

Supporting information for:

The role of orbital symmetries in enforcing ferromagnetic ground state in mixed radical dimers

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Computational details

Technical details

All DFT calculations were carried out using GAUSSIAN 09 quantum chemistry software revision D.01.^{S1} A validation study of different exchange-correlation (XC) functionals was carried out (wide infra). The tested functionals included the global hybrids B3LYP,^{S2-S5} PBE0,^{S6-S9} M06,^{S10,S11} M06-2X,^{S10,S11} and the range-separated hybrids LC- ω PBE,^{S12-S14} CAM-B3LYP,^{S15} and ω B97XD.^{S16,S17} Each functional was utilized both with and without the DFT-D3 dispersion correction,^{S18} except for ω B97XD, which includes dispersion correction in the functional definition. Both the older zero damping function and the newer Becke-Johnson (BJ)^{S19} damping function were considered, except for M06 and M06-2X functionals,

which have only been parametrized for the zero damping function. Based on the validation study, the range-separated LC- ω PBE functional with empirical dispersion correction using BJ damping (denoted as LC- ω PBE-D3BJ) was chosen for the final calculations. The “UltraFine” grid in GAUSSIAN (99 radial shells and 590 angular points per shell) was used in integration of exchange-correlation potential. In geometry optimizations, no constraints were placed on spatial or spin symmetries, and frequency calculations were carried out to ensure that all stationary points lie at true minima on the potential energy surfaces. A threshold of 10^{-7} was used for the convergence of the coupled-perturbed Hartree–Fock equations in the frequency calculations. The “Tight” convergence criteria in GAUSSIAN ($1.5 \cdot 10^{-5}$, $1.0 \cdot 10^{-5}$, $6.0 \cdot 10^{-5}$, and $4.0 \cdot 10^{-5}$ for maximum force, RMS force, maximum displacement, and RMS displacement, respectively) was used in geometry optimizations, which ensures convergence very close to numerical accuracy. Stability analyses^{S20,S21} were carried out both before and after geometry optimizations to ensure that all converged states represent a minimum in the variational space. Enthalpy corrections (including zero point energy corrections) were calculated from the partition functions constructed from electronic energies and the calculated harmonic vibrational frequencies using standard expressions. All DFT calculations, including functional validation studies, utilized the def2-TZVP basis sets.^{S22}

DLPNO-CCSD(T)^{S23–S26} calculations were carried out using ORCA software version 4.0.1^{S27} with the default parameters. Dunning’s correlation consistent basis sets^{S28} were used along with corresponding auxiliary correlation fitting basis sets.^{S29} Valence triple- ζ quality cc-pVTZ basis sets were used for atoms in the phenalenyl or oxophenalenoxyl core moieties, whereas smaller valence double- ζ quality cc-pVDZ basis sets were used for atoms in the peripheral *tert*-butyl groups to reduce the overall computational costs.

Exchange coupling constants

Exchange coupling constants were calculated using the broken symmetry (BS) formalism.^{S30–S32} A high-spin (HS) state with spin projection $M_S = 1$ and a low-spin (LS) state with spin

projection $M_S = 0$ were optimized. The corresponding exchange coupling constant was then evaluated using the Yamaguchi projection^{S33–S36}

$$J = E_S - E_T \approx \frac{2(E_{LS} - E_{HS})}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}}, \quad (1)$$

where E_S and E_T are the energies of the singlet and triplet state, respectively, E_{LS} and E_{HS} are the energies of the LS and HS states, respectively, and $\langle S^2 \rangle_{LS}$ and $\langle S^2 \rangle_{HS}$ are the expectation values of the $\hat{S}^2$ operator evaluated on the Kohn–Sham determinant. E_{LS} and E_{HS} in equation (1) are evaluated at a fixed geometry, but the equation can also be generalized into an adiabatic situation where the geometries are allowed to relax^{S37} assuming that i) the energy and geometry evaluated for the HS state are reasonable approximations of the triplet energy and geometry, and ii) the geometry optimized for the LS state is a reasonable approximation of the singlet geometry. The first assumption certainly seems valid as the HS state is single-determinantal and therefore should pose no problem to DFT; the latter assumption inevitably introduces some approximation. As J is equal to the single–triplet splitting, the energy of the singlet state is given as

$$E_S^S = E_T^S + J = E_T^S + \frac{2(E_{LS}^S - E_{HS}^T)}{\langle S^2 \rangle_{HS}^S - \langle S^2 \rangle_{LS}^T} \approx E_{HS}^{LS} + \frac{2(E_{LS}^{LS} - E_{HS}^{LS})}{\langle S^2 \rangle_{HS}^{LS} - \langle S^2 \rangle_{LS}^{LS}}, \quad (2)$$

where the subscripts indicate the state and the superscripts indicate the geometry the energy or $\langle S^2 \rangle$ value is evaluated in. Using this result, the exchange coupling constants were evaluated in the LS geometry (J_{LS}), in the HS geometry (J_{HS}), and using the adiabatic singlet–triplet splitting ($J_{\text{adiabatic}}$) as

$$J_{LS} = \frac{2(E_{LS}^{LS} - E_{HS}^{LS})}{\langle S^2 \rangle_{HS}^{LS} - \langle S^2 \rangle_{LS}^{LS}} \quad (3)$$

$$J_{HS} = \frac{2(E_{LS}^{HS} - E_{HS}^{HS})}{\langle S^2 \rangle_{HS}^{HS} - \langle S^2 \rangle_{LS}^{HS}} \quad (4)$$

$$J_{\text{adiabatic}} = E_{HS}^{LS} + \frac{2(E_{LS}^{LS} - E_{HS}^{LS})}{\langle S^2 \rangle_{HS}^{LS} - \langle S^2 \rangle_{LS}^{LS}} - E_{HS}^{HS}. \quad (5)$$

Dimerization enthalpies

The dimerization energies (ΔE) and enthalpies (ΔH) were evaluated using two different approaches; in validation studies (vide infra) all terms in the expressions were evaluated at DFT level, and in the final calculations energy terms of the HS states were evaluated at DLPNO-CCSD(T) level using the DFT optimized geometries, and the exchange coupling constants and enthalpy corrections to the energies were evaluated at the DFT level. In both cases the basis set superposition error (E_{BSSE}) was estimated using the counterpoise method^{S38} either at the DFT or DLPNO-CCSD(T) level depending on which energies were used in the expressions. Using only DFT energies, the dimerization energies and enthalpies in the LS and HS states are given as

$$\Delta E_{\text{LS}} = [E_{\text{HS}}^{\text{LS}}(\text{DFT}) + J_{\text{LS}}] - E_{\text{monomer1}}(\text{DFT}) - E_{\text{monomer2}}(\text{DFT}) + E_{\text{BSSE}}^{\text{LS}}(\text{DFT}) \quad (6)$$

$$\Delta E_{\text{HS}} = E_{\text{HS}}^{\text{HS}}(\text{DFT}) - E_{\text{monomer1}}(\text{DFT}) - E_{\text{monomer2}}(\text{DFT}) + E_{\text{BSSE}}^{\text{HS}}(\text{DFT}) \quad (7)$$

$$\begin{aligned} \Delta H_{\text{LS}} = & [E_{\text{HS}}^{\text{LS}}(\text{DFT}) + H_{\text{LS}}^{\text{LS}} + J_{\text{LS}}] - [E_{\text{monomer1}}(\text{DFT}) + H_{\text{monomer1}}] \\ & - [E_{\text{monomer2}}(\text{DFT}) + H_{\text{monomer2}}] + E_{\text{BSSE}}^{\text{LS}}(\text{DFT}) \end{aligned} \quad (8)$$

$$\begin{aligned} \Delta H_{\text{HS}} = & [E_{\text{HS}}^{\text{HS}}(\text{DFT}) + H_{\text{HS}}^{\text{HS}}] - [E_{\text{monomer1}}(\text{DFT}) + H_{\text{monomer1}}] \\ & - [E_{\text{monomer2}}(\text{DFT}) + H_{\text{monomer2}}] + E_{\text{BSSE}}^{\text{HS}}(\text{DFT}), \end{aligned} \quad (9)$$

where (2) has been used to estimate the energy of the singlet state, E_{monomer1} and E_{monomer2} are the energies of the monomers in their optimized doublet geometries, and $H_{\text{LS}}^{\text{LS}}$, $H_{\text{HS}}^{\text{HS}}$, H_{monomer1} , and H_{monomer2} are the enthalpy corrections to the LS, HS, and monomer energies evaluated at DFT level using geometries optimized for the respective states. The enthalpy correction $H_{\text{LS}}^{\text{LS}}$ is taken as a reasonable approximation to the enthalpy correction of the singlet state. Using the DLPNO-CCSD(T) energies for the HS states, the analogous expressions

are given as

$$\Delta E_{\text{LS}} = [E_{\text{HS}}^{\text{LS}}(\text{DLPNO-CCSD(T)}) + J_{\text{LS}}] \quad (10)$$

$$\begin{aligned} & - E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) - E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) \\ & + E_{\text{BSSE}}^{\text{LS}}(\text{DLPNO-CCSD(T)}) \end{aligned}$$

$$\Delta E_{\text{HS}} = E_{\text{HS}}^{\text{HS}}(\text{DLPNO-CCSD(T)}) \quad (11)$$

$$\begin{aligned} & - E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) - E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) \\ & + E_{\text{BSSE}}^{\text{HS}}(\text{DLPNO-CCSD(T)}) \end{aligned}$$

$$\Delta H_{\text{LS}} = [E_{\text{HS}}^{\text{LS}}(\text{DLPNO-CCSD(T)}) + H_{\text{LS}}^{\text{LS}} + J_{\text{LS}}] \quad (12)$$

$$\begin{aligned} & - [E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer1}}] \\ & - [E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer2}}] + E_{\text{BSSE}}^{\text{LS}}(\text{DLPNO-CCSD(T)}) \end{aligned}$$

$$\Delta H_{\text{HS}} = [E_{\text{HS}}^{\text{HS}}(\text{DLPNO-CCSD(T)}) + H_{\text{HS}}^{\text{HS}}] \quad (13)$$

$$\begin{aligned} & - [E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer1}}] \\ & - [E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer2}}] + E_{\text{BSSE}}^{\text{HS}}(\text{DLPNO-CCSD(T)}), \end{aligned}$$

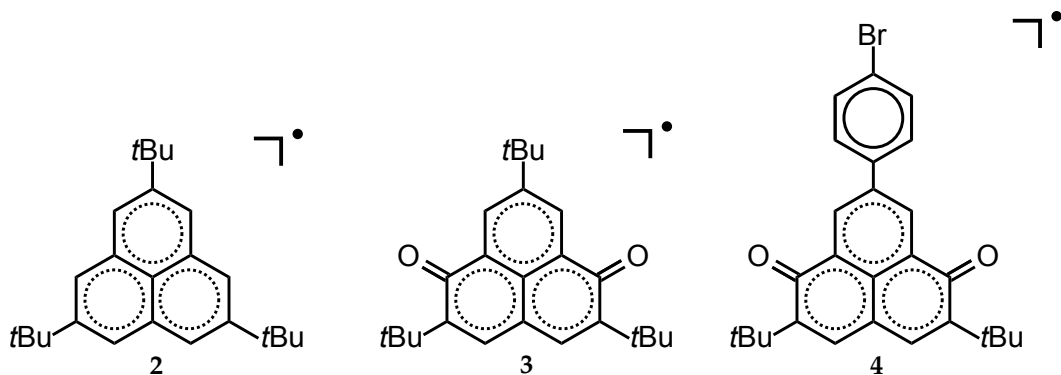
It should be noted that ΔE_{HS} is calculated purely from DLPNO-CCSD(T) energies (although using DFT optimized geometries), whereas ΔE_{LS} is evaluated using the exchange coupling constants calculated at the BS DFT level.

Validation studies

In order to produce reliable results in calculations on the hypothetical **2–3** dimer, several functionals were first validated against experimental data. Based on the results presented below, the range-separated LC- ω PBE hybrid functional with the DFT-D3 dispersion correction and BJ damping function was chosen for the final calculations.

Exchange coupling constants

The exchange coupling constants calculated using various functionals were compared to the experimentally measured values. The calculated values of the exchange coupling constants depend both on the geometry used for the calculations and the ability of the chosen XC functional to correctly estimate the energy differences between different spin states within the context of BS formalism. It is well known that values of exchange coupling constants have strong dependence on the XC functional,^{S37,S39–S48} whereas the geometry optimizations tend to compensate for the functional error.^{S49} In order to eliminate the degrees of freedom related to geometry optimizations, the calculations were carried out as single point energy evaluations on geometries extracted from experimental crystal structures. Based on SQUID measurements,^{S50–S52} the exchange coupling constant in **2–2** has been determined as roughly -1390 cm^{-1} . The measurement has, however, been carried out in the presence of paramagnetic impurities and the experimental reference should therefore be considered only as a rough estimate. The exchange coupling constant in **2–2** has also been determined from peak intensities of the EPR spectrum, giving a value of -2910 cm^{-1} , which is more than twice the magnitude of the SQUID value.^{S53} Due to the uncertainties related to the experimental value of the exchange coupling constant in **2–2**, in addition to the **2–2** dimer, validation calculations were also carried out on the dimer of 3,5-di-*tert*-butyl-8-*para*-bromophenyl-6-oxophenalenoxyl (**4**), which is structurally similar to **3–3** and for which an exchange coupling constant of -267 cm^{-1} has been reliably determined from SQUID data.^{S54}



The calculated exchange coupling constants are listed in Table S1. It is immediately clear that all values calculated for **2–2** are considerably larger in magnitude than the value estimated from SQUID measurements. The value calculated with the range-separated LC- ω PBE functional is closest to the SQUID value but its magnitude is still more than twice that of the experimental value. The LC- ω PBE value is, however, relatively close to the value extracted from EPR measurements. All functionals do correctly produce the qualitative aspects of the interaction: the strong AFM exchange. In the case of the **4–4** dimer, all calculated values are much closer to experiment. The best match is again obtained with LC- ω PBE, and the value calculated with the global hybrid PBE0 is also extremely close to experiment. However, all tested functionals provide a reasonable estimate of the exchange coupling constant in this case.

Table S1: Exchange coupling constants (J_{LS} , in cm^{-1}) calculated for **2–2** and **4–4** using various XC functionals

	2–2	4–4
B3LYP	–3669	–286
PBE0	–3531	–266
M06	–3787	–251
M06-2X	–4239	–309
LC- ω PBE	–2754	–267
CAM-B3LYP	–3323	–253
ω B97XD	–3431	–247
Experimental	–1390 ^{S50} –2910 ^{S53}	–267 ^{S54}

Geometries and dimerization enthalpies

The structures of the monomer **2** and the **2-2** dimer in its LS state were optimized using different XC functionals. The C–C distance between the central carbons of the two monomers in the dimer geometry were compared with the value in the experimental crystal structure (3.201 Å).^{S52} This was chosen as the most important structural parameter as the radical–radical exchange interaction is usually extremely sensitive to the distance between the radicals. The calculated dimerization enthalpies were also compared to those measured experimentally in solution. The enthalpy has been determined both from UV-Vis measurements ($-31.4 \text{ kJ mol}^{-1}$, $-36.8 \text{ kJ mol}^{-1}$)^{S55,S56} and from the EPR spectrum ($-39.9 \text{ kJ mol}^{-1}$).^{S56} The calculated values are listed in Table S2. Only the M06 and M06-2X functionals are able to produce reasonable estimates of the central C–C distance without the inclusion of some dispersion correction. In the case of all other functionals, the dimer dissociates if dispersion is not corrected for. The best estimate of the C–C distance is provided with the B3LYP-D3 functional, and the functionals LC- ω PBE-D3, LC- ω PBE-D3BJ, M06-2X, M06-2X-D3, PBE0-D3, and PBE0-D3BJ all give an error of less than 0.01 Å.

The calculated dimerization enthalpies are either overbinding, or repulsive in the case of dimers which dissociate. The closest estimate to the experimental values is obtained with CAM-B3LYP-D3 (with an overestimated C–C distance) and the M06-2X functional. In both cases, the magnitude of the dimerization enthalpy is still nearly double the experimental values. The large deviations could result from solvent interactions not accounted for in the calculations. Preliminary calculations were carried out using a polarizable continuum model to account for electrostatic solvent interactions, but no significant differences in the results was observed. This does not, however, rule out the possibility of stabilizing non-electrostatic solvent interactions. Based on these observations, the ability of the chosen XC functional to correctly predict the geometry was made the main criteria, and in the final calculations the dimerization enthalpy was calculated using DLPNO-CCSD(T) energies evaluated on the DFT optimized geometries. This approach should considerably reduce the dependence of

Table S2: Dimerization energies (ΔE_{LS}), enthalpies (ΔH_{LS}), and central C–C distances calculated for **2–2** using various XC functionals

XC	$\Delta E_{\text{LS}} / \text{kJ mol}^{-1}$	$\Delta H_{\text{LS}} / \text{kJ mol}^{-1}$	$d(\text{C–C}) / \text{\AA}$
B3LYP	12.9	14.2	6.897
B3LYP-D3	−90.8	−77.6	3.151
B3LYP-D3BJ	−101.2	−87.6	3.082
PBE0	−0.5	3.8	4.945
PBE0-D3	−88.9	−81.3	3.270
PBE0-D3BJ	−89.7	−80.2	3.137
M06	−95.0	−88.7	3.313
M06-D3	−149.7	−142.5	3.310
M06-2X	−83.0	−74.0	3.127
M06-2X-D3	−107.6	−98.4	3.127
LC- ω PBE	−2.8	2.2	8.223
LC- ω PBE-D3	−90.1	−82.7	3.299
LC- ω PBE-D3BJ	−99.0	−91.7	3.276
CAM-B3LYP	0.3	−4.7	9.997
CAM-B3LYP-D3	−81.5	−73.3	3.446
CAM-B3LYP-D3BJ	−89.0	−81.0	3.450
ω B97XD	−115.1	−105.5	3.310
Experimental		−31.4 ^{S55} −36.8 ^{S56} −39.9 ^{S56}	3.201 ^{S52}

the calculated dimerization enthalpies on the choice of the XC functional. See the main text for results.

It is worth noting here that Kertesz and co-workers have optimized the geometry of **2–2** using the M05-2X functional without any dispersion correction and obtained a dimerization energy (including zero point and counterpoise corrections) of $-32.9 \text{ kJ mol}^{-1}$ and a central C–C distance of $3.209 \text{ \AA}$, both in very good agreement with experiments.^{S57} In the present work, the dimerization energy calculated using the M06-2X functional (which is an improved version of M05-2X) without any dispersion correction is $-83.0 \text{ kJ mol}^{-1}$ (the respective enthalpy is $-74.0 \text{ kJ mol}^{-1}$). Thus, the value presented here is considerably larger than that calculated by Kertesz and co-workers. We own these differences to the use of spin-projection in our calculations and the larger basis sets. In the present work, initial calculations were carried out using the smaller def2-SVP^{S58} and TZVP^{S59} basis sets but after observing con-

siderable deviations between the results, all DFT data were re-calculated using the larger def2-TZVP basis.

Additional computational data

Table S3: Energies and enthalpy corrections (E and H , in Hartree atomic units), and $\langle S^2 \rangle$ values calculated for **2-2**, **3-3**, and **2-3**

	2-2	3-3	2-3
LS geometry			
$E_{\text{LS}}^{\text{LS}}(\text{DFT})^{\text{a}}$	-1944.650240	-2243.058829	-2093.858540
$E_{\text{HS}}^{\text{LS}}(\text{DFT})^{\text{a}}$	-1944.644802	-2243.058659	-2093.859392
$E_{\text{HS}}^{\text{LS}}(\text{DLPNO-CCSD(T)})$	-1940.526288	-2238.617297	-2089.579782
$H_{\text{LS}}^{\text{LS}}(\text{DFT})^{\text{a}}$	1.093329	1.070045	1.081731
$E_{\text{BSSE}}^{\text{LS}}(\text{DLPNO-CCSD(T)})$	0.010379	0.009709	0.010079
$\langle S^2 \rangle_{\text{LS}}^{\text{HS}}$	1.3553	1.3435	1.3937
$\langle S^2 \rangle_{\text{HS}}^{\text{HS}}$	2.4701	2.3405	2.4039
HS geometry			
$E_{\text{LS}}^{\text{HS}}(\text{DFT})^{\text{a}}$	-1944.648543	-2243.058788	-2093.858461
$E_{\text{HS}}^{\text{HS}}(\text{DFT})^{\text{a}}$	-1944.647337	-2243.058714	-2093.859463
$E_{\text{HS}}^{\text{HS}}(\text{DLPNO-CCSD(T)})$	-1940.528111	-2238.617177	-2089.580230
$H_{\text{HS}}^{\text{HS}}(\text{DFT})^{\text{a}}$	1.092880	1.070043	1.081750
$E_{\text{BSSE}}^{\text{HS}}(\text{DLPNO-CCSD(T)})$	0.008257	0.009716	0.010172
$\langle S^2 \rangle_{\text{LS}}^{\text{HS}}$	1.4404	1.3442	1.3933
$\langle S^2 \rangle_{\text{HS}}^{\text{HS}}$	2.4673	2.3414	2.4052

^{a)} Calculated using the LC- ω PBE-D3BJ XC functional

Table S4: Energies (in Hartree atomic units) calculated for **2** and **3**

	2	3
$E(\text{DFT})^{\text{a}}$	-972.307698	-1121.511776
$E(\text{DLPNO-CCSD(T)})$	-970.248315	-1119.291422
$H(\text{DFT})^{\text{a}}$	0.545275	0.533765

^{a)} Calculated using the LC- ω PBE-D3BJ XC functional

Table S5: Energies and enthalpy corrections (E and H , in Hartree atomic units), and $\langle S^2 \rangle$ values calculated for **2–2** and **4–4** in their crystal structure geometries using various XC functionals

XC	$E_{\text{LS}}^{\text{crystal}}(\text{DFT})$	$E_{\text{HS}}^{\text{crystal}}(\text{DFT})$	$\langle S^2 \rangle_{\text{LS}}^{\text{crystal}}$	$\langle S^2 \rangle_{\text{HS}}^{\text{crystal}}$
2–2				
B3LYP	−1945.754315	−1945.740176	0.4020	2.0935
PBE0	−1943.381490	−1943.369383	0.6382	2.1435
M06	−1944.252509	−1944.239857	0.6788	2.1451
M06-2X	−1944.905419	−1944.891334	0.6339	2.0924
LC- ω PBE	−1944.403151	−1944.395932	1.3349	2.4853
CAM-B3LYP	−1944.590798	−1944.581052	0.9348	2.2221
ω B97XD	−1945.192345	−1945.182322	0.9094	2.1919
4–4				
B3LYP	−7539.160914	−7539.160243	1.0531	2.0820
PBE0	−7535.690216	−7535.689597	1.1046	2.1249
M06	−7537.200285	−7537.199698	1.0891	2.1165
M06-2X	−7538.217784	−7538.217069	1.0955	2.1114
LC- ω PBE	−7536.683748	−7536.683139	1.3910	2.3927
CAM-B3LYP	−7538.052669	−7538.052087	1.1861	2.1960
ω B97XD	−7538.489959	−7538.489391	1.1675	2.1768

Table S6: Energies and enthalpy corrections (E and H , in Hartree atomic units), and $\langle S^2 \rangle$ values calculated for **2–2** using various XC functionals

XC	$E_{\text{LS}}^{\text{LS}}(\text{DFT})$	$E_{\text{HS}}^{\text{LS}}(\text{DFT})$	$H_{\text{LS}}^{\text{LS}}$	$E_{\text{BSSE}}^{\text{LS}}$	$\langle S^2 \rangle_{\text{LS}}^{\text{LS}}$	$\langle S^2 \rangle_{\text{HS}}^{\text{LS}}$
B3LYP	−1945.830818	−1945.830818	1.0747	0.000147	1.0933	2.0933
B3LYP-D3	−1945.999746	−1945.978884	1.0819	0.001670	0.0696	2.0962
B3LYP-D3BJ	−1946.133303	−1946.107783	1.0811	0.001730	0.0000	2.0958
PBE0	−1943.446094	−1943.446045	1.0798	0.000456	1.1383	2.1401
PBE0-D3	−1943.556615	−1943.545929	1.0825	0.001286	0.6984	2.1433
PBE0-D3BJ	−1943.615271	−1943.598315	1.0826	0.001496	0.4314	2.1437
M06	−1944.306631	−1944.296185	1.0761	0.004247	0.7677	2.1461
M06-D3	−1944.350051	−1944.339110	1.0765	0.004250	0.7477	2.1464
M06-2X	−1944.962426	−1944.943044	1.0866	0.001889	0.4278	2.0926
M06-2X-D3	−1944.979803	−1944.960358	1.0866	0.001891	0.4253	2.0925
LC- ω PBE	−1944.467966	−1944.467966	1.0916	0.000000	1.4679	2.4679
LC- ω PBE-D3	−1944.593443	−1944.588356	1.0945	0.001429	1.3644	2.4718
LC- ω PBE-D3BJ	−1944.650240	−1944.644806	1.0933	0.001443	1.3554	2.4701
CAM-B3LYP	−1944.656812	−1944.656812	1.0823	0.000008	1.2144	2.2144
CAM-B3LYP-D3	−1944.775175	−1944.770334	1.0893	0.001342	1.0774	2.2173
CAM-B3LYP-D3BJ	−1944.814095	−1944.809359	1.0879	0.001326	1.0799	2.2166
ω B97XD	−1945.251336	−1945.243474	1.0869	0.001429	0.9698	2.1901

Table S7: Energies and enthalpy corrections (E and H , in Hartree atomic units), calculated for **2** using various XC functionals

XC	$E(\text{DFT})$	H
B3LYP	−972.917786	0.537138
B3LYP-D3	−972.981600	0.538476
B3LYP-D3BJ	−973.045923	0.537974
PBE0	−971.722741	0.539091
PBE0-D3	−971.762791	0.539812
PBE0-D3BJ	−971.791225	0.539493
M06	−972.135464	0.536891
M06-D3	−972.146743	0.536898
M06-2X	−972.466415	0.541605
M06-2X-D3	−972.470413	0.541603
LC- ω PBE	−972.233455	0.544864
LC- ω PBE-D3	−972.280897	0.545867
LC- ω PBE-D3BJ	−972.307698	0.545273
CAM-B3LYP	−972.328468	0.542126
CAM-B3LYP-D3	−972.373221	0.543099
CAM-B3LYP-D3BJ	−972.391226	0.542465
ω B97XD	−972.605544	0.541658

Optimized Cartesian coordinates

Final calculations

Monomer 2

C	0.01726700	-0.01770300	0.00000000
C	1.01935500	0.97305800	0.00000000
C	0.63583900	2.33207600	0.00000000
C	-0.69242700	2.71545800	0.00000000
C	-1.66859800	1.72362400	0.00000000
C	-1.34411300	0.35634000	0.00000000
C	-2.32034600	-0.65239300	0.00000000
C	-1.98722900	-2.00293000	0.00000000
C	-0.64841400	-2.35032000	0.00000000
C	0.37264400	-1.37830100	0.00000000
C	1.73730500	-1.72609400	0.00000000
C	2.73425300	-0.76783500	0.00000000
C	2.36238100	0.57301900	0.00000000
C	-1.12085800	4.17761500	0.00000000
C	-3.10134000	-3.04222300	0.00000000
C	4.21469900	-1.12761400	0.00000000
C	-1.95721700	4.45741800	-1.24766000
C	-1.95721600	4.45741800	1.24766000
C	0.06867800	5.12775300	0.00000000
C	-3.96354700	-2.85643700	1.24763200
C	-3.96354700	-2.85643700	-1.24763200
C	-2.56260000	-4.46611500	0.00000000
C	4.87510100	-0.54297000	1.24761800
C	4.87510100	-0.54297000	-1.24761800
C	4.44297600	-2.63278900	0.00000000
H	1.98694000	-2.77911100	0.00000000
H	3.12201200	1.34654200	0.00000000
H	1.42283800	3.07475400	0.00000000
H	-2.71812500	1.99502000	0.00000000
H	-3.36144400	-0.35010900	0.00000000
H	-0.35045200	-3.39064200	0.00000000
H	4.01486600	-3.10527300	0.88558500
H	4.01486600	-3.10527400	-0.88558500
H	5.51470100	-2.83761700	0.00000000
H	4.41422000	-0.94291200	2.15224400
H	4.41422000	-0.94291200	-2.15224400
H	5.93783900	-0.79346900	1.26450800
H	5.93783900	-0.79346900	-1.26450800
H	4.78644600	0.54309700	-1.27863200

