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. A validation study of different exchange-correlation (XC) functionals was carried out (wide infra). The tested functionals included the global hybrids B3LYP, PBE0, M06, M06-2X, and the range-separated hybrids LC-ωPBE, CAM-B3LYP, and ωB97XD. Each functional was utilized both with and without the DFT-D3 dispersion correction, except for ωB97XD, which includes dispersion correction in the functional definition. Both the older zero damping function and the newer Becke–Johnson (BJ) 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-ωPBE functional with empirical dispersion correction using BJ damping (denoted as LC-ωPBE-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\textsuperscript{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.\textsuperscript{S22}

DLPNO-CCSD(T)\textsuperscript{S23–S26} calculations were carried out using ORCA software version 4.0.1\textsuperscript{S27} with the default parameters. Dunning’s correlation consistent basis sets\textsuperscript{S28} were used along with corresponding auxiliary correlation fitting basis sets.\textsuperscript{S29} Valence triple-ζ quality cc-pVTZ basis sets were used for atoms in the phenalenyl or oxophenalenoxy 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.\textsuperscript{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\(^{33-36}\)

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

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\(^{37}\) 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-determinant 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

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

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 \( (J_{adiabatic}) \) as

\[
J_{LS} = \frac{2(E_{LS} - E_{HS})}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}},
\]

\[
J_{HS} = \frac{2(E_{HS} - E_{HS})}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}},
\]

\[
J_{adiabatic} = E_{HS} + \frac{2(E_{LS} - E_{HS})}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}} - E_{HS}.
\]

S3
Dimerization enthalpies

The dimerization energies ($\Delta E$) and enthalpies ($\Delta H$) 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\textsuperscript{38} 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

\begin{align}
\Delta E_{LS} &= [E_{HS}^{LS}(DFT) + J_{LS}^{LS}] - E_{\text{monomer1}}^{DFT} - E_{\text{monomer2}}^{DFT} + E_{BSSE}^{LS}(DFT) \quad (6) \\
\Delta E_{HS} &= E_{HS}^{HS}(DFT) - E_{\text{monomer1}}^{DFT} - E_{\text{monomer2}}^{DFT} + E_{BSSE}^{HS}(DFT) \quad (7) \\
\Delta H_{LS} &= [E_{HS}^{LS}(DFT) + H_{LS}^{LS} + J_{LS}] - [E_{\text{monomer1}}^{DFT} + H_{\text{monomer1}}]
- [E_{\text{monomer2}}^{DFT} + H_{\text{monomer2}}] + E_{BSSE}^{LS}(DFT) \quad (8) \\
\Delta H_{HS} &= [E_{HS}^{HS}(DFT) + H_{HS}^{HS}] - [E_{\text{monomer1}}^{DFT} + H_{\text{monomer1}}]
- [E_{\text{monomer2}}^{DFT} + H_{\text{monomer2}}] + E_{BSSE}^{HS}(DFT), \quad (9)
\end{align}

where (2) has been used to estimate the energy of the singlet state, $E_{\text{monomer1}}$ and $E_{\text{monomer2}}$ are the energies of the monomers in their optimized doublet geometries, and $H_{LS}^{LS}$, $H_{HS}^{HS}$, $H_{\text{monomer1}}$, and $H_{\text{monomer2}}$ 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 $H_{LS}^{LS}$ 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

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

\[ - E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) - E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) \]

\[ + E_{\text{BSSE}}^{LS}(\text{DLPNO-CCSD(T)}) \]

\[ \Delta E_{HS} = E_{HS}^{HS}(\text{DLPNO-CCSD(T)}) \]

\[ - E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) - E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) \]

\[ + E_{\text{BSSE}}^{HS}(\text{DLPNO-CCSD(T)}) \]

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

\[ - \left[ E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer1}} \right] \]

\[ - \left[ E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer2}} \right] + E_{\text{BSSE}}^{LS}(\text{DLPNO-CCSD(T)}) \]

\[ \Delta H_{HS} = \left[ E_{HS}^{HS}(\text{DLPNO-CCSD(T)}) + H_{HS}^{HS} \right] \]

\[ - \left[ E_{\text{monomer1}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer1}} \right] \]

\[ - \left[ E_{\text{monomer2}}(\text{DLPNO-CCSD(T)}) + H_{\text{monomer2}} \right] + E_{\text{BSSE}}^{HS}(\text{DLPNO-CCSD(T)}), \]

It should be noted that \( \Delta E_{HS} \) is calculated purely from DLPNO-CCSD(T) energies (although using DFT optimized geometries), whereas \( \Delta E_{LS} \) 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-ωPBE 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,\textsuperscript{37,39–48} whereas the geometry optimizations tend to compensate for the functional error.\textsuperscript{49} 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,\textsuperscript{50–52} the exchange coupling constant in 2–2 has been determined as roughly $-1390\text{ cm}^{-1}$. 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 $-2910\text{ cm}^{-1}$, which is more than twice the magnitude of the SQUID value.\textsuperscript{53} 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-\textit{tert}-butyl-8-\textit{para}-bromophenyl-6-oxophenalenoxyl (4), which is structurally similar to 3–3 and for which an exchange coupling constant of $-267\text{ cm}^{-1}$ has been reliably determined from SQUID data.\textsuperscript{54}
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-\(\omega\)PBE functional is closest to the SQUID value but its magnitude is still more than twice that of the experimental value. The LC-\(\omega\)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-\(\omega\)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-\(\omega\)PBE |  2754 |  267 |
| CAM-B3LYP |  3323 |  253 |
| \(\omega\)B97XD |  3431 |  247 |
| Experimental |  1390\(^{s90}\) |  267\(^{s54}\) |
|       |      |  2910\(^{s53}\) |
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). 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 kJ mol⁻¹, −36.8 kJ mol⁻¹) and from the EPR spectrum (−39.9 kJ mol⁻¹). 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-ωPBE-D3, LC-ωPBE-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 results 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 ($\Delta E_{\text{LS}}$), enthalpies ($\Delta H_{\text{LS}}$), and central C–C distances calculated for 2–2 using various XC functionals

| XC            | $\Delta E_{\text{LS}}$ / kJ mol$^{-1}$ | $\Delta H_{\text{LS}}$ / kJ mol$^{-1}$ | $d$(C–C) / Å |
|---------------|----------------------------------------|----------------------------------------|--------------|
| 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-ωPBE      | −2.8                                   | 2.2                                    | 8.223        |
| LC-ωPBE-D3   | −90.1                                  | −82.7                                  | 3.299        |
| LC-ωPBE-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        |
| ωB97XD       | −115.1                                 | −105.5                                 | 3.310        |
| Experimental | -31.4$^{\text{S55}}$                    | 3.201$^{\text{S52}}$                   |              |
|              | -36.8$^{\text{S56}}$                   |                                        |              |
|              | -39.9$^{\text{S56}}$                   |                                        |              |

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 $−32.9$ kJ mol$^{-1}$ and a central C–C distance of 3.209 Å, both in very good agreement with experiments.$^{557}$ 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 $−83.0$ kJ mol$^{-1}$ (the respective enthalpy is $−74.0$ 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$^{558}$ and TZVP$^{559}$ 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** |              |              |              |
| $E_{\text{LS}}$(DFT)$^a$ | $-1944.650240$ | $-2243.058829$ | $-2093.858540$ |
| $E_{\text{LS}}$(DFT)$^a$ | $-1944.644802$ | $-2243.058659$ | $-2093.859392$ |
| $E_{\text{LS}}$(DLPNO-CCSD(T)) | $-1940.526288$ | $-2238.617297$ | $-2089.579782$ |
| $H_{\text{LS}}$(DFT)$^a$ | 1.093329  | 1.070045  | 1.081731  |
| $E_{\text{BSSE}}$(DLPNO-CCSD(T)) | 0.010379  | 0.009709  | 0.010079  |
| $\langle S^2 \rangle$$_{\text{LS}}$ | 1.3553  | 1.3435  | 1.3937  |
| $\langle S^2 \rangle$$_{\text{LS}}$ | 2.4701  | 2.3405  | 2.4039  |
| **HS geometry** |              |              |              |
| $E_{\text{HS}}$(DFT)$^a$ | $-1944.648543$ | $-2243.058788$ | $-2093.858461$ |
| $E_{\text{HS}}$(DFT)$^a$ | $-1944.647337$ | $-2243.058714$ | $-2093.859463$ |
| $E_{\text{HS}}$(DLPNO-CCSD(T)) | $-1940.528111$ | $-2238.617177$ | $-2089.580230$ |
| $H_{\text{HS}}$(DFT)$^a$ | 1.092880  | 1.070043  | 1.081750  |
| $E_{\text{BSSE}}$(DLPNO-CCSD(T)) | 0.008257  | 0.009716  | 0.010172  |
| $\langle S^2 \rangle$$_{\text{LS}}$ | 1.4404  | 1.3442  | 1.3933  |
| $\langle S^2 \rangle$$_{\text{LS}}$ | 2.4673  | 2.3414  | 2.4052  |

