Supplementary Information

A molecular twist on hydrophobicity

Sara Gómez*,†, Natalia Rojas–Valencia‡¶, Santiago A. Gómez‡, Chiara Cappelli†, Gabriel Merino*§ and Albeiro Restrepo*‡

†Scuola Normale Superiore, Classe di Scienze, Piazza dei Cavalieri 7, 56126, Pisa, Italy
‡Instituto de Química, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia
¶Escuela de Ciencias y Humanidades, Departamento de Ciencias Básicas, Universidad Eafit, AA 3300, Medellín, Colombia
§Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. Km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., México

*Correspondence: sara.gomezmaya@sns.it, albeiro.restrepo@udea.edu.co

Contents

1 Computational approach S2

2 Results from MD simulations S4

2.1 Entropy contributions to phase separation . . . . . . . . . . . . . . . . . . . . . . . . S6

3 NCI surfaces S8

4 Dimers S9

4.1 Global minima: Structures and NBOs . . . . . . . . . . . . . . . . . . . . . . . . . S9

4.1.1 S···Water . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . S9

4.1.2 S···S . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . S10

4.2 Optimized geometries at the MP2/6–311++G(d,p) level for all dimers . . . . S11

4.2.1 Cartesian coordinates for all S···Water dimers . . . . . . . . . . . . . . . . . . . . . S11

4.2.2 Cartesian coordinates for all S···S dimers . . . . . . . . . . . . . . . . . . . . . . . S21

Electronic Supplementary Material (ESI) for Chemical Science. This journal is © The Royal Society of Chemistry 2021
1 Computational approach

We selected 21 solvents declared by Aldrich as water–immiscible, and proceeded with the following two separate procedures:

1. We explored the potential energy surfaces for all $S \cdots S$ and for all $S \cdots$ Water dimers using a stochastic sampling algorithm\cite{1, 2, 3}. Because of the immiscibility in the macroscopic regime, high levels of electron correlation and extended basis sets are needed to treat the extremely weak bonding intermolecular interactions accurately. Accordingly, all interacting pairs were treated using second-order perturbation theory at the MP2/6–311++G($d,p$) level. Binding energies were calculated as the difference between the energy of the dimer and the energy of the isolated monomers. Highly sophisticated DLPNO–CCSD(T)/6–311++G($d,p$) interaction energies\cite{4, 5} were also computed on the optimized MP2 geometries. We then proceeded to dissect the bonding interactions using the tools provided by the NBO\cite{6, 7, 8, 9}, QTAIM\cite{10, 11, 12, 13}, NCI\cite{14, 15, 16} methods.

2. For each substance in Table S1 we constructed more realistic samples of binary systems with water contained within a $6 \times 6 \times 12$ nm$^3$ box. The box was initially filled with as many molecules of the substance as possible (not exceeding 1000) and then the available volume was filled with water molecules. We then followed standard protocols\cite{17} (minimization $\rightarrow$ equilibration $\rightarrow$ production steps) and ran 30 ns MD simulations at 298.15 K and 1 bar to explore the dynamic properties of the binary systems. It is important to remark that we chose to have the worst possible initial scenario from the point of view of intermolecular interactions, thus reducing structural bias to the minimum. Accordingly, we made sure that the starting points of our MD simulations comprise high degrees of $S$/water mixing. A detailed analysis of the quantum interactions was then carried out via NCI, NBO, and QTAIM on the interphases of randomly chosen frames of late stages of the MD trajectories following a recently suggested methodology\cite{18, 19}.

3. We chose heptane to dig deeper into the nature of $S \cdots S$ and $S \cdots$ water interactions, specifically investigating the potential for the formation of clathrate–like structures and the potential for hydrophobic clustering. For this purpose, we placed heptamer dimers at the center and at each corner of the enclosing box (a total of 18 heptane monomers), filled the box with water, ran MD simulations under the same parameters as before and followed the above procedures to investigate bonding at the interphase.

All geometry optimizations and frequency calculations were carried out using the Gaussian09 suite of programs\cite{20}. The GAFF force field\cite{21} as implemented in GROMACS\cite{22}, version 2019.4, was used for all MD runs. DLPNO–CCSD(T) energies were computed using ORCA\cite{23}.
Table S1: Binary systems studied in this work. The number of well–defined minima on each MP2/6–311++G(d,p) dimer PES is provided. Binding energies for the corresponding putative global minimum in kcal mol⁻¹. The octanol/water partition coefficients, (log $K_{ow}$) [24], are also included. $n_S, n_w$ are the numbers of organic solvent and water molecules used during the MD runs. The temperatures in °C for the experimental densities are provided inside parentheses. $I_t$ is the thickness of the interphase (see Figure S1). A three letter code is assigned to each $S$.

| Organic solvent   | Code | MD conditions | Solubility | log $K_{ow}$ | Density (g/cm³) | $I_t$ | Minima BE$_{DLPNO–CCSD(T)}$ |
|-------------------|------|---------------|------------|--------------|-----------------|-------|-----------------------------|
|                   | $n_S$ | $n_w$         | mg/L       |              | Experimental    |       | S···S       | S···W      | S···S       | S···W      |
| Isooctane         | ISC  | 910           | 6540       | 2.44         | 4.08            | 0.69  | (20)        | 0.70       | 1.30        | 4.79       | 1.95       |
| Heptane           | HPT  | 930           | 6916       | 3.40         | 4.66            | 0.67  | (25)        | 0.65       | 1.20        | 4.79       | 1.94       |
| Hexane            | HXN  | 1000          | 7273       | 9.50         | 3.90            | 0.66  | (25)        | 0.65       | 1.13        | 6.11       | 2.43       |
| Pentane           | PTN  | 1000          | 8137       | 3.80 × 10¹   | 3.39            | 0.63  | (20)        | 0.61       | 1.20        | 11.9       | 3.94       | 1.59       |
| Cyclohexane       | CYH  | 1000          | 8058       | 5.50 × 10¹   | 3.44            | 0.78  | (20)        | 0.76       | 1.48        | 2         | 2.93       | 1.68       |
| Ortho–xylene      | OXL  | 1000          | 7515       | 1.80 × 10²   | 3.12            | 0.88  | (20)        | 0.72       | 1.60        | 4         | 3.94       | 5.15       |
| Toluene           | TLN  | 1000          | 8405       | 5.26 × 10²   | 2.73            | 0.86  | (20)        | 0.76       | 1.50        | 9         | 4.75       | 4.79       |
| 1–octanol         | OTN  | 819           | 6733       | 5.40 × 10²   | 3.00            | 0.83  | (25)        | 0.82       | 1.40        | 2         | 7.95       | 1.94       |
| Carbon tetrachloride | CTC | 1000          | 10061      | 7.93 × 10²   | 2.83            | 1.59  | (20)        | 1.56       | 1.44        | 1         | 4.73       | 2.39       |
| Trichloroethylene | TCE  | 1000          | 9952       | 1.12 × 10³   | 2.61            | 1.46  | (20)        | 1.37       | 1.45        | 9         | 5.95       | 4.14       |
| Benzene           | BZN  | 1000          | 9244       | 1.79 × 10³   | 2.13            | 0.88  | (20)        | 0.83       | 1.51        | 5         | 5.33       | 3.95       |
| Chloroform        | CHL  | 1000          | 10492      | 7.95 × 10³   | 1.97            | 1.47  | (25)        | 1.41       | 1.55        | 4         | 5.83       | 5.53       |
| Butyl acetate     | BAC  | 967           | 7124       | 8.33 × 10³   | 1.78            | 0.88  | (20)        | 0.88       | 1.87        | 1         | 4.89       | 6.69       |
| Dichloroethane    | DCE  | 1000          | 9975       | 8.60 × 10³   | 1.48            | 1.25  | (25)        | 1.17       | 1.60        | 6         | 6.02       | 4.83       |
| Diisopropyl ether | DPE  | 984           | 7217       | 8.80 × 10³   | 1.52            | 0.72  | (20)        | 0.73       | 1.82        | 3         | 6.34       | 8.03       |
| Dichloromethane   | DCM  | 1000          | 11029      | 1.32 × 10⁴   | 1.25            | 1.33  | (20)        | 1.2        | 1.77        | 2         | 4.71       | 4.63       |
| Methyl tert–butyl ether | MTE | 1000          | 7878       | 4.80 × 10⁴   | 0.94            | 0.74  | (25)        | 0.71       | 2.00        | 1         | 3.80       | 7.33       |
| Diethyl ether     | DEE  | 980           | 7119       | 6.04 × 10⁴   | 0.89            | 0.71  | (20)        | 0.73       | 2.03        | 3         | 4.73       | 7.14       |
| n-butanol         | BTN  | 1000          | 8762       | 6.32 × 10⁴   | 0.88            | 0.81  | (20)        | 0.77       | 2.42        | 3         | 6.76       | 6.56       |
| Ethyl acetate     | EAC  | 1000          | 8679       | 8.00 × 10⁴   | 0.73            | 0.9   | (20)        | 0.89       | 2.28        | 3         | 7.90       | 6.52       |
| Methyl ethyl ketone | MEK | 1000          | 9071       | 2.11 × 10⁵   | 0.29            | 0.81  | (20)        | 0.67       | 3.60        | 7         | 7.62       | 6.50       |
2 Results from MD simulations

Figure S1: Densities (continuous lines) and derivatives of the densities (discontinuous lines) along the normal direction to the interphase for the chosen set of $S$. Vertical solid lines mark the boundaries of the interphase.
Table S2: NBO and QTAIM descriptors of bonding for all $S \cdots W$ and $S \cdots S$ isolated dimers. The water dimer is included for comparison. Energies in kcal mol$^{-1}$, all other quantities in a. u. All calculations on the MP2/6–311++G(d, p) optimized global minima.