H	4.78644600	0.54309800	1.27863100
H	0.69186900	4.99326400	0.88562300
H	-0.28975600	6.15831800	0.00000000
H	0.69186900	4.99326400	-0.88562300
H	-1.38054000	4.25779200	2.15225900
H	-2.27102000	5.50320300	1.26469400
H	-2.85382600	3.83816400	1.27859800
H	-2.85382600	3.83816400	-1.27859800
H	-2.27102100	5.50320300	-1.26469400
H	-1.38054100	4.25779200	-2.15225900
H	-4.41897200	-1.86648300	-1.27858700
H	-3.36572900	-2.97882100	-2.15225800
H	-4.76683600	-3.59595400	-1.26466500
H	-4.41897200	-1.86648300	1.27858700
H	-4.76683600	-3.59595400	1.26466500
H	-3.36572900	-2.97882100	2.15225800
H	-3.39643900	-5.16985800	0.00000000
H	-1.95789700	-4.66819000	0.88559200
H	-1.95789700	-4.66819000	-0.88559200

Monomer 3

C	0.01235200	0.01504900	-0.00000200
C	1.16472200	0.79199000	0.00000000
C	1.06353500	2.17372800	0.00000100
C	-0.16814800	2.80850200	0.00000000
C	-1.31094400	2.01284500	-0.00000100
C	-1.23567700	0.63639500	-0.00000100
C	-2.47601300	-0.17282800	0.00000000
C	-2.33543900	-1.64635100	-0.00000200
C	-1.08184700	-2.17534300	-0.00000400
C	0.10390300	-1.40448800	-0.00000300
C	1.37804400	-2.01641200	-0.00000300
C	2.55195700	-1.32804200	-0.00000100
C	2.49867500	0.15093300	0.00000200
C	-0.31304600	4.32254100	-0.00000100
C	-3.58281200	-2.50951100	0.00000000
C	3.90126100	-2.02105700	0.00000000
C	-1.08464800	4.75001300	-1.24782100
C	-1.08465200	4.75001500	1.24781500
C	1.03633200	5.02653200	0.00000000
C	-4.41168500	-2.21926800	1.25356100
C	-4.41170700	-2.21924400	-1.25354000
C	-3.23916000	-3.99397800	-0.00001700
C	4.68527200	-1.62518400	1.25351700

C	4.68527600	-1.62517800	-1.25351300
C	3.75416500	-3.53769500	-0.00000500
H	1.39322700	-3.09902200	-0.00000500
H	1.98810300	2.73457000	0.00000200
H	-2.29977300	2.45478700	-0.00000100
H	-0.95656200	-3.25082000	-0.00000500
H	3.22952600	-3.89718900	0.88730200
H	3.22952700	-3.89718400	-0.88731300
H	4.74683800	-3.98904100	-0.00000600
H	4.13679800	-1.90359300	2.15565900
H	4.13680600	-1.90358200	-2.15565800
H	5.64111700	-2.15241800	1.26492700
H	5.64112200	-2.15241000	-1.26492100
H	4.88010300	-0.55621800	-1.27837900
H	4.88009900	-0.55622500	1.27838900
H	1.62330200	4.77519300	0.88485400
H	0.88165300	6.10636600	-0.00000100
H	1.62330500	4.77519100	-0.88485100
H	-0.55422900	4.45101000	2.15336100
H	-1.20096200	5.83531900	1.26258200
H	-2.08018000	4.30655300	1.27826200
H	-2.08017600	4.30655100	-1.27827100
H	-1.20095700	5.83531700	-1.26259000
H	-0.55422100	4.45100700	-2.15336400
H	-4.74431800	-1.18483300	-1.27863200
H	-3.83162000	-2.42387200	-2.15565300
H	-5.29068100	-2.86655800	-1.26492100
H	-4.74429300	-1.18485600	1.27868000
H	-5.29066000	-2.86658000	1.26494300
H	-3.83158200	-2.42391700	2.15565800
H	-4.16448400	-4.57092200	-0.00001500
H	-2.67211200	-4.28197100	0.88728900
H	-2.67212800	-4.28195300	-0.88734000
O	-3.56281100	0.37901200	0.00000800
O	3.50519800	0.83942700	0.00000800

Dimer **2–2** in LS state

C	-0.11590100	0.18086900	1.62382700
C	-1.06429500	-0.86062900	1.64232500
C	-0.60905200	-2.19168000	1.74040800
C	0.73472300	-2.49884600	1.83675000
C	1.65802500	-1.46052800	1.77504500
C	1.26341700	-0.11563900	1.67633700
C	2.18174300	0.94815500	1.68428200

C	1.77174100	2.27717700	1.67443100
C	0.41700200	2.54591100	1.60946300
C	-0.54600500	1.51870700	1.59131800
C	-1.92601900	1.79064200	1.59849800
C	-2.87157900	0.78289300	1.62773900
C	-2.42848500	-0.53491900	1.62044400
C	1.22523100	-3.92374800	2.06610600
C	2.81225300	3.38748300	1.77284800
C	-4.36627300	1.07779200	1.68684400
C	2.20840500	-4.32904500	0.97292300
C	1.92825500	-3.98349000	3.42194900
C	0.08465800	-4.93154400	2.07317000
C	3.64013700	3.18613200	3.04144100
C	3.73444400	3.34379500	0.55835100
C	2.17737300	4.76967100	1.83805200
C	-4.98805200	0.33330500	2.86741200
C	-5.02733100	0.61128000	0.39312800
C	-4.65431200	2.56244300	1.86495100
C	0.11590400	-0.18086700	-1.62382600
C	1.06429700	0.86063200	-1.64232400
C	0.60905200	2.19168300	-1.74040200
C	-0.73472500	2.49884700	-1.83674000
C	-1.65802400	1.46052700	-1.77503800
C	-1.26341500	0.11563900	-1.67633100
C	-2.18174100	-0.94815600	-1.68427400
C	-1.77173800	-2.27717800	-1.67442600
C	-0.41699900	-2.54591000	-1.60946400
C	0.54600700	-1.51870500	-1.59132000
C	1.92602000	-1.79064000	-1.59850800
C	2.87157900	-0.78289000	-1.62775200
C	2.42848700	0.53492200	-1.62045100
C	-1.22523700	3.92374700	-2.06609100
C	-2.81225100	-3.38748300	-1.77283900
C	4.36627300	-1.07779200	-1.68686900
C	-2.20841400	4.32903900	-0.97290900
C	-1.92825300	3.98349300	-3.42193800
C	-0.08466500	4.93154400	-2.07314100
C	-3.64016200	-3.18611600	-3.04141200
C	-3.73442000	-3.34381300	-0.55832600
C	-2.17736700	-4.76966900	-1.83807600
C	4.98804500	-0.33330100	-2.86743800
C	5.02734200	-0.61129300	-0.39315400
C	4.65430500	-2.56244300	-1.86499000
H	-2.23244000	2.82690500	1.61247100
H	-2.71822200	1.67334800	-1.84380300

H	-3.23669800	-0.70526300	-1.73110900
H	-3.14314800	-1.34880800	1.63484200
H	-1.35445300	-2.97408100	1.77654900
H	-0.05952200	-3.56706300	-1.60241700
H	2.23244300	-2.82690200	-1.61247600
H	2.71822300	-1.67335000	1.84380800
H	3.23670000	0.70526400	1.73112600
H	3.14315400	1.34880800	-1.63485500
H	1.35445000	2.97408700	-1.77654000
H	0.05952900	3.56706500	1.60240200
H	-1.24967300	3.68227400	-4.22149600
H	-2.27232100	4.99973600	-3.62636000
H	-2.79422700	3.32159700	-3.45136400
H	-1.71473300	4.35265800	-0.00140400
H	-3.04615800	3.63524600	-0.90936300
H	-2.60911100	5.32424600	-1.17617800
H	-0.48587300	5.93606400	-2.21686400
H	0.46152500	4.92182900	-1.12870500
H	0.62156900	4.73711000	-2.88161500
H	-4.20309500	2.95066100	2.77951500
H	-4.28778700	3.15207200	1.02414800
H	-5.73237700	2.71767100	1.93134500
H	-4.51445400	0.63096000	3.80420700
H	-4.61102700	1.13948100	-0.46574300
H	-6.05417000	0.55984300	2.93459600
H	-6.10224800	0.80132900	0.42360300
H	-4.87752600	-0.45657800	0.23883700
H	-4.88389300	-0.74682400	2.76708000
H	-4.23750800	-2.38125700	-0.47817900
H	-3.17150100	-3.51052100	0.36071800
H	-4.49976800	-4.11889000	-0.63498100
H	-4.37794200	-3.98509900	-3.14121000
H	-4.17521100	-2.23662900	-3.02677800
H	-3.00039800	-3.19681000	-3.92519900
H	-1.59797200	-4.99092600	-0.94075500
H	-1.52257000	-4.87131300	-2.70487300
H	-2.95999800	-5.52555000	-1.92032400
H	-0.62156800	-4.73710200	2.88164800
H	0.48586800	-5.93606200	2.21690100
H	-0.46154300	-4.92184200	1.12874000
H	1.24967800	-3.68227200	4.22151000
H	2.27232700	-4.99973200	3.62637100
H	2.79422700	-3.32159100	3.45137000
H	3.04616100	-3.63526600	0.90939100
H	2.60908400	-5.32426200	1.17618300

H	1.71473100	-4.35264200	0.00141400
H	4.28776900	-3.15207900	-1.02419800
H	4.20309300	-2.95064800	-2.77956200
H	5.73237000	-2.71767600	-1.93137700
H	6.05416000	-0.55984800	-2.93463700
H	6.10226000	-0.80133000	-0.42364600
H	4.87752600	0.45656000	-0.23884400
H	4.88389600	0.74682700	-2.76709900
H	4.61105400	-1.13951400	0.46571200
H	4.51443400	-0.63094600	-3.80423000
H	4.23754500	2.38124300	0.47823200
H	3.17153500	3.51047600	-0.36070400
H	4.49978200	4.11888100	0.63500100
H	4.17517800	2.23663900	3.02683500
H	4.37792100	3.98511000	3.14124200
H	3.00035300	3.19684600	3.92521300
H	2.96000500	5.52555000	1.92030600
H	1.52255800	4.87133200	2.70483400
H	1.59799900	4.99091800	0.94071500

Dimer **2–2** in HS state

C	-0.56460900	0.32508300	1.65531700
C	-0.81012100	-1.06039200	1.71455100
C	0.27181800	-1.93499600	1.94359900
C	1.56207200	-1.47240400	2.11631900
C	1.79605300	-0.10656600	1.99455100
C	0.75562700	0.81075700	1.76905000
C	0.97063400	2.19596400	1.70199900
C	-0.07784900	3.10018400	1.57090100
C	-1.36756000	2.60696200	1.48761200
C	-1.63769200	1.22385900	1.52089500
C	-2.94710700	0.71160500	1.45086500
C	-3.20230700	-0.64705700	1.46631700
C	-2.12748100	-1.51986800	1.59074400
C	2.70583400	-2.39901000	2.51128600
C	0.22968600	4.59284400	1.55170100
C	-4.61183300	-1.21493000	1.35674700
C	3.87524900	-2.25383500	1.54438200
C	3.16526900	-2.01873400	3.91863400
C	2.28251400	-3.86105400	2.51910900
C	0.96297400	4.97174000	2.83779100
C	1.11762300	4.91371200	0.35156600
C	-1.02978000	5.44261700	1.45741100
C	-4.90083600	-2.10597400	2.56357800

C	-4.71357000	-2.04490600	0.07843300
C	-5.67288100	-0.12430800	1.30772600
C	0.56461100	-0.32508100	-1.65532100
C	0.81012000	1.06039400	-1.71455800
C	-0.27182000	1.93499500	-1.94361000
C	-1.56207300	1.47240000	-2.11633300
C	-1.79605000	0.10656100	-1.99456500
C	-0.75562300	-0.81075900	-1.76905900
C	-0.97062700	-2.19596700	-1.70201000
C	0.07785600	-3.10018500	-1.57090300
C	1.36756500	-2.60695900	-1.48760300
C	1.63769500	-1.22385600	-1.52088900
C	2.94710800	-0.71159900	-1.45085200
C	3.20230500	0.64706400	-1.46631200
C	2.12747800	1.51987300	-1.59074900
C	-2.70584100	2.39900100	-2.51129400
C	-0.22967700	-4.59284500	-1.55170400
C	4.61183000	1.21493900	-1.35673500
C	-3.87523600	2.25382900	-1.54436500
C	-3.16530100	2.01871600	-3.91863000
C	-2.28252300	3.86104500	-2.51913400
C	-0.96297000	-4.97174300	-2.83779100
C	-1.11761200	-4.91371400	-0.35156700
C	1.02979100	-5.44261600	-1.45742200
C	4.90084400	2.10597200	-2.56357100
C	4.71355100	2.04492700	-0.07842700
C	5.67287800	0.12431900	-1.30769400
H	-3.76216900	1.41869100	1.38327000
H	-2.79910900	-0.28592000	-2.11129700
H	-1.99177400	-2.55258500	-1.77304900
H	-2.29396800	-2.59063500	1.61323400
H	0.05277500	-2.99102200	2.01439800
H	2.20877500	-3.28244900	-1.40085700
H	3.76217100	-1.41868100	-1.38324500
H	2.79911300	0.28591200	2.11128100
H	1.99178100	2.55258400	1.77303300
H	2.29396500	2.59063900	-1.61324200
H	-0.05278000	2.99102200	-2.01441100
H	-2.20876900	3.28245500	1.40087500
H	-2.34063500	2.09822400	-4.62869900
H	-3.96892400	2.68128600	-4.24751600
H	-3.53675100	0.99388800	-3.95080400
H	-3.58934400	2.58909300	-0.54862000
H	-4.21145000	1.22039900	-1.46626000
H	-4.71913700	2.85879400	-1.88240100

H	-3.13981700	4.48858800	-2.76803800
H	-1.91278300	4.16992000	-1.54006400
H	-1.50438400	4.05442000	-3.25892300
H	-5.65602800	0.49130300	2.20856500
H	-5.54446400	0.52800400	0.44303500
H	-6.66122800	-0.58100100	1.23474700
H	-4.81438100	-1.53830300	3.49136400
H	-4.52594200	-1.42477500	-0.79954000
H	-5.91400100	-2.50855500	2.50075400
H	-5.71122600	-2.47857100	-0.01654900
H	-3.98936200	-2.85995800	0.07550500
H	-4.21035000	-2.94736400	2.62000000
H	-2.04426400	-4.34015700	-0.37713200
H	-0.60327600	-4.68243100	0.58192300
H	-1.37694700	-5.97439100	-0.34412400
H	-1.17660300	-6.04264900	-2.84881400
H	-1.90992800	-4.44048400	-2.93317900
H	-0.35556700	-4.73376700	-3.71240200
H	1.58916200	-5.23902500	-0.54333900
H	1.69075300	-5.27639700	-2.30951800
H	0.75641800	-6.49895000	-1.44908000
H	1.50437500	-4.05443700	3.25889600
H	3.13980700	-4.48860000	2.76800700
H	1.91277300	-4.16992000	1.54003600
H	2.34058700	-2.09824100	4.62868500
H	3.96888100	-2.68131100	4.24753300
H	3.53672200	-0.99390800	3.95081800
H	4.21146200	-1.22040300	1.46628200
H	4.71914500	-2.85879400	1.88244200
H	3.58938700	-2.58910600	0.54863200
H	5.54446200	-0.52797600	-0.44299000
H	5.65602600	-0.49130900	-2.20852100
H	6.66122500	0.58101500	-1.23472300
H	5.91400400	2.50856500	-2.50073500
H	5.71121300	2.47857400	0.01657600
H	3.98935900	2.85999300	-0.07552500
H	4.21034900	2.94735400	-2.62001600
H	4.52588800	1.42480800	0.79954700
H	4.81441000	1.53829000	-3.49135200
H	2.04427900	4.34016200	0.37713400
H	0.60329000	4.68242300	-0.58192400
H	1.37695200	5.97439100	0.34411900
H	1.90993000	4.44047700	2.93318200
H	1.17660900	6.04264600	2.84881700
H	0.35556700	4.73376400	3.71239900

H	-0.75640400	6.49895100	1.44906800
H	-1.69074600	5.27640400	2.30950600
H	-1.58914800	5.23902300	0.54332700

Dimer **3–3** in LS state

C	-0.88209700	-0.25767300	1.54484900
C	-2.11882900	-0.86470400	1.36395300
C	-2.20283600	-2.24682900	1.31277600
C	-1.07489000	-3.04545600	1.41821300
C	0.15144000	-2.41746300	1.61661900
C	0.25708400	-1.04545600	1.69757300
C	1.56247400	-0.42034900	2.00996900
C	1.59327400	1.04393300	2.20352300
C	0.45836600	1.74834500	1.94211500
C	-0.78215100	1.15938000	1.61368100
C	-1.93968200	1.94505400	1.41625600
C	-3.18759000	1.43004800	1.25001200
C	-3.34790700	-0.03960900	1.30010400
C	-1.13579000	-4.56532100	1.37714400
C	2.84545000	1.70106700	2.75476400
C	-4.41310100	2.31083200	1.09667400
C	-0.23666300	-5.08254100	0.25575400
C	-0.63966000	-5.11504400	2.71419300
C	-2.54973200	-5.07540000	1.13851000
C	3.12744800	1.10914800	4.13872900
C	4.05154300	1.47343100	1.84694400
C	2.66133300	3.20479400	2.91250600
C	-5.28387400	2.17454200	2.34821100
C	-5.21850400	1.91045700	-0.14061000
C	-4.02580400	3.77628200	0.93967800
C	0.88209600	0.25767400	-1.54485000
C	2.11882600	0.86470700	-1.36394900
C	2.20283000	2.24683100	-1.31276900
C	1.07488300	3.04545700	-1.41821000
C	-0.15144400	2.41746200	-1.61662300
C	-0.25708600	1.04545500	-1.69757900
C	-1.56247300	0.42034600	-2.00998500
C	-1.59327100	-1.04393800	-2.20352600
C	-0.45836300	-1.74834700	-1.94211400
C	0.78215300	-1.15937900	-1.61368200
C	1.93968600	-1.94505100	-1.41625800
C	3.18759300	-1.43004300	-1.25001300
C	3.34790600	0.03961500	-1.30009600
C	1.13578000	4.56532200	-1.37713500

C	-2.84544800	-1.70107800	-2.75475900
C	4.41310800	-2.31082300	-1.09668400
C	0.23664800	5.08253700	-0.25574700
C	0.63965500	5.11504900	-2.71418400
C	2.54972100	5.07540200	-1.13849300
C	-3.12744400	-1.10918200	-4.13873400
C	-4.05154000	-1.47342500	-1.84694200
C	-2.66133400	-3.20480800	-2.91247400
C	5.28387400	-2.17452100	-2.34822400
C	5.21851900	-1.91045500	0.14059700
C	4.02581800	-3.77627700	-0.93969600
H	-1.79891300	3.01819400	1.42373600
H	-1.06228200	2.99126300	-1.73741700
H	-3.18847000	-2.67775900	1.20281900
H	-0.46633200	-2.82571700	-2.03583400
H	1.79892000	-3.01819100	-1.42374000
H	1.06227700	-2.99126500	1.73740800
H	3.18846300	2.67776300	-1.20280600
H	0.46633600	2.82571400	2.03584100
H	1.25771600	4.74980700	-3.53574500
H	0.68340600	6.20583500	-2.71148300
H	-0.39143300	4.82091900	-2.91214400
H	0.59080400	4.73886200	0.71702600
H	-0.79479200	4.75158200	-0.38000600
H	0.23798700	6.17389900	-0.24689100
H	2.54083700	6.16536100	-1.09530700
H	2.95993600	4.70868100	-0.19616400
H	3.22574500	4.78104900	-1.94251700
H	-3.52077400	4.16879400	1.82420900
H	-3.38357400	3.92743300	0.06961200
H	-4.92992700	4.36751700	0.79153600
H	-4.72914500	2.46921100	3.24140100
H	-4.60644000	1.98269400	-1.03965400
H	-6.15358300	2.82849000	2.25878100
H	-6.06835400	2.58749900	-0.24683300
H	-5.59824400	0.89593100	-0.05472200
H	-5.63253300	1.15201800	2.47378700
H	-4.25483900	-0.41648700	-1.70830600
H	-3.89961700	-1.92623200	-0.86867800
H	-4.93158800	-1.93746600	-2.29647700
H	-3.99501500	-1.60646100	-4.57635100
H	-3.33898000	-0.04406600	-4.07552200
H	-2.27763100	-1.25996500	-4.80762500
H	-2.46341200	-3.68695300	-1.95343400
H	-1.85221700	-3.45150500	-3.60250300

H	-3.58020800	-3.63441100	-3.31255500
H	-3.22575300	-4.78104200	1.94253500
H	-2.54085000	-6.16535900	1.09532800
H	-2.95995100	-4.70868200	0.19618100
H	-1.25771700	-4.74979700	3.53575500
H	-0.68341400	-6.20583000	2.71149600
H	0.39142900	-4.82091700	2.91214700
H	0.79477800	-4.75158800	0.38000800
H	-0.23800300	-6.17390400	0.24690200
H	-0.59082200	-4.73887000	-0.71701900
H	3.38359100	-3.92743500	-0.06962900
H	3.52078500	-4.16878500	-1.82422800
H	4.92994300	-4.36750900	-0.79156100
H	6.15358700	-2.82846600	-2.25880300
H	6.06837100	-2.58749500	0.24680900
H	5.59825500	-0.89592700	0.05471300
H	5.63252700	-1.15199500	-2.47379500
H	4.60646300	-1.98269900	1.03964600
H	4.72914100	-2.46918700	-3.24141400
H	4.25483800	0.41649700	1.70828100
H	3.89962600	1.92626500	0.86869100
H	4.93159200	1.93745700	2.29649400
H	3.33898900	0.04403300	4.07549800
H	3.99501700	1.60642200	4.57635600
H	2.27763400	1.25991500	4.80762200
H	3.58020600	3.63439100	3.31259400
H	1.85221500	3.45147700	3.60253900
H	2.46341000	3.68695600	1.95347400
O	2.55597300	-1.11869400	2.12680400
O	4.44113400	0.57837600	-1.31670200
O	-2.55596900	1.11869100	-2.12684100
O	-4.44113600	-0.57836600	1.31672000

Dimer **3–3** in HS state

C	-0.83449300	-0.23661900	1.56928900
C	-2.05573300	-0.87673400	1.39885000
C	-2.10478500	-2.26110500	1.36058200
C	-0.95676300	-3.02957100	1.46846200
C	0.25450800	-2.36826100	1.65314600
C	0.32539500	-0.99372500	1.72311200
C	1.61557500	-0.33325900	2.02507900
C	1.61180200	1.13406200	2.19608700
C	0.45634000	1.80645700	1.93913500
C	-0.77109100	1.18309900	1.62713900

C	-1.95032500	1.93682800	1.43089200
C	-3.18493700	1.38829000	1.27472600
C	-3.30623000	-0.08473600	1.33404300
C	-0.98006300	-4.55093100	1.44785200
C	2.85512900	1.83058400	2.71783500
C	-4.43447500	2.23498600	1.12288800
C	-0.08021000	-5.06132100	0.32415100
C	-0.45643300	-5.06983100	2.78681600
C	-2.38331100	-5.09922400	1.23207000
C	3.17281700	1.27210500	4.10789500
C	4.05131100	1.61378400	1.79407400
C	2.63749400	3.33226400	2.85090400
C	-5.29505600	2.08247500	2.37957900
C	-5.23476700	1.80581600	-0.10808000
C	-4.08781100	3.70949500	0.95624900
C	0.83449200	0.23662100	-1.56929100
C	2.05573200	0.87673400	-1.39884900
C	2.10478700	2.26110500	-1.36057600
C	0.95676600	3.02957200	-1.46845700
C	-0.25450500	2.36826500	-1.65315100
C	-0.32539400	0.99372900	-1.72312000
C	-1.61557200	0.33326600	-2.02510400
C	-1.61180500	-1.13405800	-2.19608500
C	-0.45634400	-1.80645400	-1.93912800
C	0.77108900	-1.18309700	-1.62713900
C	1.95032200	-1.93682700	-1.43089000
C	3.18493500	-1.38829100	-1.27473000
C	3.30623000	0.08473400	-1.33405200
C	0.98006800	4.55093200	-1.44783800
C	-2.85513700	-1.83058600	-2.71781200
C	4.43447500	-2.23498800	-1.12290500
C	0.08020100	5.06131900	-0.32414700
C	0.45645800	5.06983900	-2.78680700
C	2.38331500	5.09922100	-1.23203400
C	-3.17283700	-1.27214300	-4.10788400
C	-4.05130400	-1.61375700	-1.79403900
C	-2.63750900	-3.33227000	-2.85084300
C	5.29502700	-2.08248800	-2.37961700
C	5.23480000	-1.80581200	0.10803800
C	4.08781100	-3.70949500	-0.95624600
H	-1.83788200	3.01332000	1.43075600
H	-1.18033000	2.91757800	-1.77404600
H	-3.07972100	-2.71779700	1.26007100
H	-0.43786600	-2.88453400	-2.02197900
H	1.83787700	-3.01331900	-1.43075000

H	1.18033500	-2.91757100	1.77403500
H	3.07972400	2.71779400	-1.26006000
H	0.43785800	2.88453600	2.02199400
H	1.07413500	4.70783800	-3.61008800
H	0.47433700	6.16127800	-2.79954700
H	-0.56943400	4.74885900	-2.96933200
H	0.45461800	4.74241100	0.64941000
H	-0.94311800	4.70068800	-0.43137800
H	0.05211800	6.15232500	-0.33199900
H	2.34772000	6.18913500	-1.20436800
H	2.81261800	4.75665600	-0.28918900
H	3.05783200	4.80987300	-2.03914400
H	-3.58765300	4.11992900	1.83539000
H	-3.45570000	3.87400300	0.08124300
H	-5.00846600	4.27544300	0.81128000
H	-4.74433600	2.39778200	3.26819400
H	-4.62863100	1.88465000	-1.01058100
H	-6.18288300	2.71167400	2.29058700
H	-6.10102400	2.46143500	-0.21616100
H	-5.58964100	0.78320300	-0.01258000
H	-5.61489800	1.05157700	2.51304600
H	-4.27999900	-0.55942700	-1.67573600
H	-3.87041700	-2.03900800	-0.80821500
H	-4.92638300	-2.11098700	-2.21697500
H	-4.03499800	-1.79818000	-4.52197200
H	-3.40852200	-0.21132000	-4.06145600
H	-2.33023600	-1.41596100	-4.78735300
H	-2.41195900	-3.79193700	-1.88688100
H	-1.83425900	-3.57240600	-3.54999900
H	-3.55217500	-3.79101500	-3.22750000
H	-3.05781800	-4.80987000	2.03918700
H	-2.34771500	-6.18913800	1.20441200
H	-2.81262800	-4.75666700	0.28922900
H	-1.07410000	-4.70782900	3.61010300
H	-0.47430900	-6.16127000	2.79956000
H	0.56946000	-4.74884700	2.96932600
H	0.94311100	-4.70069000	0.43136900
H	-0.05212700	-6.15232700	0.33200500
H	-0.45463800	-4.74241500	-0.64940300
H	3.45571000	-3.87399200	-0.08123100
H	3.58764100	-4.11993800	-1.83537600
H	5.00846600	-4.27544400	-0.81128300
H	6.18285400	-2.71168900	-2.29064300
H	6.10107100	-2.46142000	0.21608500
H	5.58965600	-0.78319300	0.01253300