$^a$) Calculated using the LC-ωPBE-D3BJ XC functional

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

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

$^a$) Calculated using the LC-ωPBE-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          | \(E_{\text{LS}}^{\text{crystal}}\) (DFT) | \(E_{\text{HS}}^{\text{crystal}}\) (DFT) | \(E_{\text{HS}}^{\text{LS}}\) (DFT) | \(\langle S^2 \rangle_{\text{LS}}\) | \(\langle S^2 \rangle_{\text{HS}}\) |
|-------------|---------------------------------|---------------------------------|---------------------------------|------------------|------------------|
| 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-\(\infty\)PBE | −1944.403151              | −1944.395932                   | 1.3349                          | 2.4853           |                  |
| CAM-B3LYP   | −1944.590798                   | −1944.581052                   | 0.9348                          | 2.2221           |                  |
| \(\omega\)B97XD | −1945.192345                 | −1945.182322                   | 0.9094                          | 2.1919           |                  |

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          | \(E_{\text{LS}}^{\text{crystal}}\) (DFT) | \(E_{\text{HS}}^{\text{crystal}}\) (DFT) | \(E_{\text{HS}}^{\text{LS}}\) (DFT) | \(E_{\text{BSSE}}^{\text{LS}}\) | \(\langle S^2 \rangle_{\text{LS}}\) | \(\langle S^2 \rangle_{\text{HS}}\) |
|-------------|---------------------------------|---------------------------------|---------------------------------|-------------------|------------------|------------------|
| B3LYP       | −1945.830818                   | −1945.830818                   | 1.0747                           | 0.00147           | 1.0933           | 2.0933           |
| B3LYP-D3    | −1945.999746                   | −1945.978884                   | 1.0819                           | 0.001670          | 0.6696           | 2.0962           |
| B3LYP-D3BJ  | −1946.033303                   | −1946.107783                   | 1.0811                           | 0.001730          | 0.00000          | 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                           | 0.001891          | 0.4253           | 2.0925           |
| M06-2X-D3   | −1944.979803                   | −1944.960358                   | 1.0866                           | 0.001891          | 0.4253           | 2.0925           |
| LC-\(\infty\)PBE | −1944.467966             | −1944.467966                   | 1.0916                           | 0.000000          | 1.4679           | 2.4679           |
| LC-\(\infty\)PBE-D3 | −1944.593443           | −1944.588356                   | 1.0945                           | 0.001429          | 1.3644           | 2.4718           |
| LC-\(\infty\)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           |
| \(\omega\)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                  | $E$(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-ωPBE             | -972.233455 | 0.544864 |
| LC-ωPBE-D3          | -972.280897 | 0.545867 |
| LC-ωPBE-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 |
| ωB97XD              | -972.605544 | 0.541658 |
## Optimized Cartesian coordinates

### Final calculations

**Monomer 2**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 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    | -1.34413300| 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| -3.04223000| 0.00000000 |
| 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  | -1.08468400 | 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 |
Dimer 2–2 in LS state

|   |   |   |   |
|---|---|---|---|
| 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 | -0.88731300 |
| H | -0.95656200 | -3.25082000 | -0.88731300 |
| 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 | 5.64117000 | -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 | 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 | -2.15563000 |
| 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 |

S16
H -3.2369800 -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 2.77915000
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 0.23837000
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
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 | -2.11633300 |
| 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 | -1.45085200 |
| C | 2.12748000 | 1.51987300 | -1.59074900 |
| C | 2.70584100 | 2.39900100 | -1.55170400 |
| C | -0.22967700 | -4.59284500 | -1.55170400 |
| C | 4.61183000 | 1.21493900 | -1.35673500 |
| C | -3.87523600 | 2.53829000 | -1.54436500 |
| C | -3.16530100 | 2.01871600 | -3.91863000 |
| C | -2.82523000 | 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 | -0.05277500 | 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 | -3.95084000 |
| H | -3.58934400 | 2.58909300 | -0.54862000 |
| H | -4.21145000 | 1.22039900 | -1.46626000 |
| H | -4.71913700 | 2.85879400 | -1.88240100 |
| Atoms | x        | y        | z        |
|-------|----------|----------|----------|
| H     | -3.139817| 4.488588 | -2.768038|
| H     | -1.912783| 4.169920 | -1.540064|
| H     | -1.504384| 4.054420 | -3.258923|
| H     | -5.656028| 0.491303 | 2.208565 |
| H     | -5.544464| 0.528004 | 0.443035 |
| H     | -6.661228| -0.581001| 1.234747 |
| H     | -4.814381| -1.538303| 3.491364 |
| H     | -4.525942| -1.424775| -0.799540|
| H     | -5.914001| -2.508555| 2.500754 |
| H     | -5.711226| -2.478571| -0.016549|
| H     | -3.989362| -2.859958| 0.075505 |
| H     | -4.210350| -2.947364| 2.620000 |
| H     | -2.044264| -4.340157| -0.377132|
| H     | -0.603276| -4.682431| 0.581923 |
| H     | -1.376947| -5.974391| -0.344124|
| H     | -1.766030| -6.042649| -2.848814|
| H     | -1.909928| -4.440484| -2.933179|
| H     | -0.355567| -4.733677| -3.712402|
| H     | 1.589162 | -5.239025| -0.543390|
| H     | 1.690753 | -5.276397| -2.309518|
| H     | 0.756418 | -6.498950| -1.449080|
| H     | 1.504375 | -6.054437| 3.258896 |
| H     | 3.139807 | -4.488600| 2.768007 |
| H     | 1.912773 | -4.169920| 1.540036 |
| H     | 2.340587 | -2.098241| 4.628685 |
| H     | 3.968881 | -2.681311| 4.247533 |
| H     | 3.536722 | -0.993908| 3.950818 |
| H     | 4.211462 | -1.220403| 1.466282 |
| H     | 4.719145 | -2.858794| 1.882442 |
| H     | 3.589387 | -2.589106| 0.548632 |
| H     | 5.544462 | -0.527976| -0.442990|
| H     | 5.656026 | -0.491309| -2.208521|
| H     | 6.661225 | 0.581015 | -1.234732|
| H     | 5.914004 | 2.508565 | -2.500735|
| H     | 5.711213 | 2.478574 | 0.016576 |
| H     | 3.989359 | 2.859993 | -0.075525|
| H     | 4.210349 | 2.947354 | -2.620016|
| H     | 4.525888 | 1.424808 | 0.799547 |
| H     | 4.814410 | 1.538290 | -3.491352|
| H     | 2.044279 | 4.340162 | 0.377134 |
| H     | 0.603290 | 4.682423 | -0.581924|
| H     | 1.376952 | 5.974391 | 0.344119 |
| H     | 1.909930 | 4.440477 | 2.933182 |
| H     | 1.176609 | 6.042646 | 2.848817 |
| H     | 0.355567 | 4.733764 | 3.712399 |
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  -4.14131010   2.31083200  1.09667400
C  -0.23666300  -5.08254100  0.25575400
C  -0.63966000  -5.11504400  2.71419300
C   0.54973220  -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 -1.30010400
C   1.13578000   4.56532200 -1.37713500
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     6.15357000  -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     3.38989900   0.04403300   4.07549800  
H     3.99501700   1.60642200   4.57635600  
H     2.27763400   1.25991500   4.80762200  
H     3.58026000   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    -2.05733300  -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  

