| 1.64982900 |
| N     | 1.76395100 | -0.49916300| -0.58913200|
| O     | 0.92811100 | 1.58764600 | -0.64701800|
| H     | 0.80630500 | -0.85381100| -0.62172100|
| C     | -1.90428000| -0.83423000| -0.59206500|
| C     | -3.30518700| -1.39513800| -0.49654100|
| C     | -3.97666400| -1.10083900| 0.85427000 |
| C     | -4.58490600| 0.29657200  | 0.96289700 |
| C     | -2.83738100| 1.47611200 | -0.49036900|
| C     | -3.58894300| 1.44762300 | 0.83899800 |
| H     | -3.91885100| -0.99219200| -1.30706100|
| H     | -3.25122600| -1.25725000| 1.65690700 |
| H     | -5.34521100| 0.40676100 | 0.18290100 |
| H     | -3.54224500| 1.34925600 | -1.31711100|
| H     | -3.20956400| -2.46714500| -0.64788900|
| H     | -4.76937800| -1.83472400| 1.00382100 |
| H     | -5.10660700| 0.38091200 | 1.91802900 |
| H     | -2.36660500| 2.44820100 | -0.62325600|
| H     | -4.12994200| 2.39032200 | 0.94306700 |
| H     | -2.85764500| 1.40581800 | 1.64995200 |
| N     | -1.76396100| 0.49920900 | -0.58911700|
| O     | -0.92813300| -1.58759900| -0.64718900|
| H     | -0.80631200| 0.85385300 | -0.62165700|
### A5

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -325.9205094             | -325.779034 |

**XYZ coordinates**

| Atom | X     | Y     | Z     | E     | ZPV   |
|------|-------|-------|-------|-------|-------|
| C    | 1.041 | -1.277| 0.138 | 0.138 | 0.000 |
| C    | -1.135| -0.013| 0.320 | 0.320 | 0.000 |
| C    | -0.372| 1.293 | -0.119| -0.119| 0.000 |
| C    | 1.085 | 1.202 | 0.320 | 0.320 | 0.000 |
| C    | 1.738 | -0.011| -0.329| -0.329| 0.000 |
| H    | 1.298 | -1.470| 1.184 | 1.184 | 0.000 |
| H    | 1.369 | -2.136| 0.447 | 0.447 | 0.000 |
| H    | -0.428| 1.592 | -1.170| -1.170| 0.000 |
| H    | -0.934| 2.032 | 0.448 | 0.448 | 0.000 |
| H    | 1.612 | 2.119 | 0.057 | 0.057 | 0.000 |
| H    | 1.139 | 1.102 | 1.408 | 1.408 | 0.000 |
| H    | 1.661 | 0.070 | -1.417| -1.417| 0.000 |
| H    | 2.796 | -0.077| -0.076| -0.076| 0.000 |
| H    | -0.959| -1.995| 0.097 | 0.097 | 0.000 |
| N    | -0.406| -1.157| -0.001| -0.001| 0.000 |
| O    | -2.356| -0.037| -0.002| -0.002| 0.000 |
A5 (protonated)

|          | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------|---------------------------|-------------|
|          |                           | Hartree     |
|          | -326.320572               | -326.165568 |

XYZ coordinates

| C        | -1.06970500 | -1.29904600 | -0.12710500 |
| C        | 1.01399900  | 0.00718600  | 0.00812200  |
| C        | 0.29813000  | 1.30854000  | 0.06158300  |
| C        | -1.17752700 | 1.18193700  | -0.30202300 |
| C        | -1.76879100 | -0.04977400 | 0.37091900  |
| H        | -1.33481100 | -1.52189300 | -1.16027500 |
| H        | -1.30001300 | -2.16652900 | 0.48602800  |
| H        | 0.43036800  | 1.67856300  | 1.08291200  |
| H        | 0.83946400  | 1.99822400  | -0.58670400 |
| H        | -1.69925900 | 2.08390600  | 0.00759100  |
| H        | -1.28427700 | 1.09945000  | -1.38478800 |
| H        | -1.65909400 | 0.02584400  | 1.45455300  |
| H        | -2.83046500 | -0.14536900 | 0.15338100  |
| H        | 0.95190400  | -1.97832700 | -0.14010600 |
| N        | 0.40091900  | -1.12795300 | -0.08061800 |
| O        | 2.31657900  | 0.08725300  | 0.06506800  |
| H        | 2.77048600  | -0.76927500 | 0.06222100  |
### A5 (deprotonated)

| Electronic energy ($E_e$) | $E_e + \text{ZPV}$ |
|---------------------------|----------------------|
| Hartree                   |                      |
| -325.3682475             | -325.241559          |