H	5.61486900	-1.05159200	-2.51309800
H	4.62869900	-1.88466200	1.01056200
H	4.74428500	-2.39779800	-3.26821800
H	4.28000500	0.55945800	1.67573500
H	3.87044700	2.03907200	0.80826200
H	4.92638300	2.11099600	2.21704600
H	3.40851100	0.21128400	4.06144000
H	4.03496800	1.79813600	4.52200900
H	2.33020600	1.41589600	4.78735900
H	3.55215500	3.79100300	3.22757900
H	1.83423800	3.57237800	3.55006000
H	2.41194900	3.79195600	1.88695200
O	2.62509100	-1.00616100	2.15429000
O	4.38476000	0.65198000	-1.35824400
O	-2.62507900	1.00617500	-2.15435400
O	-4.38476100	-0.65198200	1.35822300

Dimer **2–3** in LS state

C	0.00394700	0.00838000	1.75733200
C	-0.06994400	-1.40070000	1.77853900
C	1.12505400	-2.13686000	1.80531300
C	2.37249200	-1.52398500	1.81377700
C	2.42453700	-0.14171500	1.78264000
C	1.25739900	0.64619500	1.76722400
C	1.30449200	2.05353800	1.80482200
C	0.15597100	2.82216400	1.82583900
C	-1.07444900	2.17374100	1.78402600
C	-1.17881000	0.77515500	1.76014600
C	-2.42243400	0.10947800	1.78707800
C	-2.51284500	-1.27055900	1.83916200
C	-1.33609400	-2.01027400	1.82027000
C	3.62645300	-2.38353600	1.91701000
C	0.19533900	4.34186200	1.93268100
C	-3.84664600	-1.99359500	1.98548800
C	4.90049400	-1.55630600	1.82404200
C	3.60902700	-3.10598800	3.26350800
C	3.65236800	-3.41002900	0.78829000
C	-0.52559300	4.76856200	3.21078400
C	1.61798200	4.87996900	1.98630800
C	-0.50687400	4.96227900	0.72825800
C	-3.88531300	-2.65326900	3.36362600
C	-3.99189500	-3.06343700	0.90689100
C	-5.03183800	-1.04691900	1.86636500
C	0.01526400	-0.00966900	-1.59519600

C	0.03690400	1.41165200	-1.61052000
C	-1.18310900	2.12171600	-1.68408200
C	-2.40651200	1.53155100	-1.71200400
C	-2.47747800	0.05756600	-1.59830300
C	-1.20063000	-0.69148700	-1.60245600
C	-1.20567700	-2.06916800	-1.66312300
C	-0.02480000	-2.80198000	-1.74501700
C	1.17232100	-2.10720200	-1.70202800
C	1.20590200	-0.72581100	-1.61898700
C	2.50510900	-0.01988300	-1.60286200
C	2.48374400	1.45788400	-1.66330600
C	1.27799300	2.08533000	-1.64862100
C	-3.68587300	2.33132400	-1.87630600
C	-0.08452700	-4.31512100	-1.89518700
C	3.79221300	2.21908000	-1.76840900
C	-4.56073500	2.18496000	-0.63205900
C	-4.44747200	1.83399600	-3.10737800
C	-3.40020700	3.81437900	-2.07756600
C	-0.96963600	-4.67029400	-3.08921900
C	-0.68102800	-4.91914300	-0.62716900
C	1.29208100	-4.92206700	-2.12622900
C	3.56028400	3.72034300	-1.88401600
C	4.64989200	1.97072100	-0.52754700
C	4.54824100	1.76568000	-3.01974200
H	-3.31776600	0.71608600	1.78993700
H	-2.16904600	-2.56259600	-1.67419400
H	-1.37551300	-3.09225100	1.86245800
H	1.05314900	-3.21745000	1.84454500
H	2.12077700	-2.62117200	-1.75462200
H	3.37746400	0.36968100	1.78649700
H	2.27898300	2.52163300	1.83705100
H	1.23748200	3.16610600	-1.68573200
H	-1.10931700	3.19937000	-1.74281400
H	-1.99264300	2.75000300	1.79723600
H	-3.83201600	1.92677800	-4.00447100
H	-5.34334000	2.44135600	-3.24993700
H	-4.74801000	0.79553100	-2.99610300
H	-4.03732400	2.55340400	0.25196400
H	-4.83725700	1.14740300	-0.46994300
H	-5.47257100	2.77281800	-0.75367600
H	-4.34535200	4.34159100	-2.21201600
H	-2.89782900	4.25640700	-1.21613600
H	-2.79113100	3.99414900	-2.96540800
H	-5.02411300	-0.28253000	2.64491100
H	-5.04558400	-0.55919500	0.89187600

H	-5.95881000	-1.61293300	1.97042300
H	-3.78680600	-1.90664700	4.15349100
H	-3.94702200	-2.61292900	-0.08492000
H	-4.83188500	-3.17958200	3.50405700
H	-4.95395400	-3.56885400	1.01262900
H	-3.21397600	-3.82198700	0.98665900
H	-3.07608200	-3.37494200	3.48176400
H	-1.68083500	-4.52925400	-0.43949400
H	-0.05858600	-4.68998300	0.23883100
H	-0.75161000	-6.00451300	-0.72110700
H	-1.00591600	-5.75380900	-3.21699500
H	-1.99231000	-4.31722900	-2.95738300
H	-0.57636300	-4.23107400	-4.00742600
H	1.96095500	-4.74717300	-1.28351400
H	1.76197000	-4.52003600	-3.02541300
H	1.19533100	-6.00122900	-2.25370700
H	2.76789200	-4.04718900	0.80358900
H	4.52768400	-4.05486400	0.88967200
H	3.70649300	-2.90759100	-0.17760500
H	2.73806400	-3.75578900	3.35682300
H	4.50373200	-3.72255800	3.37268200
H	3.58267600	-2.38999300	4.08666500
H	4.97714900	-0.83393200	2.63829900
H	5.76657900	-2.21704500	1.88687900
H	4.95390400	-1.02480100	0.87339800
H	4.80970100	0.71213300	-2.96461200
H	3.94569700	1.93118000	-3.91510500
H	5.46697200	2.34684900	-3.11996900
H	4.52462800	4.22367200	-1.96109900
H	5.58809300	2.52180400	-0.61618200
H	4.13810400	2.32106600	0.37001400
H	3.04877100	4.12298300	-1.00835000
H	4.87853100	0.91490300	-0.41318700
H	2.98130600	3.97571200	-2.77343500
H	2.15715600	4.50585200	2.85778600
H	2.18387700	4.61326500	1.09263300
H	1.59426700	5.96883400	2.05166600
H	-0.05251300	4.32258600	4.08690400
H	-0.49375400	5.85482100	3.31832700
H	-1.57174500	4.46221600	3.20322300
H	-0.52396700	6.05029500	0.81702100
H	-1.53675400	4.61564200	0.64581900
H	0.01311900	4.70641800	-0.19606600
O	3.54682100	-0.65489100	-1.55727900
O	-3.53923600	-0.53916700	-1.52742500

Dimer **2–3** in HS state

C	-0.56460900	0.32508300	1.65531700
C	-0.81012100	-1.06039200	1.71455100
C	0.27181800	-1.93499600	1.94359900
C	1.56207200	-1.47240400	2.11631900
C	1.79605300	-0.10656600	1.99455100
C	0.75562700	0.81075700	1.76905000
C	0.97063400	2.19596400	1.70199900
C	-0.07784900	3.10018400	1.57090100
C	-1.36756000	2.60696200	1.48761200
C	-1.63769200	1.22385900	1.52089500
C	-2.94710700	0.71160500	1.45086500
C	-3.20230700	-0.64705700	1.46631700
C	-2.12748100	-1.51986800	1.59074400
C	2.70583400	-2.39901000	2.51128600
C	0.22968600	4.59284400	1.55170100
C	-4.61183300	-1.21493000	1.35674700
C	3.87524900	-2.25383500	1.54438200
C	3.16526900	-2.01873400	3.91863400
C	2.28251400	-3.86105400	2.51910900
C	0.96297400	4.97174000	2.83779100
C	1.11762300	4.91371200	0.35156600
C	-1.02978000	5.44261700	1.45741100
C	-4.90083600	-2.10597400	2.56357800
C	-4.71357000	-2.04490600	0.07843300
C	-5.67288100	-0.12430800	1.30772600
C	0.56461100	-0.32508100	-1.65532100
C	0.81012000	1.06039400	-1.71455800
C	-0.27182000	1.93499500	-1.94361000
C	-1.56207300	1.47240000	-2.11633300
C	-1.79605000	0.10656100	-1.99456500
C	-0.75562300	-0.81075900	-1.76905900
C	-0.97062700	-2.19596700	-1.70201000
C	0.07785600	-3.10018500	-1.57090300
C	1.36756500	-2.60695900	-1.48760300
C	1.63769500	-1.22385600	-1.52088900
C	2.94710800	-0.71159900	-1.45085200
C	3.20230500	0.64706400	-1.46631200
C	2.12747800	1.51987300	-1.59074900
C	-2.70584100	2.39900100	-2.51129400
C	-0.22967700	-4.59284500	-1.55170400
C	4.61183000	1.21493900	-1.35673500
C	-3.87523600	2.25382900	-1.54436500
C	-3.16530100	2.01871600	-3.91863000

C	-2.28252300	3.86104500	-2.51913400
C	-0.96297000	-4.97174300	-2.83779100
C	-1.11761200	-4.91371400	-0.35156700
C	1.02979100	-5.44261600	-1.45742200
C	4.90084400	2.10597200	-2.56357100
C	4.71355100	2.04492700	-0.07842700
C	5.67287800	0.12431900	-1.30769400
H	-3.76216900	1.41869100	1.38327000
H	-2.79910900	-0.28592000	-2.11129700
H	-1.99177400	-2.55258500	-1.77304900
H	-2.29396800	-2.59063500	1.61323400
H	0.05277500	-2.99102200	2.01439800
H	2.20877500	-3.28244900	-1.40085700
H	3.76217100	-1.41868100	-1.38324500
H	2.79911300	0.28591200	2.11128100
H	1.99178100	2.55258400	1.77303300
H	2.29396500	2.59063900	-1.61324200
H	-0.05278000	2.99102200	-2.01441100
H	-2.20876900	3.28245500	1.40087500
H	-2.34063500	2.09822400	-4.62869900
H	-3.96892400	2.68128600	-4.24751600
H	-3.53675100	0.99388800	-3.95080400
H	-3.58934400	2.58909300	-0.54862000
H	-4.21145000	1.22039900	-1.46626000
H	-4.71913700	2.85879400	-1.88240100
H	-3.13981700	4.48858800	-2.76803800
H	-1.91278300	4.16992000	-1.54006400
H	-1.50438400	4.05442000	-3.25892300
H	-5.65602800	0.49130300	2.20856500
H	-5.54446400	0.52800400	0.44303500
H	-6.66122800	-0.58100100	1.23474700
H	-4.81438100	-1.53830300	3.49136400
H	-4.52594200	-1.42477500	-0.79954000
H	-5.91400100	-2.50855500	2.50075400
H	-5.71122600	-2.47857100	-0.01654900
H	-3.98936200	-2.85995800	0.07550500
H	-4.21035000	-2.94736400	2.62000000
H	-2.04426400	-4.34015700	-0.37713200
H	-0.60327600	-4.68243100	0.58192300
H	-1.37694700	-5.97439100	-0.34412400
H	-1.17660300	-6.04264900	-2.84881400
H	-1.90992800	-4.44048400	-2.93317900
H	-0.35556700	-4.73376700	-3.71240200
H	1.58916200	-5.23902500	-0.54333900
H	1.69075300	-5.27639700	-2.30951800

H	0.75641800	-6.49895000	-1.44908000
H	1.50437500	-4.05443700	3.25889600
H	3.13980700	-4.48860000	2.76800700
H	1.91277300	-4.16992000	1.54003600
H	2.34058700	-2.09824100	4.62868500
H	3.96888100	-2.68131100	4.24753300
H	3.53672200	-0.99390800	3.95081800
H	4.21146200	-1.22040300	1.46628200
H	4.71914500	-2.85879400	1.88244200
H	3.58938700	-2.58910600	0.54863200
H	5.54446200	-0.52797600	-0.44299000
H	5.65602600	-0.49130900	-2.20852100
H	6.66122500	0.58101500	-1.23472300
H	5.91400400	2.50856500	-2.50073500
H	5.71121300	2.47857400	0.01657600
H	3.98935900	2.85999300	-0.07552500
H	4.21034900	2.94735400	-2.62001600
H	4.52588800	1.42480800	0.79954700
H	4.81441000	1.53829000	-3.49135200
H	2.04427900	4.34016200	0.37713400
H	0.60329000	4.68242300	-0.58192400
H	1.37695200	5.97439100	0.34411900
H	1.90993000	4.44047700	2.93318200
H	1.17660900	6.04264600	2.84881700
H	0.35556700	4.73376400	3.71239900
H	-0.75640400	6.49895100	1.44906800
H	-1.69074600	5.27640400	2.30950600
H	-1.58914800	5.23902300	0.54332700

Validation studies

Monomer **2** optimized with B3LYP

C	0.01567600	-0.01605500	-0.00000500
C	1.02890800	0.98665000	-0.00003800
C	0.63974100	2.35640500	-0.00005800
C	-0.70438800	2.74847600	-0.00002600
C	-1.68744200	1.74267100	-0.00000200
C	-1.36088700	0.36134600	0.00000500
C	-2.34542300	-0.65998400	0.00002000
C	-2.01223400	-2.02587500	0.00002500
C	-0.65516700	-2.37280300	0.00003400

C	0.37617300	-1.39320300	0.00001600
C	1.75459800	-1.74126700	0.00001700
C	2.76683800	-0.77356600	-0.00001700
C	2.38643600	0.58040800	-0.00004700
C	-1.13523700	4.23079700	0.00000400
C	-3.13783900	-3.08219100	-0.00000600
C	4.26597600	-1.14121900	0.00000500
C	-1.98011700	4.52036100	-1.26218800
C	-1.98005600	4.52026200	1.26227100
C	0.06896900	5.18985400	-0.00000300
C	-4.01257800	-2.90112300	1.26210500
C	-4.01232700	-2.90126000	-1.26230900
C	-2.58972000	-4.52073100	0.00013700
C	4.93897500	-0.55415100	1.26225500
C	4.93907300	-0.55404500	-1.26214800
C	4.49467700	-2.66353800	-0.00006000
H	2.00357300	-2.80272900	0.00003900
H	3.14970500	1.36237500	-0.00007800
H	1.43439500	3.10273900	-0.00011000
H	-2.74615600	2.01289100	0.00001700
H	-3.39409900	-0.35305400	0.00002400
H	-0.35160100	-3.41992500	0.00006000
H	4.06295400	-3.14450500	0.89152900
H	4.06291500	-3.14443100	-0.89167100
H	5.57511100	-2.87768100	-0.00009100
H	4.48044600	-0.95929000	2.17838100
H	4.48057700	-0.95907000	-2.17834100
H	6.01251600	-0.80524400	1.27862200
H	6.01260100	-0.80518800	-1.27847500
H	4.85320900	0.54241000	-1.30234900
H	4.85305400	0.54229700	1.30256100
H	0.70131500	5.05646000	0.89162100
H	-0.28575700	6.23262000	-0.00000600
H	0.70129900	5.05643800	-0.89163900
H	-1.40025000	4.32473500	2.17838100
H	-2.29833100	5.57582800	1.27905800
H	-2.88724000	3.89849600	1.30208600
H	-2.88720600	3.89846800	-1.30213400
H	-2.29855200	5.57588100	-1.27875600
H	-1.40028800	4.32511500	-2.17834600
H	-4.47629200	-1.90408400	-1.30243700
H	-3.41382600	-3.02856200	-2.17842300
H	-4.82393500	-3.64747700	-1.27899600
H	-4.47681700	-1.90406100	1.30186700
H	-4.82399400	-3.64754300	1.27883600

H	-3.41419600	-3.02802500	2.17834800
H	-3.42590300	-5.23764500	0.00005100
H	-1.97759500	-4.72772700	0.89181900
H	-1.97737500	-4.72782500	-0.89137200

Monomer **2** optimized with B3LYP-D3

C	0.01671300	-0.01707100	-0.00000500
C	1.02904900	0.98626300	0.00004000
C	0.63975500	2.35562100	0.00006500
C	-0.70440800	2.74561400	0.00003100
C	-1.68717100	1.73987500	0.00005100
C	-1.35989300	0.35947500	0.00002800
C	-2.34337600	-0.66182100	0.00004100
C	-2.00870000	-2.02705300	-0.00001700
C	-0.65221600	-2.37412700	-0.00006800
C	0.37795800	-1.39379800	-0.00005100
C	1.75610000	-1.74145500	-0.00007000
C	2.76654300	-0.77267600	-0.00002100
C	2.38608500	0.58101500	0.00005400
C	-1.13842100	4.22485600	-0.00001800
C	-3.13418500	-3.08047700	-0.00001900
C	4.26458600	-1.13610100	-0.00000200
C	-1.98310500	4.50979800	-1.26243500
C	-1.98384600	4.50971200	1.26192100
C	0.06222700	5.18734700	0.00037800
C	-4.00682500	-2.89639100	1.26216600
C	-4.00684000	-2.89640900	-1.26214000
C	-2.58918200	-4.51952400	0.00002200
C	4.93370000	-0.54673100	1.26227700
C	4.93385600	-0.54633300	-1.26201000
C	4.49797300	-2.65707100	-0.00023000
H	2.00405800	-2.80292100	-0.00011500
H	3.14954700	1.36254000	0.00014400
H	1.43505700	3.10091700	0.00015500
H	-2.74564500	2.01026300	0.00009300
H	-3.39229700	-0.35640200	0.00010300
H	-0.34650900	-3.42038600	-0.00011200
H	4.06653800	-3.13730400	0.89186500
H	4.06646100	-3.13705700	-0.89241800
H	5.57887500	-2.86839300	-0.00031000
H	4.47093800	-0.95173800	2.17623300
H	4.47108500	-0.95090200	-2.17615500
H	6.00738600	-0.79678300	1.28125900
H	6.00750700	-0.79653600	-1.28104000

H	4.84622300	0.54998300	-1.29910100
H	4.84588200	0.54955600	1.29979600
H	0.69345200	5.05372900	0.89274100
H	-0.29520600	6.22909900	0.00030200
H	0.69399600	5.05383600	-0.89160700
H	-1.40250600	4.31024400	2.17611300
H	-2.30298800	5.56491400	1.28134000
H	-2.89004800	3.88650400	1.29843400
H	-2.88896100	3.88614000	-1.29982200
H	-2.30273900	5.56485600	-1.28166700
H	-1.40102400	4.31096100	-2.17629400
H	-4.47024700	-1.89897100	-1.29918400
H	-3.40473500	-3.02061100	-2.17621700
H	-4.81823200	-3.64272000	-1.28146900
H	-4.47051800	-1.89908400	1.29902200
H	-4.81797600	-3.64295500	1.28166700
H	-3.40459300	-3.02024200	2.17620400
H	-3.42633700	-5.23517200	-0.00010000
H	-1.97747400	-4.72530500	0.89224900
H	-1.97722800	-4.72529300	-0.89203000

Monomer **2** optimized with B3LYP-D3BJ

C	0.01634600	-0.01669200	-0.00001500
C	1.02835000	0.98617200	0.00004200
C	0.63926100	2.35443100	0.00007100
C	-0.70412200	2.74242300	0.00002800
C	-1.68723600	1.73901900	0.00003200
C	-1.35976000	0.35963300	0.00001200
C	-2.34279100	-0.66082300	-0.00000300
C	-2.00652900	-2.02421900	-0.00005100
C	-0.65170400	-2.37250300	-0.00009700
C	0.37751000	-1.39281900	-0.00007200
C	1.75456800	-1.74022100	-0.00010000
C	2.76291700	-0.77113300	-0.00006000
C	2.38463600	0.58171400	0.00003500
C	-1.13610300	4.21876100	-0.00001200
C	-3.12866500	-3.07629100	-0.00001300
C	4.25741000	-1.13486200	-0.00000100
C	-1.97962600	4.50198300	-1.26072500
C	-1.98020200	4.50195100	1.26031300
C	0.06486500	5.17692700	0.00028300
C	-3.99946800	-2.89131500	1.26044100
C	-3.99931600	-2.89171700	-1.26057400
C	-2.58093500	-4.51168300	0.00027300

C	4.92434300	-0.54577400	1.26069600
C	4.92464700	-0.54528100	-1.26030000
C	4.48683500	-2.65395700	-0.00028600
H	2.00530600	-2.80061100	-0.00015200
H	3.14830700	1.36242900	0.00012000
H	1.43210000	3.10175200	0.00016400
H	-2.74506800	2.01017300	0.00005500
H	-3.39158000	-0.35648100	0.00004300
H	-0.34886300	-3.41916700	-0.00016300
H	4.05370700	-3.13265300	0.89129600
H	4.05358200	-3.13233500	-0.89197600
H	5.56705600	-2.86669200	-0.00039500
H	4.46096500	-0.95101400	2.17377700
H	4.46133600	-0.94996700	-2.17366000
H	5.99782000	-0.79491900	1.28024100
H	5.99807400	-0.79463900	-1.27980000
H	4.83435700	0.55050200	-1.29591200
H	4.83378600	0.54997000	1.29682500
H	0.69560700	5.04114900	0.89214100
H	-0.29106000	6.21877600	0.00013500
H	0.69611100	5.04109900	-0.89120100
H	-1.39841400	4.30196200	2.17364400
H	-2.29988200	5.55656400	1.28031100
H	-2.88466400	3.87677800	1.29539900
H	-2.88365700	3.87623800	-1.29661400
H	-2.29993100	5.55641100	-1.28045800
H	-1.39715800	4.30273900	-2.17378500
H	-4.46042300	-1.89357100	-1.29629000
H	-3.39651800	-3.01566700	-2.17376700
H	-4.81072700	-3.63740400	-1.28044000
H	-4.46092200	-1.89330800	1.29551900
H	-4.81058900	-3.63730200	1.28068300
H	-3.39663500	-3.01450300	2.17371200
H	-3.41670400	-5.22833800	0.00034100
H	-1.96842000	-4.71500600	0.89198600
H	-1.96827800	-4.71529200	-0.89127600

Monomer **2** optimized with PBE0

C	0.01578200	-0.01621300	-0.00002800
C	1.02653400	0.98270200	-0.00005100
C	0.64004100	2.34900200	-0.00005400
C	-0.70002600	2.74002000	-0.00002700
C	-1.68166500	1.73821900	-0.00001600
C	-1.35631000	0.36088200	-0.00001300

C	-2.33902300	-0.65629100	0.00001000
C	-2.00677300	-2.01844400	0.00001900
C	-0.65419000	-2.36591300	0.00002700
C	0.37428800	-1.38925900	-0.00000200
C	1.74823700	-1.73789300	-0.00000500
C	2.75754400	-0.77318900	-0.00004900
C	2.37986000	0.57751200	-0.00006600
C	-1.12797700	4.21338400	0.00000700
C	-3.12669600	-3.06706400	0.00000500
C	4.24750300	-1.13882600	0.00000800
C	-1.96755800	4.49811000	-1.25528300
C	-1.96746800	4.49803500	1.25538500
C	0.07118000	5.16426500	-0.00000900
C	-3.99432900	-2.88322400	1.25508400
C	-3.99377700	-2.88367600	-1.25552500
C	-2.58068600	-4.49672300	0.00040000
C	4.91361000	-0.55378100	1.25531900
C	4.91374900	-0.55390200	-1.25528600
C	4.47174200	-2.65266800	0.00007800
H	1.99875600	-2.79967400	0.00002000
H	3.14472400	1.35867400	-0.00007900
H	1.43416200	3.09686600	-0.00008600
H	-2.74044500	2.01032400	0.00000200
H	-3.38832100	-0.34957200	0.00002900
H	-0.35312500	-3.41444500	0.00006400
H	4.03923700	-3.13150800	0.89198900
H	4.03914400	-3.13159700	-0.89174200
H	5.55133700	-2.86816800	0.00003500
H	4.45351700	-0.95837800	2.17009700
H	4.45370800	-0.95853400	-2.17007600
H	5.98677900	-0.80367400	1.27288400
H	5.98689900	-0.80387100	-1.27273800
H	4.82613900	0.54208600	-1.29390600
H	4.82590900	0.54220600	1.29384600
H	0.70215200	5.02911700	0.89188200
H	-0.28189800	6.20700200	-0.00000100
H	0.70212300	5.02911700	-0.89192100
H	-1.38730500	4.30087000	2.17011700
H	-2.28648500	5.55271100	1.27333700
H	-2.87343700	3.87506600	1.29354000
H	-2.87338000	3.87494000	-1.29356500
H	-2.28681300	5.55271700	-1.27299400
H	-1.38736900	4.30128300	-2.17007200
H	-4.45471400	-1.88546100	-1.29413600
H	-3.39420400	-3.01065400	-2.17017900

H	-4.80658600	-3.62764200	-1.27339100
H	-4.45554800	-1.88511300	1.29298100
H	-4.80695500	-3.62738400	1.27296900
H	-3.39510500	-3.00959000	2.17004900
H	-3.41640800	-5.21332000	0.00040100
H	-1.96917000	-4.70219100	0.89240900
H	-1.96888100	-4.70258300	-0.89132200

Monomer **2** optimized with PBE0-D3

C	0.01633900	-0.01676000	-0.00002500
C	1.02675600	0.98230600	-0.00002000
C	0.64054700	2.34838400	0.00000600
C	-0.69946100	2.73833200	0.00001200
C	-1.68122300	1.73688700	-0.00001000
C	-1.35568400	0.36011300	-0.00001600
C	-2.33798800	-0.65673100	-0.00000100
C	-2.00502300	-2.01851800	0.00000400
C	-0.65291200	-2.36645900	0.00001400
C	0.37499100	-1.38961700	-0.00000900
C	1.74860000	-1.73832700	-0.00000900
C	2.75695000	-0.77312900	-0.00003300
C	2.37965900	0.57750000	-0.00003000
C	-1.12890400	4.21012500	0.00000700
C	-3.12511400	-3.06537200	0.00000400
C	4.24629300	-1.13670800	0.00000300
C	-1.96818900	4.49193600	-1.25577000
C	-1.96859800	4.49189000	1.25552300
C	0.06881800	5.16240900	0.00024300
C	-3.99124200	-2.87931000	1.25542200
C	-3.99076300	-2.87975000	-1.25580200
C	-2.58067500	-4.49536600	0.00038300
C	4.90988700	-0.55034600	1.25565600
C	4.91001000	-0.55032300	-1.25557400
C	4.47246200	-2.65001200	-0.00001300
H	1.99826900	-2.80015800	-0.00000100
H	3.14468100	1.35837000	-0.00002900
H	1.43521500	3.09544800	0.00002600
H	-2.73985200	2.00914800	-0.00000700
H	-3.38732700	-0.35051900	0.00002200
H	-0.35077300	-3.41452900	0.00005200
H	4.03973000	-3.12825400	0.89210100
H	4.03966900	-3.12823900	-0.89210700
H	5.55215800	-2.86475200	-0.00004900
H	4.44700800	-0.95486000	2.16903200

H	4.44715100	-0.95474100	-2.16900200
H	5.98317700	-0.79940300	1.27532900
H	5.98327700	-0.79947800	-1.27519300
H	4.82111000	0.54556300	-1.29266200
H	4.82087000	0.54553000	1.29279600
H	0.69919900	5.02665100	0.89245200
H	-0.28496000	6.20485600	0.00029300
H	0.69943000	5.02683100	-0.89182700
H	-1.38732400	4.29231000	2.16899200
H	-2.28846400	5.54623500	1.27549700
H	-2.87379500	3.86779600	1.29208400
H	-2.87318600	3.86758200	-1.29279600
H	-2.28833100	5.54619900	-1.27566200
H	-1.38651300	4.29268600	-2.16905600
H	-4.45064800	-1.88105300	-1.29299600
H	-3.38885000	-3.00519700	-2.16909800
H	-4.80398000	-3.62316700	-1.27571800
H	-4.45149900	-1.88075900	1.29186900
H	-4.80420200	-3.62300000	1.27545400
H	-3.38959100	-3.00403400	2.16898500
H	-3.41666400	-5.21157600	0.00030900
H	-1.96929400	-4.70003400	0.89266000
H	-1.96890000	-4.70036700	-0.89154800