| $S \cdots W$ | Interaction | $-E_{d-a}^{(2)}$ | $\rho(r_c) \times 10^2$ | $\nabla^2 \rho(r_c)$ | $|V(r_c)|/|G(r_c)|$ | $\mathcal{H}(r_c)/\rho(r_c)$ | BE |
|--------------|-------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----|
| Isooctane    | $n_O \rightarrow \sigma^*_{O-H}$ | 1.15 | 0.81 | 0.03 | 0.87 | 0.10 | 1.95 |
| Heptane      | $\sigma_{C-H} \rightarrow \sigma^*_{O-H}$ | 0.07 | 0.60 | 0.02 | 0.71 | 0.21 | 1.94 |
| Hexane       | $n_O \rightarrow \sigma^*_{C-H}$ | 0.13 | 0.56 | 0.02 | 0.84 | 0.13 | 2.43 |
| Pentane      | $n_O \rightarrow \sigma^*_{C-H}$ | 0.2 | 0.57 | 0.02 | 0.85 | 0.11 | 1.59 |
| Cyclohexane  | $n_O \rightarrow \sigma^*_{C-H}$ | 0.49 | 0.64 | 0.02 | 0.87 | 0.10 | 1.68 |
| Ortho–xylene | $\pi_{C=C} \rightarrow \sigma^*_{O-H}$ | 0.35 | 1.14 | 0.04 | 0.77 | 0.16 | 5.15 |
| Toluene      | $\pi_{C=C} \rightarrow \sigma^*_{O-H}$ | 0.41 | 0.68 | 0.02 | 0.83 | 0.11 | 4.79 |
| 1–octanol    | $n_O \rightarrow \sigma^*_{O-H}$ | 7.12 | 2.48 | 0.11 | 0.87 | 0.12 | 1.94 |
| Carbon tetrachloride | $n_O \rightarrow \sigma^*_{C-Cl}$ | 1.7 | 1.09 | 0.05 | 0.85 | 0.14 | 2.39 |
| Trichloroethylene | $\pi_{C=C} \rightarrow \sigma^*_{O-H}$ | 4.23 | 1.44 | 0.06 | 0.80 | 0.17 | 4.14 |
| Benzene      | $\pi_{C=C} \rightarrow \sigma^*_{O-H}$ | 0.58 | 7.6 | 0.03 | 0.74 | 0.17 | 3.95 |
| Chloroform   | $n_O \rightarrow \sigma^*_{C-H}$ | 3.00 | 1.66 | 0.07 | 0.81 | 0.16 | 5.53 |
| Butyl acetate | $n_O \rightarrow \sigma^*_{O-H}$ | 3.74 | 2.10 | 0.10 | 0.82 | 0.18 | 6.69 |
| Dichloroethane | $n_O \rightarrow \sigma^*_{C-H}$ | 0.72 | 1.03 | 0.04 | 0.84 | 0.13 | 4.83 |
| Diisopropyl ether | $n_O \rightarrow \sigma^*_{O-H}$ | 6.09 | 2.76 | 0.12 | 0.91 | 0.09 | 8.03 |
| Dichloromethane | $n_O \rightarrow \sigma^*_{O-H}$ | 0.72 | 1.33 | 0.05 | 0.81 | 0.16 | 4.63 |
| Methyl tert–butyl ether | $n_O \rightarrow \sigma^*_{O-H}$ | 8.39 | 2.91 | 0.12 | 0.92 | 0.08 | 7.33 |
| Diethyl ether | $n_O \rightarrow \sigma^*_{O-H}$ | 7.05 | 2.27 | 0.11 | 0.90 | 0.09 | 7.14 |
| n-butanol    | $n_O \rightarrow \sigma^*_{O-H}$ | 6.99 | 2.47 | 0.11 | 0.87 | 0.12 | 6.56 |
| Ethyl acetate | $n_O \rightarrow \sigma^*_{O-H}$ | 3.38 | 2.03 | 0.09 | 0.81 | 0.18 | 6.52 |
| Methyl ethyl ketone | $n_O \rightarrow \sigma^*_{O-H}$ | 6.11 | 2.32 | 0.10 | 0.86 | 0.13 | 6.50 |
| Water–Water  | $n_O \rightarrow \sigma^*_{O-H}$ | 7.09 | 0.02 | 0.09 | 0.89 | 0.10 | 5.60 |

| $S \cdots S$ | Interaction | $-E_{d-a}^{(2)}$ | $\rho(r_c) \times 10^2$ | $\nabla^2 \rho(r_c)$ | $|V(r_c)|/|G(r_c)|$ | $\mathcal{H}(r_c)/\rho(r_c)$ | BE |
|--------------|-------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----|
| Isooctane    | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.41 | 0.52 | 0.01 | 0.85 | 0.09 | 4.79 |
| Heptane      | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.35 | 0.69 | 0.02 | 0.88 | 0.07 | 4.79 |
| Hexane       | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.22 | 0.50 | 0.01 | 0.86 | 0.09 | 6.11 |
| Pentane      | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.22 | 0.55 | 0.02 | 0.85 | 0.10 | 3.94 |
| Cyclohexane  | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.29 | 0.44 | 0.01 | 0.86 | 0.09 | 2.93 |
| Ortho–xylene | $\sigma_{C-H} \rightarrow \sigma^{*}_{C-H}$ | 0.59 | 0.73 | 0.02 | 0.84 | 0.09 | 9.48 |
| Toluene      | $\pi_{C=C} \rightarrow \pi^{*}_{C=C}$ | 0.48 | 0.78 | 0.02 | 0.84 | 0.10 | 7.75 |
| 1–octanol    | $n_O \rightarrow \sigma^*_{O-H}$ | 5.80 | 2.30 | 0.10 | 0.86 | 0.13 | 9.05 |
| Carbon tetrachloride | $n_{Cl} \rightarrow \sigma^*_{C-Cl}$ | 0.07 | 0.43 | 0.01 | 0.67 | 0.22 | 4.73 |
| Trichloroethylene | $n_{Cl} \rightarrow \pi^{*}_{C=Cl}$ | 0.71 | 0.72 | 0.03 | 0.74 | 0.18 | 9.55 |
| Benzene      | $n_{Cl} \rightarrow \pi^{*}_{C=Cl}$ | 0.73 | 0.72 | 0.02 | 0.82 | 0.10 | 5.33 |
| Chloroform   | $n_{Cl} \rightarrow \sigma^*_{C-H}$ | 0.60 | 2.63 | 0.03 | 0.78 | 0.15 | 5.83 |
| Butyl acetate | $n_O \rightarrow \sigma^*_{C-H}$ | 0.52 | 0.76 | 0.02 | 0.86 | 0.10 | 4.89 |
| Dichloroethane | $n_{Cl} \rightarrow \sigma^*_{C-H}$ | 1.04 | 0.77 | 0.03 | 0.79 | 0.14 | 6.02 |
| Diisopropyl ether | $n_O \rightarrow \sigma^*_{C-H}$ | 1.04 | 0.83 | 0.03 | 0.87 | 0.10 | 6.34 |
| Dichloromethane | $n_{Cl} \rightarrow \sigma^*_{C-H}$ | 0.32 | 0.66 | 0.02 | 0.78 | 0.15 | 4.71 |
| Methyl tert–butyl ether | $n_O \rightarrow \sigma^*_{C-H}$ | 0.68 | 0.87 | 0.03 | 0.90 | 0.08 | 3.80 |
| Diethyl ether | $n_O \rightarrow \sigma^*_{C-H}$ | 0.88 | 0.89 | 0.03 | 0.90 | 0.07 | 4.73 |
| n-butanol    | $n_O \rightarrow \sigma^*_{O-H}$ | 7.48 | 2.50 | 0.02 | 0.84 | 0.12 | 6.76 |
| Ethyl acetate | $n_O \rightarrow \pi^{*}_{C=O}$ | 0.80 | 0.67 | 0.03 | 0.83 | 0.14 | 7.90 |
| Methyl ethyl ketone | $\pi_{C=O} \rightarrow \pi^{*}_{C=O}$ | 0.97 | 0.72 | 0.03 | 0.76 | 0.17 | 7.62 |
Figure S2: Variation of the thickness of the interphase as a function of the solubility of $S$.

2.1 Entropy contributions to phase separation

The entropy contributions to phase separation are drawn by applying the methods suggested by Menon and coworkers[25]. To this end, we identified 165 atoms within the final interphase (after 30 ns) in every case and proceeded to follow the entropy changes associated with molecules containing those atoms along the entire MD trajectory (tests choosing 900 atoms at the initial and final points of the MDs yield exactly the same trends at a considerably higher computational cost). The corresponding data is plotted in Figure S3 for the set of chosen $S$/water set in Table 1 of the main document. Clearly, the contributions to entropy change significantly during the equilibration time (to the left of the solid vertical line) and once phase separation is achieved, little entropy changes are observed. The entire entropy contributions are separated into water, $S$ (Figure S4) and $S_{mix}$, which follow exactly the same patterns.
Figure S3: Entropy changes associated with phase separation in the S/water chosen set of binary systems in Table 1 of the manuscript. The vertical solid line separates the equilibration and production stages of the MD trajectories.

Figure S4: Decomposition of the entropy changes into $S_S$ (left), $S_w$ (right) and $S_{mix}$ for phase separation in the S/water chosen set of binary systems in Table 1 of the manuscript. The vertical solid line separates the equilibration and production stages of the MD trajectories.
3 NCI surfaces

Figure S5: NCI surfaces at the $S \cdots$ Water interphases for the complete set.
4 Dimers

4.1 Global minima: Structures and NBOs

4.1.1 $S \cdots$ Water

| Compound                  | Donor Orbital Interaction | Acceptor Orbital Interaction | Orbital Interaction Energy (kcal/mol) |
|---------------------------|---------------------------|-----------------------------|--------------------------------------|
| Isooctane                | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -1.15$ |
| Hexane                   | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -0.13$ |
| Pentane                  | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -0.20$ |
| Ortho-xylene             | $\pi_{C-C} \rightarrow \sigma^*_O-H$ | $E_{d \rightarrow a}^{(2)} = -0.35$ |
| Toluene                  | $\pi_{C-C} \rightarrow \sigma^*_O-H$ | $E_{d \rightarrow a}^{(2)} = -0.41$ |
| Trichloroethylene        | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -4.23$ |
| Chloroform               | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -3.00$ |
| Dichloroethane           | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -0.72$ |
| DichloroMethane          | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -1.95$ |
| Methyl tert-butyl ether  | $n_O \rightarrow \sigma^*_O-H$ | $E_{d \rightarrow a}^{(2)} = -8.39$ |
| Diethyl ether            | $n_O \rightarrow \sigma^*_O-H$ | $E_{d \rightarrow a}^{(2)} = -7.05$ |
| n-butanol                | $n_O \rightarrow \sigma^*_C-H$ | $E_{d \rightarrow a}^{(2)} = -6.99$ |
| Ethyl acetate            | $n_O \rightarrow \sigma^*_O-H$ | $E_{d \rightarrow a}^{(2)} = -3.38$ |

Figure S6: Dimers for all hydrophobe····water pairs in this study. Explicit orbital interactions leading to the largest orbital interaction energies (there are many more) in kcal/mol are shown. Donor orbitals are shown as solid surfaces, acceptor orbitals are shown as line surfaces. All calculations on the MP2/6–311++G(d,p) optimized global minima.
Figure S7: Dimers for all hydrophobe···hydrophobe pairs in this study. Explicit orbital interactions and orbital interaction energies in kcal/mol are shown. The water dimer is included for comparison.
4.2 Optimized geometries at the MP2/6-311++G(d,p) level for all dimers

4.2.1 Cartesian coordinates for all $S \cdots$ Water dimers

| Equilibrium Geometry Benzene···Water: $E =$ -307.8663713 Hartree |
|---------------------------------------------------------------|
| 8 $ $2.726011 -0.089130 -0.001029 $ |
| 1 $ $2.625939 -1.043776 -0.002546 $ |
| 1 $ $1.813476 0.216323 -0.000075 $ |
| 6 $ -0.564457 0.677067 -1.244796 $ |
| 6 $ -0.487127 1.429391 -0.064830 $ |
| 6 $ -0.551715 0.789060 1.180247 $ |
| 6 $ -0.683617 -0.604115 1.245013 $ |
| 6 $ -0.764407 -1.355646 0.065329 $ |
| 6 $ -0.696088 -0.716064 -1.179415 $ |
| 1 $ -0.513786 1.173796 -2.209761 $ |
| 1 $ -0.384228 2.509975 -0.115280 $ |
| 1 $ -0.491436 1.372595 2.094761 $ |
| 1 $ -0.737604 -1.099782 2.210535 $ |
| 1 $ -0.875394 -2.435679 0.115837 $ |
| 1 $ -0.760593 -1.298562 -2.094530 $ |

| Equilibrium Geometry Butyl acetate···Water: $E =$ -461.6241343 Hartree |
|---------------------------------------------------------------|
| 8 $ $2.726011 -0.089130 -0.001029 $ |
| 1 $ $2.625939 -1.043776 -0.002546 $ |
| 1 $ $1.813476 0.216323 -0.000075 $ |
| 6 $ -0.564457 0.677067 -1.244796 $ |
| 6 $ -0.487127 1.429391 -0.064830 $ |
| 6 $ -0.551715 0.789060 1.180247 $ |
| 6 $ -0.683617 -0.604115 1.245013 $ |
| 6 $ -0.764407 -1.355646 0.065329 $ |
| 6 $ -0.696088 -0.716064 -1.179415 $ |
| 1 $ -0.513786 1.173796 -2.209761 $ |
| 1 $ -0.384228 2.509975 -0.115280 $ |
| 1 $ -0.491436 1.372595 2.094761 $ |
| 1 $ -0.737604 -1.099782 2.210535 $ |
| 1 $ -0.875394 -2.435679 0.115837 $ |
| 1 $ -0.760593 -1.298562 -2.094530 $ |

| Equilibrium Geometry Carbon tetrachloride···Water: $E =$ -1952.8492516 Hartree |
|---------------------------------------------------------------|
| 8 $ -4.136278 0.000268 0.067936 $ |
| 1 $ -4.642094 0.752608 -0.248541 $ |
| 1 $ -4.638211 -0.756762 -0.243570 $ |
| 6 $ 0.564012 -0.000134 0.000017 $ |
| 17 $ -1.199769 -0.001500 0.027672 $ |
| 17 $ 1.153121 1.557130 -0.617426 $ |
| 17 $ 1.148981 -1.303748 -1.054430 $ |
| 17 $ 1.190989 -0.251716 1.641156 $ |