#### XYZ coordinates

|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| C | 0.99646900  | -1.26849200 | 0.13912400  |
| C | -1.11516200 | -0.13252400 | -0.00610800 |
| C | -0.38970900 | 1.23212900  | -0.07770200 |
| C | 1.08550800  | 1.19815200  | 0.30115500  |
| C | 1.71380800  | -0.01648700 | -0.36385500 |
| H | 1.31832200  | -1.43690700 | 1.18096800  |
| H | 1.36758000  | -2.13665100 | -0.41803200 |
| H | -0.50136600 | 1.58517600  | -1.10751000 |
| H | -0.95611500 | 1.92310000  | 0.54683500  |
| H | 1.58918400  | 2.12649800  | 0.01884600  |
| H | 1.18671500  | 1.09647800  | 1.38683900  |
| H | 1.59466800  | 0.06451500  | -1.44930900 |
| H | 2.78429900  | -0.08778400 | -0.15179600 |
| N | -0.45229500 | -1.26456000 | 0.06367700  |
| O | -2.37033800 | -0.04489700 | -0.05103300 |
| XYZ coordinates |
|-----------------|
| **C** | -2.85338500 | -1.50484100 | -0.04116100 |
| **C** | -1.90793100 | 0.80968200 | 0.01913100 |
| **C** | -3.30393900 | 1.39624900 | -0.00331100 |
| **C** | -4.39305400 | 0.40767100 | -0.40514500 |
| **C** | -4.19118300 | -0.90024300 | 0.34860700 |
| **H** | -3.48707000 | 1.77104200 | 1.00723900 |
| **H** | -3.27110100 | 2.26643700 | -0.65642000 |
| **H** | -5.37540600 | 0.83288700 | -0.20192100 |
| **H** | -4.34164300 | 0.21526000 | -1.47985200 |
| **H** | -4.20784700 | -0.70969600 | 1.42458000 |
| **H** | -4.98279600 | -1.61507400 | 0.12636200 |
| **H** | -0.81761100 | -0.87629800 | 0.04989500 |
| **N** | -1.77815700 | -0.52358700 | 0.04918300 |
| **O** | -0.92662200 | 1.55877200 | 0.04137900 |
| **C** | 2.85338400 | 1.50484000 | -0.04114600 |
| **C** | 1.90793300 | -0.80968200 | 0.01913100 |
| **C** | 3.30394100 | 1.39624800 | -0.00330500 |
| **C** | 4.39305400 | -0.40766700 | -0.40515100 |
| **C** | 4.19118300 | 0.90024300 | 0.34860700 |
| **H** | 3.48707000 | -1.77105500 | 1.00723600 |
| **H** | 3.27110100 | -2.26642900 | -0.65642500 |
| **H** | 5.37540600 | -0.83288100 | -0.20194400 |
| **H** | 4.34162100 | -0.21525000 | -1.47985600 |
A8

|        | Electronic energy ($E_e$) | $E_e + ZPV$ |
|--------|---------------------------|-------------|
|        | Hartree                   |             |
|        | -247.2710398              | -247.190192 |

XYZ coordinates

|        |                  |                  |
|--------|------------------|------------------|
|        | C                |                  |
|        | -1.44686000     | 0.12673400       |
|        |                  | -0.00005500      |
|        | C                |                  |
|        | 0.64271000      | -0.01668800      |
|        |                  | 0.00000800       |
|        | C                |                  |
|        | -0.46924900     | -1.07466600      |
|        |                  | 0.00020700       |
|        | H                |                  |
|        | -2.05992900     | 0.21921900       |
|        |                  | 0.89384500       |
|        | H                |                  |
|        | -2.05981600     | 0.21889100       |
|        |                  | -0.89406800      |
|        | H                |                  |
|        | -0.48577900     | -1.69266100      |
|        |                  | 0.89340000       |
|        | H                |                  |
|        | -0.48575600     | -1.69306500      |
|        |                  | -0.89270600      |
|        | H                |                  |
|        | -0.15577200     | 1.99759100       |
|        |                  | -0.00042900      |
|        | O                |                  |
|        | 1.84558600      | -0.02869900      |
|        |                  | 0.00000030       |
|        | N                |                  |
|        | -0.26817800     | 0.99533500       |
|        |                  | -0.00014700      |
### A8 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -247.6564532             | -247.561997|

**XYZ coordinates**

|   | C   | C   | C   | C   | H   | H   | H   | H   | H   | O   | N   | H   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|   | -1.50497400 | -0.16334400 | -0.00000400 | 0.51516500 | 0.03827500 | -0.00000800 | -0.55801000 | 1.06905600 | 0.00001000 | -2.09159400 | -0.30332700 | -0.90106200 | -2.09159300 | -0.30333200 | 0.90105500 | -0.57762500 | 1.68390400 | -0.89565800 | -0.57760900 | 1.68386900 | 0.89570400 | -0.10246100 | -1.99105900 | 0.00001800 | 1.79602700 | 0.15002900 | -0.00001700 | -0.27249400 | -0.99060800 | -0.00000400 | 2.26703900 | -0.69994700 | 0.00011600 |

### A8 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -246.7323529             | -246.66468 |

**XYZ coordinates**

|   | C   | C   | C   | C   | H   | H   |
|---|-----|-----|-----|-----|-----|-----|
|   | 1.41319700 | -0.18604100 | -0.00007200 | -0.59472300 | -0.06500200 | -0.00014100 | 0.48215700 | 1.03943700 | 0.00020000 | 2.05266800 | -0.27711300 | 0.88595300 |
A8 homodimer

|                  | Electronic energy ($E_e$) | $E_e + ZPV$ |
|------------------|----------------------------|-------------|
|                  | Hartree                    |             |
|                  | -494.5582987              | -494.3938   |

