Supporting information for:

Aromaticity directs the excited-state properties of the host-guest complexes of nanohoops

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Abstract

π-Conjugated organic molecules have exciting applications, as materials for batteries, solar cells, light emitting diodes, etc. Among these systems, antiaromatic compounds are of particular interest because of their smaller HOMO–LUMO energy gap compared to aromatic compounds. A small HOMO-LUMO gap is expected to facilitate charge transfer in the systems. Here we report the ground and excited-state properties of two model nanohoops that are nitrogen-doped analogs of recently synthesized [4]cyclodibenzopentalenes – tetramers of benzene-fused aromatic 1,4-dihydropyrrolo[3,2-b]pyrrole (**[4]DHPP**) and antiaromatic pyrrolo[3,2-b]pyrrole (**[4]PP**). Their complexes with $\mathbf{C_{60}}$ fullerene show different behavior upon photoexcitation, depending on the degree of aromaticity. **[4]DHPP** acts as an electron donor, whereas **[4]PP** is a stronger electron-acceptor than $\mathbf{C_{60}}$. Ultrafast charge separation in combination with slow charge recombination we found for **[4]PP⊃$\mathbf{C_{60}}$** indicate a long lifetime of the charge transfer state.

Table of Contents

Computational Methodology

Quantum-chemical calculations

Geometry optimizations were performed employing the DFT BLYP[1, 2] exchange−correlation functional with Ahlrichs' Def2-SVP basis set,[3, 4] and using the resolution of identity approximation (RI, alternatively termed density fitting)[5, 6] implemented in the ORCA 4.2.1 program.[7-9] The empirical dispersion D3 correction with Becke–Johnson damping,[10,11] was employed. Electronic structures calculations and vertical excitation energies were calculated using TDA formalism[12] with the range-separated functional from Handy and coworkers' CAM-B3LYP[13] and Ahlrichs' Def2-SVP basis set,[3, 4] using Gaussian 16 (rev. A03).[14] The quantitative assessment of aromaticity/antiaromaticity were performed using the range-separated CAM-B3LYP.[13] The formation energy of the complexes was computed using BLYP functional coupled with def2-TZVP basis[3,4] (BLYP(D3BJ)/def2-TZVP//BLYP(D3BJ)/def2-SVP). Canonical energy decomposition analysis (EDA) was performed using the Amsterdam Density Functional (ADF) program at the BLYP-D3/TZ2P// BLYP(D3BJ)/def2-SVP level of theory.[15] The excited states have been analyzed in terms of the natural transition orbitals (NTO) concept introduced by Luzanov *et al.*[16] and implemented within modern many-body codes by Head-Gordon *et al.*[17] Molecular structures and frontier molecular orbitals were visualized by Chemcraft 1.8 program.[18]

Aromaticity

HOMA

Geometry parameters of the nanohoops (CC and CN bond lengths) were used to estimate the π-electron delocalization by applying the aromaticity index HOMA (harmonic oscillator model of aromaticity)[19,20]

$$HOMA = 1 - \frac{1}{n}\sum_{i,j=1}^{n} \alpha_i (R_{opt,i} - R_{i,j})^2 \qquad (1)$$

where n is the number of bonds taken into account when carrying out the summation and i denotes the type of bond (CC or CN), αi is a normalization constant (for CC and CN bonds, α_{CC} = 257.7 and α_{CN} = 93.52) fixed to give HOMA = 0 for a model nonaromatic system and HOMA = 1 for the system with all bonds equal to the optimal value Ropt,i assumed to be realized for full aromatic systems (for CC and CN bonds, $R_{opt,CC}$ = 1.388 Å and $R_{opt,CN}$ = 1.334 Å), and $R_{i,j}$ denotes bond lengths taken into calculation.

NICS

Nucleus independent chemical shift (NICS) values were calculated using the GIAO (Gauge Including Atomic Orbitals)[21] method at the CAM-B3LYP/Def2-TZVP[3,4] level of theory. For the $NICS(1)_{iso}$ and $NICS(1)_{ZZ}$ calculations dummy atoms were placed 1 Ångstrom above and below the respective ring planes of the five- and six-membered rings of **DHPP** and **PP** molecules. Negative NICS values indicate a diatropic ring current (associated with an aromatic character) while positive NICS values indicated a paratropic ring current (associated with antiaromatic character).

EDDB

Electron density of delocalized bonds (EDDB) is a part of the original method of one-electron density (ED) decomposition into 'layers' representing different levels of electron delocalization.[22] In the basis of natural atomic orbitals (NAO), or any other representation of well-localized orthonormalized atomic orbitals, the spinless global electron density of delocalized bonds function, $EDDB_G(r)$, for a single-determinant molecular wavefunction is defined as follows:[23,24]

$$\mathrm{EDDB_G}(r) = \sum_{\mu,\nu} \chi_\mu^\dagger(r) \mathcal{D}_{\mu,\nu}^{\Omega_G} \chi_\nu(r) \tag{2}$$

where

$$\boldsymbol{\mathcal{D}}^{\Omega_G} = 2 \sum_{\sigma=\alpha,\beta} \mathbf{P}^\sigma \left[\sum_{a,b}^{\Omega_G} \boldsymbol{\mathcal{C}}_{a,b}^\sigma \boldsymbol{\varepsilon}_{a,b}^{\Omega_G,\sigma} \left(\boldsymbol{\lambda}_{a,b}^\sigma\right)^2 \boldsymbol{\mathcal{C}}_{a,b}^{\sigma\,\dagger} \right] \mathbf{P}^\sigma \tag{3}$$

In the above equation, P^σ ($\sigma = \alpha,\beta$) stands for the σ spin-resolved charge and bond-order (CBO) matrix, $C_{a,b}^{\sigma}$ is the matrix of linear coefficients of the appropriately orthogonalized σ spin-resolved two-center bond-order orbitals (2cBO) of the chemical bond X_a–X_b (obtained by diagonalization of the appropriate off-diagonal blocks of the CBO matrix), $\lambda_{a,b}^{\sigma}$ represents the diagonal matrix collecting the corresponding 2cBO eigenvalues (occupation numbers), $E_{a,b}^{\Omega G.\sigma}$ is a diagonal matrix of the σ-spin bond-conjugation factors, and for an n-atomic molecular system, Ω_G represents the set of all n(n-1)/2 possible atomic pairs (regardless of whether the atoms are formally bonded or not). The definition of the key matrix $E_{a,b}^{\Omega G.\sigma}$ is based on the bond-orbital projection (BOP) criterion developed by one of the authors, which relies on sophisticated orbital projection cascades involving 2cBOs, their 3-center counterparts (3cBO), and canonical MOs. According to BOP, for a typical well-localized (Lewis-like) bond X_a–X_b, all diagonal elements of the $E_{a,b}^{\Omega G.\sigma}$ matrix are close to zero, which means that the 2cBOs associated with this bond do not form effectively linear combinations with 2cBOs of all other bonds in a molecule. On the other hand, when the X_a–X_b bond is effectively conjugated with any other adjacent bond in the system, the $E_{a,b}^{\Omega G.\sigma}$ matrix has at least one element on its diagonal that approaches 1 (for systems with double and higher multifaceted aromaticity, the number of non-zero diagonal elements is equal to the number of delocalization 'channels').

The trace of such defined $D^{\Omega G}$ matrix can be straightforwardly interpreted as the population of electrons delocalized through the system of all conjugated bonds in a molecule, and as such, it can be used as a 'measure' of *global* aromaticity.[23,24] However, one of the most distinctive features of the BOP technique is that one can easily restrict the set bonds/atomic pairs in Ω_G giving rise to a series of different variants of *global* and *local* EDDB functions.

Energy decomposition analysis

The interaction energy in the gas phase was examined in the framework of the Kohn-Sham MO model using a quantitative energy decomposition analysis (EDA)[25-27] into electrostatic interactions, Pauli

repulsive orbital interactions, and attractive orbital interactions, to which a term ΔE_{disp} is added to account for the dispersion correction:

$$\Delta E_{\text{int}} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp} \quad (4)$$

The term ΔV_{elstat} corresponds to the classical electrostatic interactions between the unperturbed charge distributions of the prepared (i.e. deformed) fragments and is usually attractive. The Pauli repulsion, ΔE_{Pauli}, comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interactions, ΔE_{oi}, account for electron-pair bonding, charge transfer (*i.e.*, donor–acceptor interactions between occupied orbitals on one moiety and unoccupied orbitals on the other, including HOMO-LUMO interactions), and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). The term ΔE_{disp} accounts for the dispersion corrections.[28,29]

Analysis of excited states

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out in terms of the transition density.[30-32] The analysis was done in the Löwdin orthogonalized basis, which is more convenient. The matrix ${}^{\lambda}\mathbf{C}$ of orthogonalized MO coefficients is obtained from the coefficients **C** in the original basis ${}^{\lambda}\mathbf{C} = \mathbf{S}^{1/2}\,\mathbf{C}$, where **S** is the atomic orbital overlap matrix. The transition density matrix T^{0i} for an excited state Φ^* constructed as a superposition of singly excited configurations (where an occupied MO ψ_i is replaced a virtual MO ψ_a) is computed,

$$\mathrm{T}^{0\mathrm{i}}_{\alpha\beta} = \sum_{\mathrm{ia}} \mathrm{A}_{\mathrm{i}\to\mathrm{a}}\, {}^{\lambda}\mathrm{C}_{\alpha\mathrm{i}}\, {}^{\lambda}\mathrm{C}_{\beta\mathrm{a}} \quad (5)$$

where $A_{i\to a}$ is the expansion coefficient.

A key quantity Ω (D,A) is determined by:

$$\Omega(\mathrm{D},\mathrm{A}) = \sum_{\alpha\in\mathrm{D},\,\beta\in\mathrm{A}} \left(\mathrm{T}^{0\mathrm{i}}_{\alpha\beta}\right)^2 \quad (6)$$

The weights of local excitations on D and A are Ω(D,D) and Ω(A,A). The weight of electron transfer configurations D→A and A→D is represented by Ω(D,A) and Ω(A,D), respectively. The index Δq, which describes charge separation and charge transfer between D and A, is

$$\Delta\mathrm{q}(\mathrm{CS}) = \sum \Omega(\mathrm{D},\mathrm{A}) - \Omega(\mathrm{A},\mathrm{D}) \quad (7)$$

$$\Delta\mathrm{q}(\mathrm{CT}) = \sum \Omega(\mathrm{D},\mathrm{A}) + \Omega(\mathrm{A},\mathrm{D}) \quad (8)$$

Solvent Effects

The equilibrium solvation energy $\mathrm{E}_{\mathrm{S}}^{\mathrm{eq}}$ of a molecule (in the ground or excited state) in the medium with the dielectric constant ε was estimated using a COSMO-like polarizable continuum model[33-36] in the monopole approximation:

$$E_S^{eq}(Q,\varepsilon) = -\frac{1}{2} f(\varepsilon) Q^{+} D Q \qquad (9)$$

where the $f(\varepsilon)$ is the dielectric scaling factor, $f(\varepsilon) = \frac{\varepsilon - 1}{\varepsilon}$, **Q** -the vector of *n* atomic charges in the molecular system, **D** is the *n* x *n* symmetric matrix determined by the shape of the boundary surface between solute and solvent. $\mathbf{D=B^{+}A^{-1}B}$, where the *m* x *m* matrix **A** describes electrostatic interaction between *m* surface charges and the *m* x *n* **B** matrix describes the interaction of the surface charges with *n* atomic charges of the solute.[33,37] The GEPOL93 scheme[38] was used to construct the molecular boundary surface.

The charge on atom X in the excited state Φ_i, q_X^i, was calculated as:

$$q_X^i = q_X^0 + \Delta_X^i, \quad \Delta_X^i = \sum_{Y \neq X} \sum_{\alpha \in X,\, \beta \in Y} (T_{\alpha\beta}^{0i} T_{\alpha\beta}^{0i} - T_{\beta\alpha}^{0i} T_{\beta\alpha}^{0i}), \qquad (10)$$

where q_X^0 is the atomic charge on A in the ground state and Δ_X^i is its change due to the redistribution of the electron density between the atoms X and the rest of atoms Y which is caused by the excitation $\psi_0 \rightarrow \psi_i$.

The non-equilibrium solvation energy for excited state ψ_i can be estimated as:[39]

$$E_S^{neq}(Q^0, \Delta, \varepsilon, n^2) = f(\varepsilon) \Delta^{+} D Q^0 - \frac{1}{2} f(n^2) \Delta^{+} D \Delta, \qquad (11)$$

In Eq. (8), n^2 (the refraction index squared) is the optical dielectric constant of the medium and the vector Δ describes the change of atomic charges in the molecule by excitation in terms of atomic charges, see Eq. (10). By definition, the external (solvent) reorganization energy is the difference of the non-equilibrium (Eq. 11) and equilibrium (Eq. 9) solvation energies of the excited state.

Electron transfer rates

The rate of the nonadiabatic electron transfer (ET), k_{ET}, can be expressed in terms of the electronic coupling squared, V^2, and the Franck-Condon Weighted Density of states (FCWD):

$$k_{ET} = \frac{2\pi}{\hbar} V^2 \, (FCWD) \qquad (12)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:[40]

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT \right] \qquad (13)$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD)[41,42] method was employed to calculate the electronic couplings in this work.

The Marcus expression is derived for the high-temperature condition, $\hbar\omega_l \ll kT$, for all vibrational modes *l*. The semi-classical description of ET[43,44] includes the effect of the quantum vibrational modes in an effective way, the solvent (low frequency) modes are treated classically, while a single high-frequency intramolecular mode ω_i, $\hbar\omega_i \gg kT$, is described quantum mechanically. Because ET occurs normally from the lowest vibrational level of the initial state, the rate *k* can be expressed as a sum over all channels connecting the initial state with the vibrational quantum number n = 0 to manifold vibrational levels of the final state,

$$k = \sum_{n=0}^{\infty} k_{0\to n} \text{, where } k_{0\to n} = \frac{2\pi}{\mathrm{h}} V_{0\to n}^2 \frac{1}{\sqrt{4\pi\lambda_s kT}} \exp\left[-\frac{\left(\Delta G + n\mathrm{h}\omega_i + \lambda_s\right)^2}{4\lambda_s kT} \right] \quad (14)$$

with

$$V_{0\to n}^2 = V^2 \frac{S^n}{n!} \exp\left(-S\right) \quad (15)$$

An effective value of the Huang-Rhys factor *S* is estimated from the internal reorganization energy λ_i,

$S = \lambda_i / \mathrm{h}\omega_i$

As seen, an additional parameter (as compared to the Marcus equation) enters the semi-classical expression - the frequency ω_i of a vibrational mode that effectively describes the nuclear intramolecular relaxation following the ET. Typically, in organic systems (including fullerene and nanotube derivatives) the main contribution to the internal reorganization energy is due to stretching of C=C bonds (the corresponding frequencies are found to be in the range 1400-1800 cm^{-1}). Thus, the effective frequency was set to 1600 cm^{-1}. We have demonstrated that varying the parameter ω_i within a reasonable range does not change significantly the computed ET rate (Table S4).