S24
|   | x   | y   | z   |
|---|-----|-----|-----|
| 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 | 1.12288000  |
| 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  | 2.85094000  |
| C | -5.29505600 | 2.08247500 | 2.37957900  |
| C | -5.23476700 | 1.80581600 | -0.10808000 |
| C | -4.08781100 | 3.70949500 | 0.95629400  |
| 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 | -1.27472600 |
| C | 3.30623000  | 0.08473400  | -1.33405200 |
| C | 0.98006800  | 4.55093200  | -1.44785200 |
| C | -2.85513700 | -1.83058600 | -2.71783500 |
| 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 | -4.08781100 | -3.70949500 | -1.93912800 |
| 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 | 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 | 2.11096000 | 2.21704600 |
| H | 3.40851100 | 0.21128400 | 4.06144000 |
| H | 4.03496800 | 2.11099600 | 2.21704600 |
| O | 2.62509100 | -1.00616100 | 2.15429000 |
| O | 4.38476000 | 0.65198000 | -1.35824400 |
| O | -2.62507900 | 1.00617500 | -2.15435400 |
| O | -4.38476000 | -0.65198000 | 1.35822400 |

**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 | 0.72852800 |
| C | -3.88531300 | -2.65326900 | 3.36362600 |
| C | -3.99189500 | -3.06343700 | 0.90689100 |
| C | -5.03183800 | -1.04691900 | 1.86636500 |
| C | 0.01526400 | -0.00096600 | -1.59519600 |

S27
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  1.83996600  -3.10738000
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 | 3.57241300 |
| H | 1.19533100 | -6.00122900 | -2.25707070 |
| H | 2.76789200 | -4.04718900 | 0.80358900 |
| H | 4.52768400 | -4.05486400 | 0.89672000 |
| H | 3.70649300 | -2.90759100 | -0.17760500 |
| H | 2.73064400 | -3.75578900 | 3.35682300 |
| H | 4.50372000 | -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 | -1.00358000 |
| 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 | -0.32508300 | -1.65531700 |
| C | 0.81012000 | 1.06039400 | -1.71455100 |
| C | -0.27182000 | 1.93499500 | -1.94361000 |
| C | -1.56207300 | 1.47240000 | -2.11633300 |
| C | -1.79605000 | 0.10656100 | -1.99456500 |
| C | -0.75562300 | -0.81075700 | -1.76905000 |
| C | -0.97063400 | -2.19596400 | -1.70199900 |
| C | 0.07785600 | -3.10018400 | -1.57090100 |
| C | 1.36756500 | -2.60696200 | -1.48761200 |
| C | 1.63769500 | -1.22385900 | -1.52089500 |
| C | 2.94710800 | -0.71160500 | -1.45086500 |
| C | 3.20230500 | 0.64706400 | -1.46631200 |
| C | 2.12748100 | 1.51987300 | -1.59074900 |
| C | -2.70583400 | 2.39901000 | -2.51128600 |
| C | -0.22968600 | -4.59284400 | -1.55170100 |
| C | 4.61183300 | 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 |
| Column 1 | Column 2   | Column 3   | Column 4   |
|---------|------------|------------|------------|
| H       | 0.75641800 | -6.49895000 | -1.44908000 |
| H       | 1.50437500 | -4.05443700 | 3.25889600  |
| H       | 3.13980700 | -4.48600000 | 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 | -2.85894000 | 1.88244200  |
| H       | 3.58938700 | -2.58910600 | 0.54863200  |
| H       | 5.5446200  | -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       | 5.71123000 | 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       | -1.36087000| 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  |
|   |   |   |   |
|---|---|---|---|
| H | -3.414196 | -3.028025 | 2.178348 |
| H | -3.425903 | -5.237645 | 0.000051 |
| H | -1.977595 | -4.727727 | 0.891819 |
| H | -1.977375 | -4.727825 | -0.891372 |

Monomer 2 optimized with B3LYP-D3

|   |   |   |   |
|---|---|---|---|
| C | 0.016713 | -0.017071 | -0.000005 |
| C | 1.029049 | 0.986263 | 0.000040 |
| C | 0.639755 | 2.355621 | 0.000065 |
| C | -0.704408 | 2.745614 | 0.000031 |
| C | -1.687171 | 1.739875 | 0.000051 |
| C | -1.359893 | 0.359475 | 0.000028 |
| C | -2.343376 | -0.661821 | 0.000041 |
| C | -2.008700 | -2.027053 | -0.000017 |
| C | -0.652216 | -2.374127 | -0.000068 |
| C | 0.377958 | 0.581015 | 0.000054 |
| C | 2.004058 | -2.802921 | -0.000115 |

S34
|   | x    | y    | z    |
|---|------|------|------|
| 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

|   | x    | y    | z    |
|---|------|------|------|
| 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 | -0.00001000 |
| 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 | -0.00001100 |
| C | -1.97962600 | 4.50198300 | -1.26072500 |
| C | -1.98022000 | 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 | -1.2603000 |
| C | 4.48683500 | -2.65395700 | -0.00028600 |
| H | 2.00530600 | -2.80661100 | -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 | 4.83336000 | 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 | -1.39814000 | 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 | -3.39633500 | -3.01450300 | 2.17371200 |
| H | -3.41670400 | -5.22833800 | 0.00034100 |
| H | -1.96842000 | -4.71500600 | 0.89186000 |
| 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 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -2.339023  | -0.656291  | 0.000010   |
| C       | -2.006773  | -2.018444  | -0.000020  |
| C       | -0.654190  | -2.365913  | -0.000027  |
| C       | 0.374288   | -1.389259  | -0.000002  |
| C       | 1.748237   | -1.737893  | -0.000005  |
| C       | 2.379860   | 0.577512   | -0.000066  |
| C       | -1.127977  | 4.213384   | 0.000007   |
| C       | -3.126960  | -3.067064  | -0.000050  |
| C       | 4.247503   | -1.138260  | 0.000080   |
| C       | -1.967558  | 4.498110   | -1.255283  |
| C       | -1.967468  | 4.498035   | 1.255385   |
| C       | 0.071180   | 5.164265   | -0.000090  |
| C       | -3.994329  | -2.883224  | 1.255084   |
| C       | -3.993777  | -2.883676  | -1.255525  |
| C       | -2.580686  | -4.496723  | 0.000400   |
| C       | 4.913610   | -0.553810  | 1.255319   |
| C       | 4.913749   | -0.553920  | -1.255260  |
| C       | 4.471742   | -2.652680  | 0.000780   |
| H       | 1.998756   | -2.799674  | 0.000200   |
| H       | 3.144724   | 1.358674   | -0.000079  |
| H       | 1.434162   | 3.096866   | -0.000860  |
| H       | -2.740445  | 2.010324   | 0.000020   |
| H       | -3.383321  | -0.349520  | 0.000029   |
| H       | -0.353125  | -3.414450  | 0.000640   |
| H       | 4.039237   | -3.131508  | 0.891989   |
| H       | 4.039144   | -3.131597  | -0.891742  |
| H       | 5.551337   | -2.868168  | 0.000350   |
| H       | 4.453517   | -0.958378  | 2.170097   |
| H       | 4.453708   | -0.958534  | -2.170076  |
| H       | 5.986779   | -0.803674  | 1.272884   |
| H       | 5.986899   | -0.803871  | -1.272780  |
| H       | 4.826139   | 0.542086   | -1.293906  |
| H       | 4.825909   | 0.542206   | 1.293846   |
| H       | 0.702152   | 5.029117   | 0.891820   |
| H       | 0.281888   | 6.207020   | -0.000010  |
| H       | 0.702123   | 5.029117   | -0.891921  |
| H       | -1.387350  | 4.300870   | 2.170117   |
| H       | -2.286485  | 5.552711   | 1.273370   |
| H       | -2.873437  | 3.875066   | 1.293540   |
| H       | -2.873380  | 3.874940   | -1.293565  |
| H       | -2.868130  | 5.552717   | -1.272994  |
| H       | -1.387369  | 4.301283   | -2.170072  |
| H       | -4.454714  | -1.885461  | -1.294136  |
| H       | -3.394204  | -3.010654  | -2.170179  |
Monomer 2 optimized with PBE0-D3

S38
|  |  |  |  |
|---|---|---|---|
| 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 | -2.28464400 | 5.54623500 | 1.27549700 |
| H | -2.87379500 | 3.86779600 | 1.29208400 |
| H | -2.87324000 | 3.86758200 | -1.29279600 |
| H | -2.28431000 | 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 |

