

Supporting information for:

A step towards rational design of carbon nanobelts with tunable electronic properties

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Abstract

Belt-shaped aromatic compounds are one of the most attractive classes of radial π -conjugated nanocarbon molecules with unique physical and chemical properties. In this work, we computationally studied a number of all-carbon and heteroatom-bridged nanobelts, as well as their inclusion complexes with fullerene. Our results provide a useful guide to modulating electronic properties of the nanobelts. In-depth analysis of ground and excited state properties of their complexes has allowed us to establish structure-property relationships and propose simple principles for the design of nanobelts with improved electron-donating properties suitable for photovoltaic applications.

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Computational Methodology

Quantum-chemical calculations

Geometry optimization of the complexes was performed employing the DFT B3LYP¹⁻³ exchange–correlation functional with Ahlrichs’ def2-SVP basis set.^{4,5} The empirical dispersion D3 correction was computed with the Becke–Johnson damping function.^{6,7} Vertical excitation energies were calculated using TDA formalism⁸ with the range-separated CAM-B3LYP⁹ functional and def2-SVP basis set,^{4,5} as implemented in the Gaussian16 (rev. A03) program.¹⁰ The same program was used for population analysis and calculation of Mulliken,^{11,12} Lowdin,¹³ Hirshfeld,¹⁴ CM5,¹⁵ NPA,¹⁶ and Merz-Singh-Kollman¹⁷ charges. Interaction energy was computed using the B3LYP functional coupled with def2-TZVP basis¹⁸ for the B3LYP-D3(BJ)/def2-SVP optimized geometries. Its energy decomposition analysis (EDA)^{19,20} was performed using the Amsterdam Density Functional (ADF) program.²¹ Molecular structures and frontier molecular orbitals were visualized by Chemcraft 1.8. program.²²

TD-DFT vs TDA approximation

The Tamm-Dancoff approximation (TDA) is a popular method in computational chemistry because it is formally simpler than the full Casida formalism by setting matrix **B** to zero.

Optical spectra and exciton binding energies can be obtained from the Casida equation:

$$\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{bmatrix} \vec{X}_I \\ \vec{Y}_I \end{bmatrix} = \omega_I \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \vec{X}_I \\ \vec{Y}_I \end{bmatrix} \quad (1)$$

where **A** and **B** are excitation and de-excitation matrices, respectively, X_n and Y_n are n th eigenvectors, and ω_i is the n th eigenvalue.

$$A_{ia\sigma,jb\tau} = \delta_{\sigma\tau} \delta_{ij} \delta_{ab} (\epsilon_{a\sigma} - \epsilon_{i\sigma}) + (ia | f_h + f_{XC}^{\sigma\tau} | jb) \quad (2)$$

$$B_{ia\sigma,jb\tau} = (ia | f_h + f_{XC}^{\sigma\tau} | bj) \quad (3)$$

In case of TDA formalism matrix **B** setting to 0, and thus

$$A\vec{X}_I = \omega_I \vec{X}_I \quad (4)$$

which is comparable to the CIS equation with the difference that in TD-DFT the elements of the matrix **A** depend on the exchange-correlation kernel. Setting matrix **B** to zero allow to save a lot of computational resources.²³

It is also worthwhile to note that for a long-range CT state in the TD-DFT the **B** matrix vanishes, which is equivalent to applying the Tamm-Dancoff approximation. Thus, TD-DFT and TD-DFT/TDA yield identical results for the excitation energies of long-range CT states.²³ It was also demonstrated that TDA is in a good agreement with both TD-DFT and experimental band shapes for conjugated molecules.²⁴ Isegawa and Truhlar showed that the TDA overestimates excitation energies as compared to TD-DFT, but the average absolute error changes insignificantly.²⁵ According to the systematic evaluations, the TDA performs better than the TD-DFT in calculation of nonadiabatic couplings between ground and excited states. The

correlation between TD-DFT and TDA is good when hybrid functionals are used.²⁵ Overall, the TDA is a safe way to simplify the original TD-DFT formulation.²⁶

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)²⁷⁻²⁹ 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:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp} \quad (5)$$

The term ΔE_{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 and polarization. The term ΔE_{disp} accounts for the dispersion corrections.^{30,31}

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.³²⁻³⁴ 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 \mathbf{C} in the original basis ${}^\lambda\mathbf{C} = \mathbf{S}^{1/2} \mathbf{C}$, where \mathbf{S} is the atomic orbital overlap matrix. The transition density matrix T^{0i} for an excited state Φ_i^* constructed as a superposition of singly excited configurations (where an occupied MO ψ_j is replaced a virtual MO ψ_a) is computed,

$$T_{\alpha\beta}^{0i} = \sum_{ja} A_{j \rightarrow a} {}^\lambda C_{\alpha j} {}^\lambda C_{\beta a} \quad (6)$$

where $A_{j \rightarrow a}$ is the expansion coefficient.

A key quantity $\Omega(D,A)$ is determined by:

$$\Omega(D,A) = \sum_{\alpha \in D, \beta \in A} (T_{\alpha\beta}^{0i})^2 \quad (7)$$

