Supplementary Information

A molecular twist on hydrophobicity

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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 $\mathcal{S}\cdots\mathcal{S}$ and for all $\mathcal{S}\cdots$Water dimers using a stochastic sampling algorithm[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[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[6, 7, 8, 9], QTAIM[10, 11, 12, 13], NCI[14, 15, 16] methods.

2. For each substance in Table S1 we constructed more realistic samples of binary systems with water contained within a $6\times6\times12$ 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[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 $\mathcal{S}$/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[18, 19].

3. We chose heptane to dig deeper into the nature of $\mathcal{S}\cdots\mathcal{S}$ and $\mathcal{S}\cdots$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[20]. The GAFF force field[21] as implemented in GROMACS[22], version 2019.4, was used for all MD runs. DLPNO–CCSD(T) energies were computed using ORCA[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. $n_{\mathcal{S}}, n_w$ 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 $\mathcal{S}$.

Organic solvent	Code	MD conditions		Solubility	log K_{ow}	Density (g/cm^3)		I_t	Minima		$BE_{DLPNO-CCSD(T)}$	
		$n_{\mathcal{S}}$	n_w	mg/L		Experimental	MD	nm	$\mathcal{S}\cdots\mathcal{S}$	$\mathcal{S}\cdots$ W	$\mathcal{S}\cdots\mathcal{S}$	$\mathcal{S}\cdots$ W
Isooctane	ISC	910	6540	2.44	4.08	0.69 (20)	0.70	1.30	2	9	4.79	1.95
Heptane	HPT	930	6916	3.40	4.66	0.67 (25)	0.65	1.20	4	7	4.79	1.94
Hexane	HXN	1000	7273	9.50	3.90	0.66 (25)	0.65	1.13	9	3	6.11	2.43
Pentane	PTN	1000	8137	3.80×10^1	3.39	0.63 (20)	0.61	1.20	11	9	3.94	1.59
Cyclohexane	CYH	1000	8058	5.50×10^1	3.44	0.78 (20)	0.76	1.48	2	4	2.93	1.68
Ortho–xylene	OXL	1000	7515	1.80×10^2	3.12	0.88 (20)	0.72	1.60	4	3	9.48	5.15
Toluene	TLN	1000	8405	5.26×10^2	2.73	0.86 (20)	0.76	1.50	9	4	7.75	4.79
1–octanol	OTN	819	6733	5.40×10^2	3.00	0.83 (25)	0.82	1.40	2	7	9.05	1.94
Carbon tetrachloride	CTC	1000	10061	7.93×10^2	2.83	1.59 (20)	1.56	1.44	1	3	4.73	2.39
Trichloroethylene	TCE	1000	9952	1.12×10^3	2.61	1.46 (20)	1.37	1.45	9	5	9.55	4.14
Benzene	BZN	1000	9244	1.79×10^3	2.13	0.88 (20)	0.83	1.51	5	2	5.33	3.95
Chloroform	CHL	1000	10492	7.95×10^3	1.97	1.47 (25)	1.41	1.55	4	2	5.83	5.53
Butyl acetate	BAC	967	7124	8.33×10^3	1.78	0.88 (20)	0.88	1.87	1	7	4.89	6.69
Dichloroethane	DCE	1000	9975	8.60×10^3	1.48	1.25 (25)	1.17	1.60	6	1	6.02	4.83
Diisopropyl ether	DPE	984	7217	8.80×10^3	1.52	0.72 (20)	0.73	1.82	3	2	6.34	8.03
Dichloromethane	DCM	1000	11029	1.32×10^4	1.25	1.33 (20)	1.2	1.77	2	2	4.71	4.63
Methyl tert–butyl ether	MTE	1000	7878	4.80×10^4	0.94	0.74 (25)	0.71	2.00	1	2	3.80	7.33
Diethyl ether	DEE	980	7119	6.04×10^4	0.89	0.71 (20)	0.73	2.03	3	1	4.73	7.14
n-butanol	BTN	1000	8762	6.32×10^4	0.88	0.81 (20)	0.77	2.42	3	1	6.76	6.56
Ethyl acetate	EAC	1000	8679	8.00×10^4	0.73	0.9 (20)	0.89	2.28	3	2	7.90	6.52
Methyl ethyl ketone	MEK	1000	9071	2.11×10^5	0.29	0.81 (20)	0.67	3.60	7	3	7.62	6.50