XYZ coordinates

|                  | $x$  | $y$  | $z$  |
|------------------|------|------|------|
| C                | -2.98017600 | 1.07106600 | -0.03583000 |
| C                | -1.86130900 | -0.67742600 | 0.01682200  |
| C                | -3.36790800 | -0.42948900 | -0.03130800 |
| H                | -3.29552900 | 1.63151800  | 0.84137600  |
| H                | -3.23862100 | 1.61052000  | -0.94419700 |
| H                | -3.90169100 | -0.77475400 | 0.84969500  |
| H                | -3.84660200 | -0.79537000 | -0.93527400 |
| H                | -0.69137300 | 1.14337500  | 0.03223400  |
| O                | -1.15008800 | -1.66351500 | 0.04505500  |
| N                | -1.58056100 | 0.64152900  | 0.01408000  |
| C                | 2.98001100  | -1.07116000 | -0.03584100 |
| C                | 1.86139400  | 0.67748700  | 0.01677200  |
| C                | 3.36796600  | 0.42934400  | -0.03116900 |
| H                | 3.29516900  | -1.63168700 | 0.84138600  |
| H                | 3.23852400  | -1.61058700 | -0.94420300 |
| H                | 3.90165900  | 0.77446400  | 0.84995200  |
| H                | 3.84689700  | 0.79523400  | -0.93500700 |
H 0.69117000 -1.14313900 0.03179200
O 1.15024800 1.66361400 0.04491400
N 1.58045300 -0.64142800 0.01389500

A9

|               | $E_e$       | $E_e$ + ZPV |
|---------------|-------------|-------------|
| Electronic energy ($E_e$) | $E_e$ + ZPV |
| Hartree       |             |             |
|               | -404.521883 | -404.32214  |

XYZ coordinates

C  -1.45819400  -0.06886600  -0.11588000
C   1.37127700   1.34970800  -0.45694900
C   0.36582400  -1.48290400   0.86443500
C   1.43104700  -0.06775900  -1.03719800
C   1.59870700  -1.20213600  -0.02297300
H   0.37680900  -0.88475300   1.77043600
H   0.38765100  -2.52103900   1.19234200
H   2.45533200  -1.00651400   0.62779500
H   1.83249900  -2.11264900  -0.57797900
C  -0.99776800   1.18929100   0.61406600
H  -1.46468000   1.15176900   1.60293700
H  -1.48849600   1.99489500   0.07093600
C   0.49277800   1.52601100   0.78182800
H   0.53683600   2.57488200   1.08159800
H   0.93098900   0.97460900   1.61112200
H  -1.25009700  -2.02331500  -0.38803300
N  -0.90433100  -1.27416000   0.19385900
O  -2.37974700  -0.00115200  -0.91382400
A9 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -404.9233772             | -404.710271 |

XYZ coordinates

|   |    |    |    |
|---|----|----|----|
| C | -1.41877600 | 0.00910200 | -0.02947800 |
| C | 1.69440000  | 1.19495200  | -0.24197900 |
| C | 0.38161100  | -1.47633800 | 0.85999100 |
| C | 1.53851400  | -0.12025300 | -1.00434000 |
| C | 1.51654400  | -1.39131300 | -0.16035600 |
| H | 0.53285000  | -0.82985300 | 1.71329600 |
| H | 0.28450200  | -2.48990800 | 1.23919800 |
| H | 2.44891200  | -1.48750900 | 0.39906000 |
| H | 1.45714500  | -2.25592900 | -0.82312200 |
| C | -0.83927500 | 1.36221900  | 0.23411500 |
| H | -1.55635900 | 1.82223400  | 0.92096900 |
| H | -0.97202800 | 1.89650500  | -0.71125000 |
| C | 0.58319500  | 1.55161700  | 0.75405500 |
| H | 0.66464000  | 2.61524100  | 0.97854400 |
| H | 0.71758000  | 1.05579100  | 1.71084000 |
| H | -1.47602100 | -1.96354200 | -0.01960900 |
| N | -0.92954500 | -1.15551800 | 0.26061400 |
O  -2.59111000  0.09892200  -0.61195800
H   2.64596900  1.19609700  0.29247200
H   1.75764900  1.99601600  -0.98066300
H   0.64546900  -0.08037100  -1.63633700
H   2.37039600  -0.20534600  -1.70392700
H  -3.02229400  -0.75209200  -0.78015800

A9 (deprotonated)

|                  | $E_e$ | $E_e + ZPV$ |
|------------------|-------|------------|
|                  |      | Hartree    |
|                  | -403.9682719 | -403.782855 |

XYZ coordinates

C   -1.46786700  -0.17816800  -0.13178100
C   1.37982800   1.33432100  -0.46184400
C   0.27577400  -1.46737000  0.83316700
C   1.47212700  -0.09209800  -1.01673400
C   1.57993400  -1.20594200  0.02651600
H   0.25802400  -0.83680000   1.72985500
H   0.34410600  -2.49247400   1.21267400
H   2.40806300  -1.00954400   0.71811100
H   1.82984900  -2.12653800  -0.50709600
C   -0.98595800  1.11066300   0.61776500
H  -1.43277600  1.06920000   1.61741500
H  -1.49863600  1.91639200   0.09340600
C   0.49426200  1.50227900   0.77427900
H   0.51906500  2.55945500   1.05910000
H   0.95956000  0.97079400   1.60334200
A9 homodimer

|                  | Electronic energy ($E_e$) | $E_e + ZPV$ |
|------------------|---------------------------|-------------|
|                  | Hartree                   |             |
|                  | -809.0615731             | -808.659941 |