S11
|                | Equilibrium Geometry Chloroform | Water: $E = -1493.8116489$ Hartree |
|----------------|--------------------------------|----------------------------------|
|                | 8                               | 2.824122 -0.001568 -0.976362      |
|                | 1                               | 3.311753  0.001794 -0.148735      |
|                | 1                               | 3.504955  0.009680 -1.653452      |
|                | 6                               | -0.150861 0.000104 -0.119463      |
|                | 1                               | 0.710276  0.000161 -0.776902      |
|                | 17                              | -1.087199 1.464595 -0.433012      |
|                | 17                              | -1.102084 -1.450563 -0.452237     |
|                | 17                              | 0.470787  -0.014015 1.538588       |

|                | Equilibrium Geometry Cyclohexane | Water: $E = -311.4494789$ Hartree |
|----------------|---------------------------------|----------------------------------|
|                | 8                               | -3.015677 -0.000010 -0.262650     |
|                | 1                               | -3.847891 -0.000395 0.217362      |
|                | 1                               | -3.290433 -0.000813 -1.183222     |
|                | 6                               | 1.047748 -1.263702 -0.589861      |
|                | 6                               | 0.758852 -0.001229 -1.608779      |
|                | 6                               | 1.047967 1.262580 -0.591980       |
|                | 6                               | 0.252902 1.262402 0.717944        |
|                | 6                               | 0.547989 0.001271 1.538686        |
|                | 6                               | 0.252669 -1.261172 0.720047       |
|                | 1                               | 0.811253 -2.159461 -1.176916      |
|                | 1                               | 1.350034 -0.002041 -2.332716      |
|                | 1                               | 2.122997 1.304083 -0.364326       |
|                | 1                               | 0.487151 2.160052 1.303165        |
|                | 1                               | 1.606465 0.001430 1.835742        |
|                | 1                               | -0.819569 -1.288137 0.488376      |
|                | 1                               | 0.486731 -2.157882 1.306783       |
|                | 1                               | -0.044996 0.002089 2.459458       |
|                | 1                               | -0.819338 1.289217 0.486243       |
|                | 1                               | 0.811641 2.157401 -1.180534       |
|                | 1                               | -0.300167 -0.001391 -1.701686     |
|                | 1                               | 2.122769 -1.305023 -0.362132      |

|                | Equilibrium Geometry Dichloroethane | Water: $E = -1073.9674807$ Hartree |
|----------------|-------------------------------------|-----------------------------------|
|                | 8                                   | 1.170697 2.268498 -0.028029        |
|                | 1                                   | 2.044497 1.873387 0.037559         |
|                | 1                                   | 1.343786 3.202971 -0.163776        |
|                | 6                                   | 0.196575 -0.665773 -0.557136       |
|                | 1                                   | -0.151564 -1.595660 -1.005858      |
|                | 1                                   | 0.266031 0.117277 -1.309643        |
|                | 6                                   | -0.707012 -0.230838 0.577144       |
|                | 1                                   | -0.758253 -0.995214 1.352227       |
|                | 1                                   | -0.370514 0.716610 0.991881        |
|                | 17                                  | 1.843935 -0.955744 0.078114        |
|                | 17                                  | -2.354343 0.009409 -0.066244       |

|                | Equilibrium Geometry Dichloromethane | Water: $E = -1034.7617373$ Hartree |
|----------------|-------------------------------------|-----------------------------------|

S12
| 8     | -2.503222 | -1.091896 | -0.014667 |
| 1     | -3.210150 | -1.714505 | -0.197831 |
| 1     | -2.649856 | -0.375745 | -0.637941 |
| 6     | 0.355683  | 0.002572  | 0.696140  |
| 1     | 0.745648  | 0.326723  | 1.656783  |
| 1     | -0.454808 | -0.710861 | 0.802530  |
| 17    | -0.290246 | 1.429241  | -0.135530 |
| 17    | 1.670295  | -0.770763 | -0.198766 |

Equilibrium Geometry Diethyl ether

| 8     | -0.000463 | 2.439948  | -0.272334 |
| 1     | 0.000574  | 2.913069  | 0.562024  |
| 1     | -0.000229 | 1.507539  | -0.005199 |
| 6     | -2.384624 | -0.301076 | 0.339626  |
| 6     | -1.180665 | -0.925322 | -0.338049 |
| 1     | -2.410778 | 0.775361  | 0.156084  |
| 1     | -3.304011 | -0.743740 | -0.054585 |
| 1     | -2.345918 | -0.487473 | 1.417242  |
| 1     | -1.162590 | -2.013130 | -0.179811 |
| 1     | -1.199283 | -0.736797 | -1.421340 |
| 8     | 0.000070  | -0.354312 | 0.221012  |
| 6     | 1.180878  | -0.925199 | -0.338030 |
| 6     | 2.384739  | -0.300684 | 0.339567  |
| 1     | 1.199441  | -0.736767 | -1.421338 |
| 1     | 1.162971  | -2.012991 | -0.179683 |
| 1     | 3.304200  | -0.743318 | -0.054507 |
| 1     | 2.410790  | 0.775716  | 0.155789  |
| 1     | 2.346002  | -0.477863 | 1.417217  |

Equilibrium Geometry Diisopropyl ether

| 8     | -1.274964 | 2.452221 | -0.362445 |
| 1     | -1.046292 | 2.945200 | -1.153430 |
| 1     | -0.713433 | 1.661855 | -0.411677 |
| 6     | 2.051664  | 1.178867 | 0.337744  |
| 6     | 1.390112  | -0.185764 | 0.307115  |
| 1     | 1.267694  | -0.553524 | 1.337018  |
| 1     | 1.467131  | 1.878445  | 0.940330  |
| 1     | 3.059403  | 1.103934  | 0.757762  |
| 1     | 2.130454  | 1.573894  | -0.680376 |
| 6     | 2.194490  | -1.199267 | -0.502747 |
| 1     | 1.678640  | -2.161914 | -0.561621 |
| 1     | 2.341031  | -0.820483 | -1.518878 |
| 1     | 3.174340  | -1.364848 | -0.042813 |
| 8     | 0.091541  | -0.014054 | -0.278348 |
| 6     | -0.882358 | -0.982868 | 0.151540  |
| 6     | -1.886079 | -1.128069 | -0.979835 |
| 6     | -1.355410 | -0.528654 | 1.452488  |
| 1     | -0.370265 | 1.942752  | 0.308353  |
| 1     | -1.386565 | -1.463264 | -1.892618 |
|   |   |   |   |
|---|---|---|---|
| 1 | -2.657495 | -1.856166 | -0.710252 |
| 1 | -2.367969 | -0.165233 | -1.173227 |
| 1 | -0.789669 | -0.384367 | 2.239987 |
| 1 | -2.061013 | 0.417183 | 1.291974 |
| 1 | -2.253122 | -1.280087 | 1.797982 |

Equilibrium Geometry Ethyl acetate

|   |   |   |   |
|---|---|---|---|
| 8 | -2.461478 | -1.782419 | -0.022828 |
| 1 | -2.700601 | -2.711038 | -0.037329 |
| 1 | -1.495409 | -1.794126 | 0.006432 |
| 6 | -1.062736 | 2.569181 | 0.004484 |
| 6 | -0.760086 | 0.975190 | 0.018639 |
| 1 | -0.614823 | 2.952691 | 0.868803 |
| 1 | -0.680235 | 2.920044 | -0.906993 |
| 1 | -2.145832 | 2.603128 | 0.041780 |
| 1 | -1.194081 | 0.460948 | -0.841266 |
| 1 | -1.129167 | 0.491047 | 0.925444 |
| 8 | 0.682495 | 0.835797 | -0.031193 |
| 6 | 1.140629 | -0.425196 | -0.002973 |
| 8 | 0.422256 | -1.407519 | 0.047633 |
| 6 | 2.645670 | -0.458866 | -0.016940 |
| 1 | 3.032601 | 0.225254 | -0.773914 |
| 1 | 3.016498 | -0.128931 | 0.957313 |
| 1 | 2.984010 | -1.476164 | -0.208424 |

Equilibrium Geometry Heptane

|   |   |   |   |
|---|---|---|---|
| 8 | 0.199133 | 3.278517 | -0.062154 |
| 1 | 0.392668 | 2.344237 | 0.049683 |
| 1 | -0.688316 | 3.361629 | 0.294593 |
| 6 | 3.801182 | -0.227887 | 0.024463 |
| 1 | 3.837697 | 0.459698 | -0.829755 |
| 1 | 4.700355 | -0.850550 | -0.001968 |
| 1 | 3.834038 | 0.375018 | 0.937844 |
| 6 | 2.530647 | -1.077761 | -0.017189 |
| 1 | 2.524834 | -1.693166 | -0.925573 |
| 1 | 2.519230 | -1.771456 | 0.832913 |
| 6 | 1.257446 | -0.231441 | 0.015686 |
| 1 | 1.269018 | 0.458040 | -0.841152 |
| 1 | 1.266101 | 0.383247 | 0.928291 |
| 6 | -0.028794 | -1.057440 | -0.021806 |
| 1 | -0.036790 | -1.752977 | 0.828396 |
| 1 | -0.036086 | -1.671949 | -0.932220 |
| 6 | -1.294523 | -0.200047 | 0.016194 |
| 1 | -1.284480 | 0.497733 | -0.833227 |
| 1 | -1.288447 | 0.409867 | 0.931873 |
| 6 | -2.586428 | -1.016812 | -0.025509 |
| 1 | -2.593571 | -1.717827 | 0.818591 |
| 1 | -2.594023 | -1.624391 | -0.939084 |
| 6 | -3.837578 | -0.138769 | 0.021091 |
### Equilibrium Geometry Heptane·Water 2: E= -351.8287115 Hartree

|   | X      | Y      | Z      |
|---|--------|--------|--------|
| 1 | -4.751355 | -0.739425 | -0.012811 |
| 1 | -3.859083 | 0.455564  | 0.940737  |
| 1 | -3.856568 | 0.553082  | -0.827480 |
| 8 | -0.031555 | 2.786915  | 0.029404  |
| 1 | -0.134768 | 3.370202  | 0.785662  |
| 1 | 0.047611  | 3.95578   | -0.709622 |
| 6 | 3.823433  | 0.429426  | -0.361559 |
| 1 | 3.881029  | -1.272089 | -1.058732 |
| 1 | 4.728086  | -0.438401 | 0.254482  |
| 6 | 3.824387  | 0.493622  | -0.950904 |
| 1 | 2.557773  | -0.519595 | 0.492229  |
| 1 | 2.583027  | -1.436600 | 1.095198  |
| 1 | 2.527022  | 0.320775  | 1.197242  |
| 6 | 1.280019  | -0.504182 | -0.346561 |
| 1 | 1.300494  | -1.345062 | -1.054658 |
| 1 | 1.254761  | 0.417029  | -0.942971 |
| 6 | 0.005863  | -0.578130 | 0.493268  |
| 1 | 0.004296  | 0.254994  | 1.207886  |
| 1 | 0.007993  | -1.507224 | 1.081347  |
| 6 | -1.268062 | -0.509817 | -0.347426 |
| 1 | -1.282634 | -1.348818 | -1.057906 |
| 1 | -1.248319 | 0.413738  | -0.940079 |
| 6 | -2.546375 | -0.536466 | 0.490255  |
| 1 | -2.522034 | 0.301660  | 1.198337  |
| 1 | -2.566491 | -1.455538 | 1.090278  |
| 6 | -3.811713 | -0.451216 | -0.364515 |
| 1 | -4.716994 | -0.466982 | 0.250490  |
| 1 | -3.816960 | 0.473236  | -0.951577 |
| 1 | -3.863701 | -1.292443 | -1.063850 |