2 Results from MD simulations

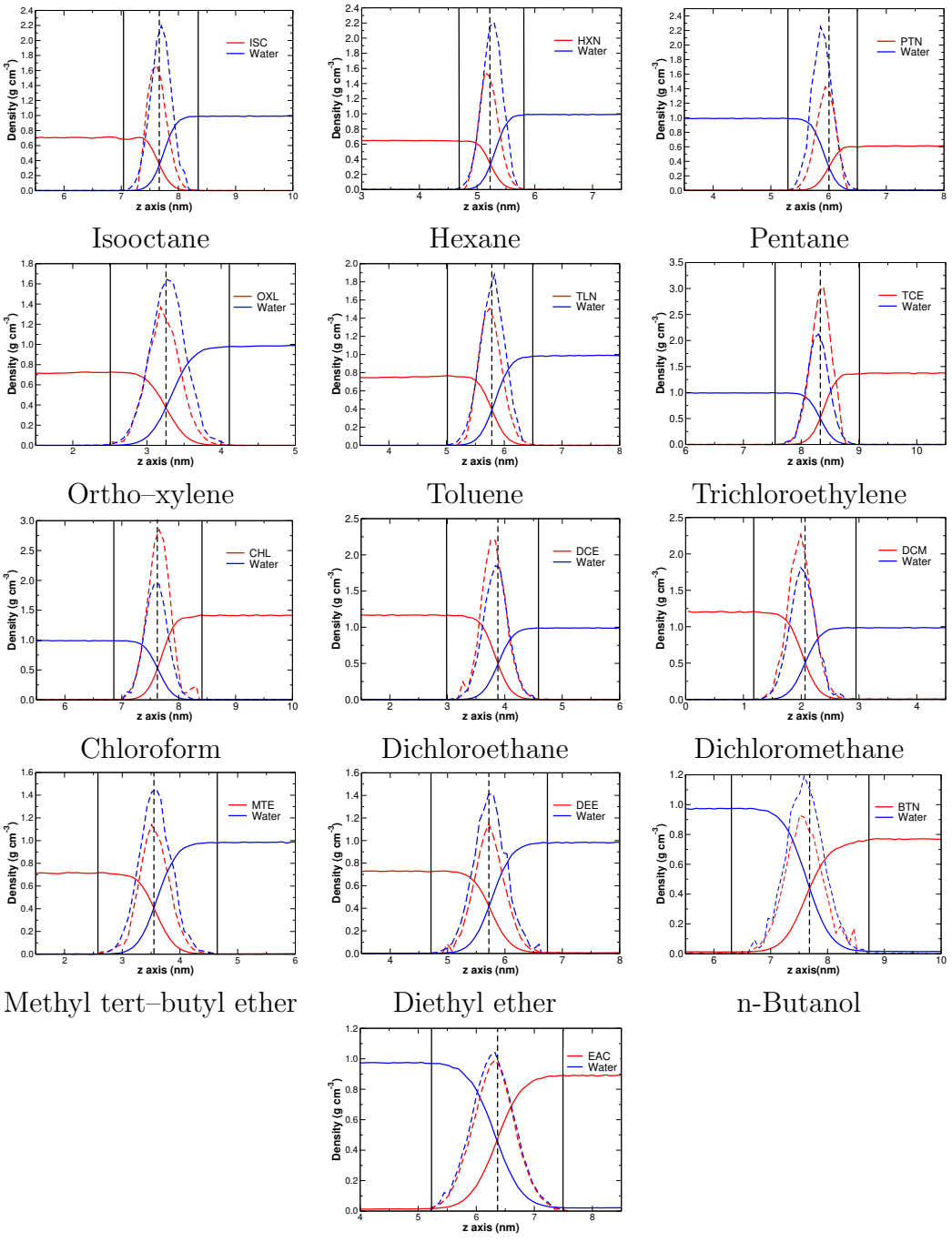


Figure S1: Densities (continuous lines) and derivatives of the densities (discontinuous lines) along the normal direction to the interphase for the chosen set of $\mathcal{S}$. Vertical solid lines mark the boundaries of the interphase.

Table S2: NBO and QTAIM descriptors of bonding for all $\mathcal{S}\cdots$Water and $\mathcal{S}\cdots\mathcal{S}$ 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.

$\mathcal{S}\cdots$ W	Interaction	-$E^{(2)}_{d\rightarrow a}$	$\rho(\mathbf{r}_c)\times 10^2$	$\nabla^2\rho(\mathbf{r}_c)$	$\lvert\mathcal{V}(\mathbf{r}_c)\rvert/\mathcal{G}(\mathbf{r}_c)$	$\mathcal{H}(\mathbf{r}_c)/\rho(\mathbf{r}_c)$	BE
Isooctane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	1.15	0.81	0.03	0.87	0.10	1.95
Heptane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma^*_{\mathrm{O-H}}$	0.07	0.60	0.02	0.71	0.21	1.94
Hexane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.13	0.56	0.02	0.84	0.13	2.43
Pentane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.2	0.57	0.02	0.85	0.11	1.59
Cyclohexane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.49	0.64	0.02	0.87	0.10	1.68
Ortho–xylene	$\pi_{\mathrm{C=C}}\rightarrow\sigma^*_{\mathrm{O-H}}$	0.35	1.14	0.04	0.77	0.16	5.15
Toluene	$\pi_{\mathrm{C=C}}\rightarrow\sigma^*_{\mathrm{O-H}}$	0.41	0.68	0.02	0.83	0.11	4.79
1–octanol	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	7.12	2.48	0.11	0.87	0.12	1.94
Carbon tetrachloride	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-Cl}}$	1.7	1.09	0.05	0.85	0.14	2.39
Trichloroethylene	$\pi_{\mathrm{C=C}}\rightarrow\sigma^*_{\mathrm{O-H}}$	4.23	1.44	0.06	0.80	0.17	4.14
Benzene	$\pi_{\mathrm{C=C}}\rightarrow\sigma^*_{\mathrm{O-H}}$	0.58	7.6	0.03	0.74	0.17	3.95
Chloroform	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	3.00	1.66	0.07	0.81	0.16	5.53
Butyl acetate	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	3.74	2.10	0.10	0.82	0.18	6.69
Dichloroethane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.72	1.03	0.04	0.84	0.13	4.83
Diisopropyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	6.09	2.76	0.12	0.91	0.09	8.03
Dichloromethane	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	0.72	1.33	0.05	0.81	0.16	4.63
Methyl tert–butyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	8.39	2.91	0.12	0.92	0.08	7.33
Diethyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	7.05	2.27	0.11	0.90	0.09	7.14
n-butanol	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	6.99	2.47	0.11	0.87	0.12	6.56
Ethyl acetate	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	3.38	2.03	0.09	0.81	0.18	6.52
Methyl ethyl ketone	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	6.11	2.32	0.10	0.86	0.13	6.50
Water$\cdots$Water	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	7.09	0.02	0.09	0.89	0.10	5.60
$\mathcal{S}\cdots\mathcal{S}$							
Isooctane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma*_{\mathrm{C-H}}$	0.41	0.52	0.01	0.85	0.09	4.79
Heptane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma*_{\mathrm{C-H}}$	0.35	0.69	0.02	0.88	0.07	4.79
Hexane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma*_{\mathrm{C-H}}$	0.22	0.50	0.01	0.86	0.09	6.11
Pentane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.22	0.55	0.02	0.85	0.10	3.94
Cyclohexane	$\sigma_{\mathrm{C-H}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.29	0.44	0.01	0.86	0.09	2.93
Ortho–xylene	$\sigma_{\mathrm{C-H}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.59	0.73	0.02	0.84	0.09	9.48
Toluene	$\pi_{\mathrm{C=C}}\rightarrow\pi^*_{\mathrm{C=C}}$	0.48	0.78	0.02	0.84	0.10	7.75
1–octanol	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	5.80	2.30	0.10	0.86	0.13	9.05
Carbon tetrachloride	$n_{\mathrm{Cl}}\rightarrow\sigma^*_{\mathrm{C-Cl}}$	0.07	0.43	0.01	0.67	0.22	4.73
Trichloroethylene	$n_{\mathrm{Cl}}\rightarrow\pi^*_{\mathrm{C=C}}$	0.71	0.72	0.03	0.74	0.18	9.55
Benzene	$\pi_{\mathrm{C=C}}\rightarrow\pi^*_{\mathrm{C=C}}$	0.73	0.72	0.02	0.82	0.10	5.33
Chloroform	$n_{\mathrm{Cl}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.60	2.63	0.03	0.78	0.15	5.83
Butyl acetate	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.52	0.76	0.02	0.86	0.10	4.89
Dichloroethane	$n_{\mathrm{Cl}}\rightarrow\sigma^*_{\mathrm{C-H}}$	1.04	0.77	0.03	0.79	0.14	6.02
Diisopropyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	1.04	0.83	0.03	0.87	0.10	6.34
Dichloromethane	$n_{\mathrm{Cl}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.32	0.66	0.02	0.78	0.15	4.71
Methyl tert–butyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.68	0.87	0.03	0.90	0.08	3.80
Diethyl ether	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{C-H}}$	0.88	0.89	0.03	0.90	0.07	4.73
n-butanol	$n_{\mathrm{O}}\rightarrow\sigma^*_{\mathrm{O-H}}$	7.48	2.50	0.02	0.84	0.12	6.76
Ethyl acetate	$n_{\mathrm{O}}\rightarrow\pi^*_{\mathrm{C=O}}$	0.80	0.67	0.03	0.83	0.14	7.90
Methyl ethyl ketone	$\pi_{\mathrm{C=O}}\rightarrow\pi^*_{\mathrm{C=O}}$	0.97	0.72	0.03	0.76	0.17	7.62