Reorganization energy

The reorganization energy is usually divided into two parts, $\lambda = \lambda_i + \lambda_s$, including the internal and solvent terms. The solvent reorganization energy corresponds to the energy required to move solvent molecules from the position they occupy in the initial state to the location they have in the CT state, but without charge transfer having occurred. The λ_s for a particular CT states was computed as a difference between the equilibrium (E^{eq}, see eq. 6) and non-equilibrium (E^{neq}, see eq. 8) solvation energies for states of interest. The internal reorganization energy λ_i corresponds to the energy of structural changes when donor/acceptor fragments going from initial-state geometries to final-state geometries.

$$\text{For CT1 } \lambda_i^{CT1} = \lambda_i^1 + \lambda_i^2, \text{ where:}$$

$$\lambda_i^1(C_{60}^{\ *} \rightarrow C_{60}^{\ -}) = \frac{1}{2}\left[\left(\left(C_{60}^{\ *}\right)_- - \left(C_{60}^{\ *}\right)_*\right) + \left(\left(C_{60}^{\ -}\right)_* - \left(C_{60}^{\ -}\right)_-\right)\right]$$

$$\lambda_i^2(\text{Nanohoop}^0 \rightarrow \text{Nanohoop}^+) = \frac{1}{2}\left[\begin{array}{l}\left(\left(\text{Nanohoop}^0\right)_+ - \left(\text{Nanohoop}^0\right)_0\right) \\ + \left(\left(\text{Nanohoop}^+\right)_0 - \left(\text{Nanohoop}^+\right)_+\right)\end{array}\right]$$

$$\text{For CT2 } \lambda_i^{CT2} = \lambda_i^1 + \lambda_i^2, \text{ where:} \qquad (16)$$

$$\lambda_i^1(C_{60}^{\ *} \rightarrow C_{60}^{\ +}) = \frac{1}{2}\left[\left(\left(C_{60}^{\ *}\right)_+ - \left(C_{60}^{\ *}\right)_*\right) + \left(\left(C_{60}^{\ +}\right)_* - \left(C_{60}^{\ +}\right)_+\right)\right]$$

$$\lambda_i^2(\text{Nanohoop}^0 \rightarrow \text{Nanohoop}^-) = \frac{1}{2}\left[\begin{array}{l}\left(\left(\text{Nanohoop}^0\right)_- - \left(\text{Nanohoop}^0\right)_0\right) \\ + \left(\left(\text{Nanohoop}^-\right)_0 - \left(\text{Nanohoop}^-\right)_-\right)\end{array}\right]$$

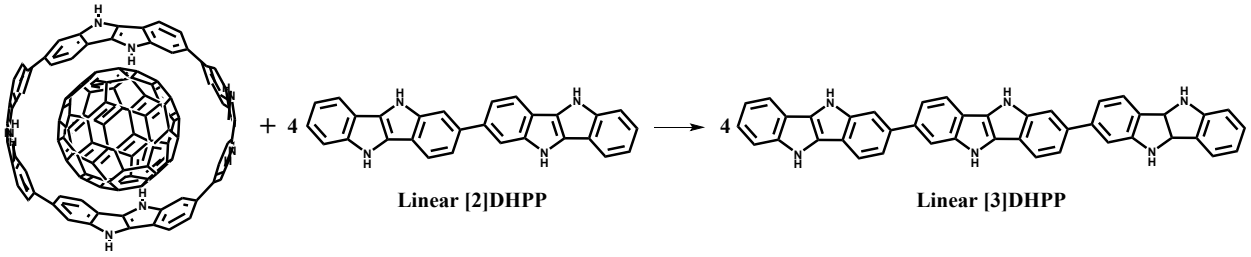
Interaction energies

The interaction energies were calculated directly from the electronic energy of complex and electronic energies of subsystems. For **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes the interaction energy can be expressed as follows:

$$E_{\text{int}} = E_{Host \supset C_{60}} - (E_{Host} + E_{C_{60}}) \qquad (17)$$

Strain energies

The strain energies of **[4]DHPP⊃C$_{60}$/[4]PP⊃C$_{60}$** tetramers were estimated using homodesmotic reaction approach. In this approach, linear dimers and trimers of **DHPP** and **PP** acting as reference molecules.



The interaction energy can be expressed as follows:

$$E_{Strain} = 4 \cdot E_{LTrimer} - (E_{[4]DHPP/[4]PP} + 4 \cdot E_{LDimer}) \qquad (18)$$

Quantum Theory of Atoms in Molecules (QTAIM)

Topological analysis of the electron distributions was conducted using the "Quantum Theory of Atoms in Molecules" (QTAIM) approach proposed by Bader.[45,46] Electron density properties measured at the bond critical point (BCP, saddle point on electron density curvature corresponding to a minimum in the direction of the atomic interaction line and a maximum in two perpendicular directions) give information about the character of different chemical bonds.[47-49] The AIMALL suite of programs[50] was applied to evaluate the BCP properties and the associated bond descriptors – the electron density [$\rho(r)$] in BCPs, its Laplacian [$\nabla^2\rho(r)$], potential energy density [$V(r)$], kinetic energy density [$G(r)$], and total electron energy density [$H(r)$].

Non-covalent interactions (NCI)

The NCI method[51-53] relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s), defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \tag{19}$$

a quantity that is essential to the design of DFT functionals. The combination of s and ρ allows a rough partition of real space into bonding regions: high-s low-ρ corresponds to non-interacting density tails, low-s high-ρ to covalent bonds, and low-s low-ρ to non-covalent interactions. The NCI analysis was carried out at the CAM-B3LYP/Def2-SVP level using Multiwfn program.[54]

Charge delocalization index

The degree of electron delocalization in the state of interest is quantified by the inverse participation ratio (IPR):

$$IPR = \Delta q^F \left(\sum_i^n \frac{1}{\left(q_i^F\right)^2} \right) \tag{20}$$

where Δq^F - indicates charge difference on the fragment in CS state compare to GS, while $\left(\Delta q_i^F\right)^2$ - corresponds to square of particular atom charge difference for denoted fragment in CS state compare to GS.

Table S1. NICS (ppm) aromaticity indices for **DHPP** and **PP** monomers.

Rings	Equilibrium monomer					
	DHPP			**PP**		
	$NICS(0)_{iso}$	$NICS(1)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{iso}$	$NICS(1)_{zz}$
Ring A	-9.9	-10.3	-28.9	-2.8	-4.9	-13.0
Ring B	-11.6	-4.9	-23.9	16.8	8.4	31.2

Table S2. NICS(ppm) and EDDB (electrons) aromaticity indices for **DHPP** and **PP** monomers in equilibrium geometry and in geometry of the corresponding **[4]DHPP** and **[4]PP** tetramers.

Rings	Equilibrium geometry		Geometry of tetramer	
	DHPP	**PP**	**DHPP**	**PP**
	$NICS(1)_{zz}$			
Ring A	-28.9	-13.0	-29.1[a]	-15.6[a]
Ring B	-23.9	31.2	-23.7[a]	31.4[a]
	π-$EDDB^{Norm}$[b]			
Ring A	0.690	0.713	0.688	0.726
Ring B	0.323	0.057	0.313	0.089
Monomer	0.754	0.675	0.739	0.683

[a] $NICS(1)_{zz}$ values computed for dummy atoms placed 1 Ångstrom inside the respective ring planes of the five- and six-membered rings of curved **DHPP** and **PP** molecules; [b] Due to inequivalent ratios of π electrons and atoms in systems, the EDDB values were normalized by the number of π electrons: $\pi\text{-}EDDB^{Norm} = \pi\text{-}EDDB/n_{\pi}$

Table S3. HOMO and LUMO energies (in eV), as well as HOMO-LUMO (HL) gap for isolated **DHPP** and **PP** linkers in equilibrium geometry, and geometries of corresponding tetramer as well as orbital energies for **[4]DHPP** and **[4]PP**.

Energy	Monomers				Tetramers	
	DHPP		**PP**		**[4]DHPP**	**[4]PP**
	Eq. geom.	Compl. geom	Eq. geom.	Compl. geom		
HOMO	-6.298	-6.298	-7.551	-7.464	-5.548	-7.081
LUMO	0.153	0.032	-2.247	-2.230	-0.827	-2.761
HL gap	6.450	6.329	5.304	5.234	4.721	4.320

Table S4. Charge separation (in electrons) between the fragments in electronic ground state for **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes. Q_{Host} - charge on host (**[4]DHPP** or **[4]PP**) , and $Q_{C_{60}}$ - charge on fullerene moiety. Total charge of the complexes $Q_{Tot} = 0$.

Charge Scheme	**[4]DHPP⊃C$_{60}$**		**[4]PP⊃C$_{60}$**	
	Q_{Host}	$Q_{C_{60}}$	Q_{Host}	$Q_{C_{60}}$
Mulliken	0.146	-0.146	0.077	-0.077
Lowdin	0.133	-0.133	0.073	-0.073
Hirshfeld	0.033	-0.033	-0.026	0.026
CM5	0.030	-0.031	-0.034	0.034

Table S5 Electronic (E_{el} in Hartree) and strain energies (ΔE_{strain}, in kcal/mol, in electronic ground state for **[4]DHPP and [4]PP** tetramers as well as their fullerene inclusion complexes **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** in the gas phase.

Energy	**DHPP**		**PP**	
	Equil. structure **[4]DHPP**	Inclusion complex **[4]DHPP⊃C$_{60}$**	Equil. structure **[4]PP**	Inclusion complex **[4]PP⊃C$_{60}$**
Linear dimer	-1942.78215		-1939.05519	
Linear. trimer	-1295.57833		-1293.09346	
System	-2588.71320	-2588.71156	-2583.75149	-2583.74816
ΔE_{strain}	-64.06	-65.09	-59.89	-61.98

Table S6. Parameters (electron density [*ρ(r)*], its Laplacian [$\nabla^2\rho(r)$], potential energy density [*V(r)*], kinetic energy density [*G(r)*], and total electron energy density [*H(r)*] for selected bond critical points related to non-covalent interactions in **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes computed in the gas phase.

Bond critical points between fragments	Interaction	*ρ(r)*, au	$\nabla^2\rho(r)$, au	*V(r)*, au	*G(r)*, au	*H(r)*, au
		[4]DHPP⊃C$_{60}$				
[4]DHPP ··· C$_{60}$	π···π C···C	9.31E-03	2.84E-02	-4.34E-03	5.72E-03	1.38E-03
		1.10E-02	3.18E-02	-4.86E-03	6.41E-03	1.55E-03
		8.08E-03	2.50E-02	-3.83E-03	5.04E-03	1.21E-03
		1.06E-02	3.30E-02	-4.86E-03	6.56E-03	1.69E-03
		9.80E-03	2.97E-02	-4.62E-03	6.02E-03	1.40E-03
		9.26E-03	3.08E-02	-4.68E-03	6.20E-03	1.52E-03
		8.63E-03	2.44E-02	-3.70E-03	4.90E-03	1.20E-03
		8.64E-03	2.45E-02	-3.71E-03	4.92E-03	1.21E-03
		9.31E-03	3.10E-02	-4.70E-03	6.22E-03	1.52E-03
		9.70E-03	2.94E-02	-4.57E-03	5.96E-03	1.39E-03

		1.06E-02	3.28E-02	-4.82E-03	6.51E-03	1.69E-03
		8.06E-03	2.49E-02	-3.83E-03	5.03E-03	1.20E-03
		1.09E-02	3.17E-02	-4.85E-03	6.39E-03	1.54E-03
		9.35E-03	2.85E-02	-4.36E-03	5.75E-03	1.38E-03
		1.10E-02	3.33E-02	-5.12E-03	6.72E-03	1.60E-03
		8.93E-03	2.93E-02	-4.64E-03	5.99E-03	1.34E-03
		9.00E-03	2.95E-02	-4.67E-03	6.02E-03	1.35E-03
		1.10E-02	3.31E-02	-5.10E-03	6.69E-03	1.59E-03
		9.22E-03	2.86E-02	-4.34E-03	5.74E-03	1.40E-03
		9.29E-03	2.88E-02	-4.39E-03	5.80E-03	1.41E-03
	π···π	4.17E-03	1.16E-02	-2.04E-03	2.47E-03	4.30E-04
	C···N	4.12E-03	1.15E-02	-2.02E-03	2.44E-03	4.27E-04
		[4]PP⊃C_{60}				
[4]PP ··· C_{60}		1.10E-02	3.35E-02	-5.21E-03	6.79E-03	1.58E-03
		1.05E-02	3.36E-02	-5.27E-03	6.83E-03	1.56E-03
		9.55E-03	2.89E-02	-4.47E-03	5.84E-03	1.37E-03
		1.12E-02	3.38E-02	-5.14E-03	6.80E-03	1.66E-03
		8.57E-03	2.66E-02	-4.05E-03	5.35E-03	1.30E-03
		1.06E-02	3.33E-02	-4.71E-03	6.52E-03	1.81E-03
		9.83E-03	3.15E-02	-4.76E-03	6.31E-03	1.55E-03
		9.32E-03	3.11E-02	-4.75E-03	6.26E-03	1.51E-03
		8.93E-03	2.62E-02	-3.87E-03	5.22E-03	1.34E-03
	π···π	8.97E-03	2.64E-02	-3.90E-03	5.25E-03	1.35E-03
	C···C	9.41E-03	3.13E-02	-4.79E-03	6.32E-03	1.52E-03
		9.78E-03	3.13E-02	-4.72E-03	6.27E-03	1.55E-03
		1.06E-02	3.31E-02	-4.67E-03	6.47E-03	1.80E-03
		8.56E-03	2.66E-02	-4.06E-03	5.35E-03	1.30E-03
		1.12E-02	3.38E-02	-5.13E-03	6.79E-03	1.66E-03
		9.57E-03	2.89E-02	-4.48E-03	5.86E-03	1.38E-03
		1.05E-02	3.37E-02	-5.30E-03	6.87E-03	1.57E-03
		1.10E-02	3.33E-02	-5.18E-03	6.75E-03	1.58E-03
		9.82E-03	3.05E-02	-4.63E-03	6.12E-03	1.49E-03
		9.90E-03	3.08E-02	-4.69E-03	6.19E-03	1.50E-03

Table S7. Excitation energies (E_x, eV) and dipole moments in ground state (μ_0, D), change in dipole moments between ground state and state of interest ($\Delta\mu = \mu_i - \mu_0$, D) and solvation energies (E_{solv}, eV) in DCM calculated for **[4]DHPP⊃C_{60}** and **[4]PP⊃C_{60}** complexes.