### Equilibrium Geometry Hexane·Water: E= -312.6328551 Hartree

|   | X      | Y      | Z      |
|---|--------|--------|--------|
| 8 | -0.007893 | 2.743664 | -0.000368 |
| 1 | -0.252260 | 3.341142 | 0.711013 |
| 1 | 0.236463  | 3.38323  | -0.714107 |
| 6 | -3.201215 | -0.548893 | -0.214379 |
| 1 | -3.250798 | 0.33027  | -0.861598 |
| 1 | -4.060367 | -0.521213 | 0.463266 |
| 1 | -3.299756 | -1.43505  | -0.848411 |
| 6 | -1.877951 | -0.575070 | 0.551656 |
| 1 | -1.806537 | 0.311428  | 1.194192 |
| 1 | -1.850353 | -1.449774 | 1.214572 |
| 6 | -0.663405 | -0.606310 | -0.375473 |
| 1 | -0.699058 | 0.270249  | -1.034558 |
| 1 | -0.719951 | -1.496722 | -1.018181 |
| 6 | 0.666611  | -0.603252 | 0.375811 |
| 1 | 0.725158  | -1.490092 | 1.022144 |
| 1 | 0.700172  | 0.276106  | 1.031234 |

S15
### Equilibrium Geometry Isooctane

| Water: E= -391.0329068 Hartree |
|-----------------------------|
| 8  | 2.171565 | 2.382174 | 0.356602 |
| 1  | 2.961896 | 2.112787 | -0.119059 |
| 1  | 2.354104 | 3.294292 | 0.057634 |
| 6  | -1.431300 | 0.130797 | -0.005036 |
| 6  | -1.402994 | 0.636349 | 1.443079 |
| 1  | -0.403045 | 0.968252 | 1.740840 |
| 1  | -2.084936 | 1.487524 | 1.557965 |
| 6  | -1.726266 | -0.152515 | 2.133444 |
| 6  | -0.994406 | 1.264817 | -0.942471 |
| 1  | -0.001234 | 1.643521 | -0.684133 |
| 1  | -0.986624 | 0.926472 | -1.985873 |
| 1  | -1.702953 | 2.099200 | -0.866529 |
| 6  | -2.852294 | -0.298450 | -0.357558 |
| 1  | -2.910291 | -0.638569 | -1.398406 |
| 1  | -3.183897 | -1.120110 | 0.288686 |
| 1  | -3.551479 | 0.537052 | -0.232543 |
| 6  | -0.507148 | -1.101532 | -0.147129 |
| 6  | -0.862338 | -1.846685 | 0.578267 |
| 1  | -0.667918 | -1.544893 | -1.142168 |
| 6  | 1.004845 | -0.871249 | 0.059687 |
| 1  | 1.150409 | 0.047916 | 0.638069 |
| 6  | 1.739087 | -0.707609 | -1.275471 |
| 1  | 1.656840 | -1.628534 | -1.866327 |
| 1  | 1.327173 | 0.112847 | -1.869992 |
| 1  | 2.806530 | -0.513024 | -1.113303 |
| 6  | 1.622360 | -2.029267 | 0.849379 |
| 1  | 2.700636 | -1.886854 | 0.984986 |
| 1  | 1.161882 | -2.119532 | 1.839048 |
| 1  | 1.470885 | -2.977671 | 0.318802 |

### Equilibrium Geometry Methyl ethyl ketone

| Water: E= -308.1374225 Hartree |
|-----------------------------|
| 8  | 3.163520 | -0.534171 | 0.068342 |
| 1  | 3.643717 | -1.314326 | -0.214956 |
| 1  | 2.235536 | -0.796617 | 0.008742 |
| 6  | -0.246095 | 0.304566 | -0.051224 |
| 8  | 0.301610 | -0.790088 | -0.091789 |
| 6  | 0.584469 | 1.594369 | 0.037769 |
| 1  | 1.580098 | 1.435606 | -0.243360 |
| 1  | 0.081200 | 2.366397 | -0.587347 |
| 1  | 0.502061 | 1.947366 | 1.074832 |
Equilibrium Geometry Methyl tert-butyl ether

Water: $E = -348.51227$ Hartree

Equilibrium Geometry n–butanol

Water: $E = -309.3226537$ Hartree
### Equilibrium Geometry of n-octanol

|   |   |   |   |
|---|---|---|---|
| 1 | -2.262167 | -1.790333 | -0.057678 |

Water: $E = -466.1057537$ Hartree

### Equilibrium Geometry of Ortho-xylene

|   |   |   |   |
|---|---|---|---|
| 8 | -4.511111 | 2.160911 | 0.362019 |
| 1 | -4.507560 | 1.245893 | 0.045412 |
| 1 | -4.820379 | 2.660814 | -0.395653 |
| 6 | 5.604768 | 0.688662 | -0.170372 |
| 1 | 5.493199 | 1.723943 | 0.168323 |
| 1 | 5.654517 | 0.697364 | -1.264214 |
| 1 | 6.559161 | 0.310388 | 0.208292 |
| 6 | 4.431197 | -0.166114 | 0.310124 |
| 1 | 4.571153 | -1.204161 | -0.017548 |
| 1 | 4.411077 | -0.183393 | 1.407250 |
| 6 | 3.083906 | 0.341680 | -0.204849 |
| 1 | 3.100920 | 0.360014 | -1.30520 |
| 1 | 2.939833 | 1.380392 | 0.123442 |
| 6 | 1.899081 | -0.502500 | 0.265319 |
| 1 | 1.880587 | -0.519781 | 1.363863 |
| 1 | 2.041856 | -1.541339 | -0.063491 |
| 6 | 0.554424 | 0.009273 | -0.252113 |
| 1 | 0.572091 | 0.027206 | -1.350458 |
| 1 | 0.409468 | 1.046790 | 0.077815 |
| 6 | -0.630551 | -0.359380 | 0.217678 |
| 1 | -0.644831 | -0.852731 | 1.316041 |
| 1 | -0.485007 | -1.873595 | -0.113473 |
| 6 | -1.969662 | -0.312381 | -0.302615 |
| 1 | -1.966334 | -0.305333 | -1.399979 |
| 1 | -2.122758 | 0.719163 | 0.033394 |
| 6 | -3.134741 | -1.160157 | 0.172641 |
| 1 | -3.179117 | -1.157282 | 1.269239 |
| 1 | -3.013887 | -2.194879 | -0.171861 |
| 8 | -4.345083 | -0.604957 | -0.369687 |
| 1 | -5.076682 | -1.162007 | -0.086959 |

Water: $E = -386.2697695$ Hartree

### Equilibrium Geometry of Ortho-xylene

|   |   |   |   |
|---|---|---|---|
| 8 | -1.134868 | -0.274503 | 2.467240 |
| 1 | -0.641846 | -0.328753 | 3.289379 |
| 1 | -0.445427 | -0.185566 | 1.799956 |
| 6 | 2.082558 | -0.710748 | -0.057823 |
| 6 | 0.891075 | -1.358794 | -0.404688 |
| 6 | -0.295719 | -0.640114 | -0.620575 |
| 6 | -0.284653 | 0.766026 | -0.471764 |
| 6 | 0.916623 | 1.406898 | -0.128485 |
| 6 | 2.094153 | 0.680799 | 0.086839 |
| 1 | 2.989379 | -1.288009 | 0.102637 |
| 1 | 0.879353 | -2.441134 | -0.517473 |
| 1 | 0.922864 | 2.489376 | -0.016542 |
| 1 | 3.011591 | 1.198438 | 0.354510 |
| 6 | -1.544939 | 1.566384 | -0.682443 |

S18
|   | 1   | 1   | 6   | 1   | 1   | 1   |
|---|-----|-----|-----|-----|-----|-----|
|   | -1.903827 | 1.474501 | -1.713858 | -2.344215 | 1.217036 | -0.020147 |
|   | -1.369483 | 2.625497 | -0.476472 | -1.575171 | -1.363235 | -0.957046 |
|   | -2.294534 | -1.281397 | -0.134206 | -2.045064 | -0.942969 | -1.852503 |
|   | -1.383568 | -2.424292 | -1.137292 | 8   | -0.302291 | 2.662006 |
|   | 0.037131 | 3.386102 | 0.514755 | 1   | -0.740045 | 3.109062 |
|   | 2.610593 | -0.508601 | -0.328547 | 1   | 2.723516 | -1.466765 |
|   | 3.508214 | -0.344903 | 0.276113 | 1   | 2.563968 | 0.280257 |
|   | 1.343887 | -0.501025 | 0.527842 | 6   | 1.415666 | -1.275121 |
|   | 1.253911 | 0.462002 | 1.043982 | 6   | 0.078142 | -0.730296 |
|   | 0.144546 | -1.704126 | -0.803296 | 1   | 0.024658 | 0.035319 |
|   | -1.201626 | 0.303194 | -1.081745 | 6   | -1.251079 | 0.300400 |
|   | -1.153105 | -1.438663 | 1.324359 | 1   | -2.459446 | -0.887368 |
|   | -2.435161 | -1.862311 | -0.805806 | 1   | -3.366858 | -0.843186 |
|   | -2.536331 | -0.117005 | -1.081872 | 8   | 0.343262 | 2.722118 |
|   | 0.115917 | 2.158587 | 0.744495 | 1   | 0.117069 | 2.158554 |
|   | 0.135019 | -0.565903 | 1.205085 | 6   | 0.135021 | -0.564511 |
|   | 0.855352 | -0.598651 | 0.000213 | 6   | -1.257300 | -0.410510 |
|   | 0.135019 | -0.565903 | 1.205085 | 6   | 0.135021 | -0.564511 |
|   | -1.257285 | -0.409150 | 1.209687 | 6   | -1.961391 | -0.364061 |
|   | -1.795345 | -0.384820 | 2.153659 | 1   | 0.674371 | -0.617565 |
|   | -1.795288 | -0.382977 | 2.153962 | 1   | 2.360020 | -0.699983 |
|   | 2.813525 | 0.297668 | 0.000316 | 1   | 0.674390 | -0.615137 |