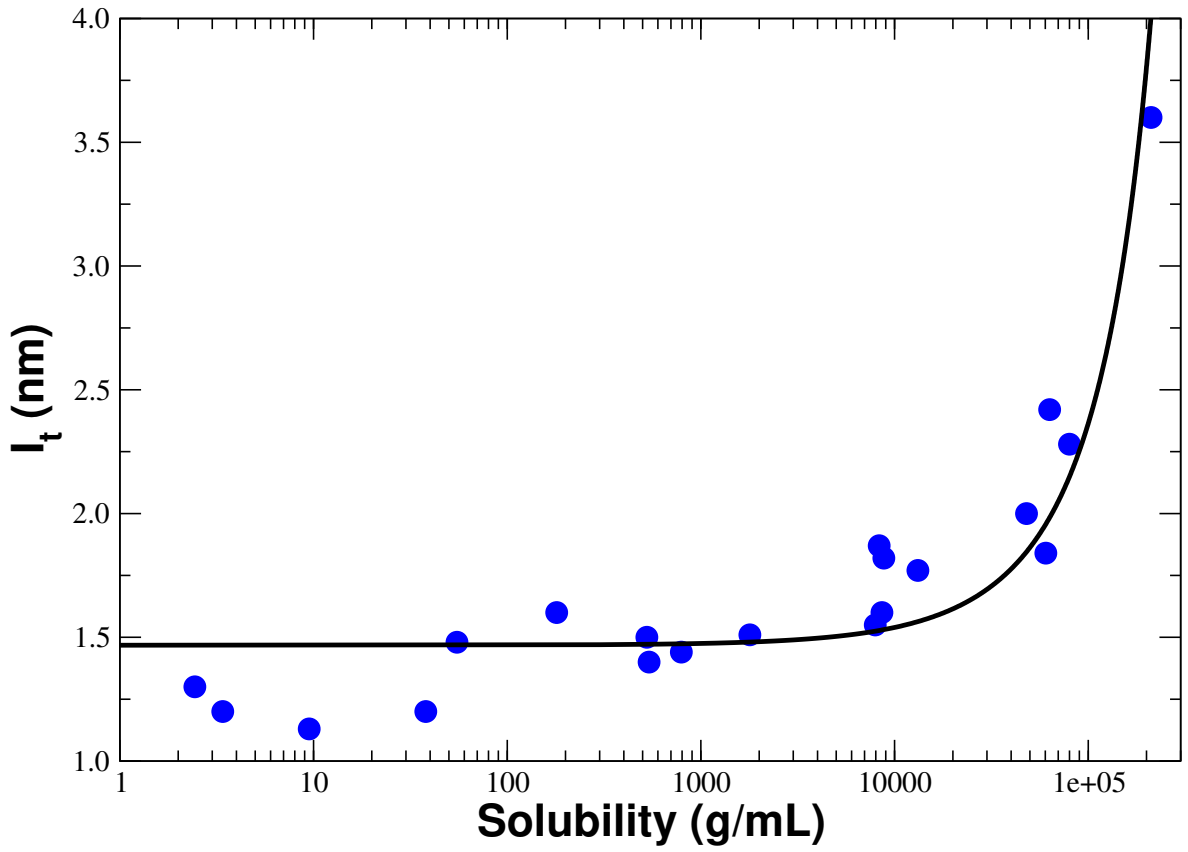


Figure S2: Variation of the thickness of the interphase as a function of the solubility of $\mathcal{S}$.

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 $\mathcal{S}$/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, $\mathcal{S}$ (Figure S4) and S_{mix}, which follow exactly the same patterns.

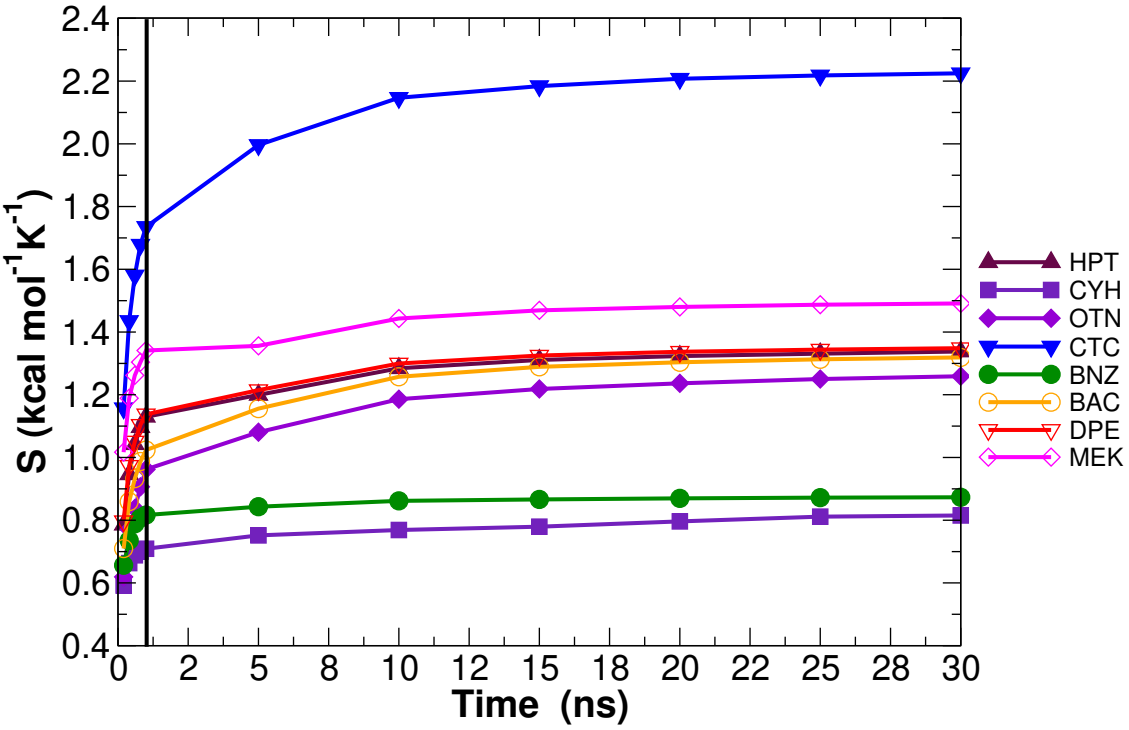


Figure S3: Entropy changes associated with phase separation in the $\mathcal{S}$/water chosen set of binary systems in Table 1 of the manuscript. The vertical solid line separates the equilibration and production stages of the MD trajectories.