S39
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 -2.16796000
H    5.97890700  -0.79870500  1.27493600
H    5.97903200  -0.79854800 -1.27470500
H    0.70025000  5.02092700  0.89190500
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   -4.80163000  -3.62142300 -1.27538200
H   -4.44705900  -1.87862800  1.29022300
H   -4.80056900  -3.62101400  1.27496900
H   -3.38587500  -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 -4.47724500  0.00031800
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   -3.90292200 -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 -0.97229900 -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
Monomer 2 optimized with M06-D3

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
H  4.02474000 -3.13949700 -0.89363300
H  5.53872700 -2.87762500 -0.00024300
H  4.43444500 -0.97207100 2.16707300
H  4.82335400  0.52834100 -1.29289000
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  1.29354300
H  -2.85974600  3.88015500 -1.29300100
H  -2.25716500  5.55409000 -1.27386300
H  -1.36512100  4.29117900 -2.16704900
H  -4.46007700 -1.86478900  1.29256900
H  -4.80877900 -3.61011500 -1.27403000
H  -3.39276900 -2.98869300  2.16695500
H  -3.43536000 -5.19127800  0.00046400
H  -1.98365100 -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  0.00001000
C  1.74689400  -1.74326100 -0.00003000
C  2.38171400  -0.77843100 -0.00003700
C  2.85439600  -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

S43
| 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    | -3.38689000 | -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    | 0.70743600  | 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 |
|  C     |          |          |          |
|--------|----------|----------|----------|
|  1.02992200 |  0.97978400 | -0.00008000 |          |
|  0.64665700 |  2.34863200 | -0.00007400 |          |
| -0.69235900 |  2.73829300 | -0.00010500 |          |
| -1.67810700 |  1.74090200 | -0.00011500 |          |
| -1.35539000 |  0.36272100 | -0.00008100 |          |
| -2.34017400 | -0.65215800 | -0.00002200 |          |
| -0.65791800 | -2.36734000 |  0.00001300 |          |
|  0.37250800 | -1.39116000 | -0.00003500 |          |
|  1.74611600 | -1.74398200 | -0.00001900 |          |
| -3.38189000 |  0.57254300 | -0.00007300 |          |
| -1.12012400 |  4.21154000 |  0.00002600 |          |
| -3.13044100 | -3.05741600 |  0.00000700 |          |
|  4.24339600 | -1.14484200 |  0.00001000 |          |
| -1.96065300 |  4.49474800 | -1.25553000 |          |
| -1.95985900 |  4.49474300 |  1.25615900 |          |
|  0.08250200 |  5.15897900 | -0.00035100 |          |
| -3.99866300 | -2.86824700 |  1.25545800 |          |
| -3.99795700 | -2.86828000 | -1.25601300 |          |
| -2.58760800 | -4.48669000 |  0.00061500 |          |
|  4.90857700 | -0.55914400 |  1.25617700 |          |
|  4.90904000 | -0.55806000 | -1.25540500 |          |
|  4.46344100 | -2.66012300 | -0.00060700 |          |
|  1.99329800 | -2.80558600 | -0.00006000 |          |
|  3.14915500 |  1.35033800 | -0.00008300 |          |
|  1.44237100 |  3.09336200 | -0.00006100 |          |
| -2.73512800 |  2.01666600 | -0.00010300 |          |
| -3.38863200 | -0.34528300 |  0.00001000 |          |
| -0.35809300 | -3.41521500 |  0.00009600 |          |
|  4.02599600 | -3.13230500 |  0.89131400 |          |
|  4.02597400 | -3.13157800 | -0.89290300 |          |
|  5.54187300 | -2.87570100 | -0.00070700 |          |
|  4.44172300 | -0.96260400 |  2.16682900 |          |
|  4.44241700 | -0.96062600 | -2.16658100 |          |
|  5.97950600 | -0.81372100 |  1.27313700 |          |
|  5.97993500 | -0.81282100 | -1.27226300 |          |
|  4.82178800 |  0.53728200 | -1.28608600 |          |
|  4.82109700 |  0.53617900 |  1.28782700 |          |
|  0.70993600 |  5.01623500 |  0.89170700 |          |
| -0.26992200 |  6.20074300 | -0.00040800 |          |
|  0.70955600 |  5.01599400 | -0.89263400 |          |
| -1.37775700 |  4.29002200 |  2.16680000 |          |
| -2.27267000 |  5.55010500 |  1.27406800 |          |
| -2.86600700 |  3.87322000 |  1.28681000 |          |
Monomer 2 optimized with LC-ωPBE
|   | X         | Y         | Z         |
|---|------------|------------|------------|
| 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  | -0.79696000 | 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-ωPBE-D3

|   | X         | Y         | Z         |
|---|------------|------------|------------|
| 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  0.00003110
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    5.54769600  -2.85378600  0.00000100
H    4.33696900  -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  1.28683200
H    4.81596100   0.55030000  1.28683200
H    0.69220700   5.01898200  0.89173900
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-ωPBE-D3BJ

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 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 | -0.00011100|
| H    | -3.38105200| -0.35153100| 0.00028000 |
| H    | -0.34812200| -3.40923700| 0.00067000 |
| 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|
Monomer 2 optimized with CAM-B3LYP

| Atom | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 | C9 | C10 | C11 | C12 | C13 | C14 | C15 | C16 | C17 | C18 | C19 | C20 | C21 | C22 | C23 | C24 | C25 | C26 | C27 | C28 | C29 | C30 |
|------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 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 | -0.00006000 |
| C    | 0.37550300 | -1.38741100 | -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 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 1.4304600 | 3.0949400 | -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 | -1.29401000 |
| H    | 4.83017200 | 0.54611100 | 1.29435000 |
| 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 | -1.29439000 |
| H    | -3.39605000 | -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

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 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 | 0.00008000 |
| 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          | H          |
|---|------------|------------|
|   | 2.75610500 | -0.76873400 | -0.00002000 |
|   | 2.37705700 | 0.58007300  | 0.00003300  |
|   | -1.13603500| 4.20800500  | -0.00001400 |
|   | -3.12066900| -3.06971600 | -0.00001600 |
|   | 4.24828300 | -1.12964200 | 0.00000200  |
|   | -1.97699600| 4.49113200  | -1.25608800 |
|   | -3.98916900| -2.88692000 | -1.25594900 |
|   | -2.57538800| -4.50132200 | 0.00012700  |
|   | 4.91396400 | -0.54276500 | 1.25601800  |
|   | 4.91410600 | -0.54241000 | -1.25577300 |
|   | 4.47899000 | -2.64408400 | -0.00020100 |
|   | 1.99954500 | -2.79508000 | -0.00008800 |
|   | 3.14001000 | 1.36126700  | 0.00010100  |
|   | 1.43043500 | 3.09376100  | 0.00011200  |
|   | -2.73987900| 2.00327600  | 0.00007700  |
|   | -3.38332500| -0.35601200 | 0.00008300  |
|   | -0.34360600| -3.41181100 | -0.00007700 |
|   | 4.04726800 | -3.12280800 | 0.89102600  |
|   | 4.04720000 | -3.12258600 | -0.89151300 |
|   | 5.55870700 | -2.85511300 | -0.00027200 |
|   | 4.45209500 | -0.94725500 | 2.16918700  |
|   | 4.45218200 | -0.94645400 | -2.16911200 |
|   | 5.98638200 | -0.79252900 | 1.27428700  |
|   | 5.98647700 | -0.79237100 | -1.27411700 |
|   | 4.82587600 | 0.55270400  | -1.29184700 |
|   | 4.82550600 | 0.55231700  | 1.29251100  |
|   | 0.69037500 | 5.03044900  | 0.89166300  |
|   | -0.29695900| 6.20555500  | 0.00017500  |
|   | 0.69073400 | 5.03050900  | -0.89093900 |
|   | -1.39680100| 4.29231600  | 2.16910600  |
|   | -2.29641500| 5.54495400  | 1.27444900  |
|   | -2.88215100| 3.86771800  | 1.29150700  |
|   | -2.88142000| 3.86741400  | -1.29243100 |
|   | -2.29639000| 5.54490400  | -1.27455200 |
|   | -1.39585800| 4.29292900  | -2.16917000 |
|   | -4.45210400| 1.89054600  | -1.29215300 |
|   | -3.38795300| -3.01084200 | -2.16918200 |
|   | -4.79907700| -3.63292100 | -1.27447600 |
|   | -4.45267100| 1.89059100  | 1.29162900  |
|   | -4.79881800| -3.63314200 | 1.27468900  |
|   | -3.38797300| -3.01001900 | 2.16913800  |
|   | -3.41108600| -5.21680100 | -0.00002400 |