Monomer **2** optimized with PBE0-D3BJ

C	0.01611400	-0.01652400	-0.00001800
C	1.02635900	0.98242100	-0.00002900
C	0.64010400	2.34794700	-0.00002600
C	-0.69960000	2.73687000	0.00000000
C	-1.68150300	1.73645700	0.00000500
C	-1.35575600	0.36016700	-0.00000300
C	-2.33780200	-0.65635200	0.00000500
C	-2.00396600	-2.01727800	-0.00000700
C	-0.65257800	-2.36571500	0.00001500
C	0.37483900	-1.38913200	0.00000100
C	1.74798200	-1.73758600	0.00000600
C	2.75530700	-0.77214300	-0.00002100
C	2.37896400	0.57809900	-0.00003700
C	-1.12804300	4.20742100	0.00000400
C	-3.12237300	-3.06377400	0.00000000
C	4.24306700	-1.13598900	0.00000400
C	-1.96695900	4.48850000	-1.25492700
C	-1.96698000	4.48850200	1.25492900
C	0.06995000	5.15762300	0.00002200

C	-3.98775000	-2.87746800	1.25463800
C	-3.98714700	-2.87808300	-1.25514800
C	-2.57635900	-4.49201100	0.00049600
C	4.90576900	-0.54987800	1.25499000
C	4.90591200	-0.54964800	-1.25480000
C	4.46725000	-2.64849700	-0.00013200
H	1.99927900	-2.79884800	0.00001900
H	3.14399100	1.35868500	-0.00005200
H	1.43340000	3.09621000	-0.00004500
H	-2.73986600	2.00896600	0.00001900
H	-3.38709400	-0.35067700	0.00003900
H	-0.35194800	-3.41403100	0.00005200
H	4.03371900	-3.12611200	0.89168900
H	4.03367500	-3.12595400	-0.89201800
H	5.54662200	-2.86387000	-0.00017900
H	4.44255900	-0.95442900	2.16796000
H	4.44275000	-0.95396900	-2.16789600
H	5.97890700	-0.79870500	1.27493600
H	5.97903200	-0.79854800	-1.27470500
H	4.81584000	0.54600700	-1.29102900
H	4.81560900	0.54576300	1.29144400
H	0.70025000	5.02092700	0.89190500
H	-0.28315300	6.20009400	0.00004900
H	0.70023900	5.02097600	-0.89187600
H	-1.38543300	4.28861300	2.16793500
H	-2.28696500	5.54260100	1.27524700
H	-2.87139500	3.86352700	1.29085100
H	-2.87119900	3.86328300	-1.29102200
H	-2.28721100	5.54252100	-1.27508700
H	-1.38529500	4.28891600	-2.16792500
H	-4.44616200	-1.87914100	-1.29162500
H	-3.38487800	-3.00322000	-2.16802900
H	-4.80016300	-3.62142300	-1.27538200
H	-4.44705900	-1.87862800	1.29022300
H	-4.80056900	-3.62101400	1.27496900
H	-3.38585700	-3.00184100	2.16786800
H	-3.41164100	-5.20874800	0.00044700
H	-1.96462500	-4.69552700	0.89255600
H	-1.96417500	-4.69597500	-0.89115200

Monomer **2** optimized with M06

C	0.01576000	-0.01666400	0.00000500
C	1.02969200	0.97742200	-0.00001500
C	0.64963900	2.34451000	-0.00003100

C	-0.68821700	2.74012400	0.00001400
C	-1.67361800	1.74285200	0.00003200
C	-1.35387800	0.36562400	0.00001700
C	-2.33990000	-0.64661400	-0.00000400
C	-2.01270500	-2.00928800	-0.00003900
C	-0.66237100	-2.36212100	0.00001400
C	0.36851700	-1.38968800	0.00001700
C	1.73975100	-1.74440900	0.00001900
C	2.75211900	-0.78406100	0.00000200
C	2.38010100	0.56750000	-0.00002200
C	-1.11175200	4.20954700	-0.00000500
C	-3.13399200	-3.04901600	-0.00001200
C	4.23668000	-1.15094200	-0.00000600
C	-1.94628400	4.49755400	-1.25148200
C	-1.94581100	4.49768000	1.25177800
C	0.08523100	5.15549700	-0.00029000
C	-3.99740400	-2.86454900	1.25145200
C	-3.99708500	-2.86501100	-1.25177300
C	-2.59752800	-4.47724500	0.00031800
C	4.90267900	-0.57192800	1.25179500
C	4.90290000	-0.57113000	-1.25131400
C	4.45908500	-2.66019600	-0.00047000
H	1.98118200	-2.81114300	0.00001200
H	3.14843200	1.34948100	-0.00005400
H	1.45219200	3.08749400	-0.00007900
H	-2.73494400	2.01743300	0.00002300
H	-3.39029200	-0.33278000	0.00001600
H	-0.36014000	-3.41326300	0.00006800
H	4.02664400	-3.14107700	0.89287000
H	4.02665900	-3.14052900	-0.89411300
H	5.54014400	-2.87755000	-0.00052500
H	4.43634400	-0.97368600	2.16719600
H	4.43666900	-0.97222900	-2.16705600
H	5.97518000	-0.83234300	1.27268300
H	5.97538300	-0.83161000	-1.27222000
H	4.82738200	0.52739900	-1.29173600
H	4.82705700	0.52656600	1.29294700
H	0.71774600	5.02036000	0.89301200
H	-0.26579300	6.20081200	-0.00027100
H	0.71736600	5.02026800	-0.89384800
H	-1.36520500	4.29314700	2.16714300
H	-2.25441900	5.55730300	1.27310500
H	-2.86055900	3.88478900	1.29245500
H	-2.86082800	3.88436000	-1.29200900
H	-2.25526400	5.55707400	-1.27253600

H	-1.36587600	4.29338300	-2.16705300
H	-4.46259600	-1.86714000	-1.29312100
H	-3.39448400	-2.99100700	-2.16712200
H	-4.80940400	-3.61215200	-1.27259400
H	-4.46325800	-1.86680400	1.29207600
H	-4.80948400	-3.61194300	1.27251700
H	-3.39496100	-2.98980400	2.16700400
H	-3.43797800	-5.19105500	0.00017100
H	-1.98650500	-4.68808800	0.89391900
H	-1.98604600	-4.68834400	-0.89290800

Monomer **2** optimized with M06-D3

C	0.01580700	-0.01669600	-0.00001500
C	1.02955900	0.97748500	-0.00003000
C	0.64956500	2.34433600	-0.00003300
C	-0.68832000	2.73934400	0.00001800
C	-1.67381400	1.74231600	0.00004300
C	-1.35381300	0.36542500	0.00001700
C	-2.33966700	-0.64660500	0.00000500
C	-2.01194800	-2.00904100	-0.00004500
C	-0.66182000	-2.36209900	0.00000200
C	0.36869400	-1.38962200	-0.00000300
C	1.73970000	-1.74426700	-0.00000500
C	2.75155000	-0.78358600	-0.00003500
C	2.37980700	0.56794000	-0.00004600
C	-1.11211000	4.20840100	-0.00000200
C	-3.13297200	-3.04864300	-0.00001000
C	4.23591100	-1.15008800	0.00000000
C	-1.94643700	4.49512300	-1.25198600
C	-1.94602700	4.49526600	1.25223600
C	0.08510300	5.15405400	-0.00025700
C	-3.99578900	-2.86323800	1.25179300
C	-3.99516800	-2.86404900	-1.25236800
C	-2.59569900	-4.47656500	0.00059000
C	4.90072900	-0.57036400	1.25216900
C	4.90095200	-0.57000300	-1.25187900
C	4.45785900	-2.65940100	-0.00020800
H	1.98120800	-2.81093000	-0.00000600
H	3.14791800	1.35009600	-0.00006000
H	1.45203600	3.08732900	-0.00006800
H	-2.73519000	2.01658200	0.00005400
H	-3.39000000	-0.33268600	0.00005400
H	-0.35944900	-3.41314300	0.00005500
H	4.02476000	-3.13974000	0.89309500

H	4.02474000	-3.13949700	-0.89363300
H	5.53872700	-2.87762500	-0.00024300
H	4.43414800	-0.97280700	2.16716100
H	4.43444500	-0.97207100	-2.16707300
H	5.97361800	-0.82900400	1.27391300
H	5.97381200	-0.82876500	-1.27357100
H	4.82335400	0.52834100	-1.29289000
H	4.82296600	0.52795600	1.29354300
H	0.71760800	5.01818600	0.89293200
H	-0.26515400	6.19961000	-0.00021700
H	0.71725100	5.01814500	-0.89368900
H	-1.36457300	4.29094100	2.16712700
H	-2.25634400	5.55434700	1.27436700
H	-2.85957100	3.88064300	1.29335100
H	-2.85974600	3.88015500	-1.29300100
H	-2.25716500	5.55409000	-1.27386300
H	-1.36512100	4.29117900	-2.16704900
H	-4.45906700	-1.86547200	-1.29428900
H	-3.39178200	-2.99055000	-2.16714900
H	-4.80842200	-3.61011500	-1.27403000
H	-4.46007700	-1.86478900	1.29256900
H	-4.80877900	-3.60957900	1.27373100
H	-3.39276900	-2.98869300	2.16695500
H	-3.43536000	-5.19127800	0.00046400
H	-1.98430100	-4.68642900	0.89415600
H	-1.98365100	-4.68695400	-0.89240500

Monomer **2** optimized with M06-2X

C	0.01681400	-0.01743700	-0.00002800
C	1.02952900	0.98025300	-0.00004500
C	0.64560600	2.34898500	-0.00003800
C	-0.69355000	2.73817200	-0.00003600
C	-1.67887300	1.74036000	-0.00003400
C	-1.35566100	0.36220400	-0.00002100
C	-2.34001600	-0.65320300	0.00000400
C	-2.00701300	-2.01486600	0.00002000
C	-0.65708100	-2.36765200	0.00003400
C	0.37305300	-1.39106000	0.00000100
C	1.74689400	-1.74326100	-0.00000300
C	2.75439600	-0.77843100	-0.00003700
C	2.38171400	0.57345600	-0.00005600
C	-1.12184200	4.21096100	0.00001000
C	-3.13059400	-3.05885400	0.00000400
C	4.24403900	-1.14325000	0.00000400

C	-1.96221800	4.49459900	-1.25559900
C	-1.96190600	4.49460200	1.25583200
C	0.08022300	5.15944000	-0.00013300
C	-3.99762600	-2.87057200	1.25546700
C	-3.99728000	-2.87080100	-1.25573000
C	-2.58605400	-4.48989500	0.00023100
C	4.90945700	-0.55695500	1.25569500
C	4.90959700	-0.55691500	-1.25559200
C	4.46494400	-2.65837500	-0.00002100
H	1.99472700	-2.80471500	0.00001600
H	3.14884100	1.35139200	-0.00006500
H	1.44085600	3.09420600	-0.00004000
H	-2.73594600	2.01596300	-0.00004000
H	-3.38868900	-0.34703600	0.00001800
H	-0.35707100	-3.41548000	0.00008800
H	4.02796900	-3.13049300	0.89214000
H	4.02785900	-3.13047400	-0.89213900
H	5.54352800	-2.87315600	-0.00008500
H	4.44309400	-0.96022600	2.16664900
H	4.44326700	-0.96006900	-2.16661500
H	5.98042000	-0.81138500	1.27221300
H	5.98053400	-0.81144800	-1.27204500
H	4.82219900	0.53840700	-1.28676300
H	4.82192900	0.53835500	1.28693500
H	0.70757100	5.01715400	0.89203300
H	-0.27299700	6.20092600	-0.00016000
H	0.70743600	5.01705900	-0.89237900
H	-1.37997700	4.29043000	2.16667300
H	-2.27494100	5.54989900	1.27317700
H	-2.86795900	3.87297600	1.28640700
H	-2.86814000	3.87277900	-1.28607600
H	-2.27548800	5.54983000	-1.27274900
H	-1.38043600	4.29067000	-2.16658900
H	-4.45526500	-1.87195200	-1.28623600
H	-3.39340900	-2.99454700	-2.16676000
H	-4.80809200	-3.61529700	-1.27295000
H	-4.45598200	-1.87187700	1.28546500
H	-4.80817700	-3.61534500	1.27276300
H	-3.39392400	-2.99376200	2.16668200
H	-3.42384500	-5.20232600	0.00020200
H	-1.97471000	-4.68962800	0.89249000
H	-1.97449800	-4.68985300	-0.89183100

Monomer **2** optimized with M06-2X-D3

C	0.01686100	-0.01746200	-0.00008400
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C	1.02992200	0.97978400	-0.00008000
C	0.64665700	2.34863200	-0.00007400
C	-0.69235900	2.73829300	-0.00010500
C	-1.67810700	1.74090200	-0.00011500
C	-1.35539000	0.36272100	-0.00008100
C	-2.34017400	-0.65215800	-0.00003200
C	-2.00770200	-2.01395800	-0.00002200
C	-0.65791800	-2.36734000	0.00001300
C	0.37250800	-1.39116000	-0.00003500
C	1.74611600	-1.74398200	-0.00001900
C	2.75396700	-0.77951000	-0.00005500
C	2.38189000	0.57254300	-0.00007300
C	-1.12012400	4.21115400	0.00002600
C	-3.13171100	-3.05741600	0.00000700
C	4.24339600	-1.14484200	0.00001000
C	-1.96065300	4.49474800	-1.25555300
C	-1.95985900	4.49474300	1.25615900
C	0.08250200	5.15897900	-0.00035100
C	-3.99866300	-2.86824700	1.25545800
C	-3.99795700	-2.86892800	-1.25601300
C	-2.58760800	-4.48866900	0.00061500
C	4.90857700	-0.55914400	1.25617700
C	4.90904400	-0.55808600	-1.25540500
C	4.46344100	-2.66012300	-0.00060700
H	1.99329800	-2.80558600	-0.00000600
H	3.14915500	1.35033800	-0.00008300
H	1.44237100	3.09336200	-0.00006100
H	-2.73512800	2.01666600	-0.00010300
H	-3.38863200	-0.34528300	0.00001000
H	-0.35809300	-3.41521500	0.00009600
H	4.02599600	-3.13230500	0.89131400
H	4.02597400	-3.13157800	-0.89290300
H	5.54187300	-2.87570100	-0.00070700
H	4.44172300	-0.96260400	2.16682900
H	4.44241700	-0.96062600	-2.16658100
H	5.97950600	-0.81372100	1.27313700
H	5.97993500	-0.81282100	-1.27226300
H	4.82178800	0.53728200	-1.28608600
H	4.82109700	0.53617900	1.28782700
H	0.70993600	5.01623500	0.89170700
H	-0.26992200	6.20074300	-0.00040800
H	0.70955600	5.01599400	-0.89263400
H	-1.37775700	4.29002200	2.16680000
H	-2.27267000	5.55010500	1.27406800
H	-2.86600700	3.87322000	1.28681000

H	-2.86660300	3.87292000	-1.28585400
H	-2.27384700	5.55000300	-1.27303000
H	-1.37900200	4.29045200	-2.16657700
H	-4.45535100	-1.86978900	-1.28665400
H	-3.39378100	-2.99280900	-2.16685500
H	-4.80915800	-3.61300100	-1.27371200
H	-4.45648300	-1.86927300	1.28506900
H	-4.80956300	-3.61263700	1.27327700
H	-3.39489100	-2.99119100	2.16669200
H	-3.42547600	-5.20102300	0.00079500
H	-1.97619600	-4.68823700	0.89288700
H	-1.97600500	-4.68894900	-0.89136400

Monomer **2** optimized with LC- ω PBE

C	0.01647400	-0.01682100	-0.00004000
C	1.02305400	0.98017800	0.00004300
C	0.63610200	2.34549300	0.00007100
C	-0.70061900	2.73391600	0.00000500
C	-1.67936100	1.73278200	-0.00001400
C	-1.35225500	0.35779800	-0.00003400
C	-2.33289400	-0.65821800	-0.00005900
C	-1.99977400	-2.01753600	-0.00009800
C	-0.65065100	-2.36245000	-0.00016400
C	0.37521100	-1.38482000	-0.00011600
C	1.74765400	-1.73261700	-0.00012900
C	2.75306300	-0.76960900	-0.00004000
C	2.37451300	0.57811400	0.00006100
C	-1.13207000	4.20443900	-0.00000900
C	-3.11887900	-3.06446900	-0.00001100
C	4.24224400	-1.13103200	0.00000900
C	-1.96949300	4.48608700	-1.25355900
C	-1.96990000	4.48602300	1.25328200
C	0.06396200	5.15610100	0.00020900
C	-3.98317700	-2.88111300	1.25359700
C	-3.98366800	-2.88114700	-1.25321100
C	-2.57278300	-4.49201700	-0.00008400
C	4.90471900	-0.54670000	1.25369400
C	4.90507300	-0.54582400	-1.25308100
C	4.46852300	-2.64260400	-0.00050400
H	1.99788800	-2.79404400	-0.00020900
H	3.13813000	1.35982000	0.00016600
H	1.43003900	3.09296300	0.00017600
H	-2.73797300	2.00360600	0.00000600
H	-3.38205100	-0.35270400	-0.00003900

H	-0.34718800	-3.40985800	-0.00027300
H	4.03732300	-3.12090600	0.89056700
H	4.03725500	-3.12030800	-0.89186100
H	5.54717600	-2.85557600	-0.00061000
H	4.44110400	-0.94853400	2.16623700
H	4.44147800	-0.94673100	-2.16604100
H	5.97569300	-0.79869600	1.27490900
H	5.97597200	-0.79813300	-1.27434900
H	4.82044800	0.54909300	-1.28807400
H	4.81971300	0.54815800	1.28960900
H	0.69326400	5.02175200	0.89163900
H	-0.29090900	6.19672600	0.00001000
H	0.69373200	5.02159300	-0.89085700
H	-1.39080100	4.28460400	2.16608600
H	-2.28633600	5.53974300	1.27475000
H	-2.87609100	3.86570600	1.28840800
H	-2.87531900	3.86527500	-1.28935200
H	-2.28648700	5.53964600	-1.27472500
H	-1.38986800	4.28536300	-2.16618200
H	-4.44847700	-1.88618400	-1.28850900
H	-3.38277900	-3.00242200	-2.16610000
H	-4.79203800	-3.62748800	-1.27442500
H	-4.44874200	-1.88649000	1.28849600
H	-4.79091900	-3.62810400	1.27570600
H	-3.38164300	-3.00132300	2.16620000
H	-3.40742500	-5.20770000	-0.00010000
H	-1.96229800	-4.69634100	0.89113200
H	-1.96228800	-4.69623900	-0.89131100

Monomer **2** optimized with LC- ω PBE-D3

C	0.01720000	-0.01758700	-0.00001400
C	1.02387400	0.97908200	-0.00002200
C	0.63798400	2.34445300	-0.00001600
C	-0.69850500	2.73244500	-0.00001700
C	-1.67785000	1.73207900	-0.00000800
C	-1.35123600	0.35749800	-0.00000700
C	-2.33198200	-0.65764600	0.00000800
C	-1.99887400	-2.01682200	0.00001200
C	-0.65039000	-2.36292500	0.00002500
C	0.37538100	-1.38553600	0.00000500
C	1.74732400	-1.73419900	0.00000500
C	2.75222700	-0.77114600	-0.00002600
C	2.37467600	0.57672000	-0.00002900
C	-1.13113700	4.20131700	0.00000500

C	-3.11890300	-3.06096000	0.00000300
C	4.24061400	-1.13066800	0.00000300
C	-1.96862200	4.48036300	-1.25359000
C	-1.96874900	4.48032200	1.25352900
C	0.06342300	5.15428800	0.00009000
C	-3.98215000	-2.87460500	1.25335200
C	-3.98172700	-2.87496100	-1.25369100
C	-2.57584800	-4.48931200	0.00031100
C	4.90091700	-0.54460200	1.25352700
C	4.90099600	-0.54465900	-1.25350900
C	4.46890700	-2.64160500	0.00003000
H	1.99564600	-2.79593000	0.00001800
H	3.13891000	1.35768800	-0.00003200
H	1.43329400	3.09025900	-0.00000900
H	-2.73618100	2.00356700	0.00000200
H	-3.38103200	-0.35214000	0.00002500
H	-0.34583200	-3.40987100	0.00006200
H	4.03736700	-3.11858200	0.89165200
H	4.03730400	-3.11861500	-0.89154500
H	5.54769600	-2.85378600	-0.00000100
H	4.43369600	-0.94517600	2.16476000
H	4.43374400	-0.94517600	-2.16475000
H	5.97171400	-0.79708300	1.27697000
H	5.97176400	-0.79726300	-1.27693200
H	4.81618100	0.55025200	-1.28681300
H	4.81596100	0.55030000	1.28683200
H	0.69220700	5.01898200	0.89173900
H	-0.29210700	6.19467000	0.00010500
H	0.69229000	5.01904000	-0.89150900
H	-1.38844100	4.27534700	2.16475000
H	-2.28471600	5.53412000	1.27719300
H	-2.87495100	3.85998500	1.28662600
H	-2.87466200	3.85980400	-1.28694500
H	-2.28484200	5.53409000	-1.27711100
H	-1.38812900	4.27569600	-2.16476200
H	-4.44567200	-1.87958200	-1.28716000
H	-3.37782600	-2.99434500	-2.16481800
H	-4.79033800	-3.62094800	-1.27726900
H	-4.44653700	-1.87940900	1.28611300
H	-4.79045300	-3.62091600	1.27709200
H	-3.37845900	-2.99323200	2.16471400
H	-3.41148700	-5.20380500	0.00018400
H	-1.96591300	-4.69285800	0.89208200
H	-1.96549700	-4.69309200	-0.89112400

Monomer **2** optimized with LC- ω PBE-D3BJ

C	0.01679300	-0.01717300	-0.00003100
C	1.02350700	0.97924300	-0.00003400
C	0.63768800	2.34400000	-0.00003200
C	-0.69841700	2.73101100	-0.00003100
C	-1.67816600	1.73201200	-0.00001600
C	-1.35150100	0.35792800	-0.00001600
C	-2.33211700	-0.65671300	-0.00000200
C	-1.99812400	-2.01496900	-0.00001000
C	-0.65050200	-2.36186300	0.00001900
C	0.37488000	-1.38497400	-0.00000500
C	1.74624000	-1.73348400	0.00000400
C	2.75012300	-0.77027900	-0.00003200
C	2.37393500	0.57726300	-0.00003800
C	-1.12937400	4.19892300	0.00000500
C	-3.11634300	-3.05900500	0.00000200
C	4.23683200	-1.13078100	0.00000400
C	-1.96622300	4.47721300	-1.25307100
C	-1.96600500	4.47722500	1.25323600
C	0.06626300	5.14896600	-0.00009500
C	-3.97859200	-2.87219700	1.25285800
C	-3.97798000	-2.87282100	-1.25337500
C	-2.57102100	-4.48544000	0.00051500
C	4.89605200	-0.54517000	1.25320400
C	4.89621700	-0.54498300	-1.25302400
C	4.46199800	-2.64119100	-0.00011000
H	1.99657600	-2.79454400	0.00002200
H	3.13817900	1.35793200	-0.00004100
H	1.43130400	3.09133000	-0.00003000
H	-2.73620500	2.00381800	-0.00001100
H	-3.38105200	-0.35153100	0.00002800
H	-0.34812200	-3.40923700	0.00006700
H	4.02940300	-3.11756900	0.89106900
H	4.02932600	-3.11743900	-0.89132300
H	5.54026500	-2.85486800	-0.00017300
H	4.42858000	-0.94599100	2.16397400
H	4.42876300	-0.94555200	-2.16391400
H	5.96678200	-0.79693900	1.27738600
H	5.96691400	-0.79689000	-1.27717200
H	4.80977500	0.54964100	-1.28594400
H	4.80944800	0.54943600	1.28634300
H	0.69510700	5.01247400	0.89108100
H	-0.28775200	6.18963000	-0.00007900
H	0.69496700	5.01246000	-0.89136500

H	-1.38535700	4.27204500	2.16396800
H	-2.28244700	5.53063900	1.27770700
H	-2.87119300	3.85570300	1.28615600
H	-2.87116700	3.85534000	-1.28606500
H	-2.28306700	5.53051300	-1.27725600
H	-1.38558400	4.27247600	-2.16390900
H	-4.44035500	-1.87689400	-1.28665500
H	-3.37371700	-2.99226100	-2.16402900
H	-4.78687500	-3.61815900	-1.27773800
H	-4.44137900	-1.87642900	1.28517300
H	-4.78720900	-3.61782800	1.27738200
H	-3.37469200	-2.99073800	2.16386800
H	-3.40557500	-5.20085800	0.00044800
H	-1.96056300	-4.68785000	0.89193800
H	-1.96007100	-4.68831100	-0.89046400

Monomer **2** optimized with CAM-B3LYP

C	0.01605900	-0.01641200	-0.00003500
C	1.02475200	0.98258300	-0.00003600
C	0.63674900	2.34846100	-0.00002400
C	-0.70201900	2.73725000	-0.00001500
C	-1.68177000	1.73543000	-0.00002400
C	-1.35528700	0.35901300	-0.00002900
C	-2.33629800	-0.65859400	-0.00002400
C	-2.00283400	-2.01912200	-0.00003200
C	-0.65178100	-2.36499000	-0.00000600
C	0.37550300	-1.38744100	-0.00002000
C	1.74926900	-1.73462600	-0.00001800
C	2.75607000	-0.76996300	-0.00004300
C	2.37742700	0.57908800	-0.00004300
C	-1.13270500	4.21224300	0.00000700
C	-3.12373600	-3.07011000	0.00000300
C	4.24876000	-1.13419900	0.00000600
C	-1.97386500	4.49868600	-1.25571900
C	-1.97340800	4.49877900	1.25602600
C	0.06610500	5.16665100	-0.00024000
C	-3.99377100	-2.88888000	1.25567500
C	-3.99335000	-2.88940800	-1.25602600
C	-2.57684400	-4.50151400	0.00041100
C	4.91718000	-0.54907600	1.25593100
C	4.91736100	-0.54894000	-1.25575900
C	4.47604900	-2.64954700	-0.00007500
H	1.99888500	-2.79524200	-0.00001000
H	3.14054300	1.36026800	-0.00003900

H	1.43034600	3.09494000	-0.00002400
H	-2.73970700	2.00594400	-0.00003200
H	-3.38470600	-0.35311800	0.00000000
H	-0.34831700	-3.41143300	0.00002800
H	4.04423200	-3.12879800	0.89082300
H	4.04414000	-3.12871100	-0.89097700
H	5.55542000	-2.86241900	-0.00013700
H	4.45816400	-0.95360900	2.17055100
H	4.45838800	-0.95326900	-2.17049100
H	5.98944100	-0.79970800	1.27231500
H	5.98959200	-0.79969900	-1.27207500
H	4.83050600	0.54626400	-1.29400100
H	4.83017200	0.54611100	1.29433500
H	0.69714800	5.03235500	0.89060200
H	-0.28923400	6.20784500	-0.00025200
H	0.69687400	5.03224300	-0.89125600
H	-1.39375600	4.30268200	2.17058400
H	-2.29150000	5.55298700	1.27275100
H	-2.87894000	3.87668300	1.29417700
H	-2.87920500	3.87630200	-1.29368900
H	-2.29229100	5.55279700	-1.27221300
H	-1.39442200	4.30289000	-2.17047500
H	-4.45641000	-1.89311800	-1.29443900
H	-3.39460500	-3.01570500	-2.17059000
H	-4.80357600	-3.63512800	-1.27261400
H	-4.45719700	-1.89272800	1.29328500
H	-4.80373600	-3.63487300	1.27249200
H	-3.39524200	-3.01437400	2.17048600
H	-3.41224700	-5.21736300	0.00037800
H	-1.96540800	-4.70641300	0.89148000
H	-1.96504200	-4.70679000	-0.89032000