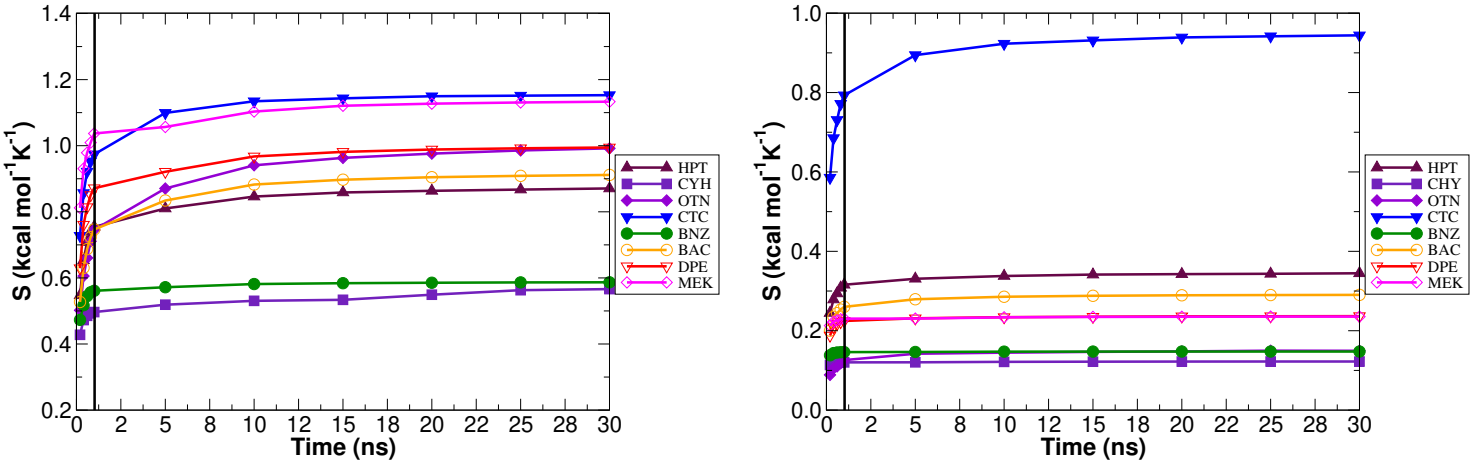
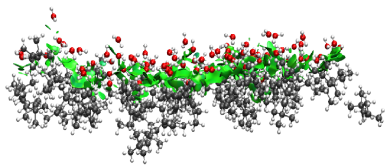
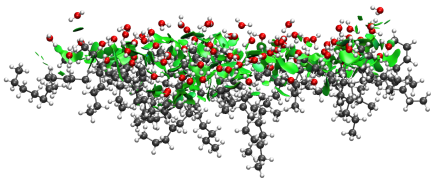


Figure S4: Decomposition of the entropy changes into $S_{\mathcal{S}}$ (left), S_w (right) and S_{mix} for phase separation in the $\mathcal{S}$/water chosen set of binary systems in Table 1 of the manuscript. The vertical solid line separates the equilibration and production stages of the MD trajectories.

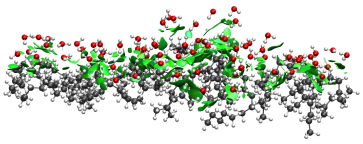
3 NCI surfaces



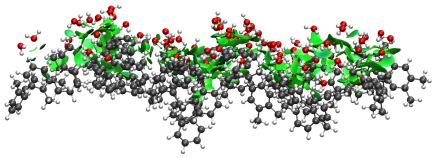
Isooctane



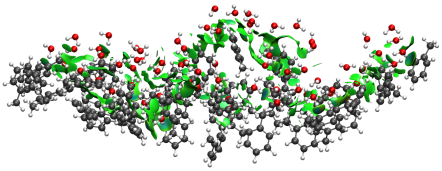
Hexane



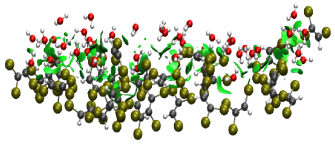
Pentane



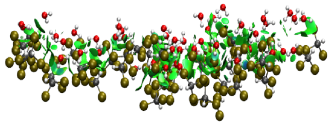
Ortho–xylene



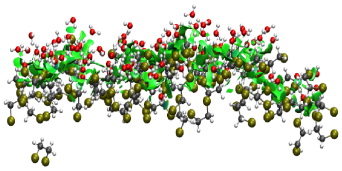
Toluene



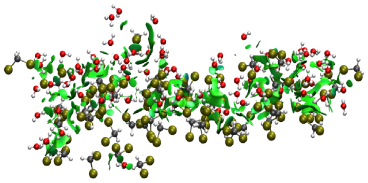
Trichloroethylene



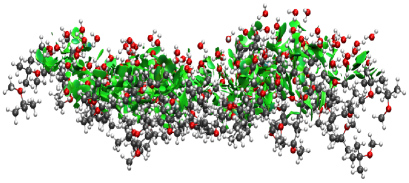
Chloroform



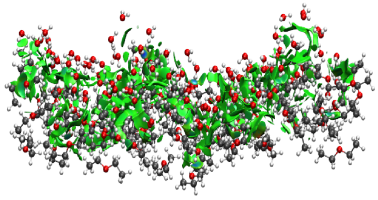
Dichloroethane



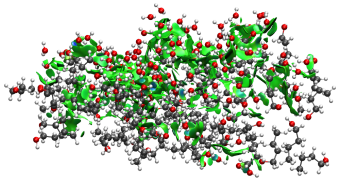
DichloroMethane



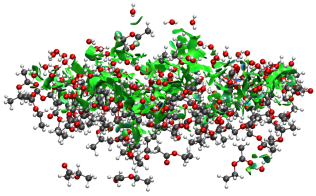
Methyl tert–butyl ether



Diethyl ether



n-Butanol



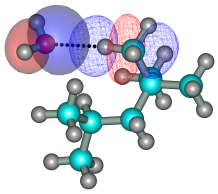
Ethyl acetate

Figure S5: NCI surfaces at the $\mathcal{S}\cdots$Water interphases for the complete set.