The weights of local excitations on donor (D) and acceptor (A) are $\Omega(D,D)$ and $\Omega(A,A)$. The weights of electron transfer configurations $D \rightarrow A$ and $A \rightarrow D$ are represented by $\Omega(D,A)$ and $\Omega(A,D)$, respectively. The index Δq , which describes charge separation and charge transfer between D and A, is

$$\Delta q(CS) = \sum \Omega(D,A) - \Omega(A,D) \quad (8)$$

$$\Delta q(CT) = \sum \Omega(D,A) + \Omega(A,D) \quad (9)$$

Solvent Effects

The equilibrium solvation energy E_S^{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 model³⁵⁻³⁸ in the monopole approximation:

$$E_S^{\text{eq}}(\mathbf{Q}, \epsilon) = -\frac{1}{2} f(\epsilon) \mathbf{Q}^+ \mathbf{D} \mathbf{Q} \quad (10)$$

where the $f(\epsilon)$ is the dielectric scaling factor, $f(\epsilon) = \frac{\epsilon - 1}{\epsilon}$, \mathbf{Q} – the vector of n atomic charges in the molecular system, \mathbf{D} is the $n \times n$ symmetric matrix determined by the shape of the boundary surface between solute and solvent. $\mathbf{D} = \mathbf{B}^+ \mathbf{A}^{-1} \mathbf{B}$, where the $m \times m$ matrix \mathbf{A} describes electrostatic interaction between m surface charges and the $m \times n$ \mathbf{B} matrix describes the interaction of the surface charges with n atomic charges of the solute.^{35,39} The GEPOL93 scheme⁴⁰ 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:

$$q_X^i = q_X^0 + \Delta_X^i, \quad \Delta_X^i = \sum_{Y \neq X} \sum_{\alpha \in X, \beta \in Y} (T_{\alpha\beta}^{0i} T_{\alpha\beta}^{0i} - T_{\beta\alpha}^{0i} T_{\beta\alpha}^{0i}), \quad (11)$$

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 $\psi_0 \rightarrow \Phi_i^*$.

The non-equilibrium solvation energy for excited state Φ_i^* can be estimated as:⁴¹

$$E_S^{\text{neq}}(\mathbf{Q}^0, \Delta, \epsilon, n^2) = f(\epsilon) \Delta^+ \mathbf{D} \mathbf{Q}^0 - \frac{1}{2} f(n^2) \Delta^+ \mathbf{D} \Delta, \quad (12)$$

In Eq. (12), 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. (11). By definition, the external (solvent) reorganization energy is the difference of the non-equilibrium (Eq. 12) and equilibrium (Eq. 10) 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):

$$k_{\text{ET}} = \frac{2\pi}{\hbar} V^2 (\text{FCWD}) \quad (13)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:⁴²

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (14)$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD)^{43,44} 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^{45,46} 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,

$$k = \sum_{n=0}^{\infty} k_{0 \rightarrow n}, \text{ where } k_{0 \rightarrow n} = \frac{2\pi}{\hbar} V_{0 \rightarrow n}^2 \frac{1}{\sqrt{4\pi\lambda_s kT}} \exp\left[-\frac{(\Delta G + n\hbar\omega_i + \lambda_s)^2}{4\lambda_s kT}\right] \quad (15)$$

with

$$V_{0 \rightarrow n}^2 = V^2 \frac{S^n}{n!} \exp(-S) \quad (16)$$

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

$$S = \lambda_i / \hbar\omega_i$$

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 of 1400-1800 cm^{-1}). It was established that varying the effective frequency from 1400 to 1800 cm^{-1} does not significantly affect the electron transfer rate for similar systems.⁴⁷⁻⁴⁹ 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.

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 state was computed as a difference between the equilibrium (E_s^{eq} , see eq. 10) and non-equilibrium (E_s^{neq} , see eq. 12) solvation energies. 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.

$\lambda_i = \lambda_i^1 + \lambda_i^2$, where :

$$\lambda_i^1(C_{60}^* \rightarrow C_{60}^-) = \frac{1}{2} \left[\left((C_{60}^*)_+ - (C_{60}^*)_- \right) + \left((C_{60}^-)_* - (C_{60}^-)_- \right) \right] \quad (17)$$

$$\lambda_i^2(CNB^0 \rightarrow CNB^+) = \frac{1}{2} \left[\left((CNB^0)_+ - (CNB^0)_0 \right) + \left((CNB^+)_0 - (CNB^+)_+ \right) \right]$$

Activation energy

The activation energies of the electron transfer reactions were computed based on the traditional Marcus theory and can be expressed as:

$$\Delta G^\ddagger = (\lambda + \Delta G^0)^2 / 4\lambda \quad (18)$$

Interaction energies

The interaction energies were calculated directly from the electronic energy of complex and electronic energies of its subsystems. For $Host \supset C_{60}$, the interaction energy can be expressed as follows:

$$E_{int} = E_{Host \supset C_{60}} - (E_{Host} + E_{C_{60}}) \quad (19)$$

Quantum Theory of Atoms in Molecules (QTAIM)

Topological analysis of the electron density distributions was conducted using the “Quantum Theory of Atoms in Molecules” (QTAIM) approach proposed by Bader.^{50,51} Electron density properties measured at the bond critical point (BCP) give information about the character of different chemical bonds.⁵²⁻⁵⁴ The AIMALL suite of programs⁵⁵ was applied to evaluate BCP properties and associated bond descriptors – 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 interaction (NCI) index

The NCI method⁵⁶⁻⁵⁸ relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s) defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla \rho|}{\rho^{4/3}} \quad (20)$$

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//B3LYP-D3(BJ)/def2-SVP level using Multiwfn program.⁵⁹