	Supramolecular host-guest systems	
	[4]DHPP⊃C_{60}	**[4]PP⊃C_{60}**
	Ground state (GS)	
E_x	0.000	0.000
μ_0	0.28	0.23
E_{solv}	-0.890	-0.620
	LE^{Guest} (Fullerene **C_{60}**)	
E_x	2.397	2.405
$\Delta\mu$	0.21	0.38
E_{solv}	-0.882	-0.612
	LE^{Host} (nanohoop)	
E_x	2.824	2.033
$\Delta\mu$	0.14	0.27
E_{solv}	-0.892	-0.732
	CT1 (nanohoop → **C_{60}**)	
E_x	1.824	3.117
$\Delta\mu$	1.75	4.24
E_{solv}	-0.912	-0.748
	CT2 (**C_{60}** → nanohoop)	
E_x	n/a	1.790
$\Delta\mu$		7.63
E_{solv}		-1.301

Table S8. Charge delocalization over the fragment index (IPR) in the CT1 and CT2 states for **[4]DHPP⊃C_{60}** and **[4]PP⊃C_{60}** complexes.

	[4]PP⊃C_{60}				**[4]DHPP⊃C_{60}**	
	CT1		**CT2**		**CT1**	
	C_{60}	**[4]PP**	**C_{60}**	**[4]PP**	**C_{60}**	**[4]DHPP**
IPR	33.4	34.8	25.4	31.2	35.9	44.6

Table S9. Gibbs energy ΔG^0 (in eV), electronic/spin-orbit coupling $|V_{ij}|$ (in eV), reorganization energy λ (in eV), Huang-Rhys factor (S_{eff}) and rates k_X (in s^{-1}) for ET, exciton transfer and ISC processes in **[4]DHPP⊃C_{60}** and **[4]PP⊃C_{60}** complexes computed in DCM.

Complex XXX⊃C_{60}	Transition	$\Delta G^{0[a]}$	$\|V_{ij}\|$	λ	$S_{eff}^{[b]}$	k_X
[4]DHPP	***$LE^{Guest} \rightarrow CT1$***	***-0.573***	***$1.96 \cdot 10^{-3}$***	***0.376***	***0.998***	***$3.60 \cdot 10^{10}$***
	$LE^{Host} \rightarrow CT1$	***-1.000***	***$6.58 \cdot 10^{-3}$***	***0.367***	***0.998***	***$3.05 \cdot 10^{10}$***
	$LE^{Host} \rightarrow LE^{Guest}$	-0.427	$1.22 \cdot 10^{-4}$	0.164	0.554	$8.72 \cdot 10^{7}$
	LE^{Guest} (S→T)	-0.538	$7.32 \cdot 10^{-5}$	0.109	0.449	$3.71 \cdot 10^{5}$
	LE^{Host} (S→T)	-0.630	$2.85 \cdot 10^{-5}$	0.089	0.348	$4.29 \cdot 10^{5}$
[4]PP	***$LE^{Guest} \rightarrow CT2$***	***-0.615***	***$1.34 \cdot 10^{-2}$***	***0.309***	***0.781***	***$9.53 \cdot 10^{11}$***
	$LE^{Host} \rightarrow CT2$	***-0.243***	***$1.71 \cdot 10^{-2}$***	***0.307***	***0.781***	***$9.58 \cdot 10^{12}$***
	$LE^{Host} \rightarrow LE^{Guest}$	-0.372	$4.59 \cdot 10^{-4}$	0.149	0.529	$6.17 \cdot 10^{8}$
	LE^{Guest} (S→T)	-0.534	$1.25 \cdot 10^{-4}$	0.112	0.464	$7.70 \cdot 10^{4}$
	LE^{Host} (S→T)	-0.783	$3.72 \cdot 10^{-5}$	0.100	0.403	$1.56 \cdot 10^{5}$

[a] Gibbs energy difference between the given states. [b] Effective value of the Huang-Rhys factor $S_{eff} = \lambda_i / \hbar\omega_{eff}$, where $\hbar\omega_{eff}$ is set to 1600 cm^{-1}

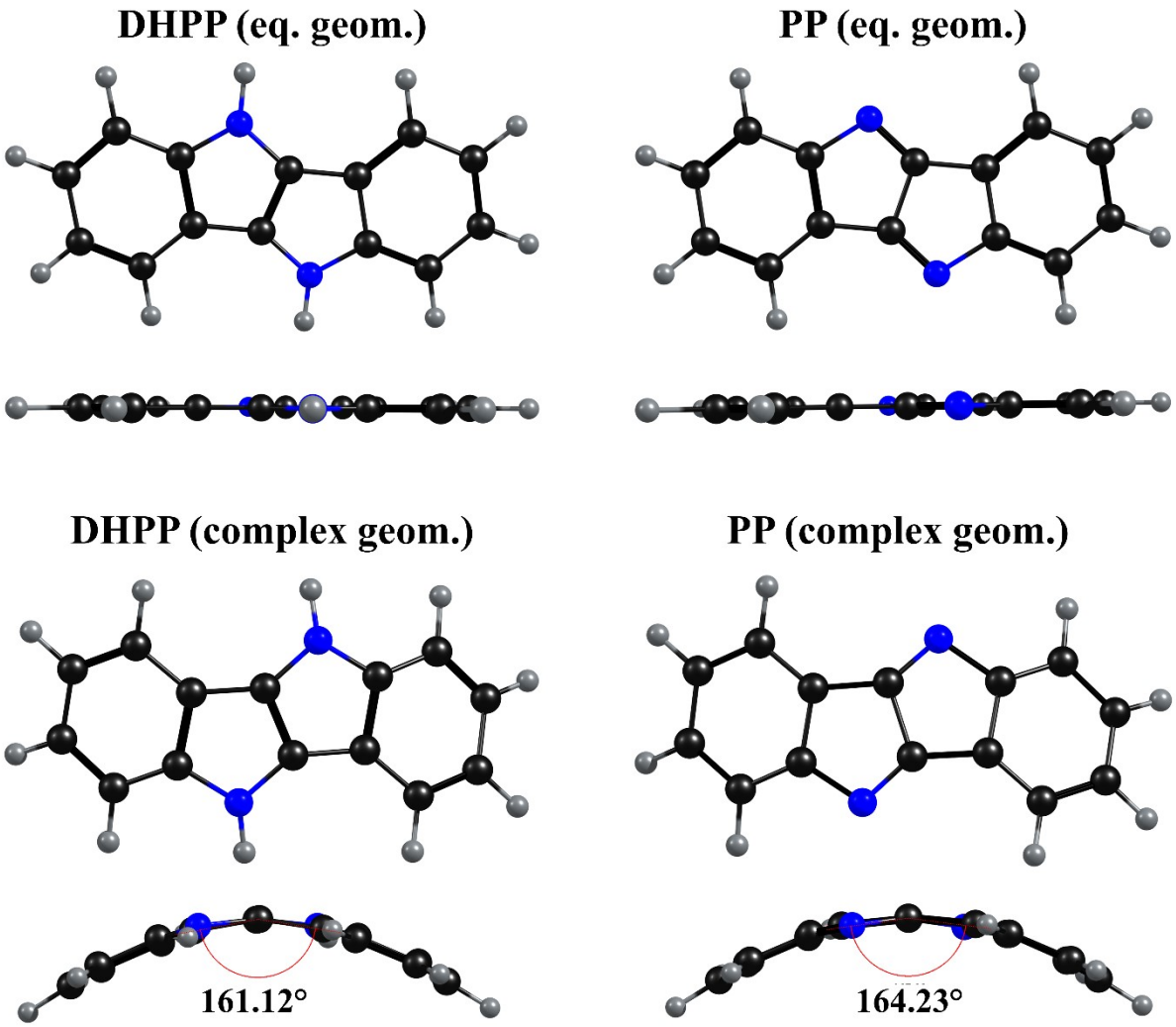


Figure S1. Graphical representations of planar and bended **DHPP** and **PP** monomer units.

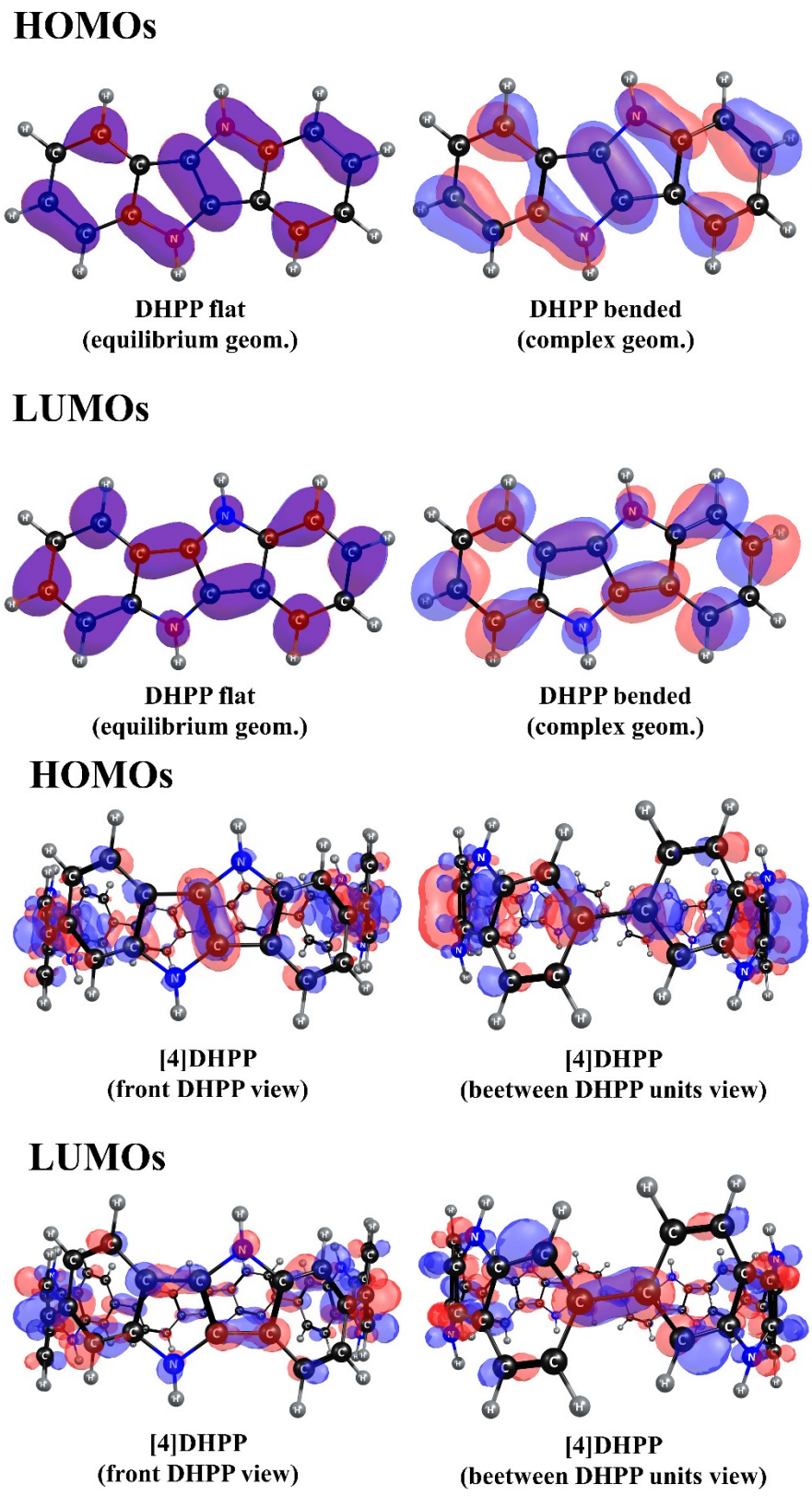


Figure S2. HOMO and LUMO for **DHPP** unit in equilibrium and complex geometries and **[4]DHPP** tetramer molecule.