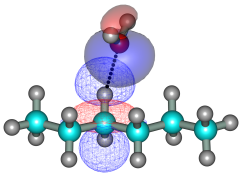
4 Dimers

4.1 Global minima: Structures and NBOs

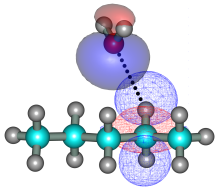
4.1.1 $\mathcal{S}\cdots$Water



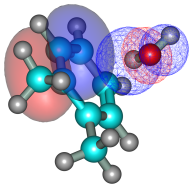
Isooctane
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -1.15



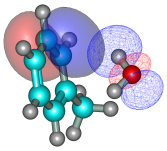
Hexane
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -0.13



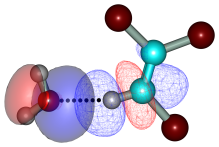
Pentane
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -0.20



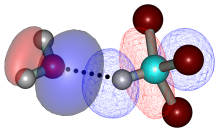
Ortho–xylene
$\pi_{\mathrm{C-C}} \rightarrow \sigma^*_{\mathrm{O-H}}$
$E^{(2)}_{d\rightarrow a}$ = -0.35



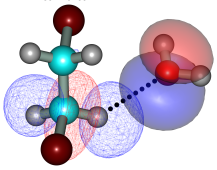
Toluene
$\pi_{\mathrm{C-C}} \rightarrow \sigma^*_{\mathrm{O-H}}$
$E^{(2)}_{d\rightarrow a}$ = -0.41



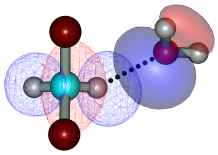
Trichloroethylene
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -4.23



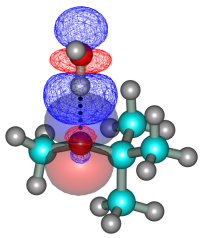
Chloroform
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -3.00



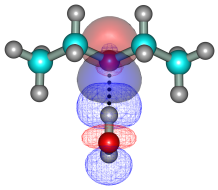
Dichloroethane
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -0.72



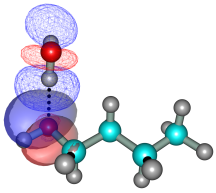
DichloroMethane
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -1.95



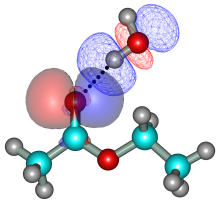
Methyl tert–butyl ether
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{O-H}}$
$E^{(2)}_{d\rightarrow a}$ = -8.39



Diethyl ether
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{O-H}}$
$E^{(2)}_{d\rightarrow a}$ = -7.05



n-butanol
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{C-H}}$
$E^{(2)}_{d\rightarrow a}$ = -6.99



Ethyl acetate
$n_{\mathrm{O}} \rightarrow \sigma^*_{\mathrm{O-H}}$
$E^{(2)}_{d\rightarrow a}$ = -3.38

Figure S6: Dimers for all hydrophobe$\cdots$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.

4.1.2 $\mathcal{S}\cdots\mathcal{S}$

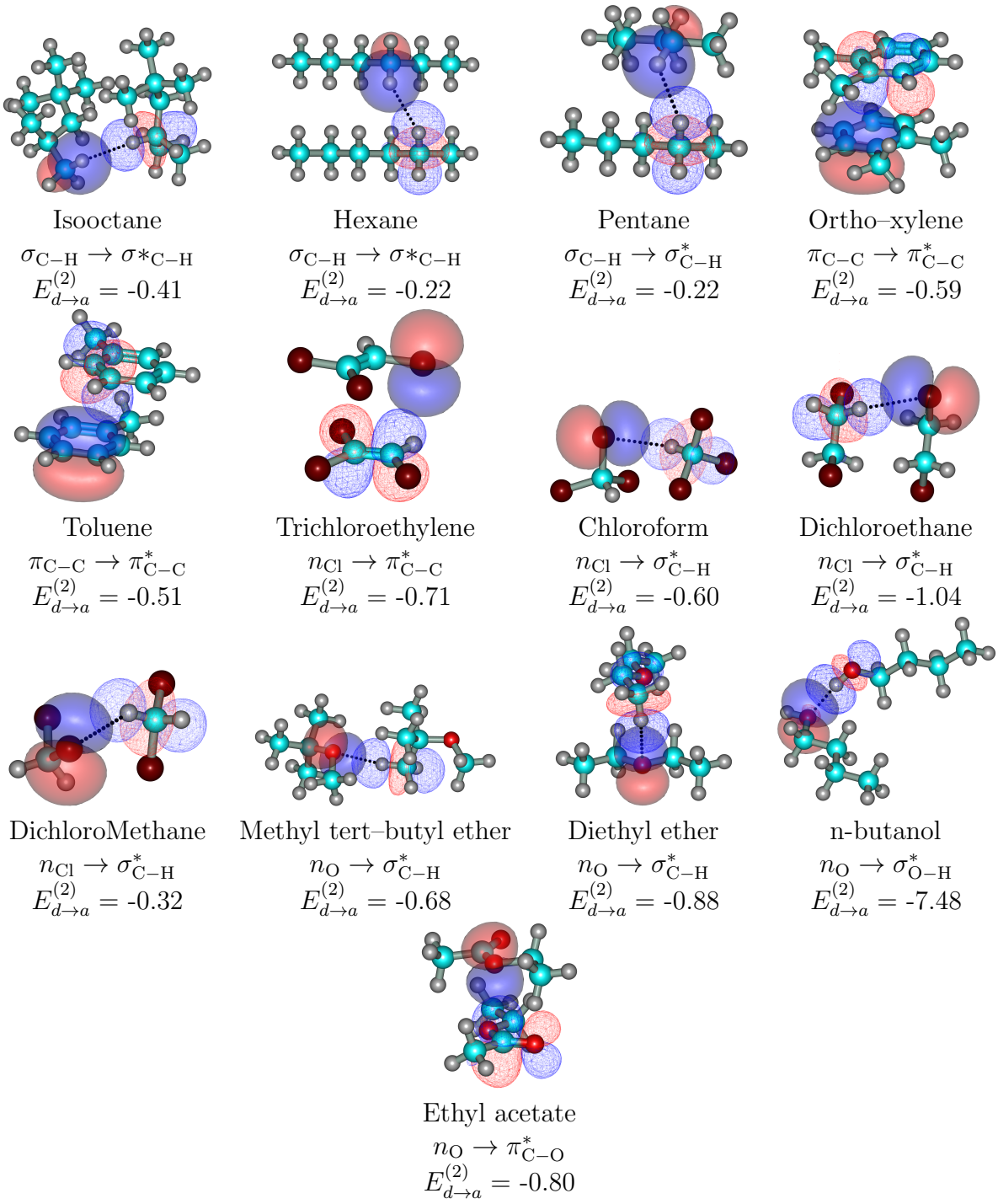


Figure S7: Dimers for all hydrophobe···hydrophobe pairs in this study. Explicit orbital interactions and orbital interaction energies in kcal/mol are shown. The water dimer is included for comparison.