XYZ coordinates

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C   | 1.92731800| -0.81330800| -0.71668300|
| C   | 4.68132500| -0.29430100| 1.14954800 |
| C   | 2.77613900| 1.56820000 | -0.62420300|
| C   | 3.49568200| 0.54047700 | 1.63296900 |
| C   | 3.19698800| 1.80535000 | 0.83260500 |
| H   | 3.63169600| 1.36881600 | -1.25943600|
| H   | 2.31834400| 2.47723300 | -1.01196600|
| H   | 4.06923400| 2.46479100 | 0.83232200 |
| H   | 2.39192600| 2.34519800 | 1.33540500 |
| C   | 3.27950300| -1.51758900| -0.64412100|
| H   | 3.38102700| -1.99105700| -1.62382700|
| H   | 3.10668400| -2.33805700| 0.05519400 |
| C   | 4.59553500| -0.82530500| -0.28648500|
| H   | 5.37611600| -1.57974200| -0.40604700|
| H   | 4.84214000| -0.05011100| -1.00670500|
S192
Electronic energy ($E_e$) | $E_e + \text{ZPV}$
|-----------------|-----------------|
| Hartree         |                 |
| -478.5775888    | -478.399648     |

XYZ coordinates

|   |      |      |      |      |
|---|------|------|------|------|
| C | 0.37823300 | 1.18768300 | -0.16209800 |
| C | 1.76021700  | -0.67578700 | -0.05173600 |
| C | 0.36189500  | -1.19362100 | 0.21441700   |
| C | -0.55700200 | 0.04223100  | 0.22684100   |
| H | 0.11209800  | -1.89581000 | -0.58174500  |
| H | 0.36223000  | -1.74702200 | 1.15202000   |
| H | 2.46068600  | 1.26355300  | -0.49536200  |
| N | 1.66172200  | 0.68562300  | -0.27348700  |
| O | 2.78632800  | -1.30242400 | -0.08346000  |
| O | 0.07707800  | 2.33982100  | -0.33385900  |
| C | -1.09318000 | 0.34337600  | 1.62954300   |
| H | -1.70032000 | 1.24833800  | 1.61967800   |
| H | -1.70253100 | -0.48532700 | 1.98766100   |
| H | -0.27503900 | 0.48791400  | 2.33690100   |
| C | -1.68458400 | -0.03300100 | -0.81335500  |
| H | -2.15844800 | 0.94793600  | -0.87242500  |
| H | -1.23710500 | -0.22524200 | -1.79220800  |
| C | -2.73018300 | -1.09952100 | -0.50886500  |
| H | -3.43942300 | -1.17947100 | -1.33185200  |
| H | -2.27618800 | -2.08225700 | -0.36779800  |
| H | -3.29763500 | -0.85930800 | 0.38961500   |
**I14 (protonated)**

| Electronic energy ($E_e$) | $E_e +$ ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -478.952086345           | -478.760912 |

**XYZ coordinates**

|        | X          | Y          | Z           |
|--------|------------|------------|-------------|
| C      | 0.40540700 | 1.08748300 | -0.13002100 |
| C      | 1.74943700 | -0.75789700| -0.04180300 |
| C      | 0.35650600 | -1.24461700| 0.25624500  |
| C      | -0.55436000| 0.00043100 | 0.24259500  |
| H      | 0.08326600 | -1.97094400| -0.50950500 |
| H      | 0.36514200 | -1.76068100| 1.21466400  |
| H      | 2.44031500 | 1.24793100 | -0.52213200 |
| N      | 1.63386000 | 0.67522500 | -0.28369100 |
| O      | 2.78942600 | -1.31433200| -0.09891600 |
| O      | -0.00589900| 2.29863600 | -0.26604700 |
| C      | -1.12700300| 0.32266200 | 1.63235800  |
| H      | -1.76225900| 1.20648800 | 1.59921100  |
| H      | -1.72297300| -0.52258000| 1.96937300  |
| H      | -0.33171200| 0.48537800 | 2.36001600  |
| C      | -1.65383700| -0.06700200| -0.84231000 |
| H      | -2.12514600| 0.91307900 | -0.92181600 |
| H      | -1.17706600| -0.27715300| -1.80278700 |
| C      | -2.70948400| -1.12298700| -0.54210300 |
| H      | -3.39874800| -1.19769100| -1.38110300 |
| H      | -2.26786900| -2.10829300| -0.38732700 |
| H      | -3.29217900| -0.86555600| 0.34069800  |
| H      | 0.68400200 | 2.94058300 | -0.50351700 |
**I14 (deprotonated)**

|          | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------|---------------------------|-------------|
|          | Hartree                   |             |
|          | -478.0603247              | -477.896067 |

**XYZ coordinates**

|      | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 0.43913600 | 1.17981500 | -0.18671200 |
| C    | 1.80101600 | -0.55580900 | -0.07788300 |
| C    | 0.42223900 | -1.17002400 | 0.20841900 |
| C    | -0.51860600 | 0.02994600 | 0.22555600 |
| H    | 0.19331900 | -1.88435900 | -0.58512400 |
| H    | 0.45854000 | -1.72574600 | 1.14617300 |
| N    | 1.72590100 | 0.77648800 | -0.31273200 |
| O    | 2.81918800 | -1.24144600 | -0.08975900 |
| O    | 0.01451900 | 2.31996400 | -0.34984100 |
| C    | -1.04927900 | 0.33836100 | 1.62664400 |
| H    | -1.64481100 | 1.25253000 | 1.61444500 |
| H    | -1.66509900 | -0.47767200 | 2.00902600 |
| H    | -0.22146800 | 0.48572400 | 2.32311800 |
| C    | -1.65612600 | -0.05940000 | -0.79751800 |
| H    | -2.13062000 | 0.92161700 | -0.86368600 |
| H    | -1.21618600 | -0.25855300 | -1.77899700 |
| C    | -2.70366400 | -1.12503600 | -0.48683600 |
| H    | -3.42163200 | -1.21421100 | -1.30344000 |
| H    | -2.24477900 | -2.10558000 | -0.34128900 |
| H    | -3.26653700 | -0.88443100 | 0.41567400 |
I14 homodimer

|                  | $E_e$     | $E_e + ZPV$ |
|------------------|-----------|-------------|
| **Electronic energy** (Hartree) | -957.1692518 | -956.811884 |