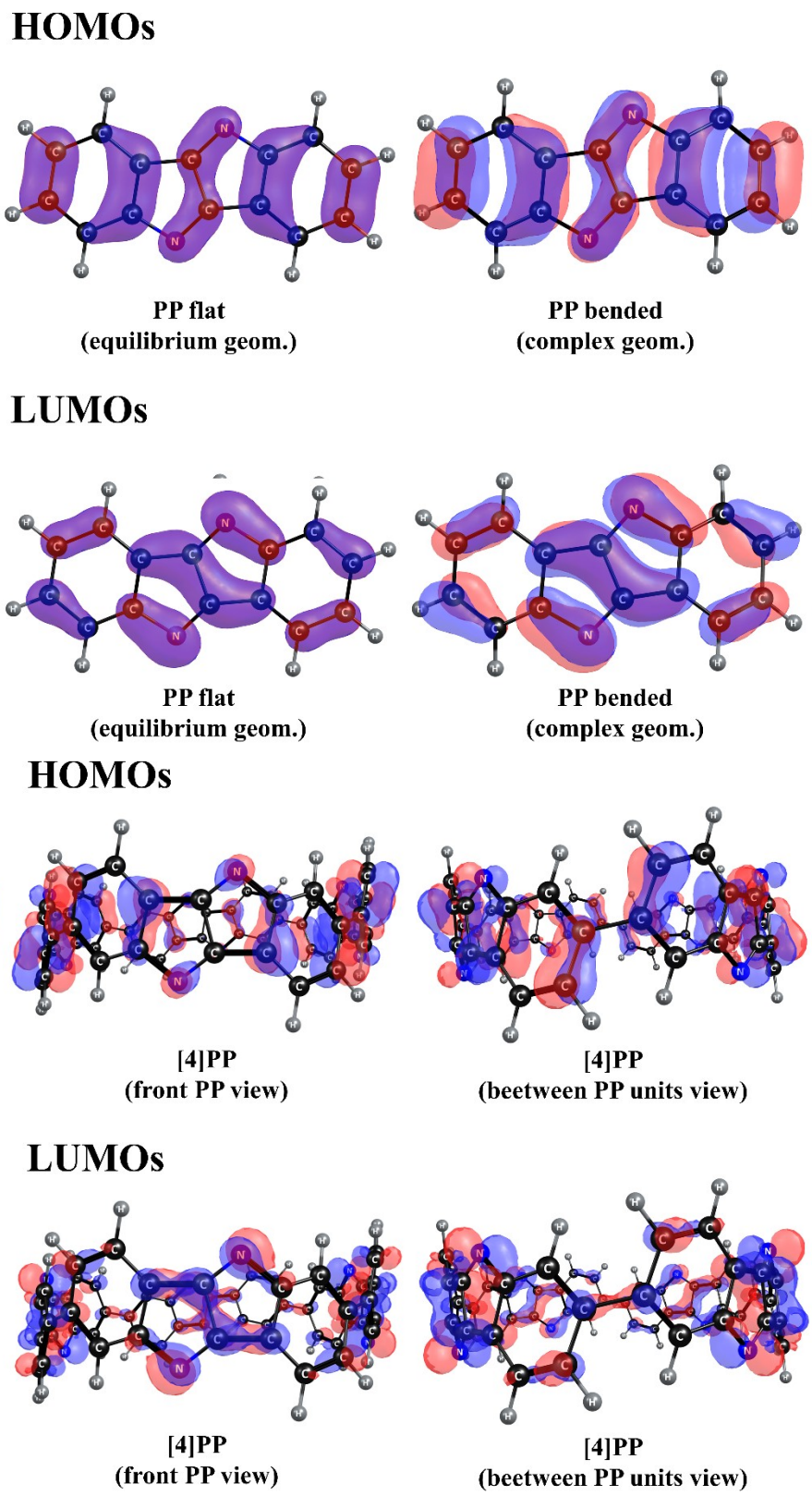


Figure S3. HOMO and LUMO for **PP** unit in equilibrium and complex geometries and **[4]PP** tetramer molecule.

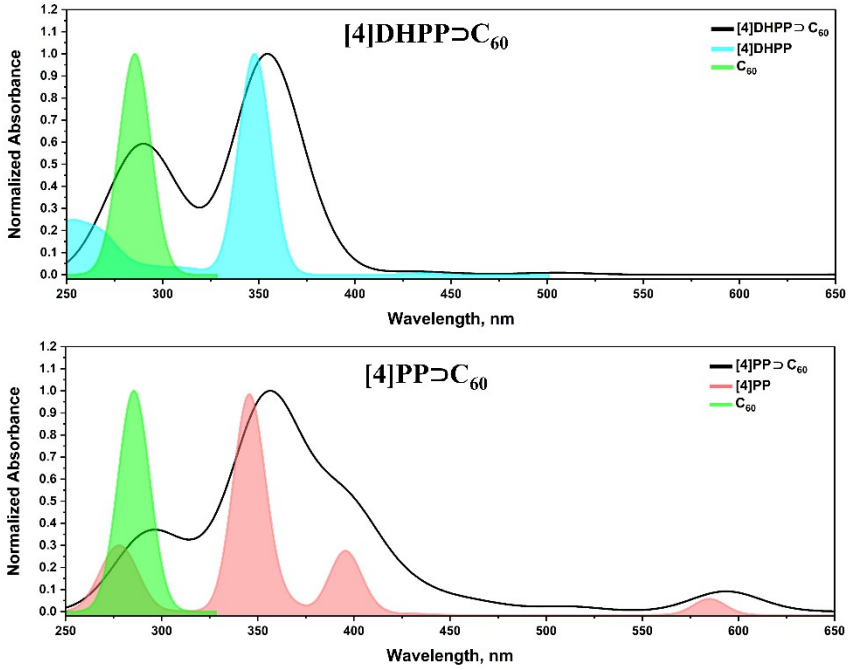


Figure S4. Simulated UV-Vis spectra of **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** and their monomers in DCM. The absorption spectra were constructed using Gaussian broadening (FWHM=0.20 eV).

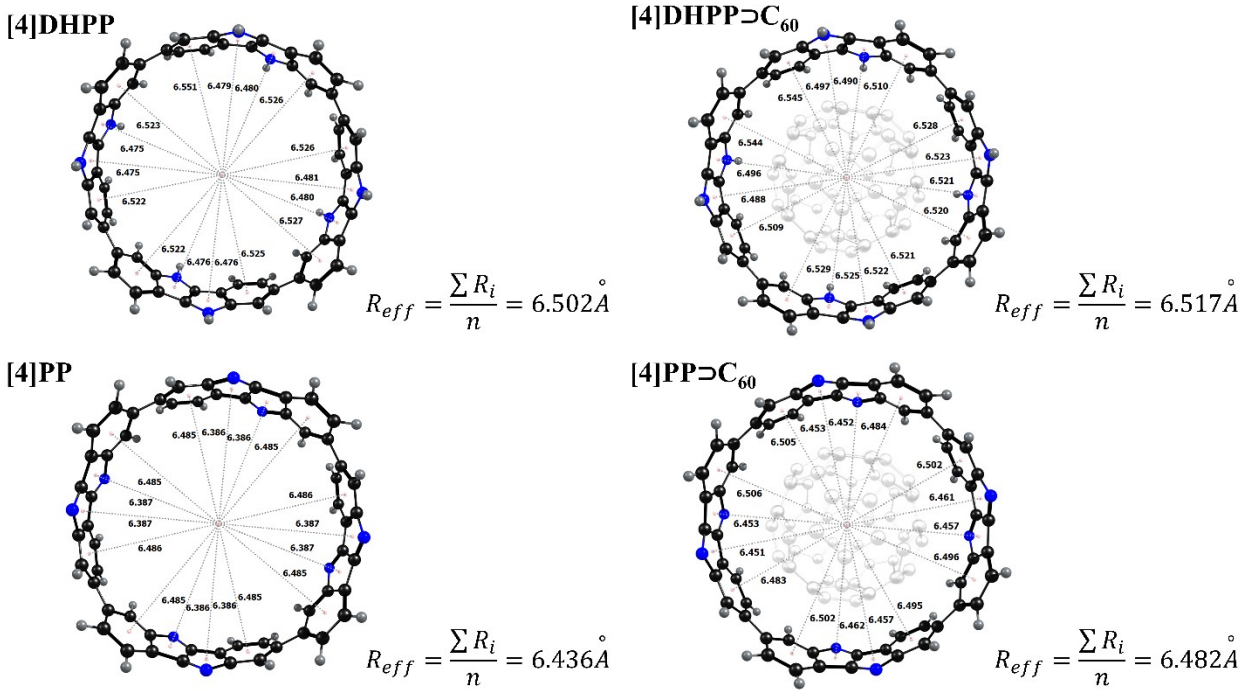


Figure S5. Effective radius of **[4]DHPP** and **[4]PP** nanohoops in free state and their complexes with **C$_{60}$** fullerene.

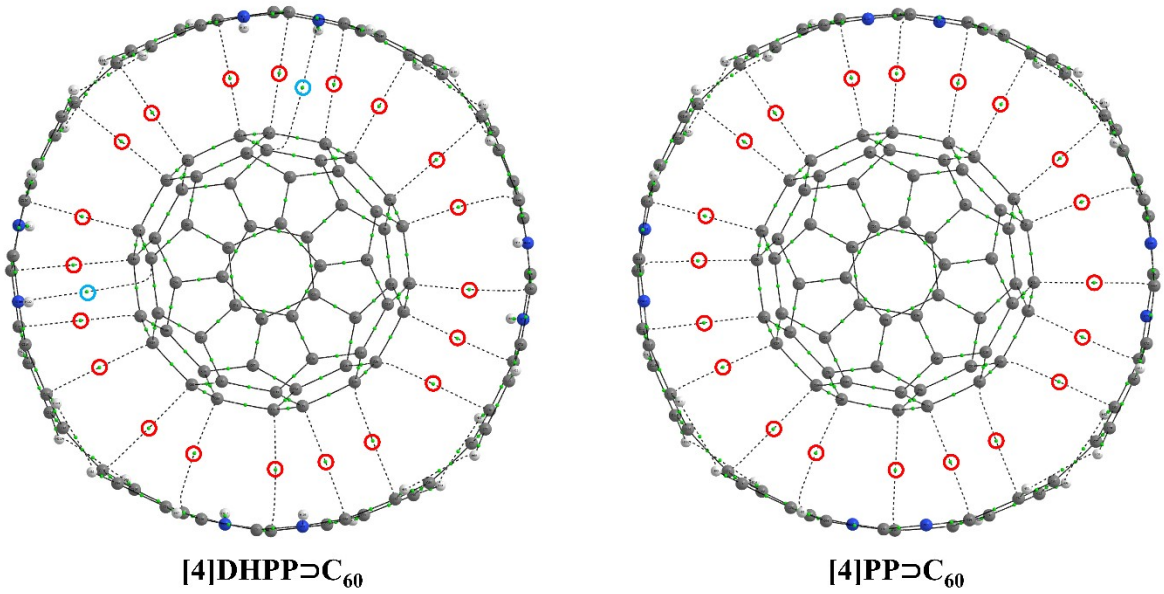


Figure S6. QTAIM molecular graph for **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs. BCPs of interest are marked by red and blue circles. Red circles correspond to C···C contacts while the blue one to C···N contacts.

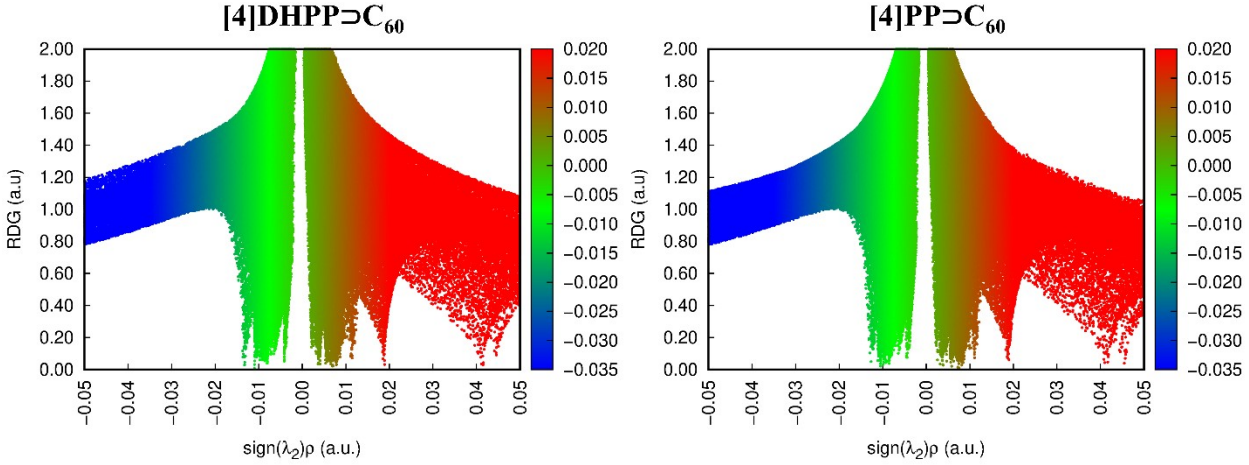


Figure S7. Plot of RDG *vs.* sign(λ2)×ρ for **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes.

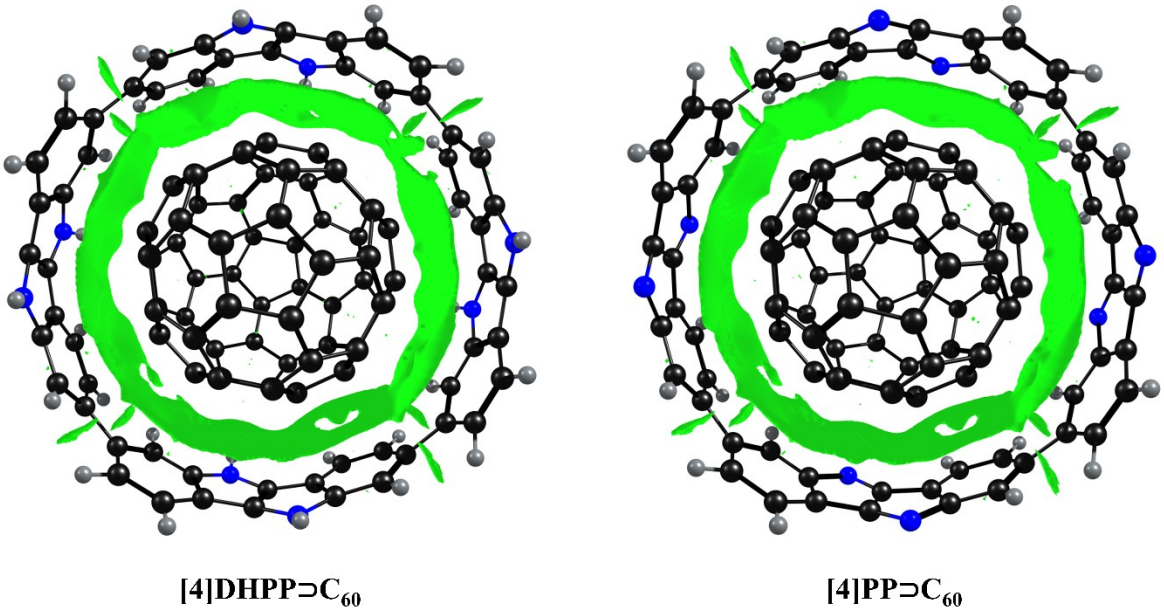


Figure S8. NCI isosurfaces of van der Waals interactions for **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes. Isosurfaces were generated for RDG = 0.65 a.u.