**Equilibrium Geometry Pentane - Water:**

**Hartree**

-273.436907

**Equilibrium Geometry Toluene - Water:**

-347.0680392

---

S19
|   |        |        |        |
|---|--------|--------|--------|
| 8 | -3.393492 | 0.650467 | -0.068345 |
| 1 | -4.167382 | 1.134834 | 0.229587  |
| 1 | -3.594990 | -0.264037 | 0.146412  |
| 6 | -0.164119 | 0.770119 | 0.011606  |
| 1 | -1.233820 | 0.940734 | 0.012540  |
| 6 | 0.329914  | -0.478084 | 0.002036  |
| 17| 1.999020  | -0.863546 | -0.009322 |
| 17| -0.751836 | -1.825752 | 0.008429  |
| 17| 0.820425  | 2.173564  | 0.005385  |
### 4.2.2 Cartesian coordinates for all $S \cdots S$ dimers

**Equilibrium Geometry (Benzene)$_2$: E = -463.1803711$ Hartree**

|   | x          | y          | z          |
|---|------------|------------|------------|
| 6 | -2.620356  | 0.000533   | 0.780720   |
| 6 | -2.201155  | -1.212572  | 0.219896   |
| 6 | -1.369209  | -1.212146  | -0.906788  |
| 6 | -0.951666  | -0.000531  | -1.470162  |
| 6 | -1.368652  | 1.211616   | -0.907526  |
| 6 | -2.200592  | 1.213105   | 0.219163   |
| 6 | -3.270773  | 0.000950   | 1.651991   |
| 6 | -2.529213  | -2.154199  | 0.653406   |
| 6 | -1.040623  | -2.153288  | -1.340496  |
| 6 | -0.295466  | -0.000944  | -2.336331  |
| 1 | -1.039610  | 2.152348   | -1.341777  |
| 1 | -2.528217  | 2.155146   | 0.652104   |
| 6 | 2.620324   | 0.000756   | -0.780742  |
| 6 | 2.200471   | 1.213217   | -0.219013  |
| 6 | 1.368552   | 1.211502   | 0.907689   |
| 6 | 0.951693   | -0.000759  | 1.470180   |
| 6 | 1.369333   | -1.212261  | 0.906642   |
| 6 | 2.201258   | -1.212462  | -0.220060  |
| 1 | 3.270722   | 0.001340   | -1.652027  |
| 1 | 2.527991   | 2.155345   | -0.651844  |
| 1 | 1.039434   | 2.152142   | 1.342080   |
| 1 | 0.295521   | -0.001337  | 2.336372   |
| 1 | 1.040846   | -2.153494  | 1.340225   |
| 1 | 2.529388   | -2.154002  | -0.653705  |

---

**Equilibrium Geometry (Butyl acetate)$_2$: E = -770.6830171625$ Hartree**

|   | x          | y          | z          |
|---|------------|------------|------------|
| 6 | -4.224777  | 0.017178   | -0.204328  |
| 8 | -3.843710  | -1.133109  | -0.277371  |
| 8 | -3.39051   | 1.069861   | -0.052272  |
| 6 | -1.994068  | 0.719783   | 0.048652   |
| 6 | -1.191378  | 2.003211   | 0.109098   |
| 1 | -1.714804  | 0.122570   | -0.825363  |
| 1 | -1.842112  | 0.107922   | 0.943647   |
| 6 | 0.297766   | 1.694938   | 0.274615   |
| 1 | -1.357094  | 2.578569   | -0.809629  |
| 1 | -1.542892  | 2.614141   | 0.948659   |
| 6 | 1.169756   | 2.949916   | 0.250762   |
| 1 | 0.442990   | 1.160925   | 1.221147   |
| 1 | 0.613567   | 1.012024   | -0.524338  |
| 1 | 2.228474   | 2.700702   | 0.377000   |
| 1 | 1.059929   | 3.482639   | -0.699693  |
| 1 | 0.886713   | 3.635769   | 1.055987   |
| 6 | -5.660060  | 0.473098   | -0.247189  |
| 1 | -5.767412  | 1.325042   | -0.920931  |
| 1 | -6.292896  | -0.353145  | -0.568496  |
| 1 | -5.960481  | 0.794638   | 0.753803   |
| 6 | 0.360606   | -2.008815  | 0.311155   |
| 8 | 0.221082   | -1.820728  | 1.501997   |
|    |        |        |        |        |
|----|--------|--------|--------|--------|
| 8  | 1.478175 | -1.656736 | -0.373759 |
| 6  | 2.539275 | -1.091256 | 0.422982  |
| 6  | 3.516772 | -0.419901 | -0.520749 |
| 1  | 3.015842 | -1.896147 | 0.993868  |
| 1  | 2.117668 | -0.375690 | 1.132568  |
| 6  | 4.679559 | 0.224066  | 0.236089  |
| 1  | 3.898196 | -1.156412 | -1.237859 |
| 1  | 2.983617 | 0.346915  | -1.096160 |
| 6  | 5.464800 | 0.949127  | -0.700551 |
| 1  | 4.282460 | 0.932112  | 0.974788  |
| 1  | 5.219220 | -0.547074 | 0.799793  |
| 1  | 6.475596 | 1.399832  | -0.147406 |
| 1  | 6.066985 | 0.255076  | -1.435362 |
| 1  | 5.130754 | 1.745655  | -1.246807 |
| 6  | -0.642279| -2.676027 | -0.592189 |
| 1  | -0.510667| -3.758909 | -0.501868 |
| 1  | -1.653458| -2.420295 | -0.273056 |
| 1  | -0.482870| -2.393072 | -1.633138 |

Equilibrium Geometry (Carbon tetrachloride)$_2$: $E = -3753.1483706$ Hartree

|    |        |        |        |        |
|----|--------|--------|--------|--------|
| 6  | -2.409399| -0.000768 | 0.000393 |
| 17 | -2.349685| 1.272594 | -1.231587 |
| 17 | -1.340502| -1.334758 | -0.473476 |
| 17 | -4.071901| -0.597590 | 0.149159 |
| 17 | -1.879146| 0.660219  | 1.555835 |
| 6  | 2.409523 | 0.000715  | 0.000365 |
| 17 | 2.349045 | -1.256229 | -1.248260 |
| 17 | 1.879472 | -0.680741 | 1.547004 |
| 17 | 1.346209 | 1.341101  | -0.455581 |
| 17 | 4.072015 | 0.595423  | 0.156639 |

Equilibrium Geometry (Chloroform)$_2$: $E = -2835.064959$ Hartree

|    |        |        |        |        |
|----|--------|--------|--------|--------|
| 6  | 1.830301| 0.000046 | -0.036682 |
| 1  | 0.933838| 0.000242 | -0.645087 |
| 17 | 1.327318| -0.000571 | 1.662544 |
| 17 | 2.743469| -1.456953 | -0.426744 |
| 17 | 2.743517| 1.457359  | -0.425667 |
| 6  | -2.026403| 0.000098 | 0.194223 |
| 1  | -1.585652| 0.000217  | 1.185953 |
| 17 | -3.778422| -0.000036 | 0.377505 |
| 17 | -1.464278| 1.456580  | -0.637654 |
| 17 | -1.464050| -1.456457 | -0.637402 |

Equilibrium Geometry (Cyclohexane)$_2$: $E = -470.3487178$ Hartree

|    |        |        |        |        |
|----|--------|--------|--------|--------|
| 6  | 1.720489| -0.422859 | -1.406749 |
| 6  | 2.685891| -1.345445 | -0.635889 |
| 6  | 2.671397| -1.050671 | 0.847485 |
| 6  | 2.991162| 0.422029  | 1.123705 |

S22
Equilibrium Geometry (Dichloroethane)₂: E = -1995.3795492 Hartree

|   | 1   | 2         | 3         | 4         | 5         | 6         | 7         | 8         | 9         |
|---|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|   | 6   | 2.026250  | 1.345696  | 0.373325  |           |           |           |           |           |
|   | 6   | 2.035868  | 1.050571  | -1.130058 |           |           |           |           |           |
|   | 1   | 1.760369  | -0.624678 | -2.483960 |           |           |           |           |           |
|   | 1   | 2.429203  | -2.395428 | -0.840502 |           |           |           |           |           |
|   | 1   | 1.675899  | -1.284360 | 1.250613  |           |           |           |           |           |
|   | 1   | 2.951128  | 0.624545  | 2.200602  |           |           |           |           |           |
|   | 1   | 1.010091  | 1.196710  | 0.763796  |           |           |           |           |           |
|   | 1   | 3.029789  | 1.287205  | -1.536281 |           |           |           |           |           |
|   | 1   | 1.318522  | 1.697718  | -1.649159 |           |           |           |           |           |
|   | 1   | 2.285345  | 2.395622  | 0.555436  |           |           |           |           |           |
|   | 1   | 4.019165  | 0.633466  | 0.796238  |           |           |           |           |           |
|   | 1   | 3.385516  | -1.69071  | 1.369065  |           |           |           |           |           |
|   | 1   | 3.703673  | -1.192138 | -1.042335 |           |           |           |           |           |
|   | 1   | 0.693526  | -0.638147 | -1.080555 |           |           |           |           |           |
|   | 6   | 2.671669  | -1.048961 | -0.849397 |           |           |           |           |           |
|   | 6   | 2.989929  | 0.424741  | -1.123462 |           |           |           |           |           |
|   | 6   | 2.024740  | 1.346350  | -0.370912 |           |           |           |           |           |
|   | 6   | 2.035664  | 1.048810  | 1.131985  |           |           |           |           |           |
|   | 6   | -1.721691 | -0.425337 | 1.406474  |           |           |           |           |           |
|   | 6   | -2.687382 | -1.345885 | 0.653489  |           |           |           |           |           |
|   | 1   | -3.386043 | -1.695601 | -1.372474 |           |           |           |           |           |
|   | 1   | -2.94856 | 0.629845  | -2.200006 |           |           |           |           |           |
|   | 1   | -1.008412 | 1.197062  | -0.760811 |           |           |           |           |           |
|   | 1   | -1.318080 | 1.694476  | 1.652591  |           |           |           |           |           |
|   | 1   | -0.694684 | -0.640934 | 1.080598  |           |           |           |           |           |
|   | 1   | -3.705283 | -1.192343 | 1.039528  |           |           |           |           |           |
|   | 1   | -2.431705 | -2.396384 | 0.836558  |           |           |           |           |           |
|   | 1   | -1.762439 | -0.628880 | 2.483273  |           |           |           |           |           |
|   | 1   | -3.029645 | 1.285637  | 1.537944  |           |           |           |           |           |
|   | 1   | -2.282756 | 2.396797  | -0.551529 |           |           |           |           |           |
|   | 1   | -4.017976 | 0.636566  | -0.796382 |           |           |           |           |           |
|   | 1   | -1.676133 | -1.282637 | -1.252274 |           |           |           |           |           |