**XYZ coordinates**

- **C**
  -2.57069400 1.99944000 -0.12589800

- **C**
  -2.02801100 -0.23996500 -0.05777300

- **C**
  -3.55018600 -0.23444800 -0.14637700

- **C**
  -3.89691200 1.26524700 -0.13076900

- **H**
  -0.56567100 1.26751300 -0.03284100

- **N**
  -1.56413000 1.04717000 -0.06186200

- **O**
  -1.32556300 -1.22890500 -0.00725000

- **C**
  2.57076100 -1.99949300 -0.12544200

- **C**
  2.02798700 0.23989100 -0.05758000

- **C**
  3.55014300 0.23440900 -0.14608900

- **C**
  3.89697000 -1.26525500 -0.12946800

- **H**
  0.56565300 -1.26762300 -0.03329000

- **N**
  1.56412400 -1.04725500 -0.06190700

- **O**
  1.32551700 1.22881500 -0.00701400

- **O**
  2.38739000 -3.18634900 -0.16047200

- **O**
  -2.38727500 3.18630200 -0.16050800

- **H**
  -4.44692800 1.56237600 0.76272000

- **H**
  -4.47594300 1.58723900 -0.99519200

- **H**
  -4.44603700 -1.56180500 0.76480100

- **H**
  4.47696900 -1.58763700 -0.99308600

- **C**
  -3.93666300 -0.90499000 -1.46802100

- **H**
  -3.63765000 -1.95299300 -1.46498400

- **H**
  -5.01324100 -0.84703800 -1.62191700
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| H  | -3.45045300 | -0.41103900 | -2.31078800 |
| C  | -4.10796700 | -0.99527700 |  1.06717500 |
| H  | -3.64876300 | -1.98477300 |  1.08936700 |
| H  | -3.78817100 | -0.47686000 |  1.97504600 |
| C  | -5.62664000 | -1.12548600 |  1.05879500 |
| H  | -5.97477900 | -1.56139600 |  1.99447100 |
| H  | -6.11335600 | -0.15486000 |  0.94511100 |
| H  | -5.96829700 | -1.76970200 |  0.24948100 |
| C  |  3.93633400 |  0.90377200 | -1.46845000 |
| H  |  3.63750700 |  1.95182700 | -1.46618000 |
| H  |  5.01284500 |  0.84547600 | -1.62268400 |
| H  |  3.44971800 |  0.40919600 | -2.31061800 |
| C  |  4.10808200 |  0.99626100 |  1.06668400 |
| H  |  3.64907500 |  1.98586300 |  1.08796900 |
| H  |  3.78824300 |  0.47874400 |  1.97504700 |
| C  |  5.62678000 |  1.12615000 |  1.05807800 |
| H  |  5.97505900 |  1.56311600 |  1.99319800 |
| H  |  6.11321600 |  0.15524700 |  0.94555900 |
| H  |  5.96852700 |  1.76928500 |  0.24794000 |

**I15**

| Electronic energy ($E_e$) | $E_e + $ZPV |
|---------------------------|------------|
|                           |            |
| Hartree                   |            |
| -1319.156376              | -1319.054065 |

**XYZ coordinates**

|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| C  | -0.77892300 |  0.68239800 |  0.98995000 |
| C  |  1.11747700 |  1.12764900 | -0.27839500 |
I15 (protonated)

|                  | $E_e$          | $E_e + ZPV$ |
|------------------|----------------|-------------|
| **Electronic energy** ($E_e$) |                |             |
| Hartree          | -1319.50671881 | -1319.392226 |
| XYZ coordinates  |                |             |
| C                | -1.08221800    | 1.05485000  | 0.10374900 |
| C                | 1.16289000     | 1.24167900  | -0.29434600 |
| C                | 0.81762200     | -0.22819500 | -0.47473500 |
| C                | -0.58032100    | -0.36633000 | 0.16963800  |
| H                | 0.74119600     | -0.39879200 | -1.54965400 |
| H                | -0.19919200    | 2.92353200  | -0.08486400 |
| N                | -0.11745300    | 1.90828700  | -0.10134200 |
| O                | 2.18738100     | 1.81624400  | -0.30930300 |
I15 (deprotonated)

| Electron energy ($E_e$) | $E_e + ZPV$ |
|-------------------------|-------------|
| Hartree                 |             |
| -1318.6615              | -1318.572541|

XYZ coordinates

C  -1.01311600  1.26751900  0.11512000
C   1.17294800  1.24701000 -0.26207100
C   0.73005200 -0.22332300 -0.46676600
C  -0.63578700 -0.24607600  0.18394800
H   0.65260200 -0.40682600 -1.53439500
N   0.09112000  2.03071000 -0.04729700
O   2.33646300  1.58949300 -0.35106600
O  -2.16004200  1.64125200  0.27278900
C  -0.67600400 -0.70230200  1.62915100
H  -1.66885100 -0.51499400  2.03371800
H  -0.44203000 -1.76191800  1.71219900
H   0.05445700 -0.13530100  2.20864500
Cl -1.80895700 -1.24749600 -0.76826600
I15 homodimer

| xyz coordinates |
|-----------------|
| Cl              | 1.91990100 -1.41714400 0.14125600 |
|                 |                                         |