Monomer **2** optimized with CAM-B3LYP-D3

C	0.01680800	-0.01713100	-0.00001200
C	1.02461300	0.98252300	0.00001800
C	0.63629500	2.34806500	0.00003800
C	-0.70264600	2.73514000	0.00000800
C	-1.68197400	1.73307200	0.00003400
C	-1.35461800	0.35737800	0.00001500
C	-2.33471100	-0.66038900	0.00002600
C	-1.99992500	-2.02044400	-0.00002000
C	-0.64912500	-2.36610300	-0.00005600
C	0.37707800	-1.38775600	-0.00004400
C	1.75071200	-1.73441500	-0.00005800

C	2.75610500	-0.76873400	-0.00002000
C	2.37705700	0.58007300	0.00003300
C	-1.13603500	4.20800500	-0.00001400
C	-3.12066900	-3.06971600	-0.00001600
C	4.24828300	-1.12964200	0.00000200
C	-1.97699600	4.49113200	-1.25608800
C	-1.97744300	4.49105900	1.25577900
C	0.06020900	5.16500400	0.00023500
C	-3.98927200	-2.88676300	1.25587200
C	-3.98916900	-2.88692000	-1.25594900
C	-2.57538800	-4.50132200	0.00012700
C	4.91396400	-0.54276500	1.25601800
C	4.91410600	-0.54241000	-1.25577300
C	4.47899000	-2.64408400	-0.00020100
H	1.99954500	-2.79508000	-0.00008800
H	3.14001000	1.36126700	0.00010100
H	1.43043500	3.09376100	0.00011200
H	-2.73987900	2.00327600	0.00007700
H	-3.38332500	-0.35601200	0.00008300
H	-0.34360600	-3.41181100	-0.00007700
H	4.04726800	-3.12280800	0.89102600
H	4.04720000	-3.12258600	-0.89151300
H	5.55870700	-2.85511300	-0.00027200
H	4.45209500	-0.94725500	2.16918700
H	4.45218200	-0.94645400	-2.16911200
H	5.98638200	-0.79252900	1.27428700
H	5.98647700	-0.79237100	-1.27411700
H	4.82587600	0.55270400	-1.29184700
H	4.82550600	0.55231700	1.29251100
H	0.69037500	5.03044900	0.89166300
H	-0.29695900	6.20555500	0.00017500
H	0.69073400	5.03050900	-0.89093900
H	-1.39680100	4.29231600	2.16910600
H	-2.29641500	5.54495400	1.27444900
H	-2.88215100	3.86771800	1.29150700
H	-2.88142000	3.86741400	-1.29243100
H	-2.29639000	5.54490400	-1.27455200
H	-1.39585800	4.29292900	-2.16921700
H	-4.45210400	-1.89054600	-1.29215300
H	-3.38795300	-3.01084200	-2.16918200
H	-4.79907700	-3.63292100	-1.27447600
H	-4.45267100	-1.89059100	1.29162900
H	-4.79881800	-3.63314200	1.27468900
H	-3.38797300	-3.01001900	2.16913800
H	-3.41108600	-5.21680100	-0.00002400

H	-1.96407900	-4.70512600	0.89153900
H	-1.96371100	-4.70520300	-0.89100700

Monomer **2** optimized with CAM-B3LYP-D3BJ

C	0.01632800	-0.01667000	-0.00004000
C	1.02463900	0.98226300	-0.00004500
C	0.63701400	2.34741800	-0.00003100
C	-0.70141600	2.73439600	-0.00001300
C	-1.68153900	1.73391800	-0.00002000
C	-1.35478000	0.35850300	-0.00002700
C	-2.33526000	-0.65834100	-0.00001600
C	-2.00043000	-2.01780900	-0.00002000
C	-0.65047900	-2.36470200	0.00000400
C	0.37585600	-1.38732300	-0.00002000
C	1.74879000	-1.73447600	-0.00002100
C	2.75386800	-0.76919500	-0.00006000
C	2.37657300	0.57951700	-0.00006000
C	-1.13239400	4.20692600	0.00000900
C	-3.12004300	-3.06684400	0.00000400
C	4.24457100	-1.13197400	0.00000700
C	-1.97290600	4.49009200	-1.25562500
C	-1.97251900	4.49017000	1.25589100
C	0.06566300	5.16058000	-0.00019700
C	-3.98799800	-2.88329800	1.25550200
C	-3.98744500	-2.88391700	-1.25596100
C	-2.57302600	-4.49706800	0.00049700
C	4.90986700	-0.54564600	1.25575700
C	4.91004300	-0.54573900	-1.25569400
C	4.47156300	-2.64629900	0.00006000
H	1.99887200	-2.79468800	-0.00000300
H	3.13974700	1.36027800	-0.00005300
H	1.43004300	3.09408000	-0.00003500
H	-2.73914600	2.00466700	-0.00002500
H	-3.38358200	-0.35350200	0.00000900
H	-0.34734600	-3.41094200	0.00004400
H	4.03880100	-3.12433100	0.89096100
H	4.03868000	-3.12440400	-0.89074400
H	5.55069000	-2.85944200	0.00000200
H	4.44797800	-0.94993600	2.16884600
H	4.44819000	-0.94999100	-2.16881800
H	5.98214700	-0.79523600	1.27464900
H	5.98229100	-0.79546400	-1.27447700
H	4.82101800	0.54917000	-1.29230500
H	4.82068100	0.54925400	1.29232800

H	0.69618400	5.02487300	0.89060600
H	-0.28933500	6.20169300	-0.00019400
H	0.69594200	5.02480000	-0.89115800
H	-1.39157800	4.29152000	2.16888900
H	-2.29156000	5.54386100	1.27510100
H	-2.87669000	3.86630000	1.29229400
H	-2.87687600	3.86592600	-1.29190500
H	-2.29228900	5.54368400	-1.27460800
H	-1.39212100	4.29175900	-2.16879200
H	-4.44869400	-1.88691800	-1.29271000
H	-3.38619300	-3.00855800	-2.16891500
H	-4.79802300	-3.62893000	-1.27505100
H	-4.44960900	-1.88643200	1.29134200
H	-4.79832900	-3.62857100	1.27477300
H	-3.38706600	-3.00709200	2.16877800
H	-3.40789800	-5.21324900	0.00048100
H	-1.96128100	-4.70029800	0.89154200
H	-1.96087700	-4.70077000	-0.89016200

Monomer **2** optimized with ω B97XD

C	0.01642800	-0.01698400	0.00002800
C	1.02305000	0.98525200	0.00002900
C	0.63189200	2.35115300	0.00003100
C	-0.70894300	2.73629000	0.00001800
C	-1.68713300	1.73137000	0.00004300
C	-1.35669000	0.35521900	0.00004600
C	-2.33578500	-0.66507500	0.00004900
C	-1.99798700	-2.02565700	0.00001100
C	-0.64531000	-2.36892100	0.00001100
C	0.37978300	-1.38787500	0.00001600
C	1.75514100	-1.73221300	-0.00000900
C	2.75977300	-0.76381900	-0.00001100
C	2.37744600	0.58538500	0.00002100
C	-1.14568300	4.20992500	-0.00001800
C	-3.11719600	-3.07890600	-0.00002200
C	4.25439400	-1.12204100	-0.00000900
C	-1.98755000	4.48934500	-1.25854300
C	-1.98742800	4.48947900	1.25856900
C	0.05081700	5.16979100	-0.00012600
C	-3.98551900	-2.89670700	1.25834900
C	-3.98496100	-2.89722400	-1.25882200
C	-2.56581700	-4.51030500	0.00040800
C	4.91723100	-0.53305400	1.25876100
C	4.91744000	-0.53240400	-1.25836400

C	4.48779900	-2.63811300	-0.00039700
H	2.00651100	-2.79333800	-0.00003500
H	3.13880400	1.36959600	0.00004000
H	1.42497500	3.09950500	0.00004000
H	-2.74677300	1.99903400	0.00004500
H	-3.38583600	-0.36182600	0.00011200
H	-0.33935200	-3.41566200	0.00000400
H	4.05792400	-3.11850500	0.89172000
H	4.05781800	-3.11806000	-0.89270200
H	5.56838100	-2.84716300	-0.00051200
H	4.45105700	-0.93534600	2.17120600
H	4.45132200	-0.93410900	-2.17109700
H	5.98962200	-0.78434500	1.28156000
H	5.98980000	-0.78382100	-1.28118200
H	4.83136500	0.56363900	-1.29231100
H	4.83099000	0.56295700	1.29332600
H	0.68157100	5.03754700	0.89213100
H	-0.30819000	6.21021600	-0.00027600
H	0.68160300	5.03730100	-0.89232200
H	-1.40639700	4.28618700	2.17113700
H	-2.30546200	5.54398800	1.28162600
H	-2.89373900	3.86712600	1.29243900
H	-2.89362300	3.86665400	-1.29248800
H	-2.30596900	5.54374200	-1.28144100
H	-1.40646000	4.28639400	-2.17115100
H	-4.45500900	-1.90335400	-1.29321200
H	-3.38035000	-3.01424200	-2.17122400
H	-4.79050100	-3.64840000	-1.28195100
H	-4.45587700	-1.90295700	1.29191700
H	-4.79083400	-3.64811400	1.28159400
H	-3.38121900	-3.01298300	2.17104700
H	-3.39936300	-5.22902600	0.00033700
H	-1.95419500	-4.71285700	0.89279900
H	-1.95374700	-4.71324000	-0.89158900

Dimer **2–2** optimized with B3LYP

C	3.03394000	0.05690300	1.19476300
C	2.49989700	-0.87291100	2.13385200
C	2.83836500	-2.25003400	2.00585400
C	3.67746400	-2.71879100	0.98807400
C	4.19317700	-1.78440700	0.07201400
C	3.89174300	-0.39943600	0.14913800
C	4.40806300	0.55036000	-0.76929900
C	4.10249800	1.92020300	-0.68556200
C	3.25736900	2.34503500	0.34756900

C	2.71179300	1.43961400	1.29932200
C	1.85635400	1.86712500	2.35123300
C	1.32053800	0.97094900	3.28493100
C	1.65157700	-0.38988900	3.16028600
C	4.04816900	-4.21000300	0.84122500
C	4.70313200	2.89711100	-1.71902400
C	0.38874100	1.42217800	4.42891000
C	3.56832200	-4.72451200	-0.53587300
C	5.58214100	-4.37230300	0.94459200
C	3.40056500	-5.08366100	1.93085600
C	6.24625100	2.85201700	-1.63057000
C	4.25739400	2.48256100	-3.14041100
C	4.25224300	4.34969400	-1.48181500
C	1.01760300	1.04089800	5.78928200
C	-0.98033200	0.71933900	4.27959200
C	0.15334600	2.94238900	4.42456400
C	-3.04144000	-0.05703100	-1.19919900
C	-2.24846600	0.81262100	-2.00330900
C	-2.28029700	2.21128900	-1.73992500
C	-3.06231700	2.75765400	-0.71570900
C	-3.83714000	1.88189300	0.06567200
C	-3.84893500	0.47931800	-0.15158500
C	-4.62985800	-0.41166500	0.62867000
C	-4.63435600	-1.79972000	0.40604300
C	-3.83121800	-2.30425800	-0.62482900
C	-3.02681400	-1.45994800	-1.43956100
C	-2.20746600	-1.96787900	-2.48449400
C	-1.41927600	-1.13225400	-3.28572800
C	-1.45508800	0.25043400	-3.03341800
C	-3.09338000	4.27087400	-0.41550000
C	-5.51127100	-2.70829800	1.29425200
C	-0.53030200	-1.67253700	-4.42565100
C	-2.58000500	4.51610900	1.02179500
C	-4.54250600	4.79434200	-0.54250300
C	-2.20758200	5.07794900	-1.38214900
C	-6.99218700	-2.28526400	1.16076000
C	-5.06737000	-2.56756300	2.76898000
C	-5.40072900	-4.19245300	0.90134600
C	-1.02769700	-1.09988900	-5.77343800
C	0.93507500	-1.23756400	-4.19272900
C	-0.56422900	-3.20906300	-4.51409200
H	1.62510800	2.93182300	2.40756800
H	-4.45984900	2.27486000	0.87294700
H	-5.24337800	0.01644800	1.42513500
H	1.24853800	-1.11670100	3.86959200

H	2.41613900	-2.93937400	2.73732900
H	-3.80321700	-3.37440600	-0.83125900
H	-2.21070500	-3.04627300	-2.64505500
H	4.85153900	-2.11581700	-0.73467800
H	5.06680700	0.18369500	-1.56022500
H	-0.85374700	0.93209900	-3.63958700
H	-1.66366300	2.85350800	-2.36901700
H	2.99258500	3.39795300	0.44798800
H	-4.93115100	4.63586300	-1.56108800
H	-4.58190800	5.87500700	-0.32708600
H	-5.22619100	4.29107500	0.15769800
H	-1.54703300	4.15009800	1.13510200
H	-3.20075900	4.00568200	1.77373300
H	-2.58891600	5.59345400	1.25675500
H	-2.27274200	6.15024100	-1.13866400
H	-1.14727600	4.78817600	-1.30900200
H	-2.52526800	4.95703000	-2.42949800
H	1.09204900	3.50445000	4.54961500
H	-0.32737200	3.28382300	3.49459200
H	-0.50985600	3.21742500	5.25997200
H	1.99806000	1.52581300	5.92093200
H	-1.45611400	0.97920200	3.32073700
H	0.36492800	1.36119000	6.61826900
H	-1.65991200	1.02422400	5.09282800
H	-0.88624900	-0.37648800	4.31790200
H	1.16653200	-0.04535800	5.88431900
H	-5.16259100	-1.53244700	3.13054000
H	-4.01566400	-2.87062600	2.89377400
H	-5.68618200	-3.20724400	3.42005200
H	-7.63322800	-2.92077500	1.79411000
H	-7.15218100	-1.24073100	1.46828300
H	-7.33841500	-2.38364800	0.11946300
H	-4.37155200	-4.57017500	1.00482500
H	-5.72763000	-4.36892400	-0.13536900
H	-6.04296800	-4.80046200	1.55803700
H	3.72177300	-4.78586700	2.94121600
H	3.69383100	-6.13573500	1.78754500
H	2.30094600	-5.03964800	1.89410200
H	5.95145000	-4.01809200	1.92030100
H	5.86541500	-5.43260900	0.83738600
H	6.11040700	-3.80628400	0.16240900
H	4.03322900	-4.17156600	-1.36616000
H	3.82397300	-5.79000200	-0.66005700
H	2.47596700	-4.62214700	-0.63578000
H	-0.20640500	-3.68098600	-3.58563100

H	-1.57675100	-3.58809300	-4.72321600
H	0.08962100	-3.54942900	-5.33257400
H	-0.40121000	-1.46614700	-6.60381100
H	1.58359400	-1.63440800	-4.99141200
H	1.04596000	-0.14265300	-4.19105200
H	-0.99301800	0.00018200	-5.78847900
H	1.31427500	-1.61023900	-3.22801100
H	-2.06784600	-1.40416900	-5.97145100
H	4.58887000	1.46486300	-3.39600600
H	3.15982500	2.50962900	-3.23248300
H	4.67987100	3.16952200	-3.89233600
H	6.64052200	1.84481800	-1.83382200
H	6.69542500	3.54095800	-2.36512000
H	6.59254000	3.15012900	-0.62810200
H	4.70069000	5.00782400	-2.24276800
H	4.56879900	4.72337300	-0.49552700
H	3.15868200	4.45790900	-1.55393600

Dimer **2–2** optimized with B3LYP-D3

C	-0.03649400	0.04094000	1.55175300
C	-1.06369200	-0.94577300	1.54462600
C	-0.69271600	-2.31670800	1.56542100
C	0.64437100	-2.72393000	1.63674300
C	1.64131700	-1.73623200	1.58853700
C	1.33525600	-0.35097500	1.56544200
C	2.32910300	0.66327600	1.57409100
C	2.00748600	2.02973000	1.61713000
C	0.65631400	2.38835600	1.55165000
C	-0.38147900	1.42038600	1.54248900
C	-1.75297200	1.78474100	1.55215600
C	-2.77792600	0.83384600	1.59884000
C	-2.41690600	-0.52118700	1.53852900
C	1.04085500	-4.20440600	1.81530300
C	3.12662200	3.08294800	1.76550700
C	-4.26270800	1.23494300	1.73161500
C	2.00872300	-4.65203500	0.70057700
C	1.73976000	-4.36074600	3.18581900
C	-0.17765100	-5.14393800	1.78805400
C	3.94971000	2.76563100	3.03503900
C	4.06085600	3.05900700	0.53786300
C	2.56811800	4.51023300	1.90759900
C	-4.89956900	0.46361500	2.90989700
C	-5.02483500	0.89376600	0.43396700
C	-4.43448800	2.73981300	2.00739100

C	0.03649400	-0.04095400	-1.55175500
C	1.06369400	0.94576200	-1.54474600
C	0.69271300	2.31669200	-1.56552400
C	-0.64437500	2.72392600	-1.63665300
C	-1.64132000	1.73622400	-1.58833100
C	-1.33524300	0.35096700	-1.56529800
C	-2.32910800	-0.66328300	-1.57379100
C	-2.00750900	-2.02973200	-1.61692000
C	-0.65632100	-2.38835700	-1.55149400
C	0.38148300	-1.42040200	-1.54242000
C	1.75298300	-1.78474800	-1.55209800
C	2.77791100	-0.83384900	-1.59907200
C	2.41689600	0.52119100	-1.53885500
C	-1.04079800	4.20441600	-1.81523300
C	-3.12664500	-3.08296500	-1.76525000
C	4.26267000	-1.23492100	-1.73197900
C	-2.00894800	4.65204000	-0.70076900
C	-1.73931800	4.36079600	-3.18595100
C	0.17771400	5.14394000	-1.78762900
C	-3.94961600	-2.76568400	-3.03486100
C	-4.06100900	-3.05897900	-0.53770600
C	-2.56819300	-4.51030000	-1.90716700
C	4.89952500	-0.46345200	-2.91017800
C	5.02478500	-0.89388900	-0.43429500
C	4.43445900	-2.73975700	-2.00801300
H	-1.98535100	2.84651000	1.58042300
H	-2.69353400	2.02230000	-1.63175100
H	-3.37196000	-0.34822000	-1.61029200
H	-3.18795300	-1.29079000	1.55325800
H	-1.49675000	-3.05004100	1.58377500
H	-0.35861800	-3.43568900	-1.56374600
H	1.98535600	-2.84651900	-1.58004400
H	2.69352300	-2.02231900	1.63212200
H	3.37196800	0.34828800	1.61094400
H	3.18796400	1.29076100	-1.55374200
H	1.49675600	3.05000800	-1.58399200
H	0.35853900	3.43567200	1.56401600
H	-1.07257800	4.04182000	-4.00252600
H	-2.01956200	5.41305300	-3.36064700
H	-2.65526500	3.75342400	-3.24551800
H	-1.52332100	4.60311100	0.28544700
H	-2.91184000	4.02612000	-0.66441300
H	-2.33069700	5.69292300	-0.86778200
H	-0.15215100	6.18833800	-1.90267800
H	0.72541500	5.07037400	-0.83565900

H	0.88211400	4.92760000	-2.60532200
H	-3.91098000	3.04638300	2.92633000
H	-4.05805300	3.35639300	1.17815500
H	-5.50264300	2.97650200	2.13387700
H	-4.36291700	0.67003800	3.84932400
H	-4.61220000	1.44808900	-0.42256300
H	-5.95182100	0.76515500	3.04134100
H	-6.09068800	1.15850900	0.52950100
H	-4.96472700	-0.17867300	0.20247100
H	-4.88606200	-0.62432200	2.74728000
H	-4.51143800	-2.06807100	-0.38878600
H	-3.51329300	-3.32318900	0.37950500
H	-4.88111800	-3.78465800	-0.66351200
H	-4.73928300	-3.52124800	-3.18092600
H	-4.43779600	-1.78165900	-2.97171900
H	-3.30548700	-2.76409300	-3.92828700
H	-1.99714000	-4.81640200	-1.01751800
H	-1.91208400	-4.60716600	-2.78590600
H	-3.39706300	-5.22527800	-2.02795800
H	-0.88206000	-4.92729600	2.60565600
H	0.15222000	-6.18829300	1.90348600
H	-0.72529400	-5.07073400	0.83602200
H	1.07321200	-4.04187500	4.00259500
H	2.02016500	-5.41297900	3.36040100
H	2.65566900	-3.75329900	3.24519000
H	2.91155600	-4.02604400	0.66396500
H	2.33056500	-5.69289800	0.86754300
H	1.52286900	-4.60318700	-0.28554000
H	4.05887700	-3.35657100	-1.17854800
H	3.91031000	-3.04633500	-2.92658000
H	5.50256300	-2.97623100	-2.13536000
H	5.95184400	-0.76480800	-3.04150200
H	6.09042500	-1.15964000	-0.52941100
H	4.96558500	0.17872100	-0.20326800
H	4.88582600	0.62447900	-2.74755500
H	4.61136000	-1.44741300	0.42234300
H	4.36302200	-0.66995400	-3.84967300
H	4.51102800	2.06800600	0.38876700
H	3.51302600	3.32345400	-0.37920800
H	4.88112700	3.78450600	0.66366200
H	4.43833800	1.78184400	2.97163200
H	4.73905700	3.52148400	3.18131600
H	3.30558100	2.76351800	3.92846300
H	3.39695500	5.22525100	2.02838300
H	1.91206600	4.60695000	2.78639900

H	1.99696700	4.81641000	1.01803600
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Dimer **2–2** optimized with B3LYP-D3BJ

C	-0.03315700	0.03603100	1.51696000
C	-1.05453900	-0.95559600	1.51000700
C	-0.67625000	-2.32326900	1.52750800
C	0.66220600	-2.72131100	1.60111800
C	1.65387100	-1.73057400	1.55100400
C	1.34004200	-0.34799300	1.53068200
C	2.32752800	0.67101700	1.54060900
C	1.99693500	2.03367900	1.58807700
C	0.64551400	2.38581100	1.52052700
C	-0.38576200	1.41280200	1.51087400
C	-1.75795000	1.76923400	1.52197300
C	-2.77586400	0.81269400	1.57151700
C	-2.40924000	-0.53916900	1.50628200
C	1.06349900	-4.19619200	1.78634900
C	3.10609600	3.09177100	1.74265500
C	-4.25848500	1.20712000	1.71212500
C	2.05278900	-4.63992200	0.69241700
C	1.73837500	-4.34383900	3.16741600
C	-0.14856800	-5.13938900	1.73978000
C	3.92444800	2.77477400	3.01242300
C	4.04477800	3.07926900	0.52095100
C	2.53555500	4.51144100	1.88707200
C	-4.88778900	0.42096000	2.88133800
C	-5.02474000	0.88096500	0.41544400
C	-4.42994000	2.70633700	2.00572500
C	0.03321900	-0.03604500	-1.51710900
C	1.05459800	0.95558700	-1.51029100
C	0.67633000	2.32326900	-1.52778900
C	-0.66212300	2.72132300	-1.60128300
C	-1.65379200	1.73057700	-1.55107000
C	-1.33997100	0.34800600	-1.53071100
C	-2.32748800	-0.67099100	-1.54038000
C	-1.99694800	-2.03365500	-1.58792900
C	-0.64553100	-2.38582600	-1.52055100
C	0.38578600	-1.41283500	-1.51096800
C	1.75795500	-1.76928700	-1.52202300
C	2.77586900	-0.81273200	-1.57178500
C	2.40928600	0.53913400	-1.50675400
C	-1.06345100	4.19619000	-1.78662400
C	-3.10619100	-3.09172300	-1.74208400
C	4.25848600	-1.20715400	-1.71229700

C	-2.05334400	4.63978000	-0.69318400
C	-1.73763400	4.34380100	-3.16804100
C	0.14850200	5.13950500	-1.73942800
C	-3.92490800	-2.77492700	-3.01163800
C	-4.04451400	-3.07894800	-0.52007000
C	-2.53575000	-4.51143300	-1.88642000
C	4.88783400	-0.42128000	-2.88168800
C	5.02456100	-0.88058200	-0.41563100
C	4.43001800	-2.70643000	-2.00553500
H	-1.99758600	2.82875300	1.55596500
H	-2.70689500	2.01131100	-1.59660400
H	-3.37157800	-0.36274300	-1.58170700
H	-3.17524200	-1.31277400	1.52651000
H	-1.47405100	-3.06272300	1.54809300
H	-0.34443900	-3.43158200	-1.53954900
H	1.99763300	-2.82880400	-1.55572700
H	2.70697200	-2.01130000	1.59663900
H	3.37163900	0.36286200	1.58234500
H	3.17536000	1.31266300	-1.52731900
H	1.47415300	3.06270200	-1.54840600
H	0.34436800	3.43155200	1.53928200
H	-1.05436900	4.02600900	-3.97072600
H	-2.02147000	5.39330400	-3.35096100
H	-2.64721600	3.72887500	-3.24010700
H	-1.58654100	4.59854600	0.30204000
H	-2.95190700	4.00741600	-0.67191100
H	-2.37859900	5.67731900	-0.87100800
H	-0.18517500	6.18203700	-1.85651600
H	0.68338200	5.06516700	-0.78078400
H	0.86482800	4.92780400	-2.54728600
H	-3.89886100	3.00306600	2.92302900
H	-4.06125000	3.33200800	1.18039700
H	-5.49729700	2.93829000	2.14379400
H	-4.34899000	0.61861300	3.82097700
H	-4.61528800	1.44380100	-0.43653800
H	-5.94034700	0.71715600	3.01883600
H	-6.08918400	1.14674700	0.51894200
H	-4.96771200	-0.18889300	0.17264900
H	-4.86889800	-0.66433800	2.70495500
H	-4.50495800	-2.09281200	-0.37174600
H	-3.49881000	-3.33999000	0.39884300
H	-4.85631600	-3.81223500	-0.65191700
H	-4.71027400	-3.53344900	-3.16245100
H	-4.41578100	-1.79283000	-2.94582700
H	-3.27732200	-2.76749500	-3.90204100

H	-1.96509700	-4.81473100	-0.99609000
H	-1.87536800	-4.59893400	-2.76238000
H	-3.35840600	-5.23198100	-2.01270100
H	-0.86459200	-4.92746300	2.54784900
H	0.18504300	-6.18193600	1.85692000
H	-0.68377000	-5.06516500	0.78130600
H	1.05558200	-4.02592200	3.97045400
H	2.02215400	-5.39337500	3.35022100
H	2.64809600	-3.72906100	3.23900500
H	2.95122500	-4.00741200	0.67042600
H	2.37832400	-5.67736000	0.87034700
H	1.58536600	-4.59913300	-0.30254500
H	4.06117100	-3.33198300	-1.18018700
H	3.89908800	-3.00334300	-2.92287000
H	5.49739700	-2.93840100	-2.14337800
H	5.94032300	-0.71769700	-3.01923600
H	6.08884900	-1.14724100	-0.51849400
H	4.96821500	0.18951400	-0.17370200
H	4.86918300	0.66404800	-2.70544600
H	4.61427900	-1.44238300	0.43661600
H	4.34890900	-0.61896100	-3.82124600
H	4.50475600	2.09298400	0.37218200
H	3.49950200	3.34122800	-0.39795600
H	4.85693200	3.81204500	0.65350800
H	4.41659900	1.79335500	2.94592700
H	4.70879400	3.53411300	3.16442400
H	3.27634700	2.76566400	3.90242900
H	3.35815900	5.23203100	2.01344200
H	1.87511100	4.59883800	2.76299600
H	1.96493600	4.81476100	0.99672800

Dimer **2–2** optimized with PBE0

C	1.09645400	-0.23400900	2.10700400
C	1.34914200	1.16407000	2.12282600
C	0.31403000	2.04290000	2.53730300
C	-0.94304200	1.57643200	2.92498900
C	-1.17247900	0.19330500	2.89899400
C	-0.17895100	-0.73016300	2.49601000
C	-0.40335900	-2.12597400	2.45999700
C	0.58711100	-3.03308200	2.05852400
C	1.83429300	-2.52516700	1.68879100
C	2.11426400	-1.13479000	1.69993900
C	3.37431700	-0.61406900	1.31253700
C	3.64132700	0.75625300	1.31261200