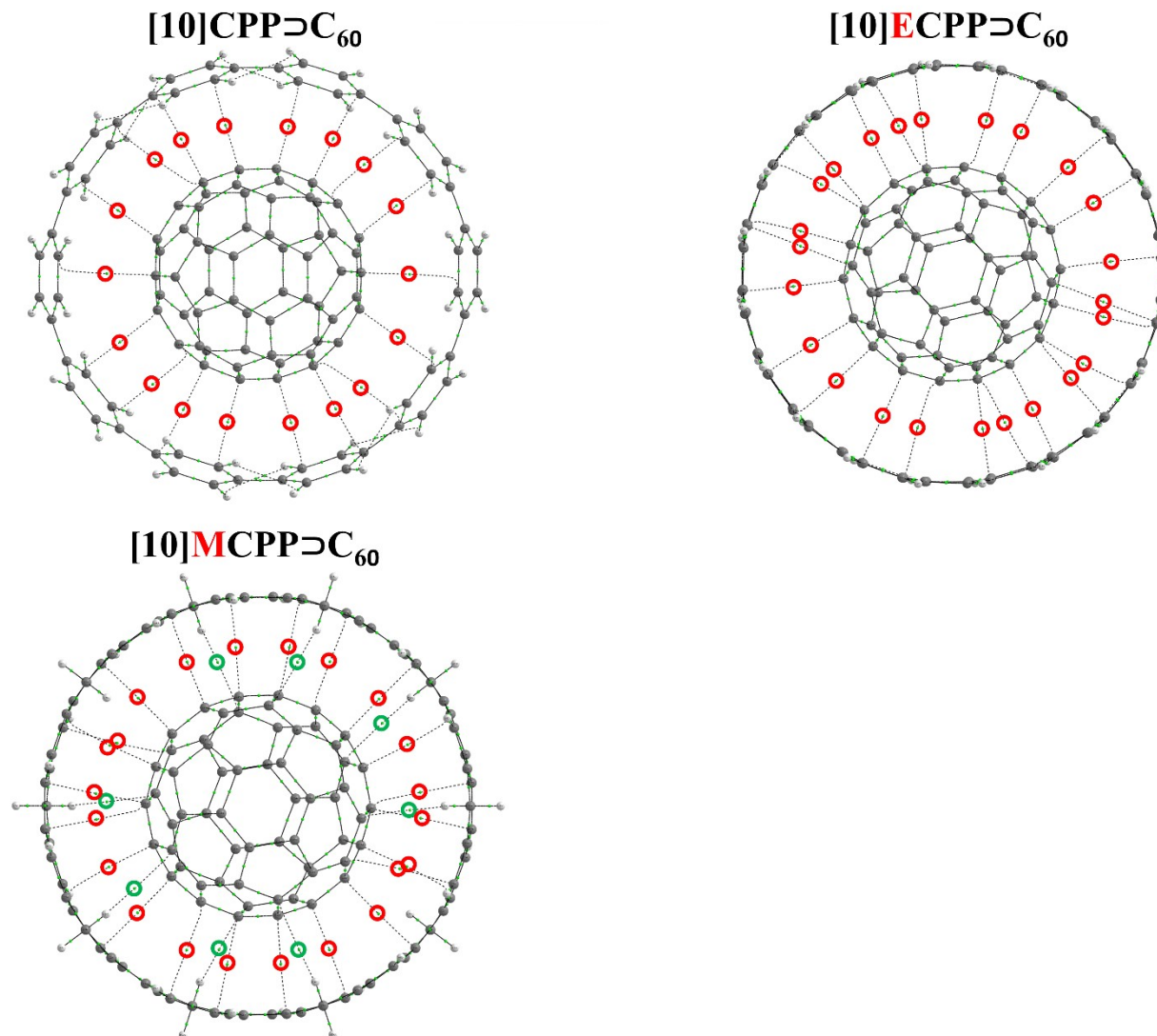


Figure S1. QTAIM molecular graph for [10]CPP⊃C₆₀, [10]MCP⊃C₆₀, and [10]ECPP⊃C₆₀ complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs. BCPs of interest are marked by red and green circles. Red circles correspond to C···C contacts, green to H···C contacts.