S23
|               |       |       |       |       |       |       |
|---------------|-------|-------|-------|-------|-------|-------|
| Equilibrium Geometry (Dichloromethane): E = -1916.9661675 Hartree |       |       |       |       |       |       |
| 6             | -1.517815 | -0.523602 | -0.602144 |       |       |       |
| 1             | -0.553543 | -0.173578 | -0.956478 |       |       |       |
| 17            | 1.287928  | 1.283639  | -0.981830  |       |       |       |
| 17            | 2.625783  | 0.849374  | -0.547456  |       |       |       |
| 6             | 2.160957  | 0.022635  | 0.615836  |       |       |       |
| 1             | 1.629849  | -0.602092 | 1.328791  |       |       |       |
| 1             | 3.176603  | 0.220940  | 0.946786  |       |       |       |
| 17            | 2.244074  | -0.845061 | -0.925731 |       |       |       |
| 17            | 1.306072  | 1.563527  | 0.483879  |       |       |       |

|               |       |       |       |       |       |       |
|---------------|-------|-------|-------|-------|-------|-------|
| Equilibrium Geometry (Diethyl ether): E = -466.0584287 Hartree |       |       |       |       |       |       |
| 6             | -1.613032 | 2.245305  | -1.107660 |       |       |       |
| 6             | -1.304797 | 0.767783  | -1.257493 |       |       |       |
| 1             | -1.230744 | 2.618581  | -0.153890 |       |       |       |
| 1             | -1.146925 | 2.814240  | -1.918372 |       |       |       |
| 1             | -2.692458 | 2.413612  | -1.138498 |       |       |       |
| 1             | -1.677105 | 0.391906  | -2.224064 |       |       |       |
| 1             | -0.220752 | 0.589230  | -1.219094 |       |       |       |
| 8             | -1.937541 | 0.072333  | -0.196368 |       |       |       |
| 6             | -1.646507 | -1.318608 | -0.240031 |       |       |       |
| 6             | -2.360890 | -1.987326 | 0.918244  |       |       |       |
| 1             | -0.560777 | -1.467288 | -0.166563 |       |       |       |
| 1             | -1.992014 | -1.736360 | -1.199243 |       |       |       |
| 1             | -2.172191 | 3.065266  | 0.904933  |       |       |       |
| 1             | -2.002487 | -1.584054 | 1.868662  |       |       |       |
| 1             | -3.438793 | -1.819702 | 0.850444  |       |       |       |
| 6             | 2.604593  | -1.382646 | -1.368195 |       |       |       |
| 6             | 2.589601  | -0.080603 | -0.590737 |       |       |       |
| 1             | 1.630702  | -1.563192 | -1.830327 |       |       |       |
| 1             | 3.362028  | -1.341785 | -2.156894 |       |       |       |
| 1             | 2.835887  | -2.217621 | -0.702314 |       |       |       |
| 1             | 3.577622  | 0.116633  | -0.146388 |       |       |       |
| 1             | 2.347179  | 0.765494  | -1.253862 |       |       |       |
| 8             | 1.613251  | -0.181935 | 0.431445  |       |       |       |
| 6             | 1.530948  | 1.011719  | 1.196057  |       |       |       |
| 6             | 0.463726  | 0.830450  | 2.257515  |       |       |       |
| 1             | 1.281178  | 1.856781  | 0.534639  |       |       |       |
| 1             | 2.509105  | 1.224562  | 1.655135  |       |       |       |
| 1             | 0.393119  | 1.732566  | 2.873612  |       |       |       |
| 1             | -0.506549 | 0.646886  | 1.790256  |       |       |       |
| 1             | 0.716450  | -0.013460 | 2.905012  |       |       |       |

|               |       |       |       |       |       |       |
|---------------|-------|-------|-------|-------|-------|-------|
| Equilibrium Geometry (Diisopropyl ether): E = -622.8614760 Hartree |       |       |       |       |       |       |
| 6             | -1.476638 | 2.468489  | -0.596564 |       |       |       |
| 6             | -1.495091 | 0.956569  | -0.755428 |       |       |       |
|   | x   | y   | z     |
|---|-----|-----|-------|
| 1 | -0.574356 | 0.533041 | -0.332639 |
| 1 | -1.346682 | 2.742879 | 0.453904 |
| 1 | -0.666194 | 2.911919 | -1.184493 |
| 1 | -2.427267 | 2.884019 | -0.946355 |
| 6 | -1.616316 | 0.549986 | -2.222102 |
| 1 | -1.706422 | -0.535023 | -2.330927 |
| 1 | -2.503863 | 1.015346 | -2.783374 |
| 1 | -0.732432 | 0.874014 | -2.783374 |
| 6 | -2.623178 | 0.494125 | -0.006673 |
| 6 | -2.536075 | -0.869582 | 0.412956 |
| 6 | -3.962267 | -1.319907 | 0.685101 |
| 6 | -1.644409 | -1.009771 | 1.643268 |
| 1 | -2.122134 | -1.477098 | -0.406464 |
| 1 | -4.571335 | -1.227122 | -0.217787 |
| 1 | -3.978538 | -2.361619 | 1.020997 |
| 1 | -4.401297 | -0.692193 | 1.466904 |
| 1 | -0.621282 | -0.685416 | 1.437374 |
| 1 | -2.056118 | -0.407478 | 2.460171 |
| 1 | -1.607613 | -2.057153 | 1.865962 |
| 6 | 1.655384 | 1.354471 | 2.031435 |
| 6 | 2.410449 | 0.791233 | 0.837585 |
| 1 | 3.403776 | 0.458795 | 1.172628 |
| 1 | 1.525376 | 0.583067 | 2.794875 |
| 1 | 2.205162 | 2.194209 | 2.467933 |
| 1 | 0.667348 | 1.706906 | 1.719460 |
| 6 | 2.570931 | 1.830467 | -0.267874 |
| 1 | 3.175580 | 1.461767 | 1.101172 |
| 1 | 1.587457 | 2.122410 | -0.649936 |
| 1 | 3.065237 | 2.720700 | 0.134353 |
| 8 | 1.649603 | -0.343674 | 0.412396 |
| 6 | 2.157652 | -1.075986 | -0.705945 |
| 6 | 1.167194 | -2.208727 | -0.925884 |
| 6 | 3.568039 | -1.604714 | -0.464114 |
| 1 | 2.157664 | -0.429575 | -1.596532 |
| 1 | 0.162969 | -1.808469 | 1.082886 |
| 1 | 1.450099 | -2.797622 | -1.804170 |
| 1 | 1.149283 | -2.846402 | -0.049876 |
| 1 | 4.306103 | -0.801671 | -0.387944 |
| 1 | 3.590597 | -2.190958 | 0.460699 |
| 1 | 3.864644 | -2.251845 | -1.295764 |

Equilibrium Geometry (Ethyl acetate)$_2$: E= -613.9047765 Hartree
|   |   |   |   |
|---|---|---|---|
|6  | 0.536445 | 1.665905 | 0.294464 |
|8  | 0.142362 | 2.169095 | -0.737577 |
|6  | 0.029157 | 1.987387 | 1.675569 |
|1  | -0.703183 | 1.225257 | 1.957020 |
|1  | 0.844327 | 1.975187 | 2.400903 |
|6  | -0.457826 | 2.962588 | 1.662366 |
|6  | -3.072438 | 0.747688 | -0.685334 |
|6  | -2.047953 | -0.335353 | -0.943358 |
|1  | 3.849129 | 0.392219 | -0.003504 |
|1  | -2.595017 | 1.633993 | -0.262326 |
|1  | -3.543352 | 1.033092 | -1.630691 |
|1  | -1.243671 | 0.021719 | -1.589989 |
|1  | -2.493724 | -1.224557 | -1.397813 |
|8  | -1.489774 | -0.706612 | 0.339678 |
|6  | -0.536526 | -1.665865 | 0.294722 |
|8  | -0.142713 | -2.169295 | -0.737314 |
|6  | 0.842544 | -1.970501 | 2.402265 |
|1  | 0.197390 | -2.869180 | -1.065977 |
|6  | 1.718336 | -1.725985 | -0.045334 |
|1  | 2.047115 | -2.572402 | 0.574329 |
|1  | 1.774029 | -0.833881 | 0.593721 |
|6  | 2.679350 | -1.558201 | -1.222555 |
|1  | 2.349478 | -0.708022 | -1.834440 |
|1  | 2.619187 | -2.445866 | -1.865594 |
|6  | 4.125288 | -1.341451 | -0.773605 |
|1  | 4.797686 | -1.216124 | -1.627942 |
|1  | 4.205618 | -0.447838 | -0.145475 |
|1  | 4.479648 | -2.195675 | -0.186943 |
|6  | -4.125180 | 1.341061 | -0.773689 |
|1  | -4.205348 | 0.447424 | -0.145572 |
|1  | -4.797525 | 1.215610 | -1.628051 |
|1  | -4.479728 | 2.195207 | -0.187028 |
|6  | -2.679261 | 1.558113 | -1.222576 |

Equilibrium Geometry (Heptane)_2: E= -551.1112096 Hartree

|   |   |   |   |
|---|---|---|---|
|6  | -3.131351 | -2.174007 | 1.453163 |
|1  | -2.900134 | -2.981848 | 2.153026 |
|1  | -4.168394 | -2.296684 | 1.125278 |
|1  | -3.059526 | -1.228283 | 2.001619 |
|6  | -2.161843 | -2.187022 | 0.270784 |
|1  | -2.267505 | -3.126307 | -0.287347 |
|1  | -2.418964 | -1.380425 | -0.427781 |
|6  | -0.704566 | -2.021725 | 0.702995 |
|1  | -0.420761 | -2.857141 | 1.358680 |
|1  | -0.608863 | -1.108374 | 1.307042 |
|6  | 0.267474 | -1.945546 | -0.474192 |
|1  | -0.040913 | -1.126956 | -1.139100 |
|1  | 0.197390 | -2.869180 | -1.065977 |
|6  | 1.718336 | -1.725985 | -0.045334 |
|1  | 2.047115 | -2.572402 | 0.574329 |
|1  | 1.774029 | -0.833881 | 0.593721 |
|6  | 2.679350 | -1.558201 | -1.222555 |
|1  | 2.349478 | -0.708022 | -1.834440 |
|1  | 2.619187 | -2.445866 | -1.865594 |
|6  | 4.125288 | -1.341451 | -0.773605 |
|1  | 4.797686 | -1.216124 | -1.627942 |
|1  | 4.205618 | -0.447838 | -0.145475 |
|1  | 4.479648 | -2.195675 | -0.186943 |
|6  | -4.125180 | 1.341061 | -0.773689 |
|1  | -4.205348 | 0.447424 | -0.145572 |
|1  | -4.797525 | 1.215610 | -1.628051 |
|1  | -4.479728 | 2.195207 | -0.187028 |
|6  | -2.679261 | 1.558113 | -1.222576 |
|   | x   | y   | z   |
|---|-----|-----|-----|
| 1 | -2.349209 | 0.708064 | -1.834540 |
| 1 | -2.619257 | 2.445855 | -1.865524 |
| 6 | -1.718326 | 1.725919 | -0.045313 |
| 1 | -1.773699 | 0.833603 | 0.593465 |
| 1 | -2.047335 | 2.572050 | 0.574580 |
| 6 | -0.267553 | 1.945999 | -0.474179 |
| 1 | -0.197754 | 2.869879 | -1.065612 |
| 1 | 0.040988  | 1.127742 | -1.139426 |
| 6 | 0.704507  | 2.019000 | 0.702981 |
| 1 | 0.608694  | 1.108433 | 1.306828 |
| 1 | 0.420822  | 2.857224 | 1.358834 |
| 6 | 2.161793  | 2.187062 | 0.270766 |
| 1 | -2.675600 | 3.126317 | -0.287397 |
| 1 | 2.418828  | 1.380412 | -0.427773 |
| 6 | 3.131318  | 2.173973 | 1.453135 |
| 1 | 4.168375  | 2.294645 | 1.125230 |
| 1 | 2.900234  | 2.984232 | 2.152947 |
| 1 | 3.059349  | 1.228293 | 2.001649 |