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

4.2.1 Cartesian coordinates for all $\mathcal{S}\cdots$Water dimers

Equilibrium Geometry Benzene$\cdots$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$\cdots$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$\cdots$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

Equilibrium Geometry Chloroform···Water: E= -1493.8116489 Hartree			
8	2.824122	-0.001568	-0.976362
1	3.311753	0.001794	-0.148735
1	3.504595	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	-0.001219	-1.408779
6	1.047967	1.262580	-0.591980
6	0.252902	1.262402	0.717944
6	0.547989	0.001271	1.536896
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

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···Water: E= -309.3115891 Hartree

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	-0.478473	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···Water: E= -387.7136812 Hartree

8	-1.274964	2.452221	-0.362445
1	-1.046292	2.944520	-1.153430
1	-0.713433	1.661855	-0.411677
6	2.051664	1.178867	0.337744
6	1.390112	-0.188764	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	-1.535410	-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 $\cdots$Water: E= -383.2312731 Hartree

8	-2.461478	-1.782419	-0.022828
1	-2.700601	-2.711038	-0.037329
1	-1.495409	-1.794126	0.006432
6	-1.062736	2.456918	0.004484
6	-0.760086	0.975190	0.018639
1	-0.614823	2.952691	0.868803
1	-0.680235	2.922044	-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$\cdots$Water **1**: E= -351.8287213 Hartree

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	0.455968	-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	-0.231414	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

1	-4.751355	-0.739425	-0.012811
1	-3.859083	0.455564	0.940737
1	-3.856568	0.553082	-0.827480

Equilibrium Geometry Heptane···Water **2**: E= -351.8287115 Hartree

8	-0.031555	2.786915	0.029404
1	-0.134768	3.370202	0.785662
1	0.047611	3.395578	-0.709622
6	3.823433	-0.429426	-0.361559
1	3.881029	-1.272089	-1.058732
1	4.728086	-0.438401	0.254482
1	3.824387	0.493622	-0.950904
6	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

8	-0.007893	2.743664	-0.000368
1	-0.252260	3.341142	0.711013
1	0.236463	3.338323	-0.714107
6	-3.201215	-0.548893	-0.214379
1	-3.250798	0.333027	-0.861598
1	-4.060367	-0.521213	0.463266
1	-3.299756	-1.436505	-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	-1.490902	1.022144
1	0.700172	0.276106	1.031234

6	1.881128	-0.573132	-0.551402
1	1.807969	0.310658	-1.197497
1	1.855377	-1.450464	-1.210907
6	3.204321	-0.541234	0.214550
1	3.304692	-1.426221	0.851947
1	4.063428	-0.514323	-0.463180
1	3.252040	0.343227	0.858435

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	0.597634
6	-1.423100	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
1	-1.726266	-0.152515	2.133344
6	-0.994406	1.264817	-0.942471
1	-0.001234	1.643521	-0.684133
1	-0.986620	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
1	-0.862338	-1.848685	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	-1.868992
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	2.233536	-0.796617	0.008742
6	-0.246095	0.304566	-0.051224
8	0.301610	-0.790088	-0.091789
6	0.538496	1.594369	0.037769
1	1.580098	1.435606	-0.243360
1	0.081120	2.366397	-0.587347
1	0.502061	1.947366	1.074832

6	-1.757114	0.431083	-0.072183
1	-2.044100	1.151135	0.704640
1	-2.018486	0.908393	-1.026756
6	-2.485299	-0.897071	0.095072
1	-2.233673	-1.357713	1.053440
1	-3.567320	-0.747802	0.054632
1	-2.197921	-1.596043	-0.692901

Equilibrium Geometry Methyl tert-butyl ether···Water: E= -348.51227 Hartree

8	-2.842519	-0.431756	0.095142
1	-1.993974	-0.098820	-0.240455
1	-3.354542	-0.596791	-0.699053
6	2.110209	0.290025	-0.223893
6	0.716877	-0.290171	0.010745
1	2.241311	0.545853	-1.280205
1	2.289995	1.182441	0.382406
1	2.864344	-0.454281	0.049750
6	0.461564	-0.541758	1.497520
6	0.541558	-1.581036	-0.781015
1	-0.561879	-0.897794	1.648358
1	1.156572	-1.303790	1.864777
1	0.615498	0.360425	2.096748
1	1.272478	-2.326872	-0.454071
1	-0.462489	-1.986013	-0.626224
1	0.686038	-1.387975	-1.848080
8	-0.301534	0.585296	-0.533790
6	-0.280883	1.933595	-0.079830
1	-1.178407	2.402212	-0.486615
1	-0.316740	1.999653	1.012880
1	0.598276	2.469508	-0.452195

Equilibrium Geometry n–butanol···Water: E= -309.3226537 Hartree

8	-2.635073	1.581540	0.246336
1	-3.081890	1.930234	-0.527180
1	-2.374712	0.688929	-0.023524
6	-0.402253	-1.249285	0.234019
1	-0.475443	-1.234567	1.328960
1	0.009238	-2.217613	-0.077555
6	0.495701	-0.123120	-0.242274
1	0.524954	-0.139119	-1.338525
1	0.054341	0.832922	0.060515
6	1.914004	-0.242381	0.316648
1	1.873116	-0.240764	1.413047
1	2.345065	-1.206205	0.017491
6	2.818594	0.893796	-0.162073
1	3.829419	0.797138	0.244671
1	2.891562	0.895387	-1.254339
1	2.417767	1.863172	0.150055
8	-1.703368	-1.063196	-0.348069

1	-2.262167	-1.790333	-0.057678

Equilibrium Geometry n–octanol···Water: E= -466.1057537 Hartree

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	0.208202
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	-1.303520
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	-0.630351	-0.835980	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	-1.399297
1	-2.122758	0.719163	0.033394
6	-3.134741	-1.160157	0.172641
1	-3.179117	-1.157282	1.269239
1	-3.013387	-2.194879	-0.171861
8	-4.345083	-0.604957	-0.369687
1	-5.076682	-1.162007	-0.086995

Equilibrium Geometry Ortho–xylene···Water: E= -386.2697695 Hartree

8	-1.134868	-0.274503	2.467240
1	-0.641846	-0.328753	3.289379
1	-0.445427	-0.185566	1.799956
6	2.082585	-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

1	-1.903827	1.474501	-1.713858
1	-2.344215	1.217036	-0.020147
1	-1.369483	2.625497	-0.476472
6	-1.575171	-1.363235	-0.957046
1	-2.294534	-1.281397	-0.134206
1	-2.045064	-0.942969	-1.852503
1	-1.383568	-2.424292	-1.137292

Equilibrium Geometry Pentane···Water: E= -273.436907 Hartree

8	-0.302291	2.662006	-0.017321
1	0.037131	3.386102	0.514755
1	-0.740045	3.109062	-0.746091
6	2.610593	-0.508601	-0.328547
1	2.723516	-1.466765	-0.847172
1	3.508214	-0.344903	0.276113
1	2.563968	0.280257	-1.086563
6	1.343887	-0.501025	0.527842
1	1.415666	-1.275121	1.303108
1	1.253911	0.462002	1.043982
6	0.078142	-0.730296	-0.296473
1	0.144546	-1.704126	-0.803296
1	0.024658	0.035319	-1.081745
6	-1.201626	-0.675562	0.536431
1	-1.251079	0.300400	1.031920
1	-1.153105	-1.438663	1.324359
6	-2.459446	-0.887368	-0.307017
1	-2.435161	-1.862311	-0.805806
1	-3.366858	-0.843186	0.303463
1	-2.536331	-0.117005	-1.081872