S52
Monomer 2 optimized with CAM-B3LYP-D3BJ

\[
\begin{align*}
\text{H} & \quad -1.96407900 \quad -4.70512600 \quad 0.89153900 \\
\text{H} & \quad -1.96371100 \quad -4.70520300 \quad -0.89100700
\end{align*}
\]
H  0.69618400  5.02487300  0.89060600
H  -0.28933500  6.20169300 -0.00019400
H   0.69594200  5.02480000 -0.89115800
H  -2.29156000  5.54386100  1.27510100
H  -2.87690000  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 ωB97XD

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
Dimer 2–2 optimized with B3LYP

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  -0.00000400
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 -3.80335000  -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

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

S55
|  | 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  | -3.84935000 | 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  | -3.09380000 | 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 |

S56
Dimer 2–2 optimized with B3LYP-D3

|   |   |   |   |
|---|---|---|---|
| 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 | -3.2348300 |
| H | 6.59542000 | 3.16952200 | -3.89236000 |
| H | 4.67987100 | 3.16952200 | -3.89236000 |
| 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 | 4.72373000 | -2.49552700 |
| H | 6.64052200 | 1.84481800 | -1.83382200 |

|   |   |   |   |
|---|---|---|---|
| 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 | 1.20440600 | 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 | 3.18519000 |
| C | -0.17765100 | -5.14393800 | 1.78805400 |
| C | 3.94971000 | 2.76563100 | 3.03503900 |
| C | 4.60886500 | 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  | -1.56524000  |
| C   | -0.64437500| 2.72392600  | -1.63665000  |
| C   | -1.64132000| 1.73622400  | -1.58831000  |
| 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 | -0.83384900 | -1.59072000  |
| C   | 2.41689600 | 0.52119100  | -1.53855000  |
| C   | -1.04079800| 4.20441600  | -1.81523300  |
| C   | -3.12645000| -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 | -3.03771000  |
| C   | -4.06100900| -3.0897900  | -0.53770600  |
| C   | -2.56819300| -4.51030000 | -1.90716700  |
| C   | 4.89552500 | -0.46345200 | -2.91017800  |
| C   | 5.02478500 | -0.89388900 | -0.43429500  |
| C   | 4.34459000 | -2.73975700 | -2.00813000  |
| 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  |

S59
| 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                 | -3.97063000| -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 | -3.35651700| -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 | 5.22521000 | 2.02838300  |
| H                 | 1.91206600 | 4.60695000 | 2.78639900  |

S60
H  1.99696700  4.81641000  1.01803600

Dimer 2–2 optimized with B3LYP-D3BJ

C  -0.03315700  0.03603100  1.51696000
C  -1.05453900  -0.95596000  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  -0.34793000  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   2.05278900  -4.63992200  0.69241700
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 -1.51067200
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

S62
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 -3.03082000  2.05852400
C  1.83429300 -2.52516700  1.68879100
C  2.11426400 -1.13479000  1.69939000
C  3.37431700 -0.61406900  1.31253700
C  3.64132700  0.75625300  1.31261200
|  C  |    |    |    |
|-----|----|----|----|
| 2.62158400 | 1.62779600 | 1.72116400 |
| -2.06906900 | 2.51827600 | 3.37062500 |
| 0.26777700 | -4.53337800 | 2.03030600 |
| 4.99496500 | 1.33151600 | 0.87642800 |
| -3.27890000 | 2.33739000 | 2.44038700 |
| -2.47354500 | 2.17970000 | 4.81397100 |
| -1.64653000 | 3.98845400 | 3.32356000 |
| -0.14090300 | -4.99608800 | 3.43744800 |
| -0.88942800 | -4.78331900 | 1.04998700 |
| 1.46584800 | -5.37236100 | 1.57984500 |
| 5.60440800 | 2.13968700 | 2.03257200 |
| 4.78434800 | 2.25022400 | -0.33774300 |
| 5.98904000 | 0.23686600 | 0.48158100 |
| -1.09651300 | 0.23400100 | -2.10719400 |
| -1.34942900 | -1.16404500 | -2.12230200 |
| -0.31467700 | -0.43200000 | -2.53698500 |
| 0.94229400 | -1.57709000 | -2.92544100 |
| 1.17201300 | -0.19400200 | -2.89996800 |
| 0.17816600 | 0.72978800 | -2.49690000 |
| 0.40348000 | 2.12557400 | -2.46148900 |
| -0.58668600 | 3.03301800 | -2.06002900 |
| -1.83383100 | 2.52546300 | -1.68967700 |
| -2.11401800 | 1.13512600 | -1.70012700 |
| -3.37983300 | 0.61477300 | -1.31196200 |
| -3.64114900 | -0.75551500 | -1.31114100 |
| -2.62172600 | -1.62740400 | -1.71975200 |
| 2.06798800 | -2.51930400 | -3.37114700 |
| -0.26704600 | 4.53325800 | -2.03236400 |
| -4.99456100 | -1.33036100 | -0.87372100 |
| 3.27756900 | -2.33929600 | -2.44039900 |
| 2.47310300 | -2.18046500 | -4.81424200 |
| 1.64474700 | -3.98930200 | -3.32472900 |
| 0.14207200 | 4.99535700 | -3.43958000 |
| 0.88996900 | 4.78331700 | -1.05184600 |
| -1.46504000 | 5.37266900 | -1.58253600 |
| -5.60445800 | -2.14005500 | -2.0285100 |
| -4.78327300 | -2.24748400 | 0.34153400 |
| -5.98855900 | -0.23529800 | -0.47981300 |
| 4.14086200 | -1.32623200 | 1.00391900 |
| 2.14638000 | 0.20411700 | -3.19511800 |
| 1.39129900 | 2.48982900 | -2.75683500 |
| 2.79637400 | 2.70692200 | 1.73301900 |
| 0.53341100 | 3.11150100 | 2.54287300 |
| -2.63332000 | 3.19826000 | -1.37583000 |
| -4.14032200 | 1.32720900 | -1.00346500 |
| Atom | X Position | Y Position | Z Position |
|------|------------|------------|------------|
| H    | -2.1468200 | -0.20509800| 3.19363400 |
| H    | -1.39118200| -2.48965600| 2.75493600 |
| H    | -2.79661100| -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 | -0.36192000| -0.36766000|
| H    | 6.94406600 | 0.69348800 | 0.17906400 |
| H    | 5.76535600 | 1.50246100 | 2.91586500 |
| 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 | 4.45346900 | -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    | -6.94387000| -0.69161900| -0.17622400|
| H    | -6.57710900| -2.56344400| -1.72988100|
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| 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 | -4.45972800 | 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  | -5.25977000 | 2.25481700 |
| H    | 1.78954200  | -5.11167200 | 0.56024100 |

Dimer 2–2 optimized with PBE0-D3

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| 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  -1.76192000
C  -1.78638100   4.28429100  -3.23354000
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  -1.66781200
H  -3.35656800   -0.41953400  -1.63719000
H  -3.16178700  -1.33758800  -1.58093700
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  -1.61886600
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  -2.99883900   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