Equilibrium Geometry (Hexane)$_2$: $E = -472.7184338$ Hartree

|   | x   | y   | z   |
|---|-----|-----|-----|
| 6 | -3.193010 | 1.936680 | -0.366922 |
| 1 | -3.250479 | 2.882628 | -0.916016 |
| 1 | -4.081804 | 1.859458 | 0.267075 |
| 1 | -3.229145 | 1.122187 | -1.098108 |
| 6 | -1.907200 | 1.868805 | 0.457963 |
| 1 | -1.899461 | 2.680155 | 1.197463 |
| 1 | -1.880363 | 0.930765 | 1.026632 |
| 6 | -0.645966 | 1.966940 | -0.400920 |
| 1 | -0.664239 | 2.910553 | -0.964639 |
| 1 | -0.651472 | 1.160019 | -1.147254 |
| 6 | 0.644973  | 1.892284 | 0.414216 |
| 1 | 0.657067  | 0.955923 | 0.989375 |
| 1 | 0.654922  | 2.708735 | 1.150343 |
| 6 | 1.909138  | 1.972979 | -0.441973 |
| 1 | 1.889453  | 2.904468 | -1.022587 |
| 1 | 1.901159  | 1.152657 | -1.171342 |
| 6 | 3.189831  | 1.912588 | 0.391744 |
| 1 | 3.232643  | 0.984087 | 0.970586 |
| 1 | 4.083314  | 1.958139 | -0.238740 |
| 1 | 3.230678  | 2.749584 | 1.096945 |
| 6 | -3.192154 | -1.937713 | 0.366919 |
| 1 | -3.249294 | -2.883655 | 0.916057 |
| 1 | -4.080983 | -1.860815 | -0.267066 |
| 1 | -3.228541 | -1.123191 | 1.098061 |
| 6 | -1.906366 | -1.869443 | -0.457975 |
| 1 | -1.898336 | -2.680841 | -1.197414 |
| 1 | 1.879833 | -0.931430 | -1.026708 |
| 6 | 0.645113  | -1.967108 | 0.400931 |
| 1 | 0.663075  | -2.910695 | 0.964704 |
| 1 | 0.650885  | -1.160153 | 1.147223 |
|   |        |        |        |
|---|--------|--------|--------|
| 6 | 0.645803 | -1.892086 | -0.414210 |
| 1 | 0.657595  | -0.955755  | -0.989434  |
| 1 | 0.656016  | -2.708578  | -1.150286  |
| 6 | 1.909995  | -1.972324  | 0.441979   |
| 1 | 1.890601  | -2.903784  | 1.022650   |
| 1 | 1.901767  | -1.151963  | 1.171300   |
| 6 | 3.190664  | -1.911591  | -0.397155  |
| 1 | 3.233198  | -0.983111  | -0.970647  |
| 1 | 4.084164  | -1.956841  | 0.238732   |
| 1 | 3.231757  | -2.748614  | -1.096906  |

Equilibrium Geometry (Isooctane)$_2$: E = -629.5138354 Hartree

|   |        |        |        |
|---|--------|--------|--------|
| 6 | -2.623715 | -0.773825 | 0.699816   |
| 6 | -4.133559  | -0.516067  | 0.740150   |
| 1 | -4.549924  | -0.383770  | -0.264056  |
| 1 | -4.649756  | -1.362542  | 1.208762   |
| 1 | -4.360388  | 0.383778   | 1.325004   |
| 6 | -2.324023  | -2.017497  | -0.149344  |
| 1 | -2.665968  | -1.915255  | -1.181329  |
| 1 | -1.245812  | -2.217491  | -0.166577  |
| 1 | -2.820612  | -2.895306  | 0.282287   |
| 6 | -2.133833  | -1.061577  | 2.127311   |
| 1 | -1.046093  | -1.202278  | 2.142875   |
| 1 | -2.379625  | -0.231352  | 2.799991   |
| 1 | -2.598935  | -1.972801  | 2.522175   |
| 6 | -1.859118  | 0.471455   | 0.196604   |
| 1 | -1.790418  | 1.172880   | 1.041986   |
| 1 | -0.824478  | 0.171572   | -0.029479  |
| 6 | -2.401593  | 1.279864   | -0.993525  |
| 1 | -3.405666  | 1.642145   | -0.733507  |
| 6 | -2.196320  | 0.497749   | -2.307038  |
| 1 | -1.541508  | 0.008432   | -2.534985  |
| 1 | -3.275617  | -0.267808  | -2.283188  |
| 1 | -2.729007  | 1.178843   | -3.133664  |
| 6 | -1.502514  | 2.505623   | -1.199552  |
| 1 | -1.909882  | 3.167084   | -1.972041  |
| 1 | -1.396504  | 3.082365   | -0.274189  |
| 1 | -0.501304  | 2.192470   | -1.520424  |
| 6 | 2.592204   | -1.024561  | -0.503218  |
| 6 | 1.852741   | -0.473281  | -1.727456  |
| 1 | 2.111872   | 0.572977   | -1.923087  |
| 1 | 2.111386   | -1.055718  | -2.620091  |
| 1 | 0.766820   | -0.536046  | -1.588948  |
| 6 | 4.108993   | -0.917810  | -0.716391  |
| 1 | 4.440677   | 0.112242   | -0.862274  |
| 1 | 4.646809   | -1.330140  | 0.145824   |
| 1 | 4.403390   | -1.492800  | -1.602862  |
| 6 | 2.248904   | -2.514353  | -0.353227  |
| 1 | 2.710443   | -2.929037  | 0.551214   |
| 1 | 1.164880   | -2.659526  | -0.278785  |

S28
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| 1 | 2.612426 | -3.086914 | -1.214913 |
| 2 | 1.33474 | -0.316903 | 0.792945 |
| 3 | 1.73181 | -0.768383 | 1.084797 |
| 4 | 2.842571 | -0.574158 | 1.596719 |
| 5 | 1.918224 | 1.204944 | 0.802925 |
| 6 | 1.164121 | 1.451004 | 0.044519 |

Equilibrium Geometry (Methyl ethyl ketone)$_2$: $E= -463.7167833$ Hartree

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| 1 | 6.158403 | -0.525346 | 0.232397 |
| 2 | -1.088369 | -0.438718 | 1.347094 |
| 3 | 1.816799 | -1.860185 | -0.440273 |
| 4 | -1.415704 | -2.666722 | 0.175100 |
| 5 | -2.891134 | -2.012868 | -0.590561 |
| 6 | -1.336006 | -1.861014 | -1.423779 |

Equilibrium Geometry (Methyl tert-butyl ether)$_2$: $E= -463.7167833$ Hartree

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| 1 | -1.585413 | -0.524414 | -0.232381 |
| 2 | 1.088765 | -0.438307 | -1.347024 |
| 3 | 1.818703 | -1.858997 | 0.440338 |
| 4 | 1.419093 | -2.666011 | -0.175378 |
| 5 | 2.893097 | -2.010311 | 0.591531 |
| 6 | 1.337700 | -1.860473 | 1.423456 |

Equilibrium Geometry (Methyl tert-butyl ether)$_2$: $E= -708.6203$ Hartree

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| 1 | -1.530577 | -0.194536 | 1.191291 |
| 2 | -2.223291 | 0.348498 | -0.058876 |
| 3 | -1.837001 | 0.385370 | 2.068026 |
| 4 | -1.770179 | -1.248326 | 1.366041 |
| 5 | -0.446998 | -0.115071 | 1.063602 |

S29
Equilibrium Geometry (n–butanol)$_2$: E= -466.085458 Hartree

\[
\begin{array}{ccc}
6 & -1.442880 & -0.981381 \\
6 & -0.868470 & -0.324453 \\
1 & -1.859990 & -1.797290 \\
6 & -2.573564 & -0.189947 \\
1 & -3.103898 & -0.842418 \\
1 & -2.141241 & 0.631599 \\
6 & -3.553789 & 0.367437 \\
1 & -3.010186 & 1.001646 \\
1 & -3.980612 & -0.460807 \\
6 & -4.681912 & 1.174577 \\
1 & -5.377073 & 1.562717 \\
1 & -5.250605 & 0.552866 \\
1 & -4.278233 & 2.024715 \\
8 & -0.613594 & -1.496436 \\
1 & 0.204173 & -1.800096 \\
6 & 2.866648 & -1.138053 \\
1 & 3.155851 & -1.292443 \\
\end{array}
\]
|   | 1       | 3.760905 | -1.233168 | -0.656038 |
|---|---------|----------|-----------|-----------|
| 6 | 2.251045 | 0.238135 | -0.199427 |
| 1 | 1.938322 | 0.352535 | -1.244662 |
|   | 1.350856 | 0.300010 | 0.422508  |
| 6 | 3.220850 | 1.358672 | 0.176421  |
| 1 | 3.550494 | 1.221473 | 1.213936  |
|   | 2.586154 | 2.741161 | 0.020247  |
| 1 | 3.290791 | 3.536439 | 0.280296  |
| 6 | 4.117917 | 1.292264 | -0.452102 |
|   | 1.709337 | 2.838170 | 0.668215  |
| 8 | 1.889016 | -2.116380 | -0.417818 |
| 1 | 2.291977 | -2.986730 | -0.343305 |

**Equilibrium Geometry (n–octanol)**: $E = -779.6578048$ Hartree

|   | 2       | 2.042100 | -2.460591 | -0.503236 |
|---|---------|----------|-----------|-----------|
| 6 | 2.243359 | -1.651012| 1.217740  |
| 1 | 1.820486 | -3.365611| 1.086373  |
|   | 0.838757 | -2.100726| 0.356062  |
| 1 | 0.699288 | -2.891492| 1.103834  |
|   | 1.061179 | -1.179110| 0.909336  |
| 6 | 0.444979 | -1.918556| 0.453496  |
| 1 | 0.285562 | -1.163965| -1.237831 |
|   | 0.691810 | -2.856923| -0.969411 |
| 6 | -1.628716| -1.495747| 0.417816  |
| 1 | -1.762198| -2.231743| 1.223172  |
| 6 | -1.391550| -0.540001| 0.906889  |
|   | 3.174358 | -2.691353| 0.329460  |
| 1 | 3.917401 | -2.198012| -0.043253 |
| 6 | 5.909034 | 0.392446 | -0.000850 |
| 1 | 5.570999 | 0.376625 | 0.985583  |
| 1 | 5.573797 | 1.162456 | -0.615899 |
| 6 | 3.609012 | 0.684926 | 0.141237  |
| 1 | 3.152727 | 0.588152 | -0.849835 |
| 1 | 3.163438 | -0.081553| 0.785071  |
| 6 | 3.324075 | 2.071773 | 0.718178  |
| 1 | 3.915463 | 2.216652 | 1.632248  |
| 1 | 3.647248 | 2.843355 | 0.005755  |
| 6 | 1.838922 | 2.272490 | 1.043755  |
| 1 | 1.692861 | 3.280778 | 1.453568  |
| 1 | 1.544005 | 1.566361 | 1.832908  |
| 8 | 5.217367 | -0.891659 | -0.635813 |
| 1 | 6.152040 | -1.116342| -0.671837 |
| 6 | -2.940493 | -1.351835 | -0.353804 |
| 1 | -3.175065 | -2.301771| -0.854288 |
| 1 | -2.816270 | -0.603517| -1.148771 |
| 6 | -4.114121 | -0.946760| 0.538601  |
| 1 | -3.844537 | -0.041390| 1.100859  |
| 1 | -4.289811 | -1.733045| 1.286244  |
| 6 | -5.405038 | -0.688744| -0.238546 |
|   |   |   |   |
|---|---|---|---|
| 1 | -5.678346 | -1.596683 | -0.791472 |
| 1 | -5.218979 | 0.090021 | -0.988349 |
| 6 | -6.562179 | -0.265868 | 0.667420 |
| 1 | -6.314703 | 0.656213 | 1.204162 |
| 1 | -7.477560 | -0.087949 | 0.094758 |
| 1 | -6.774288 | -1.040480 | 1.411892 |