Equilibrium Geometry Toluene···Water: E= -347.0680392 Hartree

8	0.343262	2.722118	-0.000934
1	0.115917	2.158587	0.744495
1	0.117069	2.158554	-0.746686
6	-1.257300	-0.410510	-1.209379
6	0.135019	-0.565903	-1.205085
6	0.855352	-0.598651	0.000213
6	0.135021	-0.564511	1.205477
6	-1.257285	-0.409150	1.209687
6	-1.961391	-0.364061	0.000131
1	-1.795345	-0.384820	-2.153659
1	0.674371	-0.617565	-2.149249
1	-1.795288	-0.382377	2.153962
1	-3.041879	-0.251535	0.000086
6	2.360020	-0.699983	0.000280
1	2.813525	0.297668	0.000316
1	2.717223	-1.231869	0.886603
1	2.717306	-1.231843	-0.886024
1	0.674390	-0.615137	2.149689

Equilibrium Geometry Trichloroethylene···Water: E= -1531.7933009 Hartree			
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 $\mathcal{S}\cdots\mathcal{S}$ dimers

Equilibrium Geometry $(Benzene)_2$: E= -463.1803711 Hartree			
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
1	-3.270773	0.000950	1.651991
1	-2.529213	-2.154199	0.653406
1	-1.040623	-2.153288	-1.340496
1	-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			
6	-4.224777	0.017178	-0.204328
8	-3.843710	-1.133109	-0.277371
8	-3.390951	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	5.646480	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 $(\text{Carbon tetrachloride})_2$: E= -3753.1483706 Hartree

6	-2.409399	-0.000768	0.000393
17	-2.349685	1.272594	-1.231587
17	-1.346052	-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 $(\text{Chloroform})_2$: 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 $(\text{Cyclohexane})_2$: E= -470.3487178 Hartree

6	1.720489	-0.422859	-1.406749
6	2.685891	-1.345445	-0.655889
6	2.671397	-1.050671	0.847485
6	2.991162	0.422029	1.123705

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	-1.699071	1.369065
1	3.703673	-1.192138	-1.042335
1	0.693526	-0.638147	-1.080555
6	-2.671669	-1.048691	-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	-2.948956	0.628945	-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	2.483327
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

Equilibrium Geometry $(Dichloroethane)_2$: E= -1995.3795492 Hartree

6	-1.783893	-0.734987	-0.183402
1	-2.687014	-1.000501	-0.732644
1	-0.911803	-1.000226	-0.780308
6	-1.784038	0.735065	0.183519
1	-2.687280	1.000445	0.732647
1	-0.912136	1.000524	0.780578
17	-1.737138	-1.709092	1.311141
17	-1.737235	1.709203	-1.310955
6	1.783941	-0.735114	0.183370
1	2.687304	-1.000392	0.732355
1	0.912113	-1.000671	0.780518
6	1.783563	0.734937	-0.183517
1	2.686351	1.000489	-0.733325
1	0.911157	1.000247	-0.779846
17	1.737025	-1.709162	-1.311147
17	1.737575	1.709091	1.310974

Equilibrium Geometry $(Dichloromethane)_2$: E= -1916.9661675 Hartree

6	-1.517815	-0.523602	-0.602144
1	-0.553543	-0.173578	-0.956478
1	-1.931175	-1.270877	-1.274112
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 $(Diethyl\ ether)_2$: 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	-1.343178	-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 $(Diisopropyl\ ether)_2$: E= -622.8614760 Hartree

6	-1.476638	2.468489	-0.596564
6	-1.495091	0.956569	-0.755428

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	-2.663333
1	-0.732432	0.874014	-2.783374
8	-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	1.963962
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	0.162696	-1.808469	-1.082886
1	1.450099	-2.797622	-1.804170
1	1.149283	-2.864602	-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 $(\text{Ethyl acetate})_2$: E= -613.9047765 Hartree

6	3.072073	-0.748046	-0.685533
6	2.048026	0.335430	-0.943569
1	3.848850	-0.392975	-0.003600
1	2.594170	-1.634163	-0.262670
1	3.542919	-1.033623	-1.630870
1	1.243789	-0.021255	-1.590477
1	2.494205	1.224557	-1.397789
8	1.489776	0.706707	0.339403

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
1	-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	-0.028601	-1.987036	1.675664
1	0.707176	-1.227266	1.954569
1	-0.842544	-1.970501	2.402265
1	0.454706	-2.964085	1.663330

Equilibrium Geometry $(\text{Heptane})_2$: E= -551.1112096 Hartree

6	-3.131351	-2.174007	1.453163
1	-2.900134	-2.984184	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

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	2.021900	0.702981
1	0.608694	1.108433	1.306828
1	0.420822	2.857224	1.358834
6	2.161793	2.187062	0.270766
1	2.267560	3.126317	-0.287397
1	2.418828	1.380412	-0.427773
6	3.131318	2.173973	1.453135
1	4.168375	2.296465	1.125230
1	2.900234	2.984232	2.152947
1	3.059349	1.228293	2.001649

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

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	0.645802	-1.892085	-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	-0.391751
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	-2.496320	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	2.111836	-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

1	2.612426	-3.086914	-1.214913
6	2.133474	-0.316903	0.792945
1	1.173181	-0.768383	1.084797
1	2.842571	-0.574158	1.596719
6	1.918224	1.204944	0.802925
1	1.164121	1.451004	0.044519
6	3.176149	2.028351	0.512309
1	4.000718	1.718367	1.166034
1	3.507966	1.932247	-0.524391
1	2.980674	3.090634	0.698133
6	1.348370	1.607253	2.168349
1	1.105012	2.675366	2.193352
1	0.439482	1.042799	2.401356
1	2.082313	1.409930	2.959809

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

6	-1.584803	-0.525346	0.232397
8	-1.088369	-0.438718	1.347094
6	-1.816799	-1.860185	-0.440273
1	-1.415704	-2.666722	0.175100
1	-2.891134	-2.012868	-0.590561
1	-1.336606	-1.861014	-1.423779
6	-1.978866	0.701764	-0.568001
1	-1.260097	0.764084	-1.396669
1	-2.956318	0.513598	-1.029478
6	-1.990191	1.986744	0.252595
1	-1.012030	2.168768	0.702194
1	-2.248389	2.842069	-0.377844
1	-2.719206	1.922180	1.064843
6	1.585413	-0.524414	-0.232381
8	1.088765	-0.438307	-1.347024
6	1.818703	-1.858997	0.440338
1	1.419093	-2.666011	-0.175378
1	2.893097	-2.010311	0.591531
1	1.337700	-1.860473	1.423456
6	1.978261	0.703128	0.567932
1	1.259431	0.764674	1.396610
1	2.955971	0.516244	1.029369
6	1.988079	1.988115	-0.252691
1	1.009657	2.169152	-0.702120
1	2.245544	2.843687	0.377719
1	2.717038	1.924284	-1.065050

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

6	-1.530577	-0.194536	1.191291
6	-2.223921	0.348498	-0.059876
1	-1.837001	0.385370	2.068026
1	-1.770179	-1.248326	1.366041
1	-0.446998	-0.115071	1.063602