S67
| H       | 2.88049600 | 2.13093100 |
|---------|------------|------------|
| H       | 0.63300800 | 3.87038600 |
| H       | 1.34552900 | -0.39641200|
| H       | 0.67832800 | 3.06742400 |
| H       | 1.03530800 | 0.56306500 |
| H       | 0.28090000 | 0.24957200 |
| H       | 0.68882400 | 2.78960500 |
| H       | -2.13475000| -0.43657300|
| H       | -3.36806100| 0.35079300 |
| H       | -3.85913500| -0.69880100|
| H       | -3.61217300| -3.20641400|
| H       | -1.86753300| -3.00794500|
| H       | -2.84208600| -3.94514500|
| H       | -4.83787900| -1.01349000|
| H       | -4.64216800| -2.78306900|
| H       | -5.28056300| -2.03174200|
| H       | -4.90661700| 2.62292300 |
| H       | -6.14806600| 1.93843100 |
| H       | -5.04977800| 0.85576700 |
| H       | -3.97630700| 4.03646600 |
| H       | -5.32806000| 3.41944100 |
| H       | -3.65451800| 3.30402100 |
| H       | -3.93638100| 0.74308100 |
| H       | -5.61433200| 0.94407600 |
| H       | -4.54728700| 0.22654300 |
| H       | -3.27418500| -1.16887600|
| H       | -2.98919000| -2.92097200|
| H       | -2.88058400| -2.13192300|
| H       | -0.67862600| -3.06744000|
| H       | -1.03695300| -0.56245400|
| H       | 0.28059700 | 0.24993800 |
| H       | 0.68884900 | 2.78900600 |
| H       | -1.34520900| 0.39654100 |
| H       | -0.63237000| -3.87027000|
| H       | 2.13430400 | 0.43701600 |
| H       | 3.36775800 | -0.35064300|
| H       | 3.85865000 | 0.69907100 |
| H       | 1.86803800 | 3.00854200 |
| H       | 3.61275100 | 3.20676800 |
| H       | 2.84258700 | 3.94533000 |
| H       | 5.28074200 | 2.03101500 |
| H       | 4.64269600 | 2.78256800 |
| H       | 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 | -5.03679900 | 0.76761000  | 0.46615600 |
| C | -4.46124000 | 2.62297300  | 2.01081400 |
| C | 0.03262900  | -0.04044700 | -1.51864200 |
| C | 1.03293800  | 0.96742200  | -1.51669800 |
| C | 0.63036700  | 2.32505900  | -1.54386200 |
| C | -0.71239800 | 2.69711700  | -1.62027400 |
| C | -1.68315700 | 1.68984500  | -1.56543000 |
| C | -1.34392200 | 0.31686300  | -1.53538000 |
| C | -2.31076900 | -0.71728800 | -1.54958900 |
| C | -1.95596300 | -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  | 0.77505600  | -1.51936900 |
| C | -1.14022000 | 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 |

S69
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -3.9932500 | -3.1399570 | -0.5652640 |
| C       | -2.4451260 | -4.5472510 | -1.8931540 |
| C       | 4.8553530  | -0.3540110 | -2.9266730 |
| C       | 5.0368960  | -0.7675890 | -0.4663010 |
| C       | 4.4612030  | -2.6230120 | -2.0109180 |
| H       | -2.0452130 | 2.7940470  | 1.5718360  |
| H       | -2.7425880 | 1.9503700  | -1.6177800 |
| H       | -3.3618080 | -0.4272530 | -1.5961780 |
| H       | -3.1447990 | -1.3667360 | 1.5462630  |
| H       | -1.4144450 | -3.0811350 | 1.5730470  |
| H       | -0.2812160 | -3.4386290 | -1.5551190 |
| H       | 2.0452010  | -2.7940490 | -1.5720100 |
| H       | 2.7426000  | -1.9503420 | 1.6179580  |
| H       | 3.3617960  | 0.4273320  | 1.5967390  |
| H       | 3.1447520  | 1.3667600  | -1.5464990 |
| H       | 1.4144850  | 3.0811110  | -1.5731260 |
| H       | 0.2811450  | 3.4386220  | 1.5550790  |
| H       | -1.1033350 | 3.9641070  | -3.9969170 |
| H       | -2.1058790 | 5.3149870  | -3.3995910 |
| H       | -2.6953410 | 3.6386380  | -3.2789900 |
| H       | -1.6856550 | 4.5622970  | 0.2541120  |
| H       | -3.0297320 | 3.9337710  | -0.7268810 |
| H       | -2.4901660 | 5.6133730  | -0.9349300 |
| H       | -0.3058150 | 6.1526660  | -1.9002490 |
| H       | 0.5753340  | 5.0620240  | -0.8082420 |
| H       | 0.7735720  | 4.9149840  | -2.5729960 |
| H       | -3.9295190 | 2.9441170  | 2.9193350  |
| H       | -4.1117160 | 3.2433320  | 1.1727490  |
| H       | -5.5314130 | 2.8364210  | 2.1545610  |
| H       | -4.3084980 | 0.5808150  | 3.8544020  |
| H       | -4.6534590 | 1.3272320  | -0.4000730 |
| H       | -5.9123770 | 0.6271180  | 3.0742110  |
| H       | -6.1058550 | 1.0087770  | 0.5803740  |
| H       | -4.9571500 | -0.3045430 | 0.2384840  |
| H       | -4.8126280 | -0.7335720 | 2.7694370  |
| H       | -4.4708320 | -2.1597050 | -0.4290350 |
| H       | -3.4592740 | -3.3892290 | 0.3638590  |
| H       | -4.7921850 | -3.8851130 | -0.7067160 |
| H       | -4.6075100 | -3.6158180 | -3.2062420 |
| H       | -4.3414050 | -1.8706080 | -2.9930470 |
| H       | -3.1730920 | -2.8330620 | -3.9236260 |
| H       | -1.8820290 | -4.8358960 | -0.9928890 |
| H       | -1.7719760 | -4.6286910 | -2.7598050 |
| H       | -3.2530850 | -5.2825240 | -2.0268160 |
| H       | -0.7736120 | -4.9150630 | 2.5725870  |
|   | X        | Y        | Z       |
|---|----------|----------|---------|
| H | 0.3059400| -6.15268400 | 1.89995400 |
| H | -0.57504400 | -5.06196600 | 0.80784600 |
| H | 1.10329400 | -3.96453600 | 3.99684300 |
| H | 2.10609700 | -5.31118800 | 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 | -3.24332000 | -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 | 3.17255000 | 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**

|   | X        | Y        | Z       |
|---|----------|----------|---------|
| 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 | -0.77246000 | 1.65039700 |
| C | 2.22727600 | 1.07642500 | 1.63916300 |
| C | 1.69537900 | 2.37205000 | 1.63569700 |
| C | 0.30632800 | 2.51003700 | 1.59433000 |
| 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 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 2.777292  | -4.164111 | 0.816832  |
| C    | 2.457721  | -3.952088 | 3.284780  |
| C    | 0.722917  | -5.026499 | 1.883476  |
| C    | 3.207212  | 3.596910  | 3.176632  |
| C    | 3.777646  | 3.491298  | 0.751000  |
| C    | 1.899804  | 4.899045  | 1.522524  |
| C    | -4.865757 | -0.260825 | 3.007466  |
| C    | -5.008897 | 0.138815  | 0.547146  |
| C    | -4.750824 | 2.039104  | 2.112608  |
| C    | 0.003071  | -0.088118 | -1.639098 |
| C    | 0.854540  | 1.048013  | -1.667946 |
| C    | 0.268788  | 2.339461  | -1.705320 |
| C    | -1.142870 | 2.522871  | -1.755845 |
| C    | -1.934230 | 1.388352  | -1.701921 |
| C    | -1.408536 | 0.077212  | -1.650542 |
| C    | -2.227329 | -1.076452 | -1.639399 |
| C    | -1.695386 | -2.372061 | -1.635797 |
| C    | -0.306341 | -2.510037 | -1.594377 |
| C    | 0.561354  | -1.390976 | -1.619376 |
| C    | 1.968393  | -1.531999 | -1.662060 |
| C    | 2.824494  | -0.432451 | -1.730151 |
| C    | 2.253178  | 0.846457  | -1.691220 |
| C    | -1.753897 | 3.903245  | -1.924254 |
| C    | -2.628599 | -3.579354 | -1.757237 |
| C    | 4.342768  | -0.591909 | -1.847729 |
| C    | -2.773500 | 4.164079  | -0.816991 |
| C    | -2.457663 | 3.952136  | -3.284860 |
| C    | -0.722873 | 5.026436  | -1.883572 |
| C    | -3.207437 | -3.596875 | -3.176529 |
| C    | -3.777314 | -3.491531 | -0.750707 |
| C    | -1.899613 | -4.899111 | -1.522819 |
| C    | 4.865438  | 0.260830  | -3.007568 |
| C    | 5.009175  | -0.138507 | -0.547249 |
| C    | 4.750841  | -2.039030 | -2.112409 |
| H    | -2.367586 | 2.549602  | 1.682962  |
| H    | -3.024918 | 1.494431  | -1.744059 |
| H    | -3.312405 | -0.926114 | -1.675567 |
| H    | -2.893015 | -1.735652 | 1.728130  |
| H    | -0.948121 | -3.197146 | 1.738963  |
| H    | 0.157151  | -3.501799 | -1.586052 |
| H    | 2.367640  | -2.549537 | -1.682981 |
| H    | 3.024869  | -1.494459 | 1.743645  |
| H    | 3.312344  | 0.925900  | 1.675119  |
| H    | 2.892850  | 1.735769  | -1.727406 |
| H    | 0.948075  | 3.197092  | -1.738837 |
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 2.22515000
H -4.38074300 0.02286700 3.95671600
H -4.67526700 0.76153000 -0.30162800
H -5.95409500 -0.12010000 3.12498300
H -6.10700200 0.22562000 0.62129000
H -4.76633100 -0.91046000 0.31221400
H -4.69104200 -1.33697700 2.84931100
H -4.41804300 -2.61206400 3.92354000
H -3.40099500 -3.44082000 0.28598400
H -4.42378800 -4.38202700 -0.83170000
H -3.88646000 -4.46177900 -3.11258000
H -3.73689000 -2.68209400 -3.39183400
H -2.40250800 -3.66858000 -3.92726800
H -1.43044700 -4.93468100 -0.52459100
H -1.11122200 -5.08167800 -2.27635400
H -2.61272500 -5.73764300 -1.58650000
H -0.10304000 -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 2.29025000 -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