XYZ coordinates

- electronic energy ($E_e$)
- $E_e + ZPV$

| Hartree         |
|-----------------|
|                |
| -2638.325484    |
| -2638.119728    |
|   |   |   |   |
|---|---|---|---|
| Cl | -5.55307200 | -1.04299900 | 0.44072900 |
| Cl | -3.93635200 | 2.11105800 | -1.02498500 |
| C  | -3.75669900 | 1.19596500 | 1.52331300 |
| H  | -3.18313900 | 2.08508200 | 1.77572200 |
| H  | -4.81769300 | 1.40260700 | 1.63787800 |
| H  | -3.48253800 | 0.38669400 | 2.20256300 |
| C  | 3.75669100 | -1.19603500 | 1.52320400 |
| H  | 3.18312300 | -2.08515800 | 1.77557500 |
| H  | 4.81768200 | -1.40269100 | 1.63776800 |
| H  | 3.48253200 | -0.38679200 | 2.20248800 |

**I16**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -858.3353243              | -858.24765  |

**XYZ coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 0.34512200 | 1.34133200 | 0.00000000 |
| C | -1.64489100 | 0.21323000 | 0.00000000 |
| C | -0.54334500 | -0.81492600 | 0.00000000 |
| C | 0.60343800 | -0.14103000 | 0.00000000 |
| H | -1.52771000 | 2.33944800 | 0.00000300 |
| N | -1.03478400 | 1.45962000 | 0.00000100 |
| O | -2.82565000 | 0.00019200 | 0.00000000 |
| O | 1.14646900 | 2.22987100 | -0.00000100 |
| Cl| 2.20330900 | -0.73482000 | 0.00000000 |
| C | -0.83814400 | -2.26542800 | 0.00000000 |
| H | 0.07772500 | -2.85084500 | 0.00000000 |
I16 (protonated)

|                     | Electronic energy ($E_e$) | $E_e + ZPV$  |
|---------------------|---------------------------|--------------|
|                     |                           | Hartree      |
|                     |                           | -858.692487938 | -858.592313 |

XYZ coordinates

|   |   |   |   |
|---|---|---|---|
|C  | -0.39731800 | -1.33819200 | -0.00021600 |
|C  | 1.53574700  | -0.21122800 | 0.00010900  |
|C  | 0.48388400  | 0.81872700  | -0.00021300 |
|C  | -0.67070300 | 0.13902800  | 0.00007400  |
|H  | 1.54815900  | -2.31416700 | 0.00241400  |
|N  | 1.04455400  | -1.43281000 | -0.00072500 |
|O  | 2.77233800  | 0.12270700  | 0.00069200  |
|O  | -1.13279200 | -2.25742300 | -0.00032600 |
|Cl | -2.25334600 | 0.70807800  | 0.00037600  |
|C  | 0.77599400  | 2.27156200  | -0.00058600 |
|H  | -0.14989100 | 2.83980000  | 0.00030800  |
|H  | 1.35841500  | 2.54322600  | 0.88024800  |
|H  | 1.35659900  | 2.54312500  | -0.88265000 |
|H  | 3.39973100  | -0.62129200 | 0.00043300  |
### I16 (deprotonated)

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -857.8277409             | -857.753285 |

**XYZ coordinates**

| Atom | X      | Y      | Z          |
|------|--------|--------|------------|
| C    | 0.30139100 | 1.37701100 | -0.00071400 |
| C    | -1.62741200 | 0.34978600 | -0.00036400 |
| C    | -0.58100700 | -0.77239400 | -0.00036500 |
| C    | 0.57258700 | -0.13029600 | -0.00034800 |
| N    | -1.04007200 | 1.57473300 | 0.00055500  |
| O    | -2.82277900 | 0.09092900 | 0.00077200  |
| O    | 1.19766100 | 2.20271700 | 0.00073300  |
| Cl   | 2.17525700 | -0.78174700 | -0.00020200 |
| C    | -0.93035800 | -2.21283400 | -0.00021900 |
| H    | -0.03916000 | -2.83892600 | -0.00104900 |
| H    | -1.53418000 | -2.45575700 | 0.87550700  |
| H    | -1.53578400 | -2.45554700 | -0.87488700 |

### I16 homodimer

| Electronic energy ($E_e$) | $E_e$ + ZPV |
|---------------------------|-------------|
| Hartree                   |             |
| -1716.683243             | -1716.507499 |

**XYZ coordinates**

| Atom | X      | Y      | Z          |
|------|--------|--------|------------|
| C    | -3.03301900 | 1.22809900 | 0.01005700 |
| C    | -1.89799000 | -0.74045100 | 0.01292800 |
| C    | -3.36263500 | -1.08010900 | -0.00445300 |
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| C   | -4.01072400 | 0.08156000 | -0.00609000 |
| H   | -0.88710900  | 1.11899000  | 0.02823300  |
| N   | -1.78058700  | 0.62923800  | 0.02148100  |
| O   | -0.98745400  | -1.53643100 | 0.01817000  |
| C   | 3.03270500  | -1.22801500 | 0.00964500  |
| C   | 1.89813100  | 0.74078000  | 0.01227200  |
| C   | 3.36285100  | 1.08010500  | -0.00459300 |
| C   | 4.01069600  | -0.08169800 | -0.00608000 |
| H   | 0.88683600  | -1.11845500 | 0.02723400  |
| N   | 1.78043400  | -0.62891200 | 0.02058400  |
| O   | 0.98778200  | 1.53697500  | 0.01737000  |
| O   | 3.27393300  | -2.39865200 | 0.01223300  |
| O   | -3.27445600 | 2.39867500  | 0.01264500  |
| C   | -3.83719100 | -2.48247300 | -0.01463500 |
| H   | -3.43809200 | -3.00658700 | -0.88367400 |
| H   | -3.47517500 | -3.00688700 | 0.87047900  |
| H   | -4.92296700 | -2.52744700 | -0.03701400 |
| C   | 3.83766300  | 2.48238900  | -0.01461600 |
| H   | 3.43951700  | 3.00636300  | -0.88418100 |
| H   | 3.47486200  | 3.00705800  | 0.87002000  |
| H   | 4.92346800  | 2.52716900  | -0.03596800 |
| Cl  | 5.68940700  | -0.38053100 | -0.02033600 |
| Cl  | -5.68950400 | 0.38005200  | -0.02081300 |
### I17