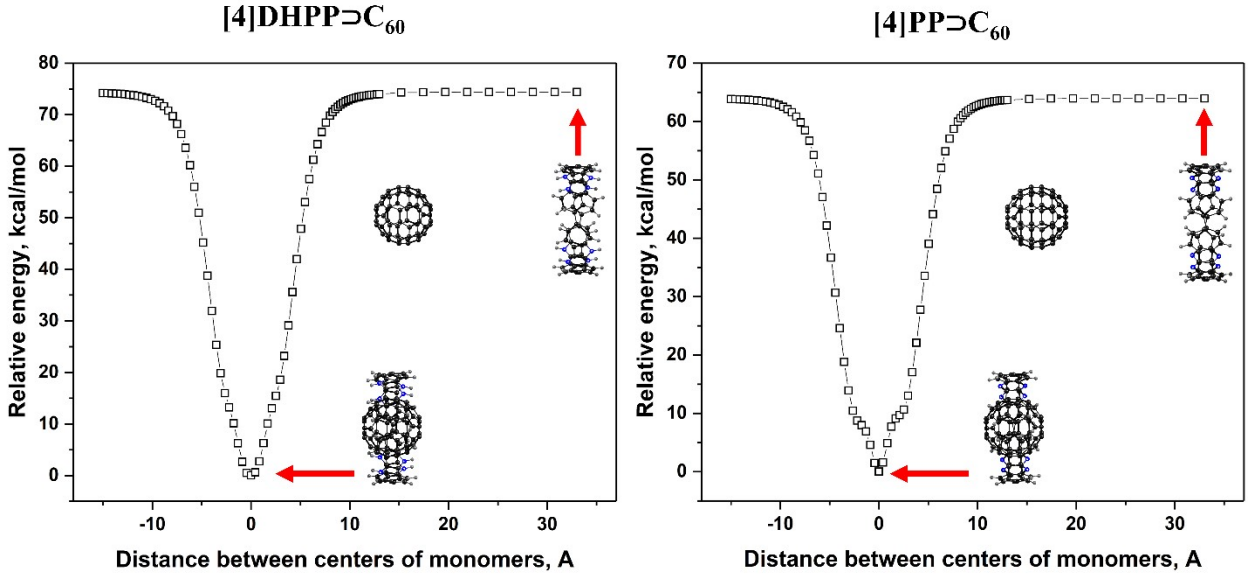


Figure S9. Energy profiles of the **[4]DHPP⊃C$_{60}$** and **[4]PP⊃C$_{60}$** complexes depending on the distance between subunits, calculated at BLYP-D3(BJ)/def2-SVP level of theory.

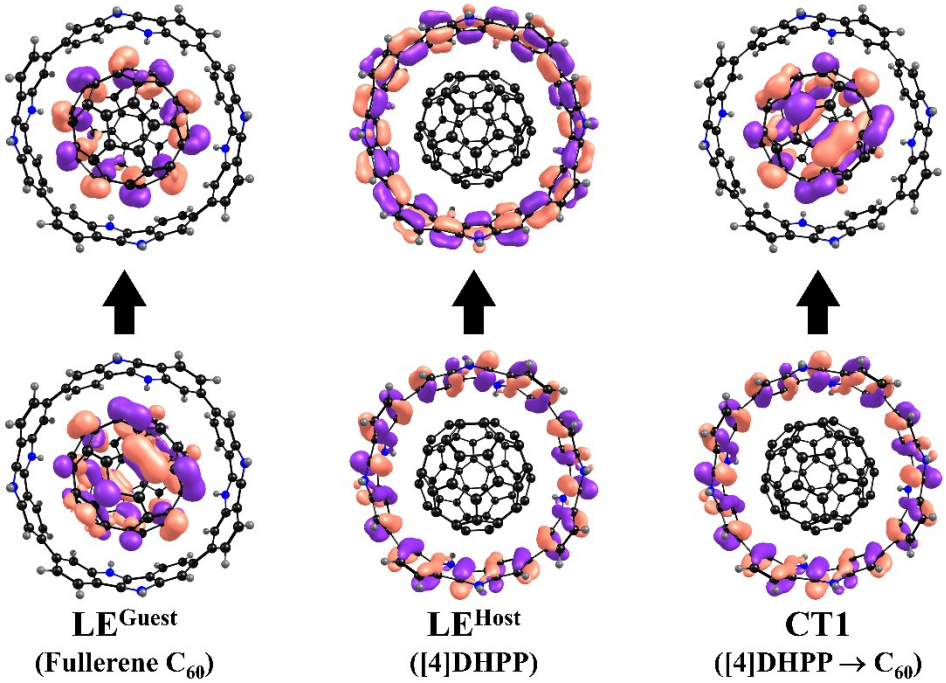


Figure S10. Natural transition molecular orbitals representing LE^{Guest}, LE^{Host}, and CT1 states in [4]DHPP⊃C_{60} complex.

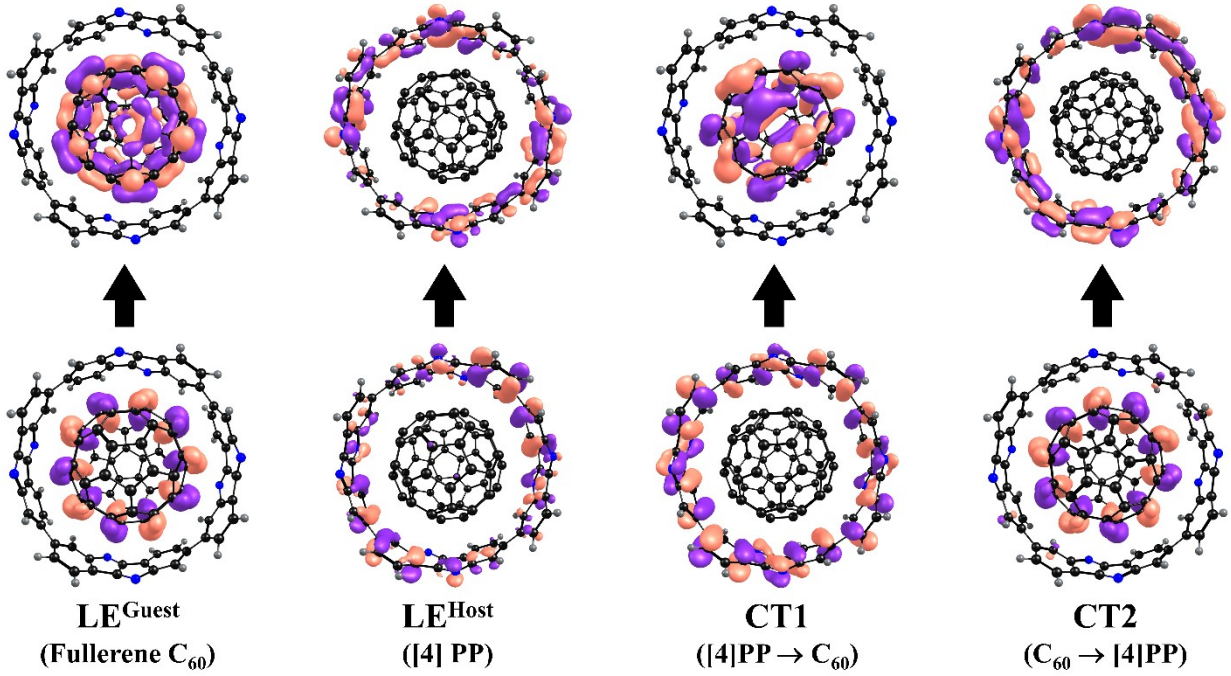


Figure S11. Natural transition molecular orbitals representing LE^{Guest}, LE^{Host}, CT1, and CT2 states in [4]PP⊃C_{60} complex.

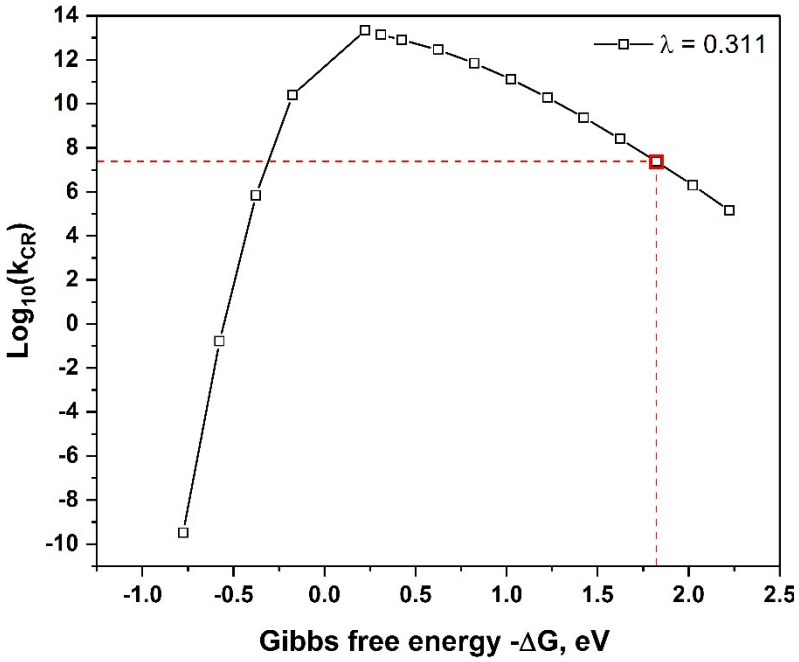


Figure S12. Dependence of the charge recombination rate on Gibbs energy for **[4]DHPP⊃C_{60}** in DCM. The electronic coupling $|V_{ij}|$ is equal to $2.38 \cdot 10^{-2}$ eV.

Cartesian coordinates

DHPP

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	4.892413000	2.730859000	4.587886000
6	4.154932000	1.919927000	5.489336000
6	2.764332000	2.053867000	5.609931000
6	2.090778000	3.014089000	4.818306000
6	4.256790000	3.694641000	3.787236000
6	2.861978000	3.838468000	3.900128000
6	0.731875000	3.448295000	4.646056000
7	1.998353000	4.708259000	3.231766000
6	0.696970000	4.474226000	3.679716000
1	4.684107000	1.175786000	6.101629000
1	2.203341000	1.419678000	6.311669000
1	4.833780000	4.320283000	3.090666000
7	-0.568523000	3.219507000	5.099533000
6	-0.661478000	4.910857000	3.510025000
6	-1.432576000	4.087020000	4.428775000
6	-2.827565000	4.229911000	4.540679000
6	-1.334812000	5.872243000	2.719625000
6	-2.725421000	6.006140000	2.840174000
6	-3.463158000	5.193837000	3.740179000
1	-0.773702000	6.507071000	2.018561000
1	-3.404706000	3.603480000	5.236414000
1	-3.254409000	6.751290000	2.228948000
1	2.281155000	5.382719000	2.525323000
1	-0.854250000	2.529524000	5.789618000
1	5.982007000	2.604119000	4.513249000
1	-4.552907000	5.319756000	3.813950000

PP

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	4.854339000	2.733040000	4.590796000
6	4.148196000	1.917575000	5.490069000
6	2.739996000	2.038271000	5.626876000
6	2.074094000	2.985763000	4.847149000
6	4.185485000	3.700810000	3.792413000
6	2.804110000	3.821480000	3.924458000
6	0.680386000	3.419242000	4.684762000
7	1.952386000	4.746852000	3.198918000
6	0.748852000	4.505293000	3.643115000
1	4.690169000	1.177218000	6.095382000
1	2.185797000	1.400960000	6.330132000
1	4.732427000	4.341312000	3.087499000
7	-0.523343000	3.176639000	5.127857000
6	-0.644949000	4.938280000	3.480209000
6	-1.375075000	4.101973000	4.402277000
6	-2.756566000	4.222022000	4.533668000
6	-1.310841000	5.885824000	2.700537000
6	-2.719157000	6.005896000	2.836686000
6	-3.425415000	5.189821000	3.735316000
1	-0.756548000	6.523633000	1.997807000
1	-3.303596000	3.581054000	5.238090000
1	-3.261139000	6.746213000	2.231330000
1	5.944700000	2.623159000	4.500435000
1	-4.515869000	5.299206000	3.825153000

[4]DHPP neutral

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.252527000	5.113746000	0.745236000
6	-4.786131000	4.321993000	1.285833000
1	-5.687876000	2.008622000	-4.113540000
7	-5.730188000	3.319002000	-0.830797000
6	-4.526813000	4.085867000	2.660957000
6	-5.560901000	3.407623000	0.557884000
6	-5.793210000	1.063703000	-3.560811000
1	-5.184292000	-0.126209000	-5.242787000
6	-6.201155000	2.034870000	-1.128366000
6	-5.504206000	-0.148951000	-4.193011000
6	-5.242019000	3.022328000	3.304216000
6	-6.150176000	1.067840000	-2.189395000
6	-6.107103000	2.216174000	1.179518000
1	-5.136608000	2.884395000	4.388097000
6	-6.004373000	2.095328000	2.587759000
6	-6.480200000	1.364543000	0.084558000
6	-5.525635000	-1.401087000	-3.494387000
6	-6.376455000	-0.210491000	-1.542130000

[4]PP neutral

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.211345000	5.022408000	0.675076000
6	-4.746226000	4.254121000	1.245173000
1	-5.663914000	2.012337000	-4.137452000
7	-5.599032000	3.263427000	-0.899997000
6	-4.498612000	4.051387000	2.644403000
6	-5.523220000	3.339125000	0.545864000
6	-5.778390000	1.072266000	-3.579713000
1	-5.163311000	-0.152966000	-5.252160000
6	-6.076815000	2.069196000	-1.139302000
6	-5.486591000	-0.161597000	-4.203588000
6	-5.219452000	3.024531000	3.310082000
6	-6.114692000	1.082093000	-2.221371000
6	-6.087916000	2.187263000	1.208834000
1	-5.102882000	2.896234000	4.393614000
6	-5.996494000	2.080934000	2.601192000
6	-6.392193000	1.272531000	0.105556000
6	-5.487010000	-1.384014000	-3.480532000
6	-6.310467000	-0.169891000	-1.528966000