S73
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 3.31133400
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

|   | X          | Y          | Z          |
|---|------------|------------|------------|
| 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 | -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| -0.01876000| 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   -2.22119000   4.03908100  -3.33027100
C   -0.58272600   5.06423900  -1.77807300
C   -3.58467000  -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   1.65635500
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     3.31519000   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    -3.17636000   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     0.79912500   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   0.83632200 -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 -3.46709000  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

S76
| 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 | 1.92247000 | 1.58312000 |
| C | -2.64261100 | 1.08339400 | 1.63096500 |
| C | 0.61185200 | -4.31726500 | 1.78624000 |
| C | 3.41557500 | 2.71905900 | 1.83034600 |
| C | -4.06996000 | 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 | -4.13309900 | -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 |

S77
| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| C       | 5.0262100   | -0.93737500 | -0.67011100 |
| C       | 4.23810300  | -3.01838100 | -1.77331300 |
| H       | -1.65164400 | 3.00369900  | 1.62614500  |
| H       | -2.54848200 | 2.22728000  | -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 2.70763000 2.20518600
H 3.02645000 3.03174100 3.95593900
H 4.01239800 4.30904300 3.19287300
H 2.25934900 4.24663200 2.90774300
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 1.62556600
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
| X      | Y      | Z      |
|--------|--------|--------|
| 3.15540300 | 3.64000900 | 3.03049800 |
| 4.73274700  | 1.98016400 | 2.07402800  |
| 3.56771400  | 3.57627400 | 0.56056800  |
| -4.76355800 | 0.93860200 | 2.95920500  |
| -4.86812300 | 1.35598100 | 0.49227600  |
| -4.08000700 | 3.13977800 | 2.03890000  |
| 0.02483400  | -0.02353400 | -1.54949900 |
| 1.11654200  | 0.88677800 | -1.55188600 |
| 0.84793000  | 2.28109000 | -1.57705100 |
| -0.45481300 | 2.77761500 | -1.64122700 |
| -1.51728100 | 1.86655600 | -1.58785000 |
| -1.31203800 | 0.46613500 | -1.55685900 |
| -2.37745900 | -0.46672400 | -1.56859100 |
| -2.15480900 | -1.84959200 | -1.62266200 |
| -0.83833400 | -2.30867200 | -1.57323600 |
| 0.26810700  | -1.42123600 | -1.55096200 |
| 1.60726500  | -1.88578800 | -1.56948200 |
| 2.69098400  | -1.00742400 | -1.61926600 |
| 2.43114300  | 0.36737000  | -1.56832000 |
| -0.75508300 | 4.27071100  | -1.83317000 |
| -3.34632000 | -2.80713800 | -1.76870500 |
| 4.13680800  | -1.49400700 | -1.78687900 |
| -1.71176800 | 4.77511500  | -0.74419000 |
| -1.41515700 | 4.45837400  | -3.20978000 |
| 0.51396700  | 5.12496400  | -1.78520700 |
| -4.13784900 | -2.43027200 | -3.03218200 |
| -4.26744500 | -2.70081000 | -0.54523900 |
| -2.89816500 | -4.26492800 | -1.90482200 |
| 4.67161400  | -0.98173000 | -3.13511000 |
| 5.01896600  | -0.94896500 | -0.65540100 |
| 4.23542000  | -3.02126200 | -1.77890600 |
| -1.65158000 | 3.00433900  | 1.62411300  |
| -2.54732500 | 2.22711500  | -1.63789300 |
| -3.39655500 | -0.07437500 | -1.59665800 |
| -3.28115900 | -0.98476700 | 1.57580600  |
| -1.78600400 | -2.90821000 | 1.60314800  |
| -0.62188000 | -3.37679000 | -1.60484700 |
| 1.76583600  | -2.96333500 | -1.59696700 |
| 2.48837100  | -2.32776300 | 1.63050800  |
| 3.40490500  | -0.06329400 | 1.68366700  |
| 3.25835500  | 1.08048500  | -1.60613200 |
| 1.70233900  | 2.95682700  | -1.60411900 |
| 0.76044900  | 3.34149400  | 1.58547000  |
| -0.75332300 | 4.09314500  | -4.00890200 |
| -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 | 5.01396600 | -0.92039200 |
| H | 0.25140900  | 6.18589900 | -1.90755500 |
| H | 1.03321600  | 5.01396600 | 2.12102000  |
| 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 | -5.89610000 | 1.73037300 | 0.59228200  |
| H | -4.91664500 | 0.27869300 | 0.27906200  |
| H | -4.85875800 | -0.14478100| 2.80143000  |
| H | -4.63336600 | -1.67379200| -0.40623700 |
| H | -3.73628000 | -3.00262000| 0.37002600  |
| H | -5.11446600 | -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 | -2.52255000 | -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 | 2.40593000  | -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| -3.29422200 |
| H | 6.06383400  | -1.26308000| -0.80182600 |
| H | 4.99883600  | 0.14983100 | -0.62262900 |
| H | 4.67382500  | 0.11702000 | -3.17489000 |
| H | 4.68120200  | -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-ωPBE

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  -0.85184100  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  3.78311100  -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  1.79552600  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  -5.20529900  1.18664600
C  5.57091500  2.74602000  1.60721200
C  4.52306700  2.84580800  -0.66778600
C  6.04263700  0.97819600  -0.06801100
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

S82
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 -2.83823000
C -9.81557000 5.09204900 -3.21295200
C 0.04534500 4.92511200 -0.93220100
C -2.40681700 5.20541400 -1.18540100
C -5.57261300 -2.74891600 -1.61065000
C -4.52580600 -2.83591600 0.66471400
C -6.04395200 -0.97691300 0.06576100
C 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 -0.62263200 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 0.06576100
H 2.95756000 -2.17055400 -5.55802000
H 2.32784800 -0.55489600 -5.18114500
H 3.02975200 -2.06608400 0.96973200
H 3.41697200 -2.06608400 -1.78711000
H 4.02873800 -2.32377000 -3.24345000
H 2.55202100 -4.09345700 -4.09345700
H 1.54081700 -3.96997600 -2.62266000
H 0.79971500 -3.87245400 -4.23704100
H 6.41645800 0.29703000 0.70970700
H 5.67651200 0.37272200 0.70970700
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 -0.33035200
H 4.85704800 3.47926000 2.00703700
### Dimer 2–2 optimized with LC-ωPBE-D3

| X    | Y    | Z    |
|------|------|------|
| 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 -4.58726600  2.66817300  1.91097500  
C  0.10628000 -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 -2.23132000 -0.84418100 -1.67361100  
C -1.86326000 -2.19410800 -1.67845800  
C -0.50784000 -2.50429300 -1.61910100  
C  0.49171100 -1.50238700 -1.59432400  
C  1.87014000 -1.81791000 -1.60761600  
C  2.85425700 -0.83469400 -1.63279700  
C  2.44641900  0.50280600 -1.61253900  
C -1.12437200  4.02904600 -2.00432400  
C -2.94495000 -3.27441100 -1.78748600  
C  4.34716900 -1.17395400 -1.69847500  
C -2.08804200  4.45217300 -0.89299400  
C -1.83556900  4.12539900 -3.35984900  
C  0.05154800  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  4.58726600 -2.66817300 -1.91097500  
H -2.14336300  2.87160900  1.62869900  