Equilibrium Geometry (Ortho-xylene)$_2$: $E = -619.9919015$ Hartree

|   |   |   |   |
|---|---|---|---|
| 6 | 1.548015 | -2.092476 | -0.542941 |
| 6 | 1.577146 | -1.485083 | 0.718390 |
| 6 | 1.652796 | -0.090414 | 0.853443 |
| 6 | 1.686951 | 0.714213 | -0.307373 |
| 6 | 1.645756 | 0.096454 | -1.565647 |
| 6 | 1.571063 | -1.295795 | -1.691750 |
| 1 | 1.502103 | -3.175890 | -0.625381 |
| 1 | 1.571382 | -2.103669 | 1.615113 |
| 1 | 1.683328 | 0.718165 | -2.459126 |
| 1 | 1.547241 | -1.752645 | -2.678383 |
| 6 | 1.837723 | 2.210225 | -0.197371 |
| 1 | 1.111018 | 2.633773 | 0.502522 |
| 1 | 2.840035 | 2.477763 | 0.160684 |
| 1 | 1.686834 | 2.685232 | -1.170998 |
| 6 | 1.693153 | 0.543786 | 2.219962 |
| 1 | 2.567764 | 1.194630 | 2.332227 |
| 1 | 0.802343 | 1.161684 | 2.387892 |
| 1 | 1.733858 | -0.218637 | 3.003431 |
| 6 | -1.571569 | 1.296223 | -1.691079 |
| 6 | -1.646509 | -0.096051 | -1.565316 |
| 6 | -1.687148 | -0.714130 | -0.307182 |
| 6 | -1.652546 | 0.090205 | 0.853836 |
| 6 | -1.576698 | 1.484895 | 0.719109 |
| 6 | -1.548008 | 2.092606 | -0.542077 |
| 1 | -1.548203 | 1.753313 | -2.677612 |
| 1 | -1.669475 | -0.71502 | -2.458971 |
| 1 | -1.570592 | 2.103252 | 1.615986 |
| 1 | -1.501886 | 3.176029 | -0.624261 |
| 6 | -1.692466 | -0.544371 | 2.220187 |
Equilibrium Geometry (Pentane):

|   | x     | y     | z     |
|---|-------|-------|-------|
| 1 | -2.566792 | -1.195621 | 2.332331 |
| 1 | -0.801391 | -1.161955 | 2.387856 |
| 1 | -1.734418 |  0.217817 | 3.003869 |
| 6 | -1.837836 | -2.210160 | -0.197384 |
| 1 | -1.110259 | -2.633825 | 0.501534 |
| 1 | -2.839711 | -2.477841 | 0.161784 |
| 1 | -1.687655 | -2.684846 | -1.171336 |

Equilibrium Geometry (Toluene):

|   | x     | y     | z     |
|---|-------|-------|-------|
| 6 | 2.859840 | 1.567473 | -0.763018 |
| 1 | 2.177448 | 2.211739 | -0.198249 |
| 1 | 3.106663 | 2.075090 | -1.700570 |
| 1 | 3.781767 | 1.465828 | -0.180659 |
| 6 | 2.226701 | 0.198195 | -1.013579 |
| 1 | 1.319233 | 0.314752 | -1.620243 |
| 1 | 2.913539 | -0.426426 | -1.599240 |
| 6 | 1.869924 | -0.528950 | 0.282778 |
| 1 | 1.203913 | 0.107987 | 0.881294 |
| 1 | 2.781589 | -0.670525 | 0.880668 |
| 6 | 1.199950 | -1.883671 | 0.054155 |
| 1 | 1.874630 | -2.524153 | -0.528609 |
| 1 | 0.301948 | -1.739566 | -0.559546 |
| 6 | 0.825813 | -2.583977 | 1.360992 |
| 1 | 0.134853 | -1.968643 | 1.947457 |
| 1 | 0.344526 | -3.549619 | 1.176979 |
| 6 | 1.716048 | -2.761738 | 1.973773 |
| 1 | -2.859626 | -1.567577 | -0.763046 |
| 1 | -2.177202 | -2.211717 | -0.198169 |
| 1 | -3.106293 | -2.075293 | -1.700587 |
| 1 | -3.781625 | -1.466025 | -0.180786 |
| 6 | -2.226630 | -0.198237 | -1.013641 |
| 1 | -1.319121 | -0.314738 | -1.620255 |
| 1 | -2.913488 |  0.426332 | -1.599334 |
| 6 | -1.869941 |  0.528973 | 0.282710 |
| 1 | -1.203845 | -0.107888 | 0.881218 |
| 1 | -2.781617 |  0.670433 | 0.880609 |
| 6 | -1.200127 |  1.883773 | 0.054097 |
| 1 | -1.874925 |  2.524240 | -0.528547 |
| 1 | -0.302182 |  1.739787 | -0.559705 |
| 6 | -0.825923 |  2.584012 | 1.360953 |
| 1 | -0.134902 |  1.968681 | 1.947339 |
| 1 | -0.344708 |  3.549695 | 1.176971 |
| 1 | -1.716132 |  2.761684 | 1.973792 |

Equilibrium Geometry (Toluene):

|   | x     | y     | z     |
|---|-------|-------|-------|
| 6 | 1.609001 | -1.607951 | 0.635573 |
| 1 | 1.139052 | -0.481855 | 1.321587 |
| 6 | 1.345223 |  0.809543 | 0.814050 |
| 6 | 2.034340 |  0.947255 | -0.402599 |
Equilibrium Geometry (Trichloroethylenes)₂: E= -2911.0397068 Hartree

References

[1] J. Pérez and A. Restrepo, “Ascec v02:annealing simulado con energía cuántica,” 2008. Property, development, and implementation: Grupo de Química–Física Teórica, Instituto de Química, Universidad de Antioquia, Medellín, Colombia.
[2] J. F. Pérez, C. Z. Hadad, and A. Restrepo, “Structural studies of the water tetramer,” *Int. J. Quant. Chem.*, vol. 108, no. 10, pp. 1653–1659, 2008.

[3] J. F. Pérez, E. Florez, C. Z. Hadad, P. Fuentenalba, and A. Restrepo, “Stochastic search of the quantum conformational space of small lithium and bimetallic lithium–sodium clusters,” *The Journal of Physical Chemistry A*, vol. 112, no. 25, pp. 5749–5755, 2008.

[4] C. Riplinger and F. Neese, “An efficient and near linear scaling pair natural orbital based local coupled cluster method,” *The Journal of Chemical Physics*, vol. 138, no. 3, p. 034106, 2013.

[5] C. Riplinger, B. Sandhoefer, A. Hansen, and F. Neese, “Natural triple excitations in local coupled cluster calculations with pair natural orbitals,” *The Journal of Chemical Physics*, vol. 139, no. 13, p. 134101, 2013.

[6] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, and F. Weinhold, “Nbo 7.0,” 2018. Theoretical Chemistry Institute, University of Wisconsin, Madison, WI.

[7] E. D. Glendening, C. R. Landis, and F. Weinhold, “Nbo 7.0: New vistas in localized and delocalized chemical bonding theory,” *Journal of Computational Chemistry*, vol. 40, no. 25, pp. 2234–2241, 2019.

[8] F. Weinhold and C. R. Landis, *Discovering Chemistry with Natural Bond Orbitals*. Wiley-VCH, Hoboken NJ, 319pp, 2012.

[9] E. D. Glendening, C. R. Landis, and F. Weinhold, “Natural bond orbital methods,” *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, vol. 2, no. 1, pp. 1–42, 2012.

[10] T. Keith, “Aimall *(version 19.10.12)*,” 2019. TK Gristmill Software, Overland Park KS, USA, aim.tkgristmill. com.

[11] R. Bader, *Atoms in Molecules: A Quantum Theory*. Oxford Univ. press Oxford, 1990.

[12] R. F. W. Bader, “A quantum theory of molecular structure and its applications,” *Chem. Rev.*, vol. 91, no. 5, pp. 893–928, 1991.

[13] P. L. Popelier, *Atoms in Molecules: An Introduction*. Prentice Hall, London, 2000.

[14] G. A. DiLabio and A. Otero-de-la Roza, *Noncovalent Interactions in Density Functional Theory*, ch. 1, pp. 1–97. John Wiley & Sons, Ltd, 2016.

[15] E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, and W. Yang, “Revealing noncovalent interactions,” *J. Am. Chem. Soc.*, vol. 132, no. 18, pp. 6498–6506, 2010.

[16] J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan, and W. Yang, “Ncplot: A program for plotting noncovalent interaction regions,” *J. Chem. Theory Comput.*, vol. 7, no. 3, pp. 625–632, 2011.

[17] N. Rojas-Valencia, I. Lans, M. Manrique-Moreno, C. Z. Hadad, and A. Restrepo, “Entropy drives the insertion of ibuprofen into model membranes,” *Phys. Chem. Chem. Phys.*, vol. 20, pp. 24869–24876, 2018.

[18] N. Rojas-Valencia, S. Gómez, S. Montillo, M. Manrique-Moreno, C. Cappelli, C. Hadad, and A. Restrepo, “Evolution of bonding during the insertion of anionic ibuprofen into model cell membranes,” *Journal of Physical Chemistry B*, vol. 124, no. 1, pp. 79–90, 2020.

[19] S. A. Gomez, N. Rojas-Valencia, S. Gomez, F. Egidi, C. Cappelli, and A. Restrepo, “Binding of sars–cov–2 to cell receptors: a tale of molecular evolution,” *ChemBioChem*, vol. 22, no. 4, pp. 724–732, 2021. DOI: 10.1002/cbic.202000618.
[20] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, “Gaussian 09 Revision E.01.” Gaussian Inc. Wallingford CT 2009.

[21] J. Wang, R. M. Wolf, J. W. Caldwell, P. A. Kollman, and D. A. Case, “Development and testing of a general amber force field,” J. Comput. Chem., vol. 25, no. 9, pp. 1157–1174, 2004.

[22] M. J. Abraham, T. Murtola, R. Schulz, S. Páll, J. C. Smith, B. Hess, and E. Lindahl, “Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers,” SoftwareX, vol. 1, pp. 19–25, 2015.

[23] F. Neese, “The orca program system,” WIREs Computational Molecular Science, vol. 2, no. 1, pp. 73–78, 2012.

[24] “National Library of Medicine - National Institutes of Health, National Center for Biotechnology Information.” https://pubchem.ncbi.nlm.nih.gov/. Accessed: 2020-04-30.

[25] S. Menon and N. Sengupta, “Perturbations in inter-domain associations may trigger the onset of pathogenic transformations in prpc: insights from atomistic simulations,” Mol. BioSyst., vol. 11, pp. 1443–1453, 2015.