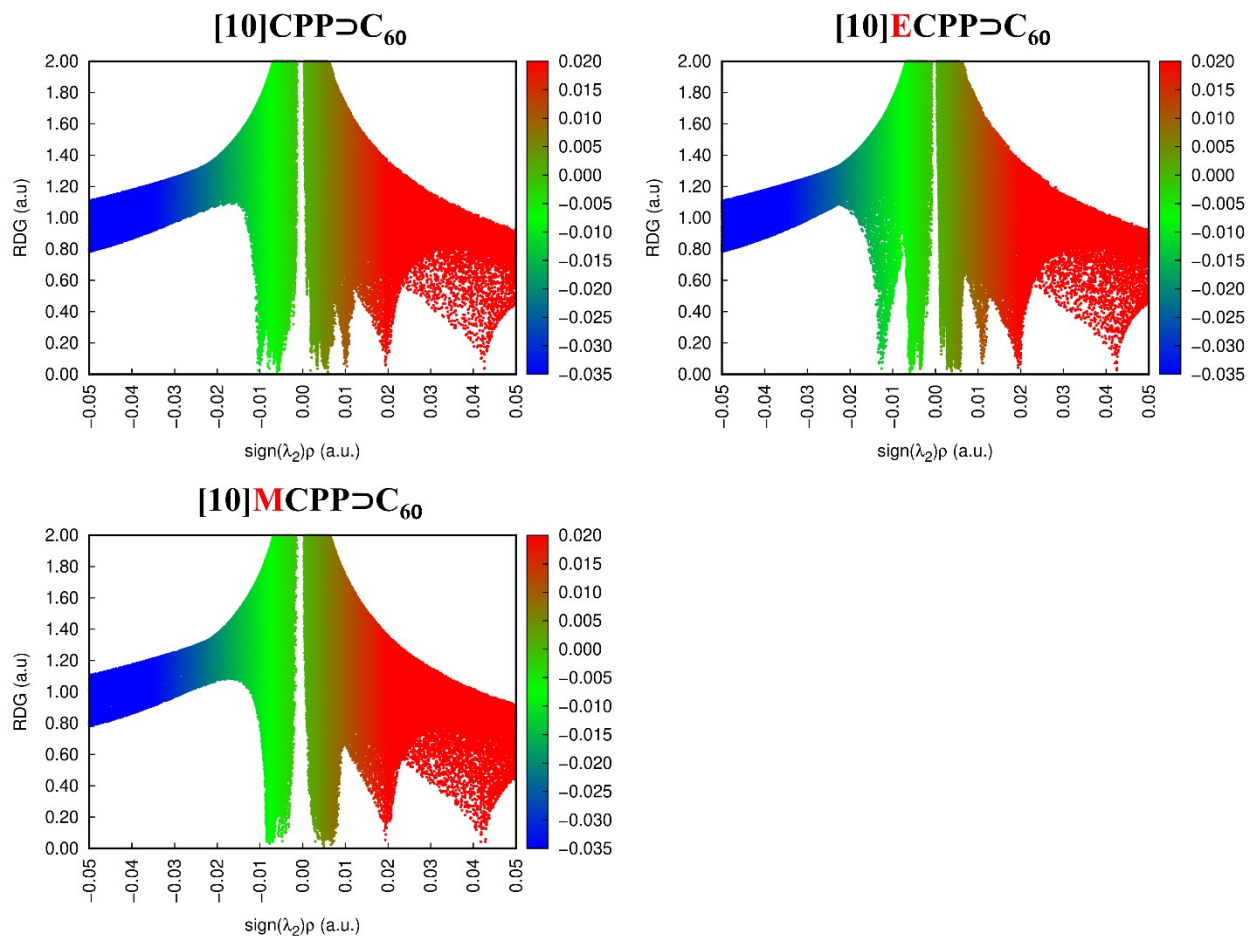


Figure S2. Plot of RDG vs. $\text{sign}(\lambda_2)\rho$ for [10]CPP \supset C₆₀, [10]MCPPE \supset C₆₀, and [10]ECPP \supset C₆₀ complexes.

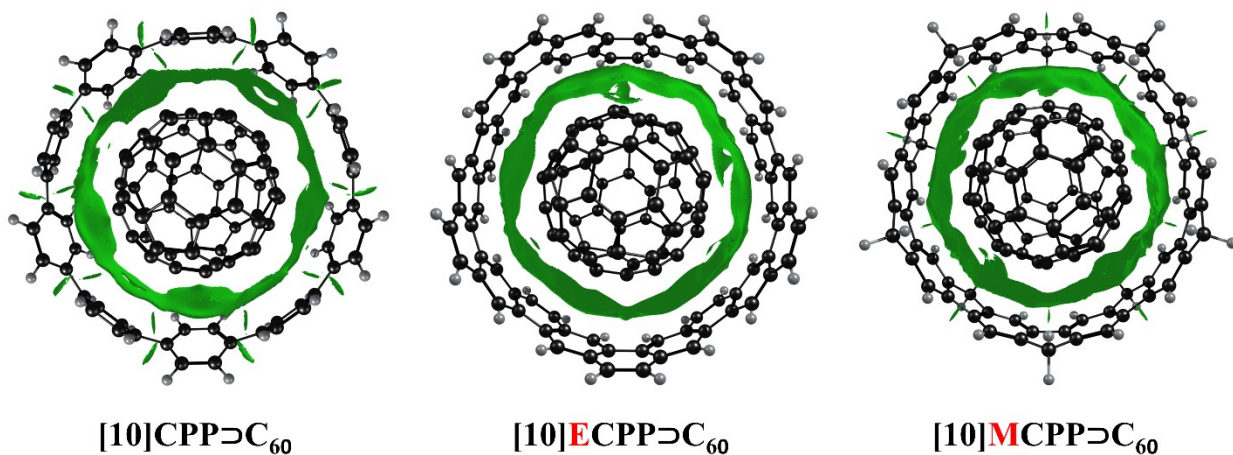


Figure S3. NCI isosurfaces of van der Waals interactions for [10]CPP \supset C₆₀, [10]MCPPE \supset C₆₀, and [10]ECPP \supset C₆₀ complexes. Isosurfaces were generated for RDG = 0.65 a.u.