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
|                           | Hartree     |
|                           | -757.5994171 | -757.538535 |

#### XYZ coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.16923300 | 0.93990700 | 0.05648900 |
| C       | 1.16925200  | 0.93984000 | -0.05648200|
| C       | 0.76631500  | -0.54411700| 0.09372000 |
| C       | -0.76633200 | -0.54411100| -0.09373000|
| H       | 0.00003400  | 2.68910900 | -0.00011900|
| N       | 0.00001200  | 1.67562600 | -0.00004300|
| O       | 2.28053700  | 1.35242000 | -0.16723700|
| O       | -2.28050800 | 1.35245000 | 0.16733100 |
| F       | -1.07580000 | -0.95110900| -1.33510500|
| F       | -1.39784300 | -1.31591700| 0.78765300 |
| F       | 1.07577200  | -0.95115800| 1.33509000 |
| F       | 1.39783000  | -1.31590800| -0.78767300|

### I17 (protonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
|                           | Hartree     |
|                           | -757.930492896 | -757.856999 |

#### XYZ coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.16172000 | 0.80406600 | 0.02729700 |
| C       | 1.13397100  | 1.01949500 | -0.03564200|
I17 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -757.1211851              | -757.072931 |

XYZ coordinates

| C           | 0.87999000  | -0.50403300 | 0.06067600 |
| C           | -0.66597800 | -0.64754000 | -0.06436500 |
| H           | -0.26746600 | 2.67078300  | 0.06527100  |
| N           | -0.17700600 | 1.65379200  | 0.03269500  |
| O           | 2.14172700  | 1.60639700  | -0.13138700 |
| O           | -2.41131000 | 1.01166900  | 0.07044300  |
| F           | -1.01823200 | -1.13305700 | -1.24780100 |
| F           | -1.19670800 | -1.36601000 | 0.90838100  |
| F           | 1.28025300  | -0.92804800 | 1.25552000  |
| F           | 1.51688600  | -1.14729300 | -0.89954100 |
| H           | -2.69420200 | 1.94588100  | 0.11657800  |
I17 homodimer

|                | $E_e$ | $E_e + ZPV$ |
|----------------|-------|-------------|
|                |       |             |
| **Electronic energy** ($E_e$) |       |             |
| **Hartree**    |       |             |
| $-1515.210257$ |       | $-1515.087036$ |

**XYZ coordinates**

|   |   |   |       |
|---|---|---|-------|
| C | 3.06800700 | 1.41527500 | -0.04708200 |
| C | 1.91163700 | -0.60541900 | -0.03033500 |
| C | 3.39976000 | -1.01233300 | -0.00003100 |
| C | 4.16806500 | 0.33311800 | 0.04432200 |
| H | 0.94519100 | 1.23977200 | -0.09413000 |
| N | 1.84587800 | 0.75877400 | -0.06661400 |
| O | 0.99593800 | -1.38143600 | -0.02966800 |
| C | -3.06819200 | -1.41530100 | -0.04683900 |
| C | -1.91157500 | 0.60525200 | -0.02995100 |
| C | -3.39964900 | 1.01234200 | 0.00039000 |
| C | -4.16811400 | -0.33301800 | 0.04471200 |
| H | -0.94536800 | -1.24006200 | -0.09395300 |
| N | -1.84597800 | -0.75894300 | -0.06631700 |
| O | -0.99578600 | 1.38116400 | -0.02924100 |
| O | -3.25402000 | -2.58878100 | -0.08471300 |
| O | 3.25369600 | 2.58878400 | -0.08483800 |
| F | -3.64912200 | 1.76643700 | 1.07279000 |
| F | -3.69792600 | 1.70711000 | -1.10223500 |
| F | -4.84090000 | -0.46693500 | 1.19228700 |
| F | -5.01950600 | -0.44996000 | -0.97667300 |
I18

|          | $E_e$     | $E_e + ZPV$ |
|----------|-----------|-------------|
|          | Hartree   |             |
|          | -611.3369802 | -611.106084 |