C	2.62158400	1.62779600	1.72116400
C	-2.06906900	2.51827600	3.37062500
C	0.26777700	-4.53337800	2.03030600
C	4.99496500	1.33151600	0.87642800
C	-3.27890000	2.33739000	2.44038700
C	-2.47354500	2.17970000	4.81397100
C	-1.64653000	3.98845400	3.32356000
C	-0.14090300	-4.99608800	3.43744800
C	-0.88942800	-4.78331900	1.04998700
C	1.46584800	-5.37236100	1.57984500
C	5.60440800	2.13968700	2.03257200
C	4.78434800	2.25022400	-0.33774300
C	5.98904000	0.23686600	0.48158100
C	-1.09651300	0.23400100	-2.10719400
C	-1.34942900	-1.16404500	-2.12230200
C	-0.31467700	-2.04320000	-2.53698500
C	0.94229400	-1.57709000	-2.92544100
C	1.17201300	-0.19400200	-2.89996800
C	0.17881600	0.72978800	-2.49690000
C	0.40348000	2.12557400	-2.46148900
C	-0.58668600	3.03301800	-2.06002900
C	-1.83383100	2.52546300	-1.68967700
C	-2.11401800	1.13512600	-1.70012700
C	-3.37398300	0.61477300	-1.31196200
C	-3.64114900	-0.75551500	-1.31114100
C	-2.62172600	-1.62740400	-1.71975200
C	2.06798800	-2.51930400	-3.37114700
C	-0.26704600	4.53325800	-2.03236400
C	-4.99456100	-1.33036100	-0.87372100
C	3.27756900	-2.33929600	-2.44039900
C	2.47310300	-2.18046500	-4.81424200
C	1.64474700	-3.98930200	-3.32472900
C	0.14207200	4.99535700	-3.43958000
C	0.88996900	4.78331700	-1.05184600
C	-1.46505400	5.37266900	-1.58253600
C	-5.60445800	-2.14005500	-2.02855100
C	-4.78327300	-2.24748400	0.34153400
C	-5.98855900	-0.23529800	-0.47981300
H	4.14086200	-1.32623200	1.00391900
H	2.14638000	0.20411700	-3.19511800
H	1.39129900	2.48892900	-2.75683500
H	2.79637400	2.70692200	1.73301900
H	0.53341100	3.11150100	2.54287300
H	-2.63332000	3.19826000	-1.37583000
H	-4.14032200	1.32720900	-1.00346500

H	-2.14688200	-0.20509800	3.19363400
H	-1.39118200	-2.48965600	2.75493600
H	-2.79666100	-2.70651400	-1.73095800
H	-0.53425300	-3.11176200	-2.54210600
H	2.63398500	-3.19771600	1.37493800
H	1.62210100	-2.30520700	-5.50161900
H	3.28573800	-2.84396700	-5.15188000
H	2.82837100	-1.14339700	-4.90739200
H	3.00503600	-2.56434900	-1.39777700
H	3.66567000	-1.31003700	-2.46614200
H	4.09630400	-3.01397200	-2.73917100
H	2.48090300	-4.62720000	-3.65031100
H	1.36560500	-4.30291900	-2.30677400
H	0.79398400	-4.19318100	-3.99290400
H	6.19942400	-0.44675500	1.31839600
H	5.62484900	-0.36169200	-0.36766000
H	6.94406600	0.69348800	0.17906400
H	5.76535600	1.50246100	2.91585600
H	4.34532100	1.69207500	-1.17957800
H	6.57714900	2.56352800	1.73483300
H	5.74501200	2.67497600	-0.67143200
H	4.11031500	3.08829200	-0.10526500
H	4.95616500	2.97483400	2.33677100
H	1.80080700	4.24055900	-1.34582700
H	0.61976400	4.45346900	-0.03650500
H	1.13617900	5.85685100	-1.01189200
H	0.37992800	6.07143200	-3.43716400
H	1.02970000	4.45872500	-3.80612600
H	-0.67219600	4.82701800	-4.16126800
H	-1.78891800	5.11261600	-0.56282400
H	-2.32638500	5.25301700	-2.25755500
H	-1.19179900	6.43914400	-1.58041300
H	-0.79597700	4.19307000	3.99177800
H	-2.48302800	4.62611100	3.64873500
H	-1.36732600	4.30174900	2.30551600
H	-1.62240400	2.30519500	5.50103800
H	-3.28648900	2.84281100	5.15164100
H	-2.82811300	1.14242800	4.90754100
H	-3.66681400	1.30808300	2.46695700
H	-4.09768200	3.01206500	2.73903200
H	-3.00684200	2.56181500	1.39750700
H	-5.62400900	0.36442100	0.36845200
H	-6.19941000	0.44720400	-1.31742800
H	-6.94338700	-0.69161900	-0.17622400
H	-6.57710900	-2.56344400	-1.72988100

H	-5.74367400	-2.67223400	0.67598600
H	-4.10890500	-3.08552600	0.10993000
H	-4.95639300	-2.97565900	-2.33186900
H	-4.34429600	-1.68806700	1.18255800
H	-5.76570200	-1.50401000	-2.91263200
H	-1.80040500	-4.24112400	1.34457400
H	-0.61968000	-4.45274200	0.03476300
H	-1.13521900	-5.85692600	1.00947600
H	-1.02852800	-4.45972800	3.80440700
H	-0.37857300	-6.07220400	3.43469600
H	0.67351600	-4.82787200	4.15899400
H	1.19275100	-6.43887400	1.57715700
H	2.32725300	-5.25297700	2.25481700
H	1.78954200	-5.11167200	0.56024100

Dimer **2–2** optimized with PBE0-D3

C	-0.04100900	0.05267800	1.55746500
C	-1.04695900	-0.95000800	1.55763500
C	-0.65201000	-2.31060400	1.59301400
C	0.68883900	-2.69106500	1.66633100
C	1.66529100	-1.68764500	1.61677300
C	1.33375400	-0.31252000	1.57860700
C	2.30677500	0.71612900	1.59553300
C	1.96038800	2.07334300	1.63473000
C	0.60662200	2.40641000	1.57030400
C	-0.41017600	1.42152600	1.55174400
C	-1.78418900	1.76037100	1.57110300
C	-2.78853600	0.79310700	1.61717600
C	-2.40417400	-0.55250800	1.56037500
C	1.11088100	-4.15396000	1.85823600
C	3.05386100	3.14056300	1.78577300
C	-4.27194300	1.16507400	1.75160600
C	2.10078100	-4.58198400	0.76745000
C	1.78573300	-4.28448000	3.23347100
C	-0.08231500	-5.11101800	1.81583500
C	3.86283900	2.84606000	3.05894300
C	3.99334600	3.12019400	0.57321200
C	2.47098600	4.55021700	1.90988800
C	-4.88214700	0.40040400	2.93654300
C	-5.02566400	0.79306300	0.46798100
C	-4.46828800	2.66168700	2.00636200
C	0.04103600	-0.05264400	-1.55737000
C	1.04700700	0.95001800	-1.55774500
C	0.65208600	2.31061700	-1.59326400

C	-0.68876600	2.69109900	-1.66644800
C	-1.66523400	1.68770500	-1.61659700
C	-1.33371600	0.31258100	-1.57838700
C	-2.30676800	-0.71605400	-1.59518300
C	-1.96041500	-2.07327200	-1.63450900
C	-0.60664700	-2.40636500	-1.57005700
C	0.41016800	-1.42150300	-1.55153600
C	1.78417000	-1.76037200	-1.57086000
C	2.78853200	-0.79313800	-1.61723600
C	2.40421800	0.55249500	-1.56060700
C	-1.11084200	4.15398000	-1.85843000
C	-3.05389200	-3.14047100	-1.78567600
C	4.27190000	-1.16521100	-1.75166900
C	-2.10013400	4.58218300	-0.76719200
C	-1.78638100	4.28429100	-3.23335400
C	0.08241300	5.11101200	-1.81684000
C	-3.86309900	-2.84561800	-3.05862100
C	-3.99318300	-3.12050600	-0.57295500
C	-2.47097700	-4.55006000	-1.91033700
C	4.88230100	-0.40033900	-2.93637900
C	5.02551900	-0.79355000	-0.46790000
C	4.46809200	-2.66179900	-2.00675700
H	-2.03812500	2.81873900	1.60481900
H	-2.72354700	1.95389500	-1.66743000
H	-3.35656800	-0.41953400	-1.63656200
H	-3.16178700	-1.33762600	1.58050800
H	-1.44160300	-3.06130900	1.61843200
H	-0.29148000	-3.44987500	-1.58799800
H	2.03808500	-2.81874900	-1.60420900
H	2.72359200	-1.95382900	1.66781200
H	3.35658600	0.41968000	1.63719000
H	3.16184800	1.33758800	-1.58093700
H	1.44170200	3.06129200	-1.61888600
H	0.29139100	3.44989300	1.58824200
H	-1.09977200	3.97579900	-4.03661600
H	-2.08855500	5.32788800	-3.41940700
H	-2.68591400	3.65449700	-3.30329200
H	-1.62916900	4.54744200	0.22653800
H	-2.98983900	3.93664900	-0.74231900
H	-2.44181900	5.61454700	-0.94368400
H	-0.26581900	6.14805900	-1.93933500
H	0.61805700	5.04988400	-0.85709700
H	0.80146500	4.90647500	-2.62434700
H	-3.95035600	2.98921200	2.92080100
H	-4.10328400	3.27391700	1.16859800

H	-5.53996800	2.88049600	2.13093100
H	-4.34761900	0.63300800	3.87038600
H	-4.62735600	1.34552900	-0.39641200
H	-5.94037800	0.67832800	3.06742400
H	-6.09635500	1.03530800	0.56306500
H	-4.94213600	-0.28090000	0.24957200
H	-4.84213600	-0.68882400	2.78960500
H	-4.45949300	-2.13475000	-0.43657300
H	-3.44884800	-3.36806100	0.35079300
H	-4.80092600	-3.85913500	-0.69880100
H	-4.64097100	-3.61217300	-3.20641400
H	-4.36383300	-1.86753300	-3.00794500
H	-3.21047600	-2.84208600	-3.94514500
H	-1.90161900	-4.83787900	-1.01349000
H	-1.80675900	-4.64216800	-2.78306900
H	-3.28544000	-5.28056300	-2.03174200
H	-0.80187200	-4.90661700	2.62292300
H	0.26587900	-6.14806600	1.93843100
H	-0.61736700	-5.04977800	0.85576700
H	1.09866500	-3.97630700	4.03646600
H	2.08802000	-5.32806000	3.41944100
H	2.68510400	-3.65451800	3.30402100
H	2.99044600	-3.93638100	0.74308100
H	2.44245000	-5.61433200	0.94407600
H	1.63035800	-4.54728700	-0.22654300
H	4.10359600	-3.27418500	-1.16887600
H	3.94968400	-2.98919000	-2.92097200
H	5.53970900	-2.88058400	-2.13192300
H	5.94041300	-0.67862600	-3.06744000
H	6.09599400	-1.03695300	-0.56245400
H	4.94304000	0.28059700	-0.24993800
H	4.84276700	0.68884900	-2.78900600
H	4.62623000	-1.34520900	0.39654100
H	4.34761200	-0.63237000	-3.87027000
H	4.45942000	2.13430400	0.43701600
H	3.44919100	3.36775800	-0.35064300
H	4.80124600	3.85865000	0.69907100
H	4.36372900	1.86803800	3.00854200
H	4.64057000	3.61275100	3.20676800
H	3.21002900	2.84258700	3.94533000
H	3.28547400	5.28074200	2.03101500
H	1.80675500	4.64269600	2.78256800
H	1.90166000	4.83769600	1.01291500

Dimer **2–2** optimized with PBE0-D3BJ

C	-0.03263300	0.04044600	1.51863200
C	-1.03293600	-0.96743600	1.51669800
C	-0.63034500	-2.32506300	1.54386200
C	0.71242200	-2.69710500	1.62028500
C	1.68317000	-1.68982200	1.56543000
C	1.34392400	-0.31684700	1.53549600
C	2.31075600	0.71731700	1.54985100
C	1.95596300	2.07110300	1.59889400
C	0.60111800	2.39699000	1.52948800
C	-0.40949700	1.40687200	1.51415900
C	-1.78481600	1.73772100	1.53216400
C	-2.78289100	0.76495600	1.58583600
C	-2.39220100	-0.57751800	1.51919100
C	1.14026600	-4.15569300	1.82124100
C	3.03976200	3.14398300	1.76590000
C	-4.26485200	1.13011000	1.74031300
C	2.14423600	-4.58475300	0.74546500
C	1.80058600	-4.27442100	3.20366600
C	-0.04698800	-5.11811900	1.77180900
C	3.83566400	2.84596300	3.04535900
C	3.99344400	3.13994300	0.56566400
C	2.44509400	4.54726400	1.89335500
C	-4.85532100	0.35395300	2.92651000
C	-5.03697900	0.76761000	0.46615600
C	-4.46124000	2.62297300	2.01081400
C	0.03262900	-0.04044700	-1.51864200
C	1.03293800	0.96742200	-1.51676700
C	0.63036700	2.32505900	-1.54390400
C	-0.71239800	2.69711700	-1.62027400
C	-1.68315700	1.68984500	-1.56531100
C	-1.34392200	0.31686300	-1.53538000
C	-2.31076900	-0.71728800	-1.54958900
C	-1.95598900	-2.07108500	-1.59872600
C	-0.60114300	-2.39698200	-1.52949600
C	0.40949100	-1.40687500	-1.51421100
C	1.78479900	-1.73772500	-1.53229800
C	2.78288400	-0.76496300	-1.58601200
C	2.39220100	0.57750600	-1.51936900
C	-1.14020200	4.15570000	-1.82134600
C	-3.03979200	-3.14397500	-1.76562400
C	4.26483800	-1.13013200	-1.74047500
C	-2.14416100	4.58494300	-0.74564800
C	-1.80054500	4.27427400	-3.20378200
C	0.04708700	5.11809800	-1.77210600
C	-3.83584200	-2.84596500	-3.04498500

C	-3.99332500	-3.13995700	-0.56526400
C	-2.44512600	-4.54725100	-1.89315400
C	4.85535300	-0.35401100	-2.92667300
C	5.03689600	-0.76758900	-0.46630100
C	4.46120300	-2.62301200	-2.01091800
H	-2.04521300	2.79404700	1.57183600
H	-2.74258800	1.95037000	-1.61778000
H	-3.36180800	-0.42725300	-1.59617800
H	-3.14479900	-1.36673600	1.54626300
H	-1.41444500	-3.08113500	1.57304700
H	-0.28121600	-3.43862900	-1.55511900
H	2.04520100	-2.79404900	-1.57201000
H	2.74260000	-1.95034200	1.61795800
H	3.36179600	0.42733200	1.59673900
H	3.14475200	1.36676000	-1.54649900
H	1.41448500	3.08111100	-1.57312600
H	0.28114500	3.43862200	1.55507900
H	-1.10333500	3.96410700	-3.99691700
H	-2.10587900	5.31498700	-3.39959100
H	-2.69534100	3.63863800	-3.27899000
H	-1.68565500	4.56229700	0.25411200
H	-3.02973200	3.93377100	-0.72688100
H	-2.49016600	5.61337300	-0.93499300
H	-0.30585100	6.15266600	-1.90024900
H	0.57533400	5.06202400	-0.80824200
H	0.77357200	4.91498400	-2.57299600
H	-3.92951900	2.94411700	2.91933500
H	-4.11171600	3.24333200	1.17274900
H	-5.53141300	2.83642100	2.15456100
H	-4.30849800	0.58081500	3.85440200
H	-4.65345900	1.32723200	-0.40007300
H	-5.91237700	0.62711800	3.07421100
H	-6.10585500	1.00877700	0.58037400
H	-4.95715000	-0.30454300	0.23848400
H	-4.81262800	-0.73357200	2.76943700
H	-4.47083200	-2.15970500	-0.42903500
H	-3.45927400	-3.38922900	0.36385900
H	-4.79218500	-3.88511300	-0.70671600
H	-4.60751000	-3.61581800	-3.20624200
H	-4.34140500	-1.87060800	-2.99304700
H	-3.17309200	-2.83306200	-3.92362600
H	-1.88202900	-4.83589600	-0.99288900
H	-1.77197600	-4.62869100	-2.75980500
H	-3.25308500	-5.28252400	-2.02681600
H	-0.77361200	-4.91506300	2.57258700

H	0.30595400	-6.15268400	1.89995400
H	-0.57504400	-5.06196600	0.80784600
H	1.10329400	-3.96453600	3.99684300
H	2.10609700	-5.31511800	3.39928300
H	2.69526100	-3.63863600	3.27903500
H	3.02974800	-3.93350500	0.72671200
H	2.49032100	-5.61317900	0.93468700
H	1.68562300	-4.56205100	-0.25424300
H	4.11163500	-3.24333200	-1.17284100
H	3.92948300	-2.94417400	-2.91943200
H	5.53137200	-2.83648600	-2.15464400
H	5.91236300	-0.62732100	-3.07443900
H	6.10567900	-1.00932500	-0.58019400
H	4.95754500	0.30468700	-0.23900900
H	4.81283600	0.73351200	-2.76952800
H	4.65287500	-1.32669500	0.40002700
H	4.30845300	-0.58074400	-3.85455100
H	4.47070300	2.15958700	0.42930700
H	3.45960500	3.38957000	-0.36348400
H	4.79248100	3.88486500	0.70736800
H	4.34156100	1.87078400	2.99330500
H	4.60705500	3.61602900	3.20692100
H	3.17275500	2.83265500	3.92387400
H	3.25302500	5.28250800	2.02734500
H	1.77167200	4.62865800	2.75979900
H	1.88228400	4.83597300	0.99293000

Dimer **2–2** optimized with M06

C	-0.00312400	0.08808500	1.63911700
C	-0.85460600	-1.04804400	1.66811300
C	-0.26884500	-2.33950000	1.70547900
C	1.11423000	-2.52289900	1.75577600
C	1.93419200	-1.38838000	1.70169200
C	1.40847500	-0.07724600	1.65039700
C	2.22727600	1.07642500	1.63916300
C	1.69537900	2.37205000	1.63569700
C	0.30632800	2.51003700	1.59443000
C	-0.56137400	1.39096900	1.61944000
C	-1.96841400	1.53202300	1.66214700
C	-2.82450300	0.43249300	1.73044100
C	-2.25322700	-0.84643400	1.69160600
C	1.75388500	-3.90326200	1.92413700
C	2.62867600	3.57927900	1.75721000
C	-4.34276700	0.59199800	1.84786900

C	2.77729200	-4.16411100	0.81683200
C	2.45772100	-3.95208800	3.28474800
C	0.72291700	-5.02649900	1.88347600
C	3.20721200	3.59691000	3.17663200
C	3.77764600	3.49129800	0.75100000
C	1.89980400	4.89904500	1.52252400
C	-4.86575700	-0.26082500	3.00746600
C	-5.00889700	0.13881500	0.54714600
C	-4.75082400	2.03910400	2.11260800
C	0.00307100	-0.08811800	-1.63909800
C	0.85454000	1.04801300	-1.66794600
C	0.26878800	2.33946100	-1.70536200
C	-1.11428700	2.52287100	-1.75584500
C	-1.93424300	1.38835200	-1.70192100
C	-1.40853600	0.07721200	-1.65054200
C	-2.22732900	-1.07645200	-1.63939900
C	-1.69538600	-2.37206100	-1.63579700
C	-0.30634100	-2.51003700	-1.59437700
C	0.56135400	-1.39097600	-1.61937600
C	1.96839300	-1.53199900	-1.66200600
C	2.82449400	-0.43245100	-1.73015100
C	2.25317800	0.84645700	-1.69122000
C	-1.75389700	3.90324500	-1.92425400
C	-2.62859900	-3.57935400	-1.75723700
C	4.34276800	-0.59190900	-1.84772900
C	-2.77735000	4.16407900	-0.81699100
C	-2.45766300	3.95213600	-3.28489600
C	-0.72287300	5.02643600	-1.88357200
C	-3.20743700	-3.59687500	-3.17652900
C	-3.77731400	-3.49153100	-0.75070700
C	-1.89961300	-4.89911100	-1.52281900
C	4.86543800	0.26083000	-3.00756800
C	5.00917500	-0.13850700	-0.54724900
C	4.75084100	-2.03900300	-2.11240900
H	-2.36758600	2.54960200	1.68296200
H	-3.02491800	1.49443100	-1.74405900
H	-3.31240500	-0.92611400	-1.67556700
H	-2.89301500	-1.73565200	1.72818300
H	-0.94812100	-3.19714600	1.73896300
H	0.15715100	-3.50179900	-1.58605200
H	2.36764000	-2.54953700	-1.68298100
H	3.02486900	-1.49445900	1.74364500
H	3.31234400	0.92599000	1.67511900
H	2.89285000	1.73576900	-1.72740600
H	0.94807500	3.19709200	-1.73883700

H	-0.15722800	3.50177800	1.58643600
H	-1.74289200	3.75925200	-4.10256700
H	-2.90898900	4.94589600	-3.45167900
H	-3.26122300	3.20165600	-3.36027600
H	-2.29214500	4.18071300	0.17428800
H	-3.57162600	3.39924900	-0.79082000
H	-3.26491000	5.14249000	-0.96925500
H	-1.22613400	6.00198800	-1.98820100
H	-0.17048600	5.03847100	-0.92853300
H	0.01020200	4.94498100	-2.70310200
H	-4.29591900	2.43022000	3.03821100
H	-4.47021300	2.70940500	1.28324800
H	-5.84593400	2.10247700	2.22551500
H	-4.38074300	0.02286700	3.95671600
H	-4.67526700	0.76155300	-0.30162800
H	-5.95409500	-0.12010000	3.12498300
H	-6.10700200	0.22562000	0.62129000
H	-4.76633100	-0.91044600	0.31221400
H	-4.69104200	-1.33697700	2.84931100
H	-4.41804300	-2.61206400	-0.92335400
H	-3.40099500	-3.44082000	0.28598400
H	-4.42378800	-4.38202700	-0.83170000
H	-3.88064600	-4.46177900	-3.31125800
H	-3.78368900	-2.68209400	-3.39183400
H	-2.40250800	-3.66865800	-3.92726800
H	-1.43044700	-4.93468100	-0.52459100
H	-1.11612200	-5.08167800	-2.27635400
H	-2.61272500	-5.73764300	-1.58650000
H	-0.01030400	-4.94499700	2.70287400
H	1.22620300	-6.00201400	1.98832300
H	0.17073100	-5.03868200	0.92831800
H	1.74290800	-3.75950000	4.10245300
H	2.90935000	-4.94572900	3.45141700
H	3.26103400	-3.20135400	3.36018700
H	3.57145000	-3.39916800	0.79039600
H	3.26498000	-5.14244200	0.96918000
H	2.29202500	-4.18098500	-0.17442400
H	4.47001700	-2.70935100	-1.28317300
H	4.29615500	-2.43005900	-3.03814800
H	5.84597800	-2.10243300	-2.22505300
H	5.95367000	0.11977500	-3.12566400
H	6.10729700	-0.22469500	-0.62188000
H	4.76617300	0.91060100	-0.31209500
H	4.69112100	1.33702100	-2.84922000
H	4.67632100	-0.76152100	0.30163600

H	4.37981800	-0.02264500	-3.95657100
H	4.41838800	2.61192200	0.92405000
H	3.40168100	3.44033400	-0.28581100
H	4.42404600	4.38185100	0.83197900
H	3.78320100	2.68203200	3.39222100
H	3.88058700	4.46168600	3.31133400
H	2.40213700	3.66902000	3.92718300
H	2.61289400	5.73758500	1.58634600
H	1.11611800	5.08164900	2.27584300
H	1.43088600	4.93454900	0.52417700

Dimer **2–2** optimized with M06-D3

C	-0.04105800	0.06471000	1.65388900
C	-0.95120400	-1.02414400	1.65590600
C	-0.43566900	-2.34334400	1.68152800
C	0.93354500	-2.60398500	1.72801500
C	1.81356800	-1.51458400	1.70629700
C	1.35726900	-0.17837000	1.67528300
C	2.24091500	0.92941800	1.67367700
C	1.78199400	2.24743300	1.66897200
C	0.39823200	2.46283500	1.63411900
C	-0.52939000	1.39694400	1.64221700
C	-1.92972700	1.60954100	1.65765500
C	-2.84196100	0.55433100	1.68621000
C	-2.33736000	-0.75203800	1.65001000
C	1.49114800	-4.02384900	1.84169500
C	2.73822300	3.43732300	1.78192300
C	-4.35406200	0.78089000	1.76054100
C	2.49685000	-4.29821300	0.72098200
C	2.19081400	-4.16811700	3.19718400
C	0.39371600	-5.08011000	1.75464500
C	2.66385400	3.96950100	3.21730500
C	4.18379600	3.04938400	1.48149500
C	2.35146300	4.55433600	0.81134300
C	-4.93545700	-0.01878600	2.93042400
C	-5.01180400	0.32028100	0.45732500
C	-4.70505400	2.25019200	1.97618100
C	0.05066500	-0.06262900	-1.62494900
C	0.92129200	1.05816800	-1.62825900
C	0.35813700	2.35767600	-1.66897900
C	-1.02062200	2.56655500	-1.73421400
C	-1.86078300	1.44758500	-1.69140500
C	-1.35788800	0.12704100	-1.64543000
C	-2.19555000	-1.01232600	-1.64823500

C	-1.68425900	-2.31673400	-1.67286600
C	-0.29883500	-2.47843400	-1.63295200
C	0.58788800	-1.37394000	-1.62022700
C	1.99228200	-1.53578200	-1.64145200
C	2.86998200	-0.44929000	-1.66994200
C	2.31802200	0.83666900	-1.62270800
C	-1.62548100	3.95970100	-1.92078800
C	-2.64232400	-3.50795200	-1.75982800
C	4.38769300	-0.64981700	-1.74045400
C	-2.72756000	4.21992800	-0.89261200
C	-2.22211900	4.03908100	-3.33027100
C	-0.58272600	5.06423900	-1.77807300
C	-3.58846700	-3.31538200	-2.94904200
C	-3.46388300	-3.61671300	-0.47306100
C	-1.90198700	-4.82726900	-1.95954100
C	5.02163000	0.38081500	-2.67785900
C	4.99583100	-0.48981100	-0.34497500
C	4.74838600	-2.04014300	-2.26253400
H	-2.27673200	2.64602500	1.68324000
H	-2.94865400	1.57262500	-1.74237900
H	-3.27802200	-0.84347800	-1.67024700
H	-3.02130300	-1.60799300	1.65635500
H	-1.16070100	-3.16157300	1.69923600
H	0.14834400	-3.47727200	-1.64840100
H	2.37533100	-2.55898800	-1.67453500
H	2.89638600	-1.67960400	1.74763000
H	3.31151900	0.71115400	1.70575600
H	2.96638200	1.72032900	-1.62828200
H	1.05124600	3.20288100	-1.69522600
H	-0.00364800	3.48296200	1.64309500
H	-1.44849500	3.85109100	-4.09370500
H	-2.65106000	5.03960300	-3.51522000
H	-3.02267200	3.29575400	-3.47744200
H	-2.32531700	4.19822100	0.13482600
H	-3.54214800	3.47917900	-0.95262200
H	-3.17663600	5.21441200	-1.05707800
H	-1.06344800	6.05081700	-1.88469000
H	-0.09065500	5.03474200	-0.79135500
H	0.20062100	4.99768300	-2.55114700
H	-4.26443200	2.64341200	2.90769500
H	-4.36314000	2.88386500	1.14153800
H	-5.79912500	2.36666900	2.04898000
H	-4.46163100	0.27481500	3.88227400
H	-4.63934200	0.90687400	-0.40055000
H	-6.02037100	0.16397800	3.01820000