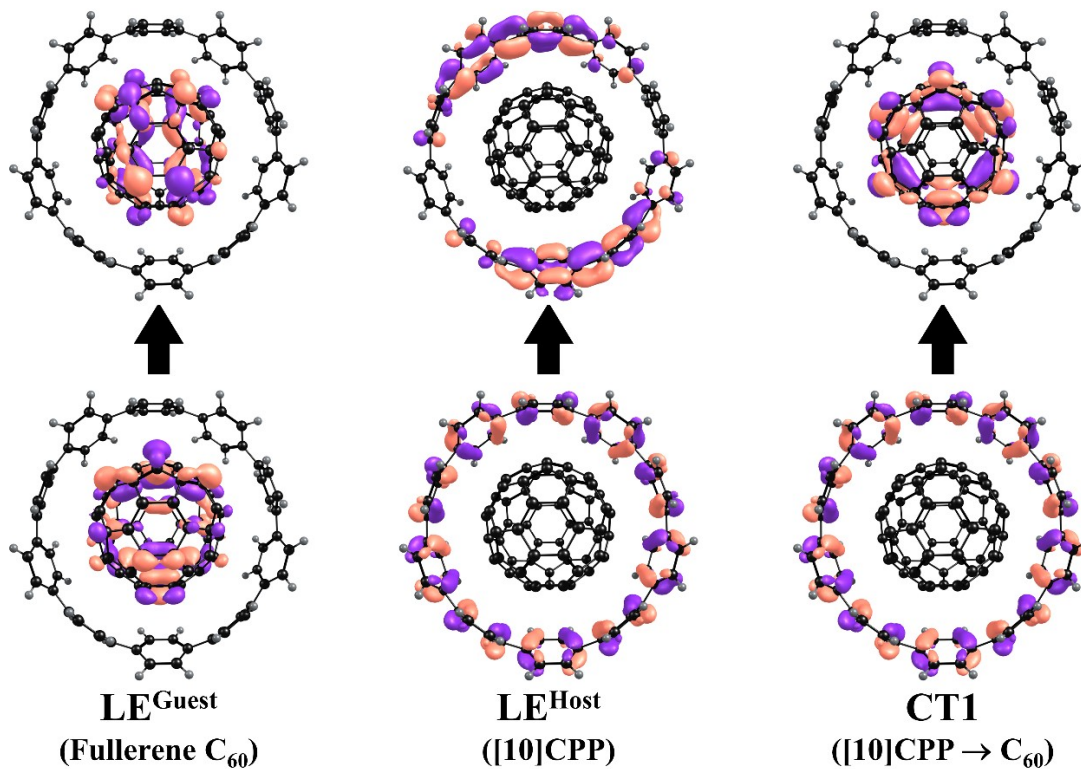


Figure S4. Frontier molecular orbitals representing LE^{Guest} , LE^{Host} , and CT states in $[10]CPP \supset C_{60}$ complex.

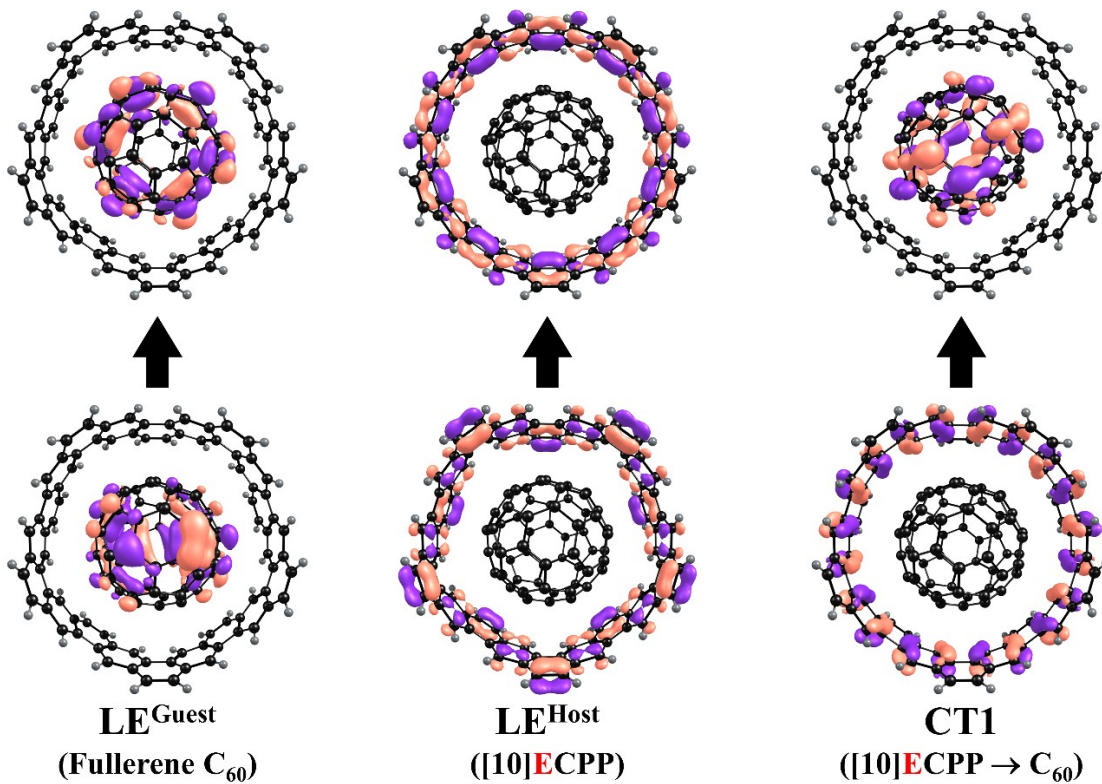


Figure S5. Frontier molecular orbitals representing LE^{Guest} , LE^{Host} , and CT states in $[10]ECPP \supset C_{60}$ complex.