XYZ coordinates

|   |        |        |        |        |
|---|--------|--------|--------|--------|
| O | -1.53597300 | 2.35527700 | 0.25927200 |
| N | -2.90572600 | 0.54367100 | 0.20261100 |
| N | -0.61321000 | 0.30601400 | -0.12612100 |
| C | -1.67761800 | 1.15919900 | 0.12114000 |
| C | -0.82126300 | -1.03350500 | -0.31075200 |
| C | -2.03089800 | -1.61694600 | -0.24313200 |
| C | -3.19947300 | -0.81149600 | 0.04137300 |
| H | -3.68596400 | 1.15901900 | 0.39065000 |
| O | -4.34231300 | -1.20727500 | 0.14115200 |
| H | 0.06294000 | -1.61447000 | -0.51857900 |
| C | 0.71291200 | 0.94547100 | -0.20974900 |
| H | 0.79722500 | 1.60522700 | 0.65247300 |
| H | -2.15383400 | -2.67628300 | -0.39109500 |
| H | 0.72778200 | 1.57997400 | -1.09682400 |
| C | 1.87904500 | -0.02594100 | -0.23289300 |
| H | 1.85717300 | -0.63832700 | -1.13831400 |
| H | 1.81229100 | -0.70176700 | 0.62236900 |
\begin{tabular}{c c c c}
C & 3.2003000 & 0.7405520 & -0.1878820 \\
H & 3.2043340 & 1.4896230 & -0.9836490 \\
H & 3.2641810 & 1.2875320 & 0.7569710 \\
C & 4.4276750 & -0.1576560 & -0.3362680 \\
H & 4.3947220 & -0.6542160 & -1.3096410 \\
H & 5.3197820 & 0.4710250 & -0.3403820 \\
C & 4.5560890 & -1.2032140 & 0.7673130 \\
H & 4.5208910 & -0.7346550 & 1.7529150 \\
H & 3.7560390 & -1.9424730 & 0.7214520 \\
H & 5.5006540 & -1.7408180 & 0.6879350 \\
\end{tabular}

**I18 (protonated)**

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|-------------|
| Hartree                   |             |
| -611.725649329            | -611.481928 |

**XYZ coordinates**

\begin{tabular}{c c c c c}
O & -1.4969470 & 2.3675820 & 0.2395950 \\
N & -2.8802880 & 0.5667940 & 0.1564230 \\
N & -0.5648190 & 0.3029700 & -0.0957460 \\
C & -1.6242640 & 1.1854260 & 0.1099900 \\
C & -0.7706960 & -1.0111670 & -0.2459730 \\
C & -2.0112060 & -1.5907210 & -0.2015700 \\
C & -3.0938000 & -0.7488900 & 0.0130110 \\
H & -3.6500410 & 1.2119400 & 0.3099540 \\
O & -4.3031860 & -1.2397910 & 0.0739070 \\
H & 0.1097980 & -1.6135560 & -0.4087800 \\
C & 0.7782220 & 0.9434580 & -0.1396450 \\
\end{tabular}
H     0.84811000  1.55372000  0.75934900
H     -2.15598200 -2.65028300 -0.32275700
H     0.77125600  1.62086400 -0.99289900
C     1.93516300 -0.03097300  0.21961800
H     1.89104300 -0.60974900 -1.14641600
H     1.88997500 -0.73184000  0.61718200
H     3.25602300  0.73949200 -0.99289900
C     3.24745800  1.50463400 -0.32275700
C     4.47936500 -0.15698700 -0.99289900
H     4.43604700 -0.62594000 -1.34851000
H     5.36865400  0.47452400 -0.36015800
H     4.62267800 -1.23019700  0.71190200
H     4.59454700 -0.79004400  1.71064200
H     3.83087000 -1.97783600  0.65202400
H     5.57076500 -1.75655800  0.60899000
H     -4.99605400 -0.58134300  0.22972100

I18 (deprotonated)

| Electronic energy ($E_e$) | $E_e + ZPV$ |
|---------------------------|------------|
| Hartree                   |            |
| -610.8125614              | -610.595737|

XYZ coordinates

O     -1.49378200  2.35349600  0.26960500
N     -2.98205600  0.62038100  0.25946500
N     -0.64982600  0.29641900 -0.13832900
C     -1.75661800  1.15183900  0.14396000
## I18 homodimer

|                | Electronic energy ($E_e$) | $E_e + ZPV$ |
|----------------|---------------------------|-------------|
|                | Hartree                   |             |
|                | -1222.689185              | -1222.225625|

### XYZ coordinates

|   | x          | y          | z          |
|---|------------|------------|------------|
| O | -3.15651700| -2.12801600| -0.08286100|
| O | -0.60355400| 1.61872700 | 0.13522600 |
| N | -4.22761700| -0.11988300| -0.11100600|
| N | -1.89913900| -0.23726400| 0.03210600 |
| C | -3.09035900| -0.91880000| -0.05580200|
| C | -1.72670500| 1.13345200 | 0.06056000 |
| C | -2.95181200| 1.89249700 | -0.00316500|
| C | -4.12654100| 1.23998200 | -0.08537600|
| H | -1.04771100| -0.80987200| 0.07735700 |
| H | -5.05944200| 1.77884500 | -0.13479400|
| O | 3.15654700 | 2.12799100 | -0.08284800|
| N | 1.89914100 | 0.23726900 | 0.03223200 |
| N | 4.22760300 | 0.11983400 | -0.11110000|
| C | 3.09036900 | 0.91877600 | -0.05579700|
| C | 4.12649400 | -1.24003100| -0.08553900|
| C | 2.95175300 | -1.89251600| -0.00325600|
| C | 1.72667100 | -1.13341000| 0.06062800 |
| H | 1.04773700 | 0.80990600 | 0.07748000 |
| C | -5.50409500| -0.84958000| -0.20954800|
| H | -5.47966100| -1.43328500| -1.13002500|
| O | 0.60351600 | -1.61869500| 0.13538200 |
| H | 5.05937400 | -1.77891900| -0.13508100|
| C | 5.50408400 | 0.84951800 | -0.20973300|
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