H	-6.10657100	0.45157700	0.50709600
H	-4.81044200	-0.74383400	0.24940800
H	-4.79435400	-1.10441300	2.80694200
H	-4.03151100	-2.69395800	-0.26763800
H	-2.81127600	-3.81226200	0.39563900
H	-4.18715400	-4.44735400	-0.54442900
H	-4.25877400	-4.18624300	-3.05104800
H	-4.22434700	-2.42278900	-2.83695500
H	-3.02221900	-3.20787000	-3.88952800
H	-1.23627100	-5.06023900	-1.11157400
H	-1.29458700	-4.82259200	-2.87996600
H	-2.62643700	-5.65447800	-2.04067900
H	-0.33232600	-4.99175700	2.57966500
H	0.83632200	-6.08834900	1.81185600
H	-0.16158800	-5.01318800	0.80285800
H	1.48828100	-3.96812400	4.02368400
H	2.58634700	-5.19118100	3.32298400
H	3.03468500	-3.46670900	3.30004600
H	3.33017600	-3.57584700	0.71723400
H	2.93181100	-5.30606300	0.83464400
H	2.00713200	-4.25318700	-0.26713600
H	4.43262500	-2.84136200	-1.57419500
H	4.29179900	-2.23662600	-3.24725200
H	5.84220100	-2.12576300	-2.37302300
H	6.10335600	0.18840700	-2.77764200
H	6.08917200	-0.63909800	-0.37786500
H	4.80416800	0.51518000	0.06502300
H	4.91281400	1.41197200	-2.30511200
H	4.57319700	-1.22891400	0.35743800
H	4.57214000	0.33570500	-3.68419500
H	4.57719400	2.30324700	2.19098300
H	4.28926700	2.64170500	0.46085500
H	4.83265600	3.93794700	1.55368300
H	2.95213400	3.18796300	3.94035700
H	3.34257200	4.83011000	3.35172700
H	1.64250800	4.29766600	3.47193600
H	3.05470000	5.39923100	0.90474200
H	1.34219200	4.95279700	1.00323600
H	2.38433400	4.20361200	-0.23474800

Dimer **2–2** optimized with M06-2X

C	-0.00916800	0.00803300	1.56243100
C	-1.13239600	-0.86229300	1.55425600
C	-0.90907900	-2.26295500	1.57765000

C	0.37422500	-2.80798600	1.63614900
C	1.46906200	-1.93393000	1.59580000
C	1.30693000	-0.52847000	1.58177500
C	2.40691900	0.36839100	1.62675400
C	2.23446800	1.75194300	1.66528300
C	0.93067700	2.26053400	1.57742700
C	-0.20310900	1.41605700	1.55910500
C	-1.52919000	1.92224700	1.58312000
C	-2.64261100	1.08339400	1.63073200
C	-2.43149200	-0.30022200	1.56096500
C	0.61185200	-4.31726500	1.78624000
C	3.41557500	2.71905900	1.83034600
C	-4.06999600	1.63044100	1.77856100
C	1.44647400	-4.84542000	0.61141100
C	1.36981100	-4.57073200	3.10031000
C	-0.70066600	-5.10418800	1.83166900
C	3.15893800	3.63005100	3.04254900
C	4.73469900	1.97890400	2.06918000
C	3.56334400	3.58404100	0.57076400
C	-4.75863900	0.94325700	2.96939000
C	-4.87295600	1.34868200	0.50086200
C	-4.08074100	3.14033700	2.03577500
C	0.02485000	-0.02235500	-1.54858100
C	1.11618900	0.88854700	-1.55051500
C	0.84671800	2.28278500	-1.57563600
C	-0.45628400	2.77878100	-1.64086200
C	-1.51827700	1.86713700	-1.58737100
C	-1.31235400	0.46668500	-1.55624800
C	-2.37732800	-0.46684800	-1.56918800
C	-2.15402200	-1.84961000	-1.62431000
C	-0.83731500	-2.30800900	-1.57364200
C	0.26881600	-1.42003400	-1.55032500
C	1.60831200	-1.88385700	-1.56908200
C	2.69172000	-1.00499900	-1.61946600
C	2.43118900	0.36965700	-1.56804400
C	-0.75680400	4.27156200	-1.83647600
C	-3.34494400	-2.80764500	-1.77378000
C	4.13732600	-1.49127300	-1.79165200
C	-1.72150800	4.77733500	-0.75514000
C	-1.40754300	4.45691300	-3.21819100
C	0.51090000	5.12752400	-1.78169300
C	-4.13300900	-2.43149100	-3.03973400
C	-4.26983600	-2.70171800	-0.55314400
C	-2.89649500	-4.26547400	-1.90891900
C	4.66335200	-0.98853600	-3.14704300

C	5.02662100	-0.93737500	-0.67011100
C	4.23810300	-3.01838100	-1.77331300
H	-1.65164400	3.00369900	1.62614500
H	-2.54848200	2.22727800	-1.63781700
H	-3.39676800	-0.07522800	-1.59762900
H	-3.28184200	-0.98503400	1.57599500
H	-1.78623100	-2.90944000	1.60242000
H	-0.62046500	-3.37606500	-1.60539700
H	1.76763100	-2.96134200	-1.59675300
H	2.48808400	-2.32910800	1.63138300
H	3.40501200	-0.06447200	1.68446000
H	3.25812400	1.08315500	-1.60544800
H	1.70059500	2.95930400	-1.60208500
H	0.76113300	3.34059100	1.58819300
H	-0.73956500	4.09205400	-4.01213500
H	-1.61891200	5.52184400	-3.40220500
H	-2.35430300	3.90261700	-3.29231800
H	-1.26612600	4.69967900	0.24366400
H	-2.66129700	4.20669800	-0.75002100
H	-1.97128800	5.83430100	-0.93471600
H	0.24737300	6.18797800	-1.90642700
H	1.02522400	5.01814200	-0.81557400
H	1.21731200	4.86081300	-2.58094300
H	-3.51854300	3.39536600	2.94623000
H	-3.64670600	3.70008700	1.19546000
H	-5.11695500	3.48452600	2.16776300
H	-4.18883900	1.10859900	3.89557400
H	-4.41271200	1.84645100	-0.36605400
H	-5.77157500	1.35179400	3.10716200
H	-5.90395200	1.72077700	0.60437600
H	-4.91978300	0.27060300	0.29134100
H	-4.85292500	-0.14108300	2.81772700
H	-4.63603400	-1.67474900	-0.41467500
H	-3.74168200	-3.00430500	0.36362100
H	-5.14361900	-3.35966800	-0.67773000
H	-4.97805900	-3.12295400	-3.18083300
H	-4.53784400	-1.41153400	-2.97714000
H	-3.48716000	-2.48588100	-3.92837900
H	-2.34923000	-4.60383900	-1.01690500
H	-2.24926200	-4.40922800	-2.78630400
H	-3.77727900	-4.91333300	-2.02694700
H	-1.32364000	-4.80356400	2.68653200
H	-0.48495900	-6.17794500	1.93142200
H	-1.28587400	-4.96209900	0.91105100
H	0.79645700	-4.18839000	3.95750800

H	1.53338500	-5.65003800	3.24416400
H	2.35121100	-4.07547400	3.10198800
H	2.40894600	-4.32093200	0.53222800
H	1.65489800	-5.91824300	0.74376200
H	0.90695200	-4.71686700	-0.33918600
H	3.86386200	-3.43299300	-0.82606200
H	3.66877100	-3.47276200	-2.59707200
H	5.28955900	-3.32141100	-1.88369600
H	5.69491200	-1.33758600	-3.31005800
H	6.07035700	-1.25315000	-0.82111200
H	5.00792400	0.16164600	-0.64585300
H	4.66329900	0.10988400	-3.19532900
H	4.69559600	-1.30873300	0.31160900
H	4.03525800	-1.36297100	-3.96862900
H	4.68509000	1.35254200	2.97202700
H	4.99996600	1.33556600	1.21863300
H	5.54716800	2.70763100	2.20518600
H	3.02645000	3.03174100	3.95593900
H	4.01239800	4.30904300	3.19287300
H	2.25934900	4.24663200	2.90774300
H	4.38957300	4.30151900	0.69216200
H	2.64510900	4.15304400	0.36696000
H	3.77873000	2.95744900	-0.30808800

Dimer **2–2** optimized with M06-2X-D3

C	-0.00903300	0.00897600	1.56143900
C	-1.13209100	-0.86138400	1.55390300
C	-0.90880900	-2.26189700	1.57767100
C	0.37453000	-2.80673700	1.63540900
C	1.46933800	-1.93270300	1.59504300
C	1.30706200	-0.52735500	1.58094600
C	2.40689000	0.36957200	1.62555600
C	2.23413400	1.75312200	1.66309200
C	0.93034400	2.26154300	1.57508000
C	-0.20321400	1.41687600	1.55752100
C	-1.52922900	1.92292700	1.58136400
C	-2.64252900	1.08391200	1.62905900
C	-2.43121800	-0.29963300	1.56027500
C	0.61216500	-4.31603400	1.78347200
C	3.41536200	2.72029700	1.82574000
C	-4.06996100	1.63111800	1.77446800
C	1.44238200	-4.84302200	0.60502600
C	1.37497100	-4.57052500	3.09440200
C	-0.70067200	-5.10213000	1.83248600

C	3.15540300	3.64000900	3.03049800
C	4.73274700	1.98016400	2.07402800
C	3.56771400	3.57627400	0.56056800
C	-4.76355800	0.93860200	2.95920500
C	-4.86812300	1.35598100	0.49227600
C	-4.08000700	3.13977800	2.03889000
C	0.02483400	-0.02353400	-1.54949900
C	1.11654200	0.88677800	-1.55188600
C	0.84793000	2.28109000	-1.57705100
C	-0.45481300	2.77761500	-1.64122700
C	-1.51728100	1.86655600	-1.58785000
C	-1.31203800	0.46613500	-1.55685900
C	-2.37745900	-0.46672400	-1.56859100
C	-2.15480900	-1.84959200	-1.62266200
C	-0.83833400	-2.30867200	-1.57323600
C	0.26810700	-1.42123600	-1.55096200
C	1.60726500	-1.88578800	-1.56948200
C	2.69098400	-1.00742400	-1.61926600
C	2.43114300	0.36737000	-1.56883200
C	-0.75508300	4.27071100	-1.83317000
C	-3.34632000	-2.80713800	-1.76870500
C	4.13680800	-1.49400700	-1.78687900
C	-1.71176800	4.77511500	-0.74411900
C	-1.41515700	4.45837400	-3.20997800
C	0.51396700	5.12496400	-1.78520700
C	-4.13784900	-2.43027200	-3.03218200
C	-4.26744500	-2.70081000	-0.54523900
C	-2.89816500	-4.26492800	-1.90482200
C	4.67161400	-0.98173000	-3.13511000
C	5.01896600	-0.94896500	-0.65540100
C	4.23542000	-3.02126200	-1.77890600
H	-1.65158000	3.00433900	1.62411300
H	-2.54732500	2.22711500	-1.63789300
H	-3.39655500	-0.07437500	-1.59665800
H	-3.28115900	-0.98476700	1.57580600
H	-1.78600400	-2.90821000	1.60314800
H	-0.62188000	-3.37676900	-1.60484700
H	1.76583600	-2.96333500	-1.59696700
H	2.48837100	-2.32776300	1.63050800
H	3.40490500	-0.06329400	1.68366700
H	3.25835500	1.08048500	-1.60613200
H	1.70233900	2.95682700	-1.60411900
H	0.76044900	3.34149400	1.58547000
H	-0.75332300	4.09314500	-4.00890200
H	-1.62636500	5.52372900	-3.39158800

H	-2.36319400	3.90546600	-3.27788400
H	-1.24853100	4.69647500	0.25100100
H	-2.65077700	4.20326600	-0.73231200
H	-1.96370900	5.83209900	-0.92039200
H	0.25140900	6.18589900	-1.90755500
H	1.03321600	5.01396600	-0.82194000
H	1.21567100	4.85734000	-2.58830200
H	-3.51762000	3.39004800	2.95054800
H	-3.64557300	3.70338600	1.20136600
H	-5.11601200	3.48405500	2.17210200
H	-4.19667500	1.09815700	3.88820100
H	-4.40268900	1.85523900	-0.37099900
H	-5.77646200	1.34759600	3.09562200
H	-5.89861000	1.73037300	0.59228200
H	-4.91664500	0.27869300	0.27906200
H	-4.85875800	-0.14478100	2.80143000
H	-4.63333600	-1.67379200	-0.40623700
H	-3.73628000	-3.00262000	0.37002600
H	-5.14144600	-3.35905200	-0.66645100
H	-4.98337900	-3.12148400	-3.17148200
H	-4.54232600	-1.41028000	-2.96758800
H	-3.49437400	-2.48387200	-3.92260400
H	-2.34910800	-4.60300300	-1.01380100
H	-2.25225500	-4.40847200	-2.78320700
H	-3.77895900	-4.91304600	-2.02104100
H	-1.32123100	-4.80088400	2.68888300
H	-0.48568100	-6.17608600	1.93127700
H	-1.28818300	-4.95925500	0.91346200
H	0.80514900	-4.18818500	3.95396800
H	1.53881800	-5.64991400	3.23719300
H	2.35649800	-4.07549700	3.09230500
H	2.40459300	-4.31845300	0.52332800
H	1.65091600	-5.91610200	0.73489900
H	0.89956300	-4.71277700	-0.34345400
H	3.85767300	-3.44178600	-0.83569400
H	3.66752400	-3.46887300	-2.60737400
H	5.28670500	-3.32526200	-1.88794300
H	5.70351100	-1.33123200	-3.29482200
H	6.06383400	-1.26308000	-0.80182600
H	4.99883600	0.14983100	-0.62262900
H	4.67382500	0.11702000	-3.17489000
H	4.68142000	-1.32813800	0.32111500
H	4.04761900	-1.34862400	-3.96321700
H	4.67804900	1.35754900	2.97917300
H	5.00155400	1.33292000	1.22757300

H	5.54531500	2.70864900	2.21055000
H	3.01836500	3.04830600	3.94752900
H	4.00916300	4.31890200	3.17937000
H	2.25729100	4.25695300	2.88777600
H	4.39532000	4.29273800	0.67832700
H	2.65093000	4.14570100	0.35152300
H	3.78304400	2.94316400	-0.31361100

Dimer **2–2** optimized with LC- ω PBE

C	1.43731100	-0.18733200	1.96760200
C	1.50942800	1.22619200	2.02527300
C	0.41813800	1.94655800	2.57620200
C	-0.72063400	1.30731500	3.05756000
C	-0.77373800	-0.08958800	2.98606200
C	0.28373900	-0.85814100	2.44956900
C	0.23797000	-2.26719300	2.37425800
C	1.29187500	-3.02097100	1.84599300
C	2.41703200	-2.34279400	1.38431600
C	2.51412800	-0.92967800	1.43010100
C	3.65311100	-0.23660500	0.95389500
C	3.74193000	1.15209000	0.99428900
C	2.66506400	1.86614500	1.53258600
C	-1.90536200	2.07281300	3.65627800
C	1.16919000	-4.54751000	1.79282800
C	4.96248400	1.91613300	0.47018800
C	-3.16717300	1.76952600	2.83937200
C	-2.11200300	1.62983300	5.10986900
C	-1.68056800	3.58452400	3.64385400
C	0.98350900	-5.09210300	3.21435200
C	-0.04370900	-4.92563800	0.93368600
C	2.40856300	-5.20525900	1.18664600
C	5.57091500	2.74602000	1.60721200
C	4.52306700	2.84580800	-0.66778600
C	6.04263700	0.97819600	-0.06808100
C	-1.43720900	0.18732600	-1.96740500
C	-1.50991900	-1.22614400	-2.02563500
C	-0.41867000	-1.94678700	-2.57628000
C	0.72062600	-1.30786800	-3.05682300
C	0.77432700	0.08898400	-2.98474200
C	-0.28309700	0.85780900	-2.44852900
C	-0.23678800	2.26682200	-2.37276000
C	-1.29069400	3.02087600	-1.84489500
C	-2.41634400	2.34301100	-1.38395700
C	-2.51398800	0.92995000	-1.43020800

C	-3.65351200	0.23720300	-0.95483000
C	-3.74293700	-1.15143600	-0.99581400
C	-2.66610900	-1.86576700	-1.53381600
C	1.90530100	-2.07367900	-3.65525000
C	-1.16756100	4.54737500	-1.79149900
C	-4.96416000	-1.91512200	-0.47275300
C	3.16674800	-1.77156000	-2.83735900
C	2.11311600	-1.63000900	-5.10846500
C	1.67965400	-3.58526900	-3.64382300
C	-0.98155700	5.09204900	-3.21295200
C	0.04534500	4.92511200	-0.93220100
C	-2.40681700	5.20541400	-1.18540100
C	-5.57261300	-2.74379900	-1.61065000
C	-4.52580600	-2.84591600	0.66471400
C	-6.04395200	-0.97691300	0.06576100
H	4.47044000	-0.83183700	0.54530900
H	1.65553400	0.62177500	-3.35000400
H	0.66174000	2.76664300	-2.74262100
H	2.70189500	2.95728600	1.58027700
H	0.50059200	3.03329200	2.61216500
H	-3.26247200	2.89255400	-0.96973200
H	-4.47078700	0.83265500	-0.54646100
H	-1.65451500	-0.62263300	3.35198900
H	-0.66009800	-2.76729100	2.74485900
H	-2.70345200	-2.95686900	-1.58199700
H	-0.50159100	-3.03347100	-2.61269900
H	3.26318200	-2.89211600	0.96984500
H	1.21762600	-1.83396800	-5.71318900
H	2.95975600	-2.17055400	-5.55802000
H	2.32784800	-0.55489600	-5.18114500
H	3.02975200	-2.06608400	-1.78711000
H	3.41697200	-0.70175300	-2.85122400
H	4.02873800	-2.32237700	-3.24345000
H	2.55202100	-4.09345700	-4.07936100
H	1.54801700	-3.96997600	-2.62226600
H	0.79971500	-3.87245400	-4.23704100
H	6.41645800	0.29703000	0.70970700
H	5.67651200	0.37272200	-0.90958900
H	6.89742300	1.56683600	-0.43114600
H	5.88760800	2.09961200	2.43844900
H	4.07526600	2.27045800	-1.49120100
H	6.45224500	3.29963700	1.24974400
H	5.38554000	3.40083600	-1.06674900
H	3.77947800	3.58120000	-0.33063200
H	4.85704800	3.47926000	2.00703700

H	0.98067600	4.52354300	-1.34586200
H	-0.06256300	4.53227500	0.08918200
H	0.14821200	6.01911700	-0.87150700
H	-0.89340900	6.18885700	-3.19588600
H	-0.07559100	4.69246600	-3.68908200
H	-1.83839700	4.82798700	-3.84952100
H	-2.58098400	4.87499300	-0.15127500
H	-3.31150600	4.99193800	-1.77244800
H	-2.27504200	6.29683500	-1.16614700
H	-0.80047000	3.87255600	4.23642400
H	-2.55298000	4.09247100	4.07958300
H	-1.54970800	3.96871400	2.62200300
H	-1.21625600	1.83465900	5.71391600
H	-2.95868400	2.17012100	5.55965800
H	-2.32604300	0.55463000	5.18327100
H	-3.41690000	0.69961500	2.85416400
H	-4.02916400	2.32022100	3.24562700
H	-3.03102800	2.06335100	1.78881500
H	-5.67775900	-0.37224100	0.90781500
H	-6.41709700	-0.29499600	-0.71169200
H	-6.89922400	-1.56529100	0.42810700
H	-6.45433300	-3.29727700	-1.25393000
H	-5.38882800	-3.40057900	1.06299700
H	-3.78266400	-3.58164300	0.32730200
H	-4.85895300	-3.47705300	-2.01082200
H	-4.07781500	-2.27151000	1.48868100
H	-5.88870500	-2.09656900	-2.44147600
H	-0.97907300	-4.52407500	1.34728100
H	0.06412300	-4.53302400	-0.08779000
H	-0.14642700	-6.01967100	0.87325100
H	0.07733800	-4.69296500	3.69046400
H	0.89593800	-6.18895900	3.19741600
H	1.84022500	-4.82751700	3.85086900
H	2.27709000	-6.29671800	1.16750700
H	3.31326000	-4.99146400	1.77356800
H	2.58251500	-4.87489300	0.15246800

Dimer **2–2** optimized with LC- ω PBE-D3

C	-0.10061800	0.14428700	1.61402000
C	-1.08529400	-0.87325100	1.62591700
C	-0.66916700	-2.22539900	1.70721400
C	0.67300800	-2.58023900	1.79391700
C	1.63085300	-1.56175900	1.73981000
C	1.27578600	-0.19672800	1.65849200

C	2.23133600	0.84412300	1.67381100
C	1.86332900	2.19406100	1.67865600
C	0.50790900	2.50428000	1.61935600
C	-0.49165700	1.50238700	1.59453300
C	-1.87008500	1.81791000	1.60792100
C	-2.85421400	0.83478800	1.63275700
C	-2.44641700	-0.50273900	1.61229900
C	1.12437200	-4.02904600	2.00435000
C	2.94495000	3.27441100	1.78748600
C	-4.34712000	1.17395400	1.69847500
C	2.08804200	-4.45234500	0.89299400
C	1.83556900	-4.12543200	3.35984900
C	-0.05175300	-5.00421900	2.00850700
C	3.77115700	3.02935000	3.05589200
C	3.86259400	3.21834000	0.56312700
C	2.34990100	4.67936100	1.87281600
C	-4.99380600	0.42026200	2.86662100
C	-5.02051000	0.75668200	0.38791700
C	-4.58872600	2.66817300	1.91097500
C	0.10062800	-0.14428000	-1.61397600
C	1.08527400	0.87326700	-1.62604700
C	0.66911200	2.22540100	-1.70743800
C	-0.67307200	2.58020900	-1.79397400
C	-1.63089400	1.56170500	-1.73971500
C	-1.27578900	0.19669900	-1.65839400
C	-2.23131200	-0.84418100	-1.67361100
C	-1.86326000	-2.19410800	-1.67845800
C	-0.50784000	-2.50429300	-1.61910100
C	0.49171100	-1.50236400	-1.59432400
C	1.87014000	-1.81784100	-1.60761600
C	2.85425700	-0.83469400	-1.63279700
C	2.44641900	0.50280600	-1.61253900
C	-1.12451500	4.02900400	-2.00432400
C	-2.94484200	-3.27447200	-1.78750700
C	4.34716900	-1.17384500	-1.69857600
C	-2.08795700	4.45217300	-0.89272600
C	-1.83604100	4.12539900	-3.35964300
C	0.05154800	5.00425300	-2.00874200
C	-3.77074600	-3.02928700	-3.05609700
C	-3.86275800	-3.21856800	-0.56335300
C	-2.34975800	-4.67940500	-1.87279800
C	4.99384000	-0.42013900	-2.86670900
C	5.02053600	-0.75657400	-0.38801600
C	4.58877100	-2.66806800	-1.91111300
H	-2.14336300	2.87160900	1.62869900

H	-2.69295000	1.80796300	-1.80133800
H	-3.28591100	-0.56448100	-1.71408000
H	-3.19054300	-1.30100500	1.62148700
H	-1.44699400	-2.98756900	1.73743100
H	-0.17570700	-3.54255000	-1.62063900
H	2.14344000	-2.87154100	-1.62784600
H	2.69289600	-1.80804300	1.80160100
H	3.28593000	0.56440800	1.71434200
H	3.19045600	1.30115200	-1.62186600
H	1.44691700	2.98758000	-1.73787300
H	0.17579800	3.54254600	1.62095300
H	-1.16866500	3.80691000	-4.17331300
H	-2.15118400	5.16121500	-3.55734300
H	-2.73161200	3.48955000	-3.39323400
H	-1.58356600	4.44242900	0.08292600
H	-2.95754100	3.78453700	-0.83032800
H	-2.45931600	5.47178300	-1.07426200
H	-0.31657500	6.03142600	-2.14358300
H	0.60673400	4.97060000	-1.06073900
H	0.75402500	4.79351100	-2.82736700
H	-4.12180600	3.02462300	2.84029800
H	-4.19965700	3.26980700	1.07836900
H	-5.66840700	2.86356000	1.98130900
H	-4.50496400	0.67908000	3.81685900
H	-4.58511100	1.29770200	-0.46393100
H	-6.05986300	0.68088100	2.94601700
H	-6.09846100	0.97532600	0.41794300
H	-4.89945600	-0.31839700	0.20195300
H	-4.92924400	-0.66896800	2.74103000
H	-4.33574500	-2.23380700	-0.45831700
H	-3.29869100	-3.42286500	0.35718300
H	-4.66315400	-3.96884600	-0.64654100
H	-4.53713800	-3.81040100	-3.17230400
H	-4.28579000	-2.05938200	-3.02769000
H	-3.12817500	-3.04214100	-3.94819100
H	-1.76766900	-4.93018000	-0.97512600
H	-1.69695200	-4.79210000	-2.74999200
H	-3.15726000	-5.42040900	-1.95978500
H	-0.75444400	-4.79335500	2.82691800
H	0.31626000	-6.03140600	2.14351300
H	-0.60662900	-4.97055100	1.06032900
H	1.16797200	-3.80696900	4.17334800
H	2.15069200	-5.16124000	3.55762700
H	2.73110000	-3.48954000	3.39367000
H	2.95780200	-3.78490600	0.83085800

H	2.45916000	-5.47202600	1.07462000
H	1.58396700	-4.44248400	-0.08282700
H	4.20036700	-3.26963800	-1.07815000
H	4.12123400	-3.02464300	-2.84007200
H	5.66842200	-2.86335200	-1.98217300
H	6.05994200	-0.68061200	-2.94598800
H	6.09834000	-0.97600200	-0.41766200
H	4.90020700	0.31867300	-0.20251800
H	4.92912500	0.66908800	-2.74119300
H	4.58449600	-1.29690900	0.46393300
H	4.50513200	-0.67908600	-3.81698200
H	4.33570700	2.23361600	0.45832700
H	3.29824600	3.42220700	-0.35732800
H	4.66287300	3.96879000	0.64588700
H	4.28600400	2.05933800	3.02759400
H	4.53775400	3.81032500	3.17167200
H	3.12885500	3.04257200	3.94817500
H	3.15741100	5.42032200	1.96008200
H	1.69690100	4.79194500	2.74987900
H	1.76802000	4.93028800	0.97504400

Dimer **2–2** optimized with LC- ω PBE-D3BJ

C	-0.09220500	0.14581600	1.60431200
C	-1.08185200	-0.86663400	1.61816000
C	-0.67203500	-2.22012400	1.69775900
C	0.66819300	-2.58021700	1.78576000
C	1.63117900	-1.56758800	1.73346900
C	1.28237200	-0.20139900	1.65076800
C	2.24219800	0.83485100	1.66731500
C	1.87969600	2.18558500	1.66834400
C	0.52669300	2.50254500	1.60515000
C	-0.47677600	1.50549400	1.58334200
C	-1.85287100	1.82741800	1.59920800
C	-2.84095600	0.84936600	1.62956500
C	-2.44083000	-0.48979100	1.60892700
C	1.10901300	-4.02951400	2.00515800
C	2.96365300	3.26122400	1.78162600
C	-4.32983000	1.19804900	1.70620300
C	2.10842500	-4.45504200	0.92810300
C	1.77373900	-4.12686800	3.38314200
C	-0.06932900	-4.99980200	1.96786400
C	3.77710000	3.01555300	3.05707200
C	3.89093200	3.19895100	0.56601900
C	2.37200900	4.66701500	1.85823300