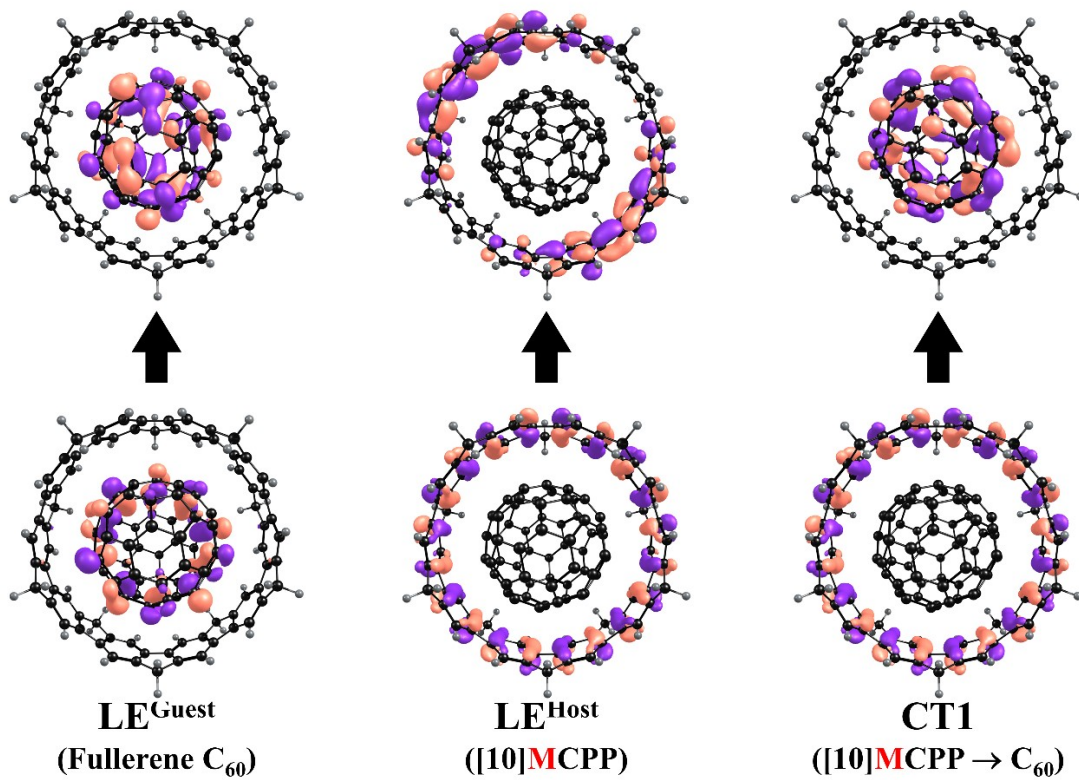


Figure S6. Frontier molecular orbitals representing LE^{Guest}, LE^{Host}, and CT states in [10]MCPP⊃C₆₀ complex.

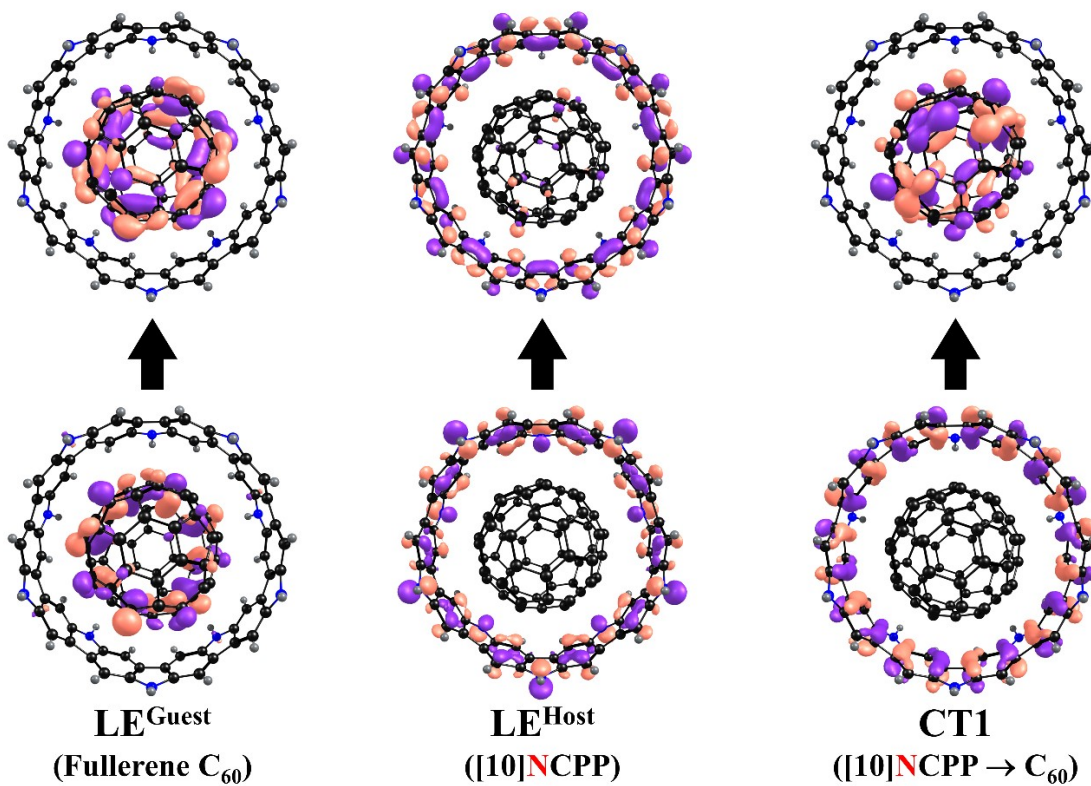


Figure S7. Frontier molecular orbitals representing LE^{Guest}, LE^{Host}, and CT states in [10]NCPP⊃C₆₀ complex.