S85
|   |   |   |   |
|---|---|---|---|
| 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  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 2.4591600 | -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    | 6.09942200 | 0.68061200  | -2.94598800 |
| H    | 6.09834000 | -0.97600200 | -0.41766200 |
| H    | 4.90020700 | 0.31867300  | 0.46393300  |
| H    | 4.50513200 | -0.67908600 | -3.81698200 |
| H    | 4.35707000 | 2.23361600  | 0.45832700  |
| H    | 3.29824600 | 3.42207000  | -0.35732800 |
| H    | 4.66287300 | 3.96879000  | 0.64588700  |
| H    | 4.28600400 | 2.05933800  | 3.02759400  |
| H    | 4.57775400 | 3.81032500  | 3.17167200  |
| H    | 3.12855000 | 3.04257200  | 3.94817500  |
| H    | 3.17541100 | 5.42032200  | 1.96008200  |
| H    | 1.76020000 | 4.93028800  | 0.97504400  |

Dimer 2–2 optimized with LC-\(\omega\)PBE-D3BJ

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 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    | 2.24198000  | 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  | 3.01553000  | 3.05707200 |
| C    | 3.89093200  | 3.19895100  | 0.56601900 |
| C    | 2.37200900  | 4.66701500  | 1.85823300 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| 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       | -2.42205000 | -0.83485500 | -1.66709700 |
| C       | -1.87969000 | -2.18590000 | -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       | -1.10895000 | 4.02948800  | -2.00530800 |
| C       | -2.96365400 | -3.26121600 | -1.78156400 |
| C       | 4.32837700  | -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       | 4.96992200  | -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 |
|    |     X     |     Y     |     Z     |
|----|----------|----------|----------|
| H  | -2.471070 | 5.474714 | -1.124652 |
| H  | -0.291588 | 6.029209 | -2.102978 |
| H  | 0.598690  | 4.953690 | -1.006423 |
| H  | 0.793231  | 4.795099 | -2.769369 |
| H  | -4.079885 | 3.048177 | 2.842538  |
| H  | -4.171790 | 3.290623 | 1.081438  |
| H  | -5.635249 | 2.896306 | 1.998520  |
| H  | -4.470980 | 0.708397 | 3.826101  |
| H  | -4.588552 | 1.322440 | -0.452991 |
| H  | -6.032210 | 0.716568 | 2.969359  |
| H  | -6.094147 | 1.009792 | 0.444125  |
| H  | -4.906005 | -0.291613 | 0.216886 |
| H  | -4.910337 | -0.639103 | 2.756422 |
| H  | -4.360569 | -2.212104 | -0.466955 |
| H  | -3.336199 | -3.404710 | 0.359623  |
| H  | -4.693704 | -3.945942 | -0.654955 |
| H  | -4.546741 | -3.792229 | -3.177570 |
| H  | -4.285368 | -2.042042 | -3.035438 |
| H  | -3.170380 | -3.034560 | -3.943500 |
| H  | -1.797325 | -4.916414 | -0.955719 |
| H  | -1.712850 | -4.784392 | -2.729695 |
| H  | -3.181146 | -5.405497 | -1.949054 |
| H  | -0.793374 | -4.795272 | 2.768715  |
| H  | 0.291681  | -6.029280 | 2.102519  |
| H  | -0.598328 | -4.953700 | 1.005794  |
| H  | 1.079117  | -3.808819 | 4.173569  |
| H  | 2.082895  | -5.162253 | 3.591319  |
| H  | 2.666090  | -3.488889 | 3.446132  |
| H  | 2.981335  | -3.789894 | 0.894458  |
| H  | 2.471265  | -5.474663 | 1.124646  |
| H  | 1.638727  | -4.447624 | -0.064532 |
| H  | 4.172447  | -3.290316 | -1.080510 |
| H  | 4.079186  | -3.048630 | -2.841670 |
| H  | 5.635177  | -2.896298 | -1.998891 |
| H  | 6.033026  | -0.716864 | -2.969796 |
| H  | 6.094132  | -1.010263 | -0.444041 |
| H  | 4.906980  | 0.292239  | -0.217931 |
| H  | 4.910182  | 0.638858  | -2.756976 |
| H  | 4.588138  | -1.320867 | 0.453060  |
| H  | 4.470652  | -0.708810 | -3.826293 |
| H  | 4.360626  | 2.212057  | 0.467186  |
| H  | 3.335980  | 3.404260  | -0.359659 |
| H  | 4.693465  | 3.946014  | 0.654667  |
| H  | 4.285542  | 2.042187  | 3.035457  |
| H  | 4.546896  | 3.792385  | 3.177387  |
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 1.16693000
C 2.76299000 -3.45965900 1.84589900
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 -1.50205800
C 2.76657300 1.15301200 -1.73916700
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 -2.1190900
H -0.01823100 -4.73145900 3.47925700
H 1.46139200 -5.55814700 2.95429800
H 0.61525300 -5.31857300 -2.78709500
H 1.38992500 -3.27517500 5.03905800
H 2.81545500 -4.19977800 4.50170000
H 2.82502000 -2.42470100 4.42306900
H 3.41412200 -2.57609500 1.90874300
H 3.38706900 -4.34966700 2.03284400
H 2.37118800 -3.51103100 0.81934400
H 5.27499600 -1.73567400 0.37166500
H 5.67253500 -1.82444300 0.95924700
H 6.78433500 -1.02464000 -2.10952900
H 6.81815000 0.99943200 0.37166500
H 4.75615800 2.00803000 -0.00235500
H 5.32868200 1.87706900 -2.51900400
H 4.67800200 0.51627700 0.95924700
H 5.65542000 0.29764600 -3.26318500
H 3.04219900 3.85942200 1.44146900
H 1.88616300 4.03266800 0.25990800
H 2.80561600 5.14309400 1.31087400
H 2.49774200 3.52361900 3.96681800
H 2.75431000 5.27821700 3.79917100
H 0.97763700 4.27351320 4.49500760
H 0.71390700 6.23570100 2.11868400
H -0.61184400 5.31890100 2.78439100
H -0.28745100 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

S92
|   |   |   |   |
|---|---|---|---|
| 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 | -1.28567100 | 3.87233100 | -4.16729700 |
| H | -2.30266600 | 5.17788200 | -3.50210900 |
| H | -2.83186500 | 3.48402700 | -3.38348000 |
| H | -1.68645500 | 4.37789700 | 0.11746700 |
| H | -3.05188800 | 3.72601400 | -0.80894900 |
| H | -2.58054400 | 5.28674000 | -1.00803600 |
| H | -0.46750900 | 6.05827900 | -2.09250900 |
| H | 0.48905700 | 5.00160100 | -1.03341000 |
| 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 | -6.11689000 | 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 | -4.25777700 | -2.16830100 | -3.04580100 |
| H | -3.08934300 | -3.14279900 | -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 |
| 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 | -0.16718000 | 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 | 3.0744900 |
| 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 |
| 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| 1.51032000 | -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     | -4.59222500| -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 | 5.51497500 | 1.93527000  |
| H     | 1.56369100 | 4.85936500 | 2.74215000  |
Dimer 2–2 optimized with $\omega$B97XD

|     | X   | Y   | Z   |
|-----|-----|-----|-----|
| H   | 1.62410400 | 4.96544700 | 0.96578200 |
| 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   | -4.33316000 | 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 | 4.08328200  | -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   | -2.27537700 | 1.84703400 | -1.75762100 |
| H   | -3.31457700 | -0.53346200| -1.69262700 |
| H   | -3.16786600 | -1.34486000| 1.60803300  |
| H   | -1.41773500 | -3.03407500| 1.68488500  |
| H   | -0.19459800 | -3.50824700| -1.60847900 |
| H   | 2.12432200  | -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  | -1.31344000 | 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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