C	-4.96947400	0.45039100	2.88086400
C	-5.01817300	0.78421200	0.40338900
C	-4.55783900	2.69348700	1.91840500
C	0.09219800	-0.14581900	-1.60424100
C	1.08183900	0.86661800	-1.61819700
C	0.67203300	2.22010800	-1.69789400
C	-0.66818800	2.58019800	-1.78585500
C	-1.63118500	1.56757500	-1.73340900
C	-1.28238200	0.20140000	-1.65065500
C	-2.24220500	-0.83485500	-1.66709700
C	-1.87969000	-2.18559000	-1.66814600
C	-0.52669300	-2.50254800	-1.60491900
C	0.47678600	-1.50548800	-1.58314400
C	1.85287300	-1.82739800	-1.59893600
C	2.84097100	-0.84934400	-1.62950500
C	2.44083000	0.48979500	-1.60900100
C	-1.10899500	4.02948800	-2.00530800
C	-2.96365400	-3.26121600	-1.78156400
C	4.32983700	-1.19802800	-1.70624700
C	-2.10820000	4.45510900	-0.92810700
C	-1.77397100	4.12678800	-3.38317900
C	0.06940300	4.99971900	-1.96834400
C	-3.77694700	-3.01542000	-3.05708100
C	-3.89104100	-3.19905200	-0.56604000
C	-2.37205900	-4.66702700	-1.85820200
C	4.96929200	-0.45066500	-2.88119100
C	5.01832600	-0.78381400	-0.40363900
C	4.55781400	-2.69353500	-1.91804700
H	-2.12213600	2.88195500	1.62066500
H	-2.69173800	1.81858000	-1.79843100
H	-3.29515900	-0.55114200	-1.71461800
H	-3.18855300	-1.28423000	1.62547700
H	-1.45189500	-2.98007300	1.72715200
H	-0.20092500	-3.54265100	-1.60404400
H	2.12213100	-2.88194400	-1.62001100
H	2.69173100	-1.81858900	1.79859300
H	3.29515000	0.55114800	1.71495500
H	3.18845600	1.28432400	-1.62555900
H	1.45190000	2.98004600	-1.72741400
H	0.20091500	3.54264500	1.60436100
H	-1.07957600	3.80849900	-4.17370800
H	-2.08295900	5.16221000	-3.59142100
H	-2.66647800	3.48900200	-3.44591800
H	-1.63831000	4.44776200	0.06443000
H	-2.98108200	3.78993800	-0.89425300

H	-2.47108700	5.47471400	-1.12465200
H	-0.29158800	6.02920900	-2.10297800
H	0.59869000	4.95369000	-1.00642300
H	0.79323100	4.79509900	-2.76936900
H	-4.07988500	3.04817700	2.84253800
H	-4.17179000	3.29062300	1.08143800
H	-5.63524900	2.89630600	1.99852000
H	-4.47098000	0.70839700	3.82610100
H	-4.58855200	1.32224400	-0.45299100
H	-6.03322100	0.71656800	2.96935900
H	-6.09414700	1.00979200	0.44412500
H	-4.90600500	-0.29161300	0.21688600
H	-4.91033700	-0.63910300	2.75642200
H	-4.36056900	-2.21210400	-0.46695500
H	-3.33619900	-3.40474100	0.35962300
H	-4.69370400	-3.94594200	-0.65495500
H	-4.54674100	-3.79222900	-3.17756700
H	-4.28536800	-2.04204200	-3.03543800
H	-3.12703800	-3.03456000	-3.94350000
H	-1.79732500	-4.91641400	-0.95571900
H	-1.71285000	-4.78439200	-2.72969500
H	-3.18114600	-5.40549700	-1.94905400
H	-0.79337400	-4.79527200	2.76871500
H	0.29168100	-6.02928000	2.10251900
H	-0.59832800	-4.95370000	1.00579400
H	1.07911700	-3.80881900	4.17356900
H	2.08289500	-5.16225300	3.59131900
H	2.66609000	-3.48888900	3.44613200
H	2.98133500	-3.78989400	0.89445800
H	2.47126500	-5.47466300	1.12464600
H	1.63872700	-4.44762400	-0.06453200
H	4.17244700	-3.29031600	-1.08051000
H	4.07918600	-3.04863000	-2.84167000
H	5.63517700	-2.89629800	-1.99889100
H	6.03302600	-0.71686400	-2.96979600
H	6.09413200	-1.01026300	-0.44404100
H	4.90698000	0.29223900	-0.21793100
H	4.91018200	0.63885800	-2.75697600
H	4.58813800	-1.32086700	0.45306000
H	4.47065200	-0.70888100	-3.82629300
H	4.36062600	2.21205700	0.46718600
H	3.33598000	3.40426000	-0.35965900
H	4.69346500	3.94601400	0.65466700
H	4.28554200	2.04218700	3.03545700
H	4.54689600	3.79238500	3.17738700

H	3.12730600	3.03476300	3.94357500
H	3.18104900	5.40549200	1.94944200
H	1.71252700	4.78425200	2.72953700
H	1.79753700	4.91648900	0.95560000

Dimer **2–2** optimized with CAM-B3LYP

C	-0.77374500	0.19688300	2.10993000
C	-1.39150000	-1.07940800	2.04437900
C	-0.60453500	-2.23492600	2.29190700
C	0.75416800	-2.15419200	2.59288900
C	1.34536700	-0.88521100	2.64720700
C	0.61141100	0.30092800	2.41235300
C	1.19814400	1.58558400	2.46905800
C	0.46091700	2.75476400	2.24314400
C	-0.89706500	2.62995700	1.95157400
C	-1.53770500	1.36722700	1.87575600
C	-2.91600900	1.23602100	1.57517200
C	-3.54141900	-0.00776500	1.50012900
C	-2.76750900	-1.15120300	1.73765100
C	1.61343000	-3.39839400	2.86610300
C	1.16534700	4.11797700	2.32164700
C	-5.03329400	-0.16183000	1.16669300
C	2.76299000	-3.45965900	1.84598900
C	2.19352400	-3.31619600	4.28844400
C	0.80727700	-4.69667300	2.75327200
C	1.76369700	4.30571800	3.72625600
C	2.29050400	4.17030700	1.27403000
C	0.20748500	5.28317200	2.05145000
C	-5.74755100	-0.87486300	2.32756300
C	-5.18442200	-0.99650300	-0.11673000
C	-5.72011400	1.18925000	0.94096700
C	0.77374300	-0.19689300	-2.10983400
C	1.39038800	1.07996000	-2.04480400
C	0.60219400	2.23476600	-2.29173600
C	-0.75663400	2.15278900	-2.59183200
C	-1.34671100	0.88327000	-2.64572600
C	-0.61153300	-0.30219500	-2.41126500
C	-1.19715300	-1.58737600	-2.46742900
C	-0.45869600	-2.75588200	-2.24205300
C	0.89939900	-2.62985200	-1.95153200
C	1.53893800	-1.36653400	-1.87613900
C	2.91732100	-1.23405500	-1.57645000
C	3.54167200	0.01030500	-1.50202800
C	2.76657300	1.15301200	-1.73916700

C	-1.61710700	3.39618400	-2.86491400
C	-1.16206900	-4.11969800	-2.31966100
C	5.03369700	0.16577700	-1.16992500
C	-2.76776600	3.45553600	-1.84594800
C	-2.19572900	3.31415000	-4.28787900
C	-0.81256300	4.69531900	-2.75049900
C	-1.76364300	-4.30734900	-3.72289600
C	-2.28460900	-4.17348100	-1.26929800
C	-0.20253400	-5.28418800	-2.05236400
C	5.74651200	0.87753900	-2.33246700
C	5.18541100	1.00248000	0.11210400
C	5.72151500	-1.18454300	-0.94272000
H	-3.48069900	2.15093700	1.39919800
H	-2.40942900	0.78377000	-2.87618800
H	-2.26316400	-1.64975600	-2.69577400
H	-3.22564000	-2.14118400	1.68729300
H	-1.10407300	-3.20186300	2.24015200
H	1.51160200	-3.51341800	-1.77314500
H	3.48295800	-2.14844200	-1.40074000
H	2.40803700	-0.78669300	2.87831500
H	2.26402000	1.64696200	2.69832600
H	3.22385900	2.14341500	-1.68941900
H	1.10087200	3.20216300	-2.24024900
H	-1.50832800	3.51406900	1.77266000
H	-1.39134500	3.27476500	-5.03773800
H	-2.81872000	4.19698300	-4.50115400
H	-2.82325800	2.42180400	-4.42365500
H	-2.37717400	3.50615100	-0.81881300
H	-3.41824000	2.57159300	-1.91030900
H	-3.39233200	4.34524000	-2.02304800
H	-1.46755400	5.55618200	-2.95129300
H	-0.39021300	4.82767600	-1.74333400
H	0.01336800	4.73169500	-3.47591800
H	-5.67101800	1.82795200	1.83505900
H	-5.27296200	1.74117100	0.10105000
H	-6.78295400	1.03035900	0.70520600
H	-5.65676100	-0.29647300	3.25924900
H	-4.67661800	-0.50889500	-0.96282200
H	-6.81909500	-0.99558900	2.10356400
H	-6.24810700	-1.11370800	-0.37701100
H	-4.75516000	-2.00221400	-0.00365100
H	-5.33068600	-1.87501000	2.51291600
H	-3.03698900	-3.38920400	-1.43410800
H	-1.87769400	-4.03667600	-0.25609200
H	-2.79942600	-5.14644400	-1.30574500

H	-2.27428100	-5.28047400	-3.79510900
H	-2.49933600	-3.52611800	-3.96121100
H	-0.97953000	-4.27530200	-4.49427000
H	0.24181900	-5.22686400	-1.04764200
H	0.61525300	-5.31857300	-2.78709500
H	-0.74820600	-6.23718200	-2.11910900
H	-0.01823100	-4.73145900	3.47925700
H	1.46139200	-5.55814700	2.95429800
H	0.38414100	-4.82933800	1.74648700
H	1.38992500	-3.27517500	5.03905800
H	2.81545500	-4.19977800	4.50170000
H	2.82250200	-2.42470100	4.42306900
H	3.41414200	-2.57609500	1.90874300
H	3.38706900	-4.34966700	2.02328400
H	2.37118800	-3.51103100	0.81934400
H	5.27499600	-1.73567400	-0.10194600
H	5.67253500	-1.82444300	-1.83595900
H	6.78433500	-1.02464000	-0.70756000
H	6.81815000	0.99943200	-2.10952900
H	6.24922700	1.12008000	0.37166500
H	4.75615800	2.00803000	-0.00235500
H	5.32868200	1.87706900	-2.51900400
H	4.67800200	0.51627700	0.95924700
H	5.65540200	0.29764600	-3.26318500
H	3.04219900	3.38594200	1.44146900
H	1.88616300	4.03266800	0.25990800
H	2.80561600	5.14309400	1.31087400
H	2.49774200	3.52361900	3.96681800
H	2.27543100	5.27821700	3.79917100
H	0.97763700	4.27513900	4.49570600
H	0.75390700	6.23570100	2.11868400
H	-0.61184400	5.31890100	2.78439100
H	-0.23475800	5.22548700	1.04581200

Dimer **2–2** optimized with CAM-B3LYP-D3

C	-0.10466000	0.12411300	1.66403400
C	-1.06576500	-0.91959800	1.66929500
C	-0.61471000	-2.26223800	1.73574100
C	0.73842800	-2.58472100	1.81215000
C	1.67140800	-1.54132700	1.76906800
C	1.28258100	-0.18318100	1.70291100
C	2.21217000	0.88294700	1.71304100
C	1.81016300	2.22438800	1.71706100
C	0.44527000	2.50121700	1.66635300

C	-0.53018200	1.47482300	1.64604200
C	-1.91708500	1.75560400	1.64877700
C	-2.87800200	0.74688800	1.66430200
C	-2.43682000	-0.58137200	1.64892400
C	1.22655000	-4.03082200	1.98747500
C	2.86642600	3.33715900	1.80394300
C	-4.38323300	1.05255600	1.70313600
C	2.19434000	-4.40883000	0.85650500
C	1.95458800	-4.14598200	3.33775100
C	0.07224700	-5.03798900	1.97756800
C	3.71893200	3.12822600	3.06681700
C	3.77499900	3.29642100	0.56598400
C	2.23485500	4.73097700	1.88215100
C	-5.03836800	0.28475100	2.86313000
C	-5.02857200	0.61766000	0.37821200
C	-4.66511100	2.54508700	1.90689500
C	0.10468300	-0.12409900	-1.66400600
C	1.06573300	0.91965600	-1.66949300
C	0.61462200	2.26226200	-1.73614000
C	-0.73853900	2.58467200	-1.81249700
C	-1.67146600	1.54123800	-1.76928100
C	-1.28257200	0.18312900	-1.70298000
C	-2.21210600	-0.88304100	-1.71307500
C	-1.81005600	-2.22446700	-1.71679600
C	-0.44516600	-2.50123400	-1.66580600
C	0.53025900	-1.47478800	-1.64569200
C	1.91716600	-1.75550900	-1.64830900
C	2.87804600	-0.74673900	-1.66417500
C	2.43681200	0.58148900	-1.64914100
C	-1.22675500	4.03072900	-1.98789200
C	-2.86629600	-3.33725600	-1.80380000
C	4.38329100	-1.05235600	-1.70291100
C	-2.19433400	4.40876200	-0.85674000
C	-1.95506500	4.14574100	-3.33802800
C	-0.07248100	5.03793200	-1.97826000
C	-3.71836500	-3.12850300	-3.06700900
C	-3.77531100	-3.29637900	-0.56617200
C	-2.23469600	-4.73107800	-1.88162900
C	5.03842300	-0.28501800	-2.86319200
C	5.02854900	-0.61688100	-0.37813000
C	4.66523800	-2.54496700	-1.90605800
H	-2.21544300	2.80146900	1.66018200
H	-2.73890900	1.76167400	-1.82136600
H	-3.27272600	-0.63033700	-1.74477600
H	-3.16045200	-1.39689400	1.64959600

H	-1.37263300	-3.04315700	1.75675900
H	-0.08720400	-3.52967700	-1.66451600
H	2.21557900	-2.80135900	-1.65930600
H	2.73883500	-1.76183200	1.82118300
H	3.27278900	0.63018300	1.74445300
H	3.16040900	1.39704900	-1.65010400
H	1.37250600	3.04321600	-1.75733600
H	0.08735800	3.52968000	1.66549900
H	-1.28567100	3.87233100	-4.16729700
H	-2.30286600	5.17788200	-3.50210900
H	-2.83186500	3.48402700	-3.38348000
H	-1.68645500	4.37789700	0.11746700
H	-3.05518800	3.72801400	-0.80894900
H	-2.58054400	5.42867000	-1.00803600
H	-0.46750900	6.05827900	-2.09250900
H	0.48905700	5.00160100	-1.03334100
H	0.63265700	4.86069400	-2.80314000
H	-4.22262400	2.91704300	2.84270100
H	-4.27575400	3.15392300	1.07894400
H	-5.75093700	2.71448600	1.95787200
H	-4.58077000	0.56247500	3.82441400
H	-4.59049800	1.16574800	-0.46871100
H	-6.11374900	0.51580000	2.91514200
H	-6.11168900	0.81567600	0.39111500
H	-4.88391400	-0.45529300	0.19446600
H	-4.93947800	-0.80336800	2.74571100
H	-4.27820900	-2.32583200	-0.46398800
H	-3.19528300	-3.47353300	0.35089100
H	-4.55294600	-4.07290900	-0.63367000
H	-4.47054400	-3.92761000	-3.15928600
H	-4.25277700	-2.16830100	-3.04580100
H	-3.08934300	-3.14278900	-3.96961200
H	-1.63653300	-4.95850500	-0.98739500
H	-1.58677900	-4.83695900	-2.76388800
H	-3.02444500	-5.49354000	-1.95304800
H	-0.63298600	-4.86080100	2.80238000
H	0.46723400	-6.05835500	2.09179300
H	-0.48921800	-5.00163000	1.03260100
H	1.28503900	-3.87259300	4.16690100
H	2.30229500	-5.17815500	3.50182300
H	2.83141300	-3.48431600	3.38342200
H	3.05526200	-3.72815000	0.80897100
H	2.58044300	-5.42877700	1.00779700
H	1.68670100	-4.37782100	-0.11782400
H	4.27635500	-3.15342200	-1.07760400

H	4.22234800	-2.91744600	-2.84146100
H	5.75105900	-2.71425400	-1.95746200
H	6.11393600	-0.51557700	-2.91469000
H	6.11155500	-0.81553800	-0.39059600
H	4.88446700	0.45629200	-0.19523300
H	4.93896100	0.80313300	-2.74657100
H	4.58990400	-1.16406100	0.46908300
H	4.58129400	-0.56362900	-3.82444600
H	4.27829600	2.32607500	0.46387300
H	3.19452700	3.47304400	-0.35089200
H	4.55231000	4.07331900	0.63300200
H	4.25334500	2.16803200	3.04526800
H	4.47113900	3.92732100	3.15895900
H	3.09023100	3.14236300	3.96964700
H	3.02462300	5.49339400	1.95381500
H	1.58692600	4.83663600	2.76442800
H	1.63671400	4.95865700	0.98795900

Dimer **2–2** optimized with CAM-B3LYP-D3BJ

C	-0.10124600	0.13544500	1.67064500
C	-1.05916200	-0.91098200	1.67901400
C	-0.60384100	-2.25152000	1.74725100
C	0.75006900	-2.56875800	1.82603300
C	1.68003700	-1.52346700	1.78406900
C	1.28671000	-0.16717800	1.71316700
C	2.21247300	0.90166400	1.72231300
C	1.80569300	2.24109800	1.71801100
C	0.44063200	2.51387000	1.66402200
C	-0.53092800	1.48455300	1.64819200
C	-1.91802200	1.76086300	1.65109400
C	-2.87528600	0.74945900	1.67088700
C	-2.43092700	-0.57728200	1.66017300
C	1.23926200	-4.01204700	2.01253900
C	2.85641600	3.35782100	1.80337400
C	-4.37995100	1.05252900	1.71426100
C	2.25213500	-4.38324500	0.92043400
C	1.91483300	-4.12479200	3.38958800
C	0.09110400	-5.02365700	1.95475900
C	3.69859500	3.16137300	3.07444900
C	3.77472900	3.31107900	0.57358700
C	2.21782700	4.74847800	1.86532900
C	-5.02583900	0.29235500	2.88360300
C	-5.03246700	0.60737100	0.39692900
C	-4.66177100	2.54573800	1.90795200

C	0.10132700	-0.13546100	-1.67060400
C	1.05920800	0.91099500	-1.67929300
C	0.60383300	2.25151800	-1.74761200
C	-0.75009700	2.56869200	-1.82621300
C	-1.68001300	1.52335900	-1.78415300
C	-1.28663700	0.16711700	-1.71311200
C	-2.21237400	-0.90174100	-1.72207400
C	-1.80559800	-2.24116700	-1.71750600
C	-0.44053800	-2.51390200	-1.66331700
C	0.53102200	-1.48455100	-1.64778600
C	1.91811700	-1.76084000	-1.65062900
C	2.87535400	-0.74941300	-1.67100500
C	2.43098600	0.57732100	-1.66064200
C	-1.23943300	4.01195400	-2.01249500
C	-2.85636800	-3.35785000	-1.80303700
C	4.38002200	-1.05238600	-1.71474000
C	-2.25210500	4.38285100	-0.92007800
C	-1.91531900	4.12489300	-3.38935400
C	-0.09130600	5.02360400	-1.95476400
C	-3.69784800	-3.16160900	-3.07461100
C	-3.77537400	-3.31081600	-0.57377400
C	-2.21786700	-4.74856600	-1.86435900
C	5.02496700	-0.29431600	-2.88595700
C	5.03326300	-0.60462500	-0.39866800
C	4.66194400	-2.54592100	-1.90572300
H	-2.22064000	2.80550400	1.66049400
H	-2.74796800	1.73979700	-1.84003900
H	-3.27355700	-0.65289700	-1.76058600
H	-3.15171000	-1.39519300	1.66782800
H	-1.35788800	-3.03611900	1.76802700
H	-0.08075600	-3.54156400	-1.65715000
H	2.22070800	-2.80549300	-1.65946300
H	2.74798800	-1.73996000	1.84000800
H	3.27367500	0.65285200	1.76087400
H	3.15177400	1.39524500	-1.66875300
H	1.35785600	3.03613700	-1.76859700
H	0.08088000	3.54154600	1.65836000
H	-1.21228500	3.85887900	-4.19257200
H	-2.26544600	5.15418200	-3.56515300
H	-2.78305300	3.45462300	-3.46939700
H	-1.78366800	4.35546100	0.07362100
H	-3.11128500	3.69854000	-0.90599000
H	-2.63741300	5.40050900	-1.08651300
H	-0.48761700	6.04322800	-2.06938600
H	0.44085900	4.97778900	-0.99358300

H	0.64047600	4.86060200	-2.75880100
H	-4.21631000	2.92566100	2.83895700
H	-4.27607400	3.14861300	1.07413100
H	-5.74743400	2.71409200	1.96218700
H	-4.56478000	0.57971900	3.84026200
H	-4.60190500	1.15103200	-0.45649600
H	-6.10169700	0.51948400	2.93946200
H	-6.11572600	0.80334300	0.41565600
H	-4.88729600	-0.46643800	0.21876300
H	-4.92218600	-0.79609600	2.77476100
H	-4.28315400	-2.34161900	-0.48319100
H	-3.20293700	-3.47904800	0.34965600
H	-4.54922500	-4.09085900	-0.64174300
H	-4.44820700	-3.96225900	-3.16634900
H	-4.23269700	-2.20158000	-3.06619100
H	-3.06167600	-3.18294100	-3.97188900
H	-1.62428800	-4.96521800	-0.96464900
H	-1.56361100	-4.85984200	-2.74104000
H	-3.00369100	-5.51497500	-1.93409000
H	-0.64082000	-4.86048500	2.75863400
H	0.48737000	-6.04326300	2.06967500
H	-0.44090400	-4.97805700	0.99348300
H	1.21158900	-3.85864500	4.19257700
H	2.26491300	-5.15405500	3.56564100
H	2.78252500	-3.45448100	3.46971300
H	3.11154400	-3.69921100	0.90659900
H	2.63711600	-5.40100200	1.08701100
H	1.78407000	-4.35572800	-0.07344400
H	4.27758400	-3.14703400	-1.07001600
H	4.21532400	-2.92795200	-2.83529500
H	5.74757300	-2.71410400	-1.96111200
H	6.10096700	-0.52080900	-2.94173600
H	6.11628700	-0.80192800	-0.41700700
H	4.88942500	0.46981600	-0.22325900
H	4.92053400	0.79429100	-2.77942900
H	4.60208900	-1.14548300	0.45622300
H	4.56375600	-0.58408000	-3.84182000
H	4.28302800	2.34215900	0.48300700
H	3.20160200	3.47864800	-0.34953400
H	4.54814400	4.09161300	0.64088300
H	4.23353300	2.20139800	3.06552400
H	4.44893800	3.96206300	3.16595300
H	3.06291600	3.18245200	3.97208500
H	3.00362000	5.51489700	1.93527000
H	1.56369100	4.85936500	2.74215000

H	1.62410400	4.96544700	0.96578200
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Dimer **2–2** optimized with ω B97XD

C	-0.07556600	0.10544100	1.61405100
C	-1.06158500	-0.91553200	1.61654200
C	-0.64170900	-2.26918600	1.66853000
C	0.70458000	-2.62414400	1.74286900
C	1.66203600	-1.60207900	1.70484500
C	1.30476600	-0.23412700	1.64766600
C	2.25922400	0.81120000	1.65780200
C	1.88843600	2.16251900	1.66494200
C	0.52924700	2.47054800	1.61072300
C	-0.46972900	1.46621100	1.59790000
C	-1.85006900	1.77931200	1.60965700
C	-2.83578000	0.79356400	1.63410000
C	-2.42546300	-0.54506100	1.60431600
C	1.15715300	-4.08328600	1.91583400
C	2.96955700	3.25247000	1.76134200
C	-4.33331600	1.13770800	1.69875400
C	2.14058000	-4.47810500	0.80231800
C	1.85385400	-4.21981800	3.28279100
C	-0.02156300	-5.06367700	1.87460600
C	3.82035000	3.00825400	3.02135000
C	3.87438100	3.20929600	0.51914400
C	2.36588900	4.65925900	1.86030700
C	-4.99541300	0.35485800	2.84713200
C	-5.00564800	0.75738600	0.36914600
C	-4.57110600	2.63298400	1.94842000
C	0.07557500	-0.10543200	-1.61404100
C	1.06155500	0.91555500	-1.61682400
C	0.64164900	2.26919300	-1.66903600
C	-0.70464800	2.62411000	-1.74318100
C	-1.66207900	1.60201900	-1.70489800
C	-1.30477200	0.23410100	-1.64763700
C	-2.25919300	-0.81126300	-1.65766700
C	-1.88835600	-2.16257400	-1.66474000
C	-0.52917700	-2.47056600	-1.61034300
C	0.46978600	-1.46618700	-1.59757800
C	1.85011600	-1.77923600	-1.60907400
C	2.83581800	-0.79344500	-1.63394700
C	2.42547000	0.54514700	-1.60467600
C	-1.15729600	4.08322800	-1.91606800
C	-2.96945800	-3.25251900	-1.76143400
C	4.33334900	-1.13761100	-1.69845800

C	-2.14011100	4.47813200	-0.80205300
C	-1.85468700	4.21970800	-3.28267700
C	0.02148400	5.06358100	-1.87547700
C	-3.81977100	-3.00827700	-3.02178700
C	-3.87478300	-3.20939600	-0.51961300
C	-2.36576400	-4.65930100	-1.86018500
C	4.99543000	-0.35521900	-2.84715900
C	5.00563800	-0.75673500	-0.36900500
C	4.57115000	-2.63299100	-1.94750000
H	-2.12432500	2.83278100	1.63061500
H	-2.72537700	1.84703400	-1.75762100
H	-3.31457700	-0.53346200	-1.69262700
H	-3.16786600	-1.34488600	1.60803300
H	-1.41773500	-3.03407500	1.68488500
H	-0.19459800	-3.50824700	-1.60847900
H	2.12443200	-2.83271200	-1.62924100
H	2.72531800	-1.84713100	1.75775900
H	3.31460000	0.53334400	1.69271600
H	3.16780100	1.34504600	-1.60889700
H	1.41767500	3.03407700	-1.68569300
H	0.19471100	3.50824900	1.60894700
H	-1.17586500	3.92656600	-4.09795400
H	-2.16984100	5.26158800	-3.45396800
H	-2.74929300	3.58254700	-3.34644700
H	-1.64886400	4.44705600	0.18173800
H	-3.01169400	3.80853600	-0.76572900
H	-2.51121900	5.50255100	-0.96345300
H	-0.34771300	6.09547100	-1.97664200
H	0.56999600	4.99748600	-0.92348700
H	0.73319300	4.88527700	-2.69542600
H	-4.10171500	2.96757300	2.88606100
H	-4.18197300	3.25513500	1.12921800
H	-5.65131500	2.82979100	2.02480800
H	-4.51281500	0.58690100	3.80878200
H	-4.55950600	1.31476700	-0.46837200
H	-6.06184000	0.61958100	2.92497700
H	-6.08270800	0.98684300	0.39790100
H	-4.89511100	-0.31552900	0.15710400
H	-4.93638100	-0.73254800	2.69465800
H	-4.35580700	-2.22820800	-0.40233500
H	-3.29660900	-3.41432200	0.39397600
H	-4.67084000	-3.96690700	-0.59542300
H	-4.58385400	-3.79477200	-3.12834000
H	-4.34138100	-2.04078700	-2.98348800
H	-3.19070400	-3.01526900	-3.92493700

H	-1.77281200	-4.91318000	-0.96864000
H	-1.72017000	-4.76629100	-2.74490400
H	-3.17120600	-5.40480600	-1.94223500
H	-0.73364200	-4.88546100	2.69425400
H	0.34761500	-6.09556400	1.97585100
H	-0.56965300	-4.99753400	0.92238000
H	1.17458700	-3.92679000	4.09773800
H	2.16900700	-5.26168400	3.45416800
H	2.74836400	-3.58257000	3.34705900
H	3.01225600	-3.80859200	0.76668100
H	2.51150700	-5.50258000	0.96375800
H	1.64995300	-4.44674200	-0.18177600
H	4.18286700	-3.25471700	-1.12757200
H	4.10109000	-2.96818900	-2.88458100
H	5.65133400	-2.82965500	-2.02462100
H	6.06186500	-0.61994300	-2.92488500
H	6.08263600	-0.98651900	-0.39746400
H	4.89538200	0.31633500	-0.15759400
H	4.93637700	0.73224700	-2.69512500
H	4.55919000	-1.31344400	0.46879800
H	4.51285100	-0.58766900	-3.80871900
H	4.35562700	2.22821100	0.40199000
H	3.29566100	3.41367700	-0.39421000
H	4.67023700	3.96707300	0.59435600
H	4.34192600	2.04075000	2.98289100
H	4.58451100	3.79472100	3.12754600
H	3.19165900	3.01531700	3.92476200
H	3.17135800	5.40473600	1.94236400
H	1.72037300	4.76614400	2.74509400
H	1.77287100	4.91326900	0.96883800

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