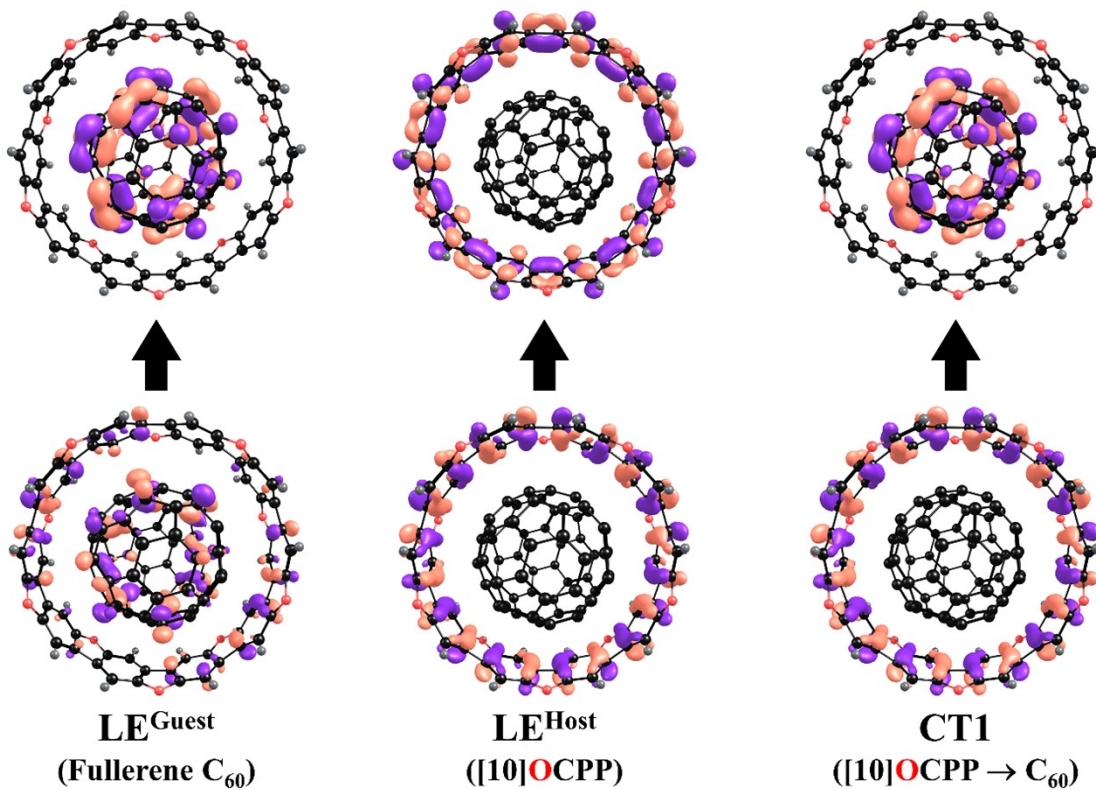


Figure S8. Frontier molecular orbitals representing LE^{Guest}, LE^{Host}, and CT states in [10]OCPP \rightarrow C₆₀ complex.

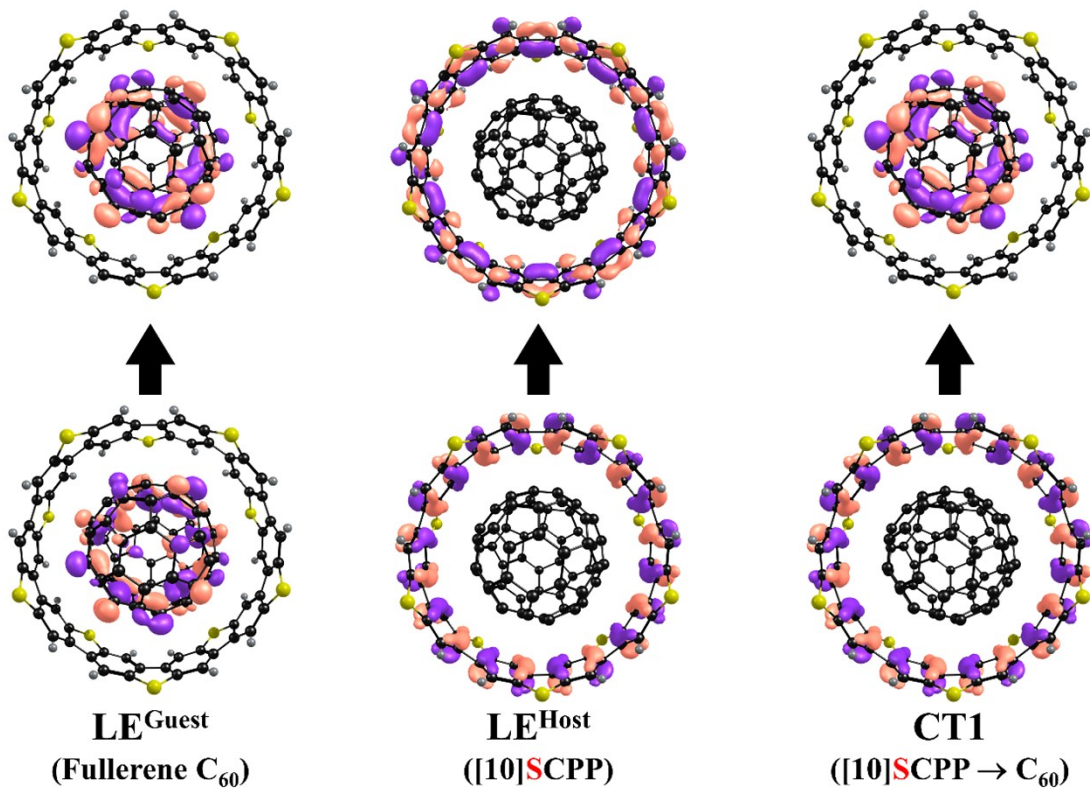


Figure S9. Frontier molecular orbitals representing LE^{Guest}, LE^{Host}, and CT states in [10]SCPP \rightarrow C₆₀ complex.