6	-1.847251	-0.477956	-1.290412
6	-1.835706	1.805791	-0.278409
1	-2.417642	-0.135671	-2.160470
1	-0.779031	-0.353379	-1.492534
1	-2.042240	-1.545022	-1.141888
1	-0.754897	1.890665	-0.423603
1	-2.346606	2.198936	-1.162418
1	-2.130427	2.404756	0.588650
8	-3.651251	0.401998	0.124651
6	-4.309142	-0.845213	0.240858
1	-5.356286	-0.616027	0.447157
1	-4.255776	-1.429630	-0.685887
1	-3.915738	-1.449894	1.067479
6	2.991857	-0.063172	1.528428
6	2.736620	0.211749	0.045846
1	2.079893	0.112845	2.108404
1	3.328578	-1.089094	1.704319
1	3.771479	0.610608	1.897733
6	3.958874	-0.153009	-0.798518
6	2.376273	1.678515	-0.158941
1	3.746566	0.024029	-1.857306
1	4.813278	0.464923	-0.503736
1	4.247721	-1.199903	-0.667497
1	3.223004	2.321274	0.101776
1	2.108879	1.853246	-1.205351
1	1.523502	1.948876	0.470625
8	1.570219	-0.493123	-0.423014
6	1.559802	-1.893843	-0.205513
1	0.667760	-2.271042	-0.709118
1	2.438439	-2.389460	-0.635550
1	1.491012	-2.144957	0.859919

Equilibrium Geometry $(n\text{–butanol})_2$: E= -466.0854548 Hartree

6	-1.442880	-0.981381	-0.204280
1	-0.868470	-0.324453	-0.874525
1	-1.859990	-1.797290	-0.813542
6	-2.573564	-0.189947	0.429589
1	-3.103898	-0.842418	1.133920
1	-2.141241	0.631599	1.014077
6	-3.553789	0.367437	-0.602183
1	-3.010186	1.001646	-1.314341
1	-3.980612	-0.460807	-1.181818
6	-4.681912	1.174577	0.041873
1	-5.377073	1.562717	-0.708735
1	-5.250605	0.552866	0.740936
1	-4.278233	2.024715	0.601383
8	-0.613594	-1.496436	0.828694
1	0.204173	-1.800096	0.408989
6	2.866648	-1.138053	-0.027193
1	3.155851	-1.292443	1.020263

1	3.760905	-1.233168	-0.656038
6	2.251045	0.238135	-0.199427
1	1.938322	0.352535	-1.244662
1	1.350856	0.300010	0.422508
6	3.220850	1.358672	0.176421
1	3.550494	1.221473	1.213936
1	4.117917	1.292264	-0.452102
6	2.586154	2.741161	0.020247
1	3.290791	3.536439	0.280296
1	2.261002	2.901893	-1.012743
1	1.709337	2.838170	0.668215
8	1.889016	-2.116380	-0.417818
1	2.291977	-2.986730	-0.343305

Equilibrium Geometry $(\text{n–octanol})_2$: E= -779.6578048 Hartree

6	2.042100	-2.460591	-0.503236
1	2.243359	-1.651012	-1.217740
1	1.820486	-3.365611	-1.086373
6	0.838757	-2.100726	0.356062
1	0.699288	-2.891492	1.103834
1	1.061179	-1.179110	0.909336
6	-0.444979	-1.918556	-0.453496
1	-0.285562	-1.163965	-1.237831
1	-0.691810	-2.856923	-0.969411
6	-1.628716	-1.495747	0.417816
1	-1.762198	-2.231743	1.223172
1	-1.391550	-0.540001	0.906889
8	3.174358	-2.691353	0.329460
1	3.917401	-2.198012	-0.043253
6	5.090324	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	-0.891569	-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	0.090921	-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
6	0.919115	2.089583	-0.165400
1	0.954698	1.047291	-0.507612
1	1.288365	2.707195	-0.997777
6	-0.536588	2.455872	0.124380
1	-0.593257	3.506388	0.442953
1	-0.901527	1.854034	0.969084
6	-1.451126	2.241591	-1.082130
1	-1.088128	2.853691	-1.918247
1	-1.372398	1.195838	-1.405366
6	-2.912045	2.583596	-0.788029
1	-3.548225	2.416865	-1.663161
1	-3.296419	1.966754	0.030939
1	-3.012634	3.633705	-0.492961

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	1.668328	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	1.686384	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	-0.717502	-2.458971
1	-1.570592	2.103252	1.615986
1	-1.501886	3.176029	-0.624261
6	-1.692466	-0.544371	2.220187

1	-2.566792	-1.195621	2.332331
1	-0.801391	-1.161955	2.387856
1	-1.733418	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 $(Pentane)_2$: E= -394.3245324 Hartree

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
1	1.716048	-2.761738	1.973773
6	-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 $(Toluene)_2$: E= -541.5859167 Hartree

6	1.609001	-1.607951	0.635573
6	1.139052	-0.481855	1.321587
6	1.345223	0.809543	0.814050
6	2.034340	0.947255	-0.402599

6	2.503312	-0.174383	-1.096145
6	2.291902	-1.458135	-0.576765
1	1.436057	-2.600285	1.045288
1	0.597197	-0.607457	2.256750
1	3.038420	-0.046593	-2.034307
1	2.658773	-2.331368	-1.110390
6	0.877017	2.024392	1.575690
1	1.704458	2.479831	2.132379
1	0.475575	2.783501	0.896473
1	0.094112	1.756576	2.290942
1	2.215722	1.943487	-0.803710
6	-1.340822	-1.703532	-0.744276
6	-1.092380	-0.477200	-1.367888
6	-1.497737	0.729620	-0.773667
6	-2.148476	0.677544	0.468310
6	-2.403569	-0.548465	1.097261
6	-1.998940	-1.743442	0.491985
1	-1.019235	-2.626374	-1.220937
1	-0.576782	-0.453802	-2.326373
1	-2.921056	-0.569133	2.053670
1	-2.200650	-2.696923	0.973863
6	-1.238301	2.043529	-1.466849
1	-1.650917	2.038170	-2.481300
1	-1.692702	2.875327	-0.920340
1	-0.161516	2.229800	-1.547923
1	-2.475186	1.603716	0.938318

Equilibrium Geometry (Trichloroethylene)$_2$: E= -2911.0397068 Hartree			
6	-1.674894	0.732311	0.571874
1	-1.510781	1.254997	1.504473
6	-1.448456	-0.589621	0.485058
17	-1.692093	-1.517733	-0.930744
17	-0.897667	-1.452016	1.873313
17	-2.250624	1.693011	-0.720516
6	1.779383	0.458261	0.908186
1	2.119685	-0.109366	1.764099
6	1.693379	-0.112849	-0.305494
17	1.176005	0.709549	-1.712409
17	2.123610	-1.768117	-0.503108
17	1.381630	2.095645	1.215446

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