7	-6.681544000	0.007052000	-0.191312000	7	-6.550151000	-0.008489000	-0.108294000
6	-6.069120000	-1.418958000	-2.183505000	6	-6.005764000	-1.378604000	-2.142216000
1	-6.471906000	1.248833000	3.111536000	1	-6.453761000	1.233953000	3.131704000
1	-6.093815000	-2.349144000	-1.602139000	1	-6.020434000	-2.288218000	-1.530848000
1	-6.678391000	-0.729690000	0.511102000	1	-3.523399000	-1.407732000	-5.424031000
1	-5.254034000	3.925994000	-1.494879000	6	-3.632133000	-2.353746000	-4.881243000
1	-3.627281000	-1.413602000	-5.482637000	1	2.059387000	-2.937449000	-6.332595000
6	-3.698470000	-2.361802000	-4.935185000	7	-1.340813000	-3.048033000	-5.641754000
1	2.045654000	-2.961977000	-6.335999000	6	-4.696781000	-2.559501000	-3.940809000
7	-1.430304000	-3.146902000	-5.720382000	6	-2.601752000	-3.281722000	-4.965535000
6	-4.723928000	-2.566258000	-3.975637000	6	2.075857000	-3.600710000	-5.456393000
6	-2.644121000	-3.281131000	-5.032084000	1	4.174978000	-3.257328000	-5.066642000
6	2.069693000	-3.618155000	-5.453767000	6	-0.535680000	-3.956322000	-5.153407000
1	4.158722000	-3.262663000	-5.098111000	6	3.272239000	-3.780048000	-4.726174000
6	-0.527854000	-4.077210000	-5.191638000	6	-4.761090000	-3.806622000	-3.264288000
6	3.262238000	-3.788374000	-4.744744000	6	0.899962000	-4.197511000	-4.987961000
6	-4.749174000	-3.819903000	-3.279844000	6	-2.588774000	-4.452873000	-4.120869000
6	0.884562000	-4.237578000	-4.984631000	1	-5.605121000	-4.016651000	-2.595259000
6	-2.573935000	-4.444755000	-4.168756000	6	-3.707472000	-4.745740000	-3.332820000
1	-5.588376000	-4.043617000	-2.608571000	6	-1.188751000	-4.883492000	-4.154568000
6	-3.697417000	-4.737350000	-3.356107000	6	3.304166000	-4.515023000	-3.511292000
6	-1.218232000	-4.906780000	-4.278638000	6	0.962272000	-5.106240000	-3.867450000
6	3.329497000	-4.549082000	-3.531002000	7	-0.340862000	-5.564263000	-3.426993000
6	0.997475000	-5.173882000	-3.882405000	6	2.137150000	-5.265291000	-3.143343000
7	-0.279714000	-5.645315000	-3.548498000	1	-3.736688000	-5.652794000	-2.712891000
6	2.196515000	-5.324192000	-3.171126000	1	2.097719000	-5.841377000	-2.211706000
1	-3.721697000	-5.650928000	-2.744336000	1	5.077528000	-2.398291000	-3.411037000
1	2.193187000	-5.910711000	-2.243853000	6	5.109832000	-3.055873000	-2.534719000
1	-0.485983000	-6.147522000	-2.687444000	1	6.976709000	1.874611000	0.119645000
1	-1.159875000	-2.304334000	-6.223496000	7	6.252650000	-1.243406000	-1.223443000
1	5.126139000	-2.469729000	-3.491175000	6	4.359747000	-4.278734000	-2.487632000
6	5.160619000	-3.099025000	-2.593034000	6	5.730039000	-2.586191000	-1.383778000
1	6.990658000	1.855567000	0.132244000	6	6.584717000	1.378711000	1.018718000
7	6.368495000	-1.343117000	-1.238595000	1	6.194705000	3.243291000	2.042362000
6	4.398424000	-4.293818000	-2.519013000	6	6.364357000	-1.089394000	0.070978000
6	5.788757000	-2.603056000	-1.441619000	6	6.129566000	2.150109000	2.111683000
6	6.592280000	1.365532000	1.032600000	6	4.440365000	-5.068847000	-1.310209000
1	6.221984000	3.232251000	2.029692000	6	6.434313000	-0.011916000	1.061371000
6	6.464030000	-1.127542000	0.141056000	6	5.632471000	-3.313736000	-0.140227000
6	6.149935000	2.139799000	2.108949000	1	3.935442000	-6.042489000	-1.275832000
6	4.470534000	-5.060130000	-1.309072000	6	5.054505000	-4.588174000	-0.131846000
6	6.455212000	-0.044046000	1.084109000	6	5.969050000	-2.308718000	0.871354000
6	5.676802000	-3.284934000	-0.166093000	6	5.489284000	1.555906000	3.231544000
1	3.972940000	-6.037496000	-1.263306000	6	5.967352000	-0.639117000	2.275380000
6	5.079543000	-4.569992000	-0.150364000	7	5.760342000	-2.067653000	2.140251000
6	6.090271000	-2.315601000	0.809958000	6	5.505405000	0.124719000	3.339842000
6	5.528311000	1.560992000	3.264381000	1	5.005771000	-5.177458000	0.794587000
6	6.023786000	-0.639643000	2.334516000	1	5.017163000	-0.391081000	4.174666000
7	5.916832000	-2.027424000	2.168684000	6	4.558133000	2.332103000	4.096736000
6	5.569348000	0.149042000	3.401177000	6	3.982056000	1.762688000	5.263352000
1	5.042998000	-5.157709000	0.778478000	6	2.765389000	2.239300000	5.801255000
1	5.094398000	-0.342570000	4.259415000	6	2.133527000	3.327204000	5.188452000
1	5.442458000	-2.637651000	2.831062000	6	3.996082000	3.551979000	3.590505000
1	6.368883000	-0.604596000	-1.939077000	6	2.808920000	4.035107000	4.126374000
6	4.596844000	2.357094000	4.119123000	6	0.765277000	3.848070000	5.130495000

6	3.979081000	1.779589000	5.277264000
6	2.772860000	2.257977000	5.796685000
6	2.142521000	3.370540000	5.185758000
6	4.073104000	3.582206000	3.630459000
6	2.870955000	4.081346000	4.152033000
6	0.827462000	3.948369000	5.176533000
7	2.067865000	5.116958000	3.654605000
6	0.789712000	4.977392000	4.207889000
1	4.427185000	0.888468000	5.735545000
1	2.293074000	1.736340000	6.637623000
1	4.501167000	4.055701000	2.738041000
7	-0.486359000	3.618486000	5.528749000
6	-0.581420000	5.256272000	3.883153000
6	-1.352445000	4.319194000	4.678077000
6	-2.698493000	4.051404000	4.390445000
6	-1.272696000	6.043092000	2.928477000
6	-2.618795000	5.776956000	2.662163000
6	-3.328981000	4.707744000	3.301571000
1	-0.744668000	6.821102000	2.358054000
1	-3.194300000	3.216725000	4.901642000
1	-3.123583000	6.366690000	1.886060000
1	2.271404000	5.622520000	2.794877000
1	-0.753822000	2.776617000	6.034520000
7	1.994730000	5.068391000	3.517115000
6	0.822944000	4.936713000	4.083992000
1	4.437713000	0.871057000	5.712206000
1	2.288387000	1.710458000	6.638333000
1	4.389957000	4.031217000	2.686867000
7	-0.449342000	3.488767000	5.458112000
6	-0.580868000	5.268116000	3.826880000
6	-1.305771000	4.297784000	4.613175000
6	-2.637727000	4.011888000	4.341056000
6	-1.269991000	6.052058000	2.894756000
6	-2.629637000	5.768747000	2.634253000
6	-3.302168000	4.687150000	3.262710000
1	-0.747144000	6.824781000	2.313859000
1	-3.101114000	3.162510000	4.856022000
1	-3.143918000	6.347742000	1.856838000

[4]DHPP cation

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.265297000	5.127072000	0.748979000
6	-4.785212000	4.324815000	1.286153000
1	-5.674582000	2.006280000	-4.116591000
7	-5.697795000	3.304789000	-0.832099000
6	-4.521935000	4.084720000	2.664262000
6	-5.544110000	3.402098000	0.560164000
6	-5.774957000	1.061183000	-3.564556000
1	-5.190184000	-0.127813000	-5.251349000
6	-6.149421000	2.022430000	-1.128954000
6	-5.497177000	-0.148778000	-4.198297000
6	-5.233588000	3.016037000	3.310713000
6	-6.122552000	1.062390000	-2.187661000
6	-6.079500000	2.204180000	1.183339000
1	-5.136973000	2.885736000	4.395740000
6	-5.984887000	2.085185000	2.595226000
6	-6.429519000	1.346491000	0.094712000
6	-5.522278000	-1.403573000	-3.497397000
6	-6.359245000	-0.216479000	-1.540796000
7	-6.645418000	0.000142000	-0.183265000
6	-6.069406000	-1.423695000	-2.183480000
1	-6.454949000	1.240174000	3.117744000
1	-6.108123000	-2.356212000	-1.607793000
1	-6.703063000	-0.740693000	0.512928000
1	-5.273858000	3.946713000	-1.499220000
1	-3.638011000	-1.416106000	-5.495378000
6	-3.700596000	-2.357877000	-4.937109000
1	2.050398000	-2.945206000	-6.326448000
7	-1.419573000	-3.121843000	-5.694324000

[4]PP cation

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.214506000	5.033142000	0.671628000
6	-4.740435000	4.258291000	1.240712000
1	-5.664431000	2.014819000	-4.138679000
7	-5.587541000	3.261336000	-0.897278000
6	-4.489530000	4.047794000	2.637476000
6	-5.510592000	3.338087000	0.541245000
6	-5.768718000	1.075475000	-3.578623000
1	-5.165676000	-0.152046000	-5.249664000
6	-6.067559000	2.065857000	-1.138331000
6	-5.477993000	-0.157270000	-4.197938000
6	-5.213608000	3.016332000	3.305575000
6	-6.098192000	1.081692000	-2.216647000
6	-6.073020000	2.179250000	1.206546000
1	-5.105188000	2.896642000	4.390756000
6	-5.989872000	2.073391000	2.601355000
6	-6.382525000	1.270850000	0.106019000
6	-5.478453000	-1.385188000	-3.472184000
6	-6.299884000	-0.175054000	-1.522551000
7	-6.539035000	-0.012437000	-0.109275000
6	-6.003643000	-1.384869000	-2.137138000
1	-6.455893000	1.232286000	3.132648000
1	-6.029206000	-2.295660000	-1.528311000
1	-3.526436000	-1.404871000	-5.435034000
6	-3.630290000	-2.345981000	-4.883315000
1	2.058983000	-2.936500000	-6.335278000
7	-1.341439000	-3.039970000	-5.633058000
6	-4.688489000	-2.551882000	-3.936744000
6	-2.596604000	-3.270478000	-4.960409000

6	-4.727027000	-2.563516000	-3.972598000	6	2.073753000	-3.591215000	-5.453214000
6	-2.642409000	-3.267737000	-5.019705000	1	4.172213000	-3.259436000	-5.067402000
6	2.075260000	-3.598531000	-5.442949000	6	-0.534238000	-3.950270000	-5.145752000
1	4.165983000	-3.261674000	-5.100687000	6	3.265646000	-3.771941000	-4.722188000
6	-0.517730000	-4.035611000	-5.157408000	6	-4.752523000	-3.804390000	-3.257308000
6	3.266612000	-3.777371000	-4.741829000	6	0.897105000	-4.184716000	-4.976901000
6	-4.752426000	-3.818437000	-3.271930000	6	-2.581713000	-4.443382000	-4.108387000
6	0.887595000	-4.213805000	-4.966040000	1	-5.602895000	-4.017727000	-2.597715000
6	-2.569766000	-4.426910000	-4.147349000	6	-3.703150000	-4.743600000	-3.323651000
1	-5.597774000	-4.047694000	-2.611285000	6	-1.187662000	-4.876145000	-4.148026000
6	-3.698488000	-4.728039000	-3.339906000	6	3.298249000	-4.510105000	-3.502114000
6	-1.214715000	-4.872871000	-4.237677000	6	0.960219000	-5.101063000	-3.855208000
6	3.332726000	-4.544911000	-3.528199000	7	-0.337228000	-5.556340000	-3.418787000
6	1.000024000	-5.160836000	-3.870372000	6	2.136352000	-5.267505000	-3.135362000
7	-0.281347000	-5.619067000	-3.524555000	1	-3.736587000	-5.655517000	-2.711936000
6	2.198169000	-5.325977000	-3.169269000	1	2.099142000	-5.852837000	-2.209695000
1	-3.723089000	-5.643820000	-2.732645000	1	5.085057000	-2.396850000	-3.419918000
1	2.199944000	-5.926173000	-2.251531000	6	5.107635000	-3.050099000	-2.540357000
1	-0.484096000	-6.175146000	-2.695995000	1	6.978487000	1.875346000	0.117520000
1	-1.167885000	-2.306005000	-6.249215000	7	6.241055000	-1.242123000	-1.225396000
1	5.141077000	-2.478393000	-3.499538000	6	4.352859000	-4.268968000	-2.486937000
6	5.161169000	-3.099319000	-2.595913000	6	5.720181000	-2.577694000	-1.386772000
1	6.978861000	1.862539000	0.129842000	6	6.576928000	1.380556000	1.012415000
7	6.336797000	-1.330690000	-1.235885000	1	6.196145000	3.240061000	2.042048000
6	4.393022000	-4.295249000	-2.519547000	6	6.354975000	-1.087138000	0.071019000
6	5.772003000	-2.599584000	-1.441979000	6	6.121457000	2.147251000	2.104429000
6	6.576218000	1.374828000	1.028757000	6	4.433982000	-5.062095000	-1.304206000
1	6.228042000	3.238159000	2.032684000	6	6.418167000	-0.011002000	1.056066000
6	6.415617000	-1.109781000	0.135769000	6	5.617498000	-3.306189000	-0.137513000
6	6.144557000	2.146710000	2.106098000	1	3.938516000	-6.040558000	-1.275316000
6	4.459451000	-5.063179000	-1.306179000	6	5.046122000	-4.585642000	-0.126928000
6	6.428598000	-0.036635000	1.079908000	6	5.959948000	-2.305940000	0.869713000
6	5.648088000	-3.279029000	-0.164076000	6	5.478493000	1.550903000	3.229342000
1	3.971743000	-6.045028000	-1.264695000	6	5.954202000	-0.641362000	2.276411000
6	5.057434000	-4.570324000	-0.147596000	7	5.749554000	-2.062848000	2.140295000
6	6.037562000	-2.307905000	0.809804000	6	5.499714000	0.121060000	3.344727000
6	5.524666000	1.564735000	3.265164000	1	5.006764000	-5.178936000	0.796845000
6	6.006123000	-0.635205000	2.334209000	1	5.021505000	-0.395832000	4.184361000
7	5.880859000	-2.023239000	2.162904000	6	4.551865000	2.330429000	4.086533000
6	5.567710000	0.148880000	3.405377000	6	3.972854000	1.758768000	5.258020000
1	5.024264000	-5.158020000	0.780596000	6	2.759224000	2.231978000	5.797396000
1	5.106617000	-0.341795000	4.270897000	6	2.126245000	3.317153000	5.176668000
1	5.459941000	-2.646971000	2.848928000	6	3.997578000	3.553948000	3.582582000
1	6.393435000	-0.608189000	-1.951146000	6	2.806290000	4.031179000	4.113838000
6	4.598605000	2.352674000	4.116796000	6	0.764545000	3.841842000	5.123041000
6	3.978856000	1.770565000	5.275865000	7	1.994961000	5.059441000	3.509353000
6	2.770852000	2.241721000	5.787208000	6	0.821081000	4.929635000	4.077592000
6	2.137276000	3.350815000	5.166617000	1	4.436138000	0.874151000	5.712472000
6	4.076326000	3.583011000	3.627257000	1	2.287121000	1.709843000	6.640839000
6	2.869341000	4.069445000	4.138149000	1	4.397060000	4.040336000	2.685535000
6	0.821893000	3.909697000	5.142380000	7	-0.452683000	3.481668000	5.449125000
7	2.057873000	5.094953000	3.626750000	6	-0.577862000	5.255893000	3.815361000
6	0.783081000	4.946720000	4.164722000	6	-1.306339000	4.285233000	4.608500000
1	4.433741000	0.887501000	5.741583000	6	-2.640399000	4.004255000	4.343086000
1	2.292103000	1.724431000	6.630557000	6	-1.266113000	6.047762000	2.886470000

1	4.513691000	4.064566000	2.744468000
7	-0.484260000	3.594509000	5.504373000
6	-0.582462000	5.238820000	3.859466000
6	-1.354339000	4.308404000	4.664827000
6	-2.701032000	4.050800000	4.391943000
6	-1.274783000	6.034054000	2.908208000
6	-2.619938000	5.775239000	2.650565000
6	-3.331228000	4.706133000	3.296713000
1	-0.746724000	6.813399000	2.340928000
1	-3.202625000	3.227759000	4.914892000
1	-3.128658000	6.371770000	1.883127000
1	2.285814000	5.644166000	2.800160000
1	-0.761191000	2.786753000	6.059035000
6	-2.622503000	5.762309000	2.628721000
6	-3.298381000	4.676229000	3.259691000
1	-0.745632000	6.827209000	2.313350000
1	-3.106762000	3.161842000	4.866242000
1	-3.141951000	6.347816000	1.859918000

[4]DHPP anion

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.281352000	5.122551000	0.736962000
6	-4.805448000	4.326441000	1.281463000
1	-5.676568000	2.012860000	-4.113561000
7	-5.769766000	3.335788000	-0.833348000
6	-4.516827000	4.082142000	2.659895000
6	-5.580688000	3.414094000	0.560046000
6	-5.787995000	1.068465000	-3.559601000
1	-5.146083000	-0.118149000	-5.228344000
6	-6.224538000	2.040474000	-1.131577000
6	-5.484327000	-0.143380000	-4.183683000
6	-5.227056000	3.007737000	3.298117000
6	-6.165677000	1.077751000	-2.189125000
6	-6.125751000	2.215762000	1.177000000
1	-5.106609000	2.858401000	4.379600000
6	-6.002731000	2.089095000	2.587613000
6	-6.503572000	1.371698000	0.084490000
6	-5.514820000	-1.402669000	-3.491310000
6	-6.395774000	-0.206161000	-1.547009000
7	-6.723823000	0.012628000	-0.194960000
6	-6.087984000	-1.412835000	-2.181885000
1	-6.465087000	1.240150000	3.113631000
1	-6.123752000	-2.341898000	-1.598348000
1	-6.634853000	-0.718974000	0.508063000
1	-5.221803000	3.894356000	-1.485381000
1	-3.626440000	-1.432029000	-5.507474000
6	-3.697882000	-2.374904000	-4.949936000
1	2.044708000	-2.950804000	-6.333655000
7	-1.438927000	-3.172035000	-5.753631000
6	-4.720013000	-2.558885000	-3.967788000
6	-2.650022000	-3.295091000	-5.045357000
6	2.067014000	-3.612145000	-5.454278000
1	4.145129000	-3.230260000	-5.077795000
6	-0.529021000	-4.093650000	-5.209187000
6	3.253134000	-3.771421000	-4.734439000
6	-4.734793000	-3.812120000	-3.263996000
6	0.878685000	-4.246449000	-4.999801000
6	-2.572028000	-4.459758000	-4.178665000
1	-5.564967000	-4.027753000	-2.577922000

[4]PP anion

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
1	-4.225268000	5.028778000	0.681077000
6	-4.757915000	4.258313000	1.250876000
1	-5.641841000	2.016005000	-4.128816000
7	-5.611300000	3.276656000	-0.894475000
6	-4.498452000	4.051414000	2.646743000
6	-5.531834000	3.343325000	0.543772000
6	-5.766524000	1.074175000	-3.575080000
1	-5.147926000	-0.144980000	-5.248802000
6	-6.074746000	2.066902000	-1.134924000
6	-5.479197000	-0.155640000	-4.202495000
6	-5.213894000	3.013750000	3.310355000
6	-6.112376000	1.086513000	-2.215841000
6	-6.086766000	2.179853000	1.204809000
1	-5.089987000	2.879226000	4.392552000
6	-5.984529000	2.070754000	2.599425000
6	-6.388326000	1.271020000	0.103044000
6	-5.487613000	-1.384867000	-3.482893000
6	-6.320269000	-0.170967000	-1.527294000
7	-6.565264000	-0.016354000	-0.114771000
6	-6.016573000	-1.378070000	-2.149260000
1	-6.432127000	1.216470000	3.127694000
1	-6.032599000	-2.288627000	-1.538824000
1	-3.532833000	-1.415501000	-5.431663000
6	-3.640044000	-2.361351000	-4.887718000
1	2.052010000	-2.914297000	-6.318021000
7	-1.352862000	-3.050476000	-5.654880000
6	-4.699382000	-2.559722000	-3.940680000
6	-2.602615000	-3.284576000	-4.974809000
6	2.071956000	-3.587279000	-5.448589000
1	4.168761000	-3.237751000	-5.060674000
6	-0.537770000	-3.953900000	-5.149365000
6	3.268637000	-3.768461000	-4.724926000
6	-4.756033000	-3.807590000	-3.256190000
6	0.893320000	-4.192041000	-4.987729000
6	-2.581466000	-4.453357000	-4.119190000
1	-5.595679000	-4.014859000	-2.580425000
6	-3.700321000	-4.740098000	-3.323432000
6	-1.185574000	-4.878943000	-4.154890000

6	-3.693160000	-4.738311000	-3.350169000
6	-1.222800000	-4.922988000	-4.295519000
6	3.328904000	-4.541672000	-3.523232000
6	0.998672000	-5.187377000	-3.897990000
7	-0.281592000	-5.677916000	-3.575944000
6	2.191267000	-5.338041000	-3.184687000
1	-3.717569000	-5.649049000	-2.732811000
1	2.184845000	-5.933816000	-2.262752000
1	-0.486062000	-6.103483000	-2.673451000
1	-1.149299000	-2.293861000	-6.180623000
1	5.157140000	-2.471941000	-3.489633000
6	5.180507000	-3.101492000	-2.590694000
1	6.982279000	1.859010000	0.124721000
7	6.409895000	-1.354834000	-1.241184000
6	4.388725000	-4.289303000	-2.518848000
6	5.807457000	-2.611910000	-1.441283000
6	6.588959000	1.365771000	1.026493000
1	6.186240000	3.230579000	2.008987000
6	6.487414000	-1.132488000	0.143680000
6	6.131225000	2.137122000	2.096868000
6	4.454597000	-5.048524000	-1.300100000
6	6.472162000	-0.050062000	1.079993000
6	5.693743000	-3.288549000	-0.159434000
1	3.940908000	-6.017996000	-1.248540000
6	5.076055000	-4.568896000	-0.145100000
6	6.113028000	-2.323603000	0.810960000
6	5.517294000	1.561739000	3.262303000
6	6.043934000	-0.641659000	2.337133000
7	5.957206000	-2.038189000	2.177597000
6	5.587559000	0.140913000	3.401679000
1	5.033443000	-5.156889000	0.784218000
1	5.122037000	-0.356458000	4.262407000
1	5.407976000	-2.621236000	2.806694000
1	6.325838000	-0.600433000	-1.920267000
6	4.593299000	2.350514000	4.110633000
6	3.963726000	1.768904000	5.264571000
6	2.766924000	2.254012000	5.796049000
6	2.139344000	3.381744000	5.199843000
6	4.073312000	3.597269000	3.643384000
6	2.876140000	4.092996000	4.167816000
6	0.831861000	3.963955000	5.194021000
7	2.078349000	5.147217000	3.682617000
6	0.791238000	4.994647000	4.224393000
1	4.401537000	0.866205000	5.711610000
1	2.286345000	1.726953000	6.634156000
1	4.502775000	4.080664000	2.756339000
7	-0.486191000	3.646228000	5.561481000
6	-0.574058000	5.269161000	3.893942000
6	-1.352690000	4.335126000	4.690980000
6	-2.693833000	4.063329000	4.405768000
6	-1.268213000	6.042213000	2.923586000
6	-2.608626000	5.762985000	2.648620000
6	-3.328585000	4.699575000	3.294343000
1	-0.741004000	6.817772000	2.347611000
1	-3.188130000	3.233326000	4.927032000
6	3.306325000	-4.514128000	-3.511863000
6	0.960802000	-5.114172000	-3.872506000
7	-0.332270000	-5.578732000	-3.434981000
6	2.141873000	-5.272080000	-3.153975000
1	-3.723319000	-5.642545000	-2.695520000
1	2.103279000	-5.850894000	-2.223659000
1	5.090340000	-2.408800000	-3.412693000
6	5.119857000	-3.065299000	-2.535112000
1	6.955970000	1.873182000	0.108648000
7	6.266577000	-1.253735000	-1.232032000
6	4.359006000	-4.280767000	-2.487975000
6	5.739976000	-2.587410000	-1.384781000
6	6.573525000	1.377907000	1.012891000
1	6.182796000	3.244485000	2.029762000
6	6.360760000	-1.092905000	0.072355000
6	6.124734000	2.150961000	2.103633000
6	4.431881000	-5.066450000	-1.302067000
6	6.431958000	-0.016821000	1.056302000
6	5.630444000	-3.309122000	-0.133502000
1	3.918825000	-6.035976000	-1.264270000
6	5.041189000	-4.581935000	-0.126248000
6	5.966112000	-2.305122000	0.871557000
6	5.490187000	1.557913000	3.232546000
6	5.974880000	-0.643980000	2.279578000
7	5.772726000	-2.065987000	2.152836000
6	5.517101000	0.127673000	3.343132000
1	4.982086000	-5.165441000	0.803929000
1	5.029690000	-0.387437000	4.179233000
6	4.560161000	2.331114000	4.097691000
6	3.974583000	1.756941000	5.262250000
6	2.757832000	2.232676000	5.793205000
6	2.126398000	3.328247000	5.186376000
6	4.002539000	3.555913000	3.600250000
6	2.811727000	4.043798000	4.129492000
6	0.764140000	3.849512000	5.125413000
7	2.008714000	5.076753000	3.523545000
6	0.824168000	4.932247000	4.082326000
1	4.425132000	0.860266000	5.706777000
1	2.274230000	1.698195000	6.623671000
1	4.398017000	4.035411000	2.697110000
7	-0.458932000	3.500500000	5.469600000
6	-0.573352000	5.265428000	3.823984000
6	-1.305357000	4.302768000	4.621511000
6	-2.640565000	4.023902000	4.346540000
6	-1.264882000	6.042533000	2.883119000
6	-2.623199000	5.765519000	2.624647000
6	-3.303654000	4.688256000	3.261421000
1	-0.738102000	6.807011000	2.293815000
1	-3.104994000	3.176253000	4.864011000
1	-3.134202000	6.338591000	1.840373000

1	-3.107786000	6.340751000	1.859044000
1	2.251428000	5.584831000	2.779344000
1	-0.743862000	2.759692000	5.991587000

[4]DHPP⊃C_{60}

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-1.613592000	2.130998000	2.367882000
6	-2.736472000	1.694095000	1.543045000
6	-0.641003000	2.992881000	1.826819000
6	-2.849253000	2.145175000	0.214169000
6	-0.758564000	3.470159000	0.449628000
6	-1.845998000	3.055760000	-0.345445000
6	-1.211125000	1.006237000	3.218480000
6	-3.035071000	0.302382000	1.877236000
6	-2.090109000	-0.128060000	2.912706000
6	0.772720000	2.762997000	2.109205000
6	-3.255264000	1.216599000	-0.838733000
6	0.154019000	0.786884000	3.493235000
6	-3.429413000	-0.594929000	0.863351000
6	0.590333000	3.535293000	-0.122815000
6	-1.626067000	2.682401000	-1.746589000
6	1.164492000	1.684218000	2.923820000
6	-3.528135000	-0.126982000	-0.519805000
6	1.539728000	3.102630000	0.909974000
6	-2.502158000	1.547236000	-2.052196000
6	-1.568709000	-1.439120000	2.889482000
6	0.802367000	3.175634000	-1.470151000
6	-0.327042000	2.741598000	-2.298850000
6	0.696171000	-0.575955000	3.472237000
6	-2.888671000	-1.959166000	0.839651000
6	-0.148889000	-1.667151000	3.174074000
6	-1.976309000	-2.373398000	1.833737000
6	2.328147000	0.881149000	2.556868000
6	-3.062358000	-1.195851000	-1.398686000
6	2.665405000	2.328578000	0.557852000
6	-2.049330000	0.515967000	-2.899198000
6	2.044891000	-0.514183000	2.897004000
6	-2.666959000	-2.331245000	-0.561658000
6	3.059478000	1.194169000	1.394764000
6	-2.332452000	-0.880833000	-2.560003000
6	1.972470000	2.370187000	-1.837166000
6	0.144041000	1.668433000	-3.178429000
6	2.887079000	1.956428000	-0.844191000
6	-0.701252000	0.577472000	-3.474146000
6	0.320662000	-2.742342000	2.293212000
6	-0.808505000	-3.178206000	1.465185000
6	1.565004000	1.438412000	-2.892920000
6	2.495078000	-1.548093000	2.049133000
6	-1.543642000	-3.104349000	-0.916606000
6	3.529613000	0.124024000	0.518752000
6	-1.166169000	-1.680134000	-2.924967000
6	1.617664000	-2.684245000	1.741848000
6	-0.596527000	-3.537395000	0.115334000
6	3.427064000	0.592795000	-0.867008000

[4]PP⊃C_{60}

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-1.607395000	2.110614000	2.373227000
6	-2.729699000	1.677208000	1.550422000
6	-0.641552000	2.979200000	1.833088000
6	-2.840497000	2.135201000	0.225549000
6	-0.760993000	3.468701000	0.460321000
6	-1.847232000	3.055102000	-0.333920000
6	-1.207311000	0.987723000	3.225067000
6	-3.031524000	0.285363000	1.885992000
6	-2.085505000	-0.145959000	2.920392000
6	0.770721000	2.750786000	2.111862000
6	-3.245528000	1.211918000	-0.829460000
6	0.156775000	0.770509000	3.494614000
6	-3.421489000	-0.607060000	0.868809000
6	0.586873000	3.542709000	-0.112511000
6	-1.630379000	2.690543000	-1.737383000
6	1.161038000	1.670472000	2.923475000
6	-3.514516000	-0.131137000	-0.510682000
6	1.535096000	3.103526000	0.916466000
6	-2.501004000	1.552837000	-2.043684000
6	-1.560694000	-1.455867000	2.891569000
6	0.797118000	3.188248000	-1.461555000
6	-0.332741000	2.753977000	-2.290405000
6	0.702850000	-0.589275000	3.473066000
6	-2.881937000	-1.970058000	0.841290000
6	-0.139833000	-1.681671000	3.173483000
6	-1.967099000	-2.386217000	1.832282000
6	2.325583000	0.873929000	2.552172000
6	-3.050128000	-1.195012000	-1.393075000
6	2.661248000	2.336562000	0.559809000
6	-2.048351000	0.526496000	-2.894992000
6	2.049534000	-0.521978000	2.894032000
6	-2.658485000	-2.335366000	-0.561087000
6	3.052107000	1.197360000	1.391170000
6	-2.324570000	-0.870970000	-2.553143000
6	1.968454000	2.387605000	-1.834558000
6	0.139859000	1.685084000	-3.175150000
6	2.884117000	1.971552000	-0.843768000
6	-0.702707000	0.592795000	-3.474010000
6	0.332211000	-2.751456000	2.287568000
6	-0.797313000	-3.186790000	1.458890000
6	1.561819000	1.458473000	-2.893167000
6	2.500135000	-1.548791000	2.041487000
6	-1.533944000	-3.103229000	-0.919179000
6	3.522551000	0.133850000	0.510389000
6	-1.157429000	-1.664751000	-2.919861000
6	1.628744000	-2.688155000	1.735669000
6	-0.586363000	-3.541355000	0.108537000
6	3.421733000	0.608594000	-0.871303000

6	-0.158166000	-0.785891000	-3.495892000	6	-0.157045000	-0.767951000	-3.496821000
6	3.240767000	-1.216856000	0.834206000	6	3.236808000	-1.206700000	0.825951000
6	-0.779238000	-2.769605000	-2.121782000	6	-0.771731000	-2.755701000	-2.120437000
6	2.086976000	0.127556000	-2.915703000	6	2.086994000	0.148733000	-2.921477000
6	3.034625000	-0.303474000	-1.881801000	6	3.032744000	-0.283202000	-1.888063000
6	1.206985000	-1.005585000	-3.218882000	6	1.207877000	-0.984914000	-3.226263000
6	1.835272000	-3.054978000	0.339359000	6	1.842860000	-3.050806000	0.330832000
6	0.751902000	-3.475937000	-0.457775000	6	0.760756000	-3.470912000	-0.465621000
6	2.837456000	-2.146658000	-0.216551000	6	2.836119000	-2.132965000	-0.225533000
6	0.636426000	-2.996504000	-1.838150000	6	0.642993000	-2.978639000	-1.840200000
6	2.733704000	-1.699349000	-1.547325000	6	2.729927000	-1.676762000	-1.552030000
6	1.607495000	-2.128128000	-2.372028000	6	1.607448000	-2.106928000	-2.376372000
1	-4.300511000	5.147157000	0.745037000	1	-4.324059000	5.066848000	0.679662000
6	-4.810982000	4.340811000	1.285064000	6	-4.816394000	4.274429000	1.254499000
1	-5.636675000	2.010334000	-4.123330000	1	-5.583781000	2.026679000	-4.113874000
7	-5.751465000	3.336935000	-0.841222000	7	-5.706896000	3.298726000	-0.890017000
6	-4.514828000	4.082916000	2.649673000	6	-4.492714000	4.040932000	2.637070000
6	-5.578924000	3.421112000	0.550444000	6	-5.603076000	3.359233000	0.556616000
6	-5.779499000	1.068220000	-3.575196000	6	-5.751481000	1.086729000	-3.570006000
1	-5.127846000	-0.119238000	-5.237729000	1	-5.048363000	-0.122795000	-5.212756000
6	-6.211058000	2.047603000	-1.146804000	6	-6.142151000	2.087052000	-1.141713000
6	-5.485572000	-0.147353000	-4.200865000	6	-5.436345000	-0.146834000	-4.187181000
6	-5.193364000	2.988338000	3.280246000	6	-5.153054000	2.967076000	3.290224000
6	-6.172207000	1.080480000	-2.213393000	6	-6.164419000	1.100190000	-2.232531000
6	-6.101253000	2.214640000	1.162143000	6	-6.115713000	2.175879000	1.206856000
1	-5.051753000	2.815323000	4.354171000	1	-4.974141000	2.788543000	4.357288000
6	-5.961178000	2.066876000	2.563245000	6	-5.942997000	2.027403000	2.586898000
6	-6.478276000	1.369247000	0.064863000	6	-6.441051000	1.274372000	0.094662000
6	-5.544072000	-1.404661000	-3.513228000	6	-5.491059000	-1.380896000	-3.486110000
6	-6.408057000	-0.198181000	-1.572781000	6	-6.389066000	-0.156911000	-1.558533000
7	-6.688135000	0.014586000	-0.213766000	7	-6.627623000	-0.002313000	-0.136005000
6	-6.110076000	-1.411623000	-2.211915000	6	-6.068877000	-1.366905000	-2.169139000
1	-6.390729000	1.196167000	3.078466000	1	-6.337858000	1.145515000	3.109867000
1	-6.149844000	-2.336344000	-1.623718000	1	-6.111168000	-2.273914000	-1.555750000
1	-6.631027000	-0.723438000	0.485634000	1	-3.557989000	-1.470924000	-5.489779000
1	-5.261743000	3.939801000	-1.499703000	6	-3.663261000	-2.402487000	-4.922540000
1	-3.653040000	-1.458238000	-5.518508000	1	2.021716000	-2.819054000	-6.255338000
6	-3.728404000	-2.396963000	-4.956595000	7	-1.377833000	-3.098663000	-5.697612000
1	2.007782000	-2.892102000	-6.272740000	6	-4.701346000	-2.566628000	-3.940562000
7	-1.448323000	-3.163622000	-5.714307000	6	-2.636978000	-3.338941000	-5.018326000
6	-4.746140000	-2.579166000	-3.984573000	6	2.048989000	-3.536104000	-5.423342000
6	-2.671615000	-3.316424000	-5.043093000	1	4.118457000	-3.120895000	-4.979224000
6	2.043471000	-3.582077000	-5.417905000	6	-0.553864000	-3.983217000	-5.190945000
1	4.113437000	-3.176142000	-5.036692000	6	3.241291000	-3.707724000	-4.681273000
6	-0.542459000	-4.086144000	-5.180684000	6	-4.730255000	-3.790429000	-3.220407000
6	3.235209000	-3.744399000	-4.706339000	6	0.887629000	-4.200446000	-5.015232000
6	-4.751589000	-3.815940000	-3.258314000	6	-2.599297000	-4.494074000	-4.152625000
6	0.870128000	-4.238728000	-4.974399000	1	-5.534274000	-3.975078000	-2.497646000
6	-2.592364000	-4.472529000	-4.172390000	6	-3.686562000	-4.741827000	-3.306589000
1	-5.569520000	-4.022308000	-2.556687000	6	-1.194600000	-4.927797000	-4.203211000
6	-3.704239000	-4.739244000	-3.334886000	6	3.294977000	-4.504757000	-3.507469000
6	-1.229415000	-4.926612000	-4.274294000	6	0.966179000	-5.153851000	-3.933156000
6	3.321752000	-4.543295000	-3.518729000	7	-0.335543000	-5.637229000	-3.510675000
6	0.994787000	-5.193997000	-3.890672000	6	2.141993000	-5.308931000	-3.200486000
7	-0.283172000	-5.671862000	-3.555720000	1	-3.692937000	-5.619099000	-2.644930000

6	2.201273000	-5.349875000	-3.186953000
1	-3.717318000	-5.630906000	-2.692064000
1	2.200367000	-5.958248000	-2.274653000
1	-0.482998000	-6.157242000	-2.683087000
1	-1.173124000	-2.299040000	-6.176592000
1	5.172113000	-2.490746000	-3.495661000
6	5.191212000	-3.112576000	-2.592989000
1	6.940164000	1.875352000	0.098732000
7	6.398333000	-1.345101000	-1.251000000
6	4.393644000	-4.286774000	-2.505263000
6	5.834188000	-2.614338000	-1.448654000
6	6.572509000	1.376678000	1.006667000
1	6.127630000	3.236425000	1.978144000
6	6.520223000	-1.126541000	0.127312000
6	6.101807000	2.144202000	2.077187000
6	4.438240000	-5.026196000	-1.279116000
6	6.486914000	-0.036217000	1.067710000
6	5.724570000	-3.283092000	-0.167861000
1	3.892197000	-5.974504000	-1.203096000
6	5.073870000	-4.541326000	-0.132015000
6	6.156815000	-2.314608000	0.801955000
6	5.514201000	1.559955000	3.248212000
6	6.064812000	-0.631720000	2.322124000
7	5.969464000	-2.020184000	2.159573000
6	5.593655000	0.149887000	3.387361000
1	5.006930000	-5.107763000	0.807776000
1	5.133362000	-0.355465000	4.244601000
1	5.462292000	-2.620181000	2.807435000
1	6.392987000	-0.609962000	-1.954840000
6	4.579220000	2.343964000	4.114422000
6	3.943539000	1.741682000	5.250561000
6	2.751017000	2.230466000	5.794618000
6	2.137599000	3.372631000	5.223252000
6	4.066206000	3.586119000	3.658551000
6	2.871984000	4.088370000	4.196192000
6	0.826330000	3.968479000	5.230726000
7	2.074289000	5.131097000	3.706479000
6	0.796401000	5.003561000	4.268223000
1	4.364922000	0.822464000	5.675955000
1	2.262306000	1.685123000	6.614340000
1	4.490213000	4.077187000	2.774723000
7	-0.493090000	3.629989000	5.557891000
6	-0.572165000	5.275545000	3.924147000
6	-1.355022000	4.346922000	4.714314000
6	-2.699090000	4.077782000	4.410707000
6	-1.243115000	6.022637000	2.924298000
6	-2.581648000	5.743982000	2.631658000
6	-3.314050000	4.705016000	3.292292000
1	-0.701092000	6.772616000	2.330773000
1	-3.199920000	3.255688000	4.935233000
1	-3.055710000	6.298409000	1.812449000
1	2.263727000	5.606722000	2.826192000
1	-0.766580000	2.786990000	6.058315000

1	2.101782000	-5.926428000	-2.296162000
1	5.173449000	-2.445485000	-3.408470000
6	5.171800000	-3.096649000	-2.527551000
1	6.923280000	1.877051000	0.083646000
7	6.330716000	-1.285432000	-1.224479000
6	4.353921000	-4.279452000	-2.472973000
6	5.808467000	-2.632328000	-1.379355000
6	6.568139000	1.376185000	0.994824000
1	6.098503000	3.238482000	1.978908000
6	6.431488000	-1.112613000	0.070876000
6	6.084962000	2.146214000	2.077788000
6	4.385658000	-5.039308000	-1.273604000
6	6.478877000	-0.020529000	1.053917000
6	5.683814000	-3.335467000	-0.125932000
1	3.814323000	-5.973077000	-1.207276000
6	5.029265000	-4.573257000	-0.103355000
6	6.042502000	-2.325960000	0.882743000
6	5.481021000	1.552898000	3.219663000
6	6.039461000	-0.643197000	2.281583000
7	5.854524000	-2.076965000	2.155915000
6	5.553800000	0.121447000	3.338849000
1	4.930739000	-5.137786000	0.834206000
1	5.085571000	-0.405047000	4.177928000
6	4.544982000	2.325965000	4.093586000
6	3.942875000	1.733552000	5.236765000
6	2.740567000	2.225203000	5.795573000
6	2.131298000	3.351160000	5.227116000
6	4.002968000	3.575764000	3.632253000
6	2.825985000	4.072645000	4.185538000
6	0.766690000	3.896827000	5.180542000
7	2.022055000	5.123663000	3.590133000
6	0.838866000	4.987657000	4.137611000
1	4.362925000	0.809126000	5.651575000
1	2.248140000	1.670952000	6.606471000
1	4.399797000	4.075118000	2.741406000
7	-0.455439000	3.557735000	5.511032000
6	-0.568726000	5.313890000	3.858500000
6	-1.308511000	4.372261000	4.662752000
6	-2.638483000	4.075248000	4.376194000
6	-1.242967000	6.038194000	2.867506000
6	-2.594291000	5.732144000	2.582678000
6	-3.290733000	4.689988000	3.250302000
1	-0.708281000	6.771878000	2.248447000
1	-3.102176000	3.244687000	4.919462000
1	-3.075319000	6.259824000	1.750249000

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