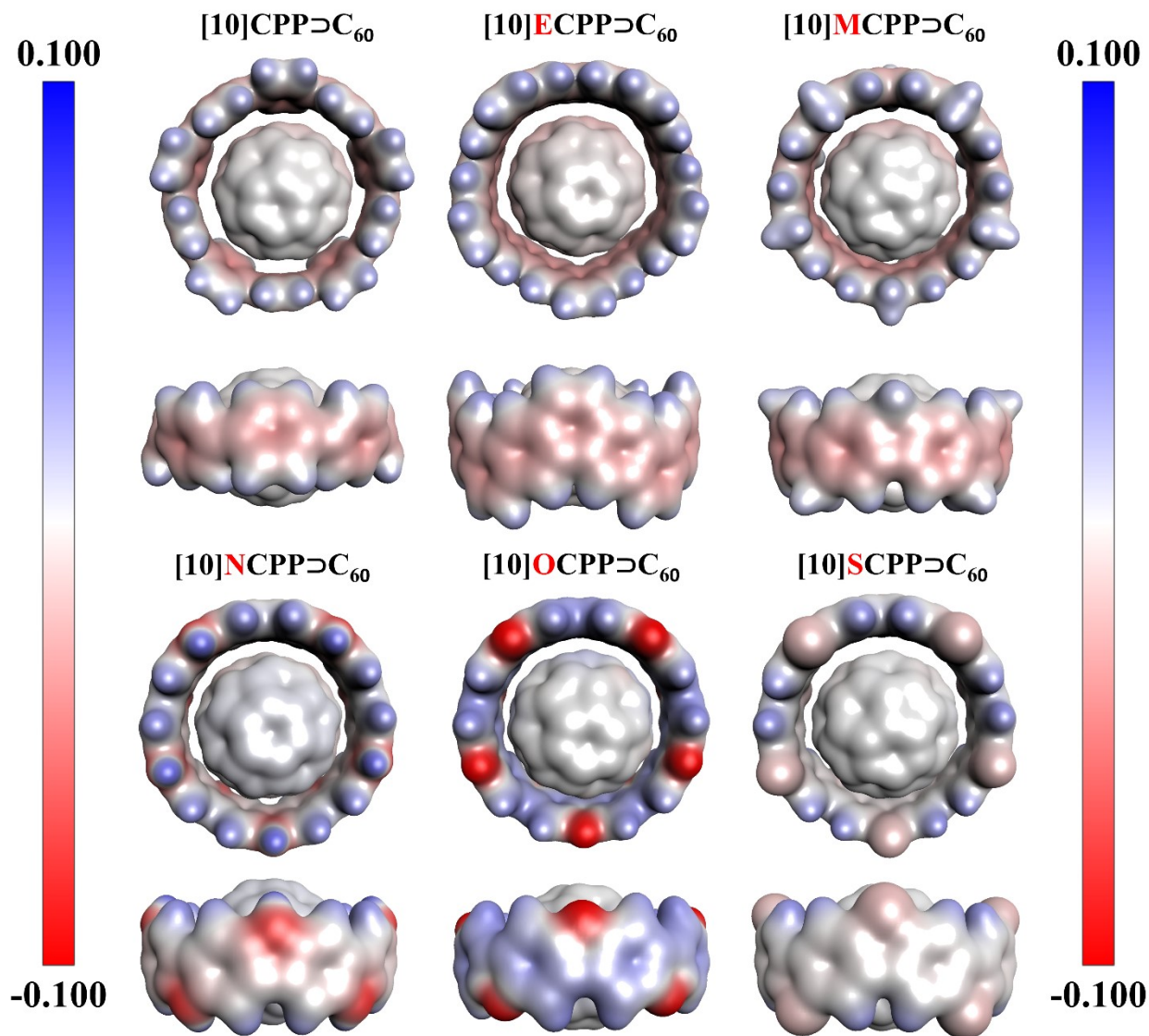


Figure S10. Calculated molecular electrostatic potential (MEP) surfaces for [10]CPP⊃C₆₀, [10]ECPP⊃C₆₀, [10]MCPPE⊃C₆₀, [10]NCPPE⊃C₆₀, [10]OCPPE⊃C₆₀, and [10]SCPPE⊃C₆₀ complexes. The surfaces are drawn at electron density contours of 0.02 e/Å³ and colored according to the electrostatic potential value.

Table S1. Charge separation (in electrons) between the fragments in electronic ground state for [10]CPP \supset C₆₀, [10]MCP \supset C₆₀, and [10]ECP \supset C₆₀ complexes. Q_{Host} - charge on host ([10]CPP, [10]MCP or [10]ECP), and $Q_{C_{60}}$ - charge on fullerene moiety. Total charge of the complexes $Q_{Tot} = 0$.

Charge Scheme	[10]CPP \supset C ₆₀		[10]MCP \supset C ₆₀		[10]ECP \supset C ₆₀	
	Q_{Host}	$Q_{C_{60}}$	Q_{Host}	$Q_{C_{60}}$	Q_{Host}	$Q_{C_{60}}$
Mulliken	0.024	-0.024	0.029	-0.029	0.011	-0.011
Lowdin	0.011	-0.011	0.033	-0.033	0.028	-0.028
Hirshfeld	-0.084	0.084	-0.120	0.120	-0.040	0.040
CM5	-0.073	0.073	-0.106	0.106	-0.036	0.036
NPA	0.073	-0.073	0.133	-0.133	0.097	-0.097

Table S2. Interaction energy (in kcal/mol) for [10]CPP \supset C₆₀, [10]ECP \supset C₆₀, and [10]MCP \supset C₆₀, complexes computed using B3LYP functional and different basis sets.

System	DZP	TZP	TZ2P	QZ4P
[10]CPP \supset C ₆₀	-95.24	-52.2	-51.94	-52.89
[10]ECP \supset C ₆₀	-115.18	-65.11	-65.26	-66.93
[10]MCP \supset C ₆₀	-123.66	-67.45	-66.94	-68.03

Table S3. Parameters (electron density [$\rho(r)$], 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 [10]CPP \supset C₆₀, [10]MCP \supset C₆₀, and [10]ECP \supset C₆₀ complexes computed in the gas phase.

Bond critical points between fragments	Interaction	$\rho(r)$, au	$\nabla^2\rho(r)$, au	$V(r)$, au	$G(r)$, au	$H(r)$, au
		[10]CPP \supset C ₆₀				
[10]CPP ... C ₆₀	C...C	6.88E-03	1.83E-02	-2.82E-03	3.70E-03	8.84E-04
		5.59E-03	1.45E-02	-2.41E-03	3.01E-03	6.05E-04
		5.67E-03	1.50E-02	-2.46E-03	3.11E-03	6.48E-04
		5.56E-03	1.55E-02	-2.52E-03	3.20E-03	6.81E-04
		8.15E-03	2.33E-02	-3.57E-03	4.70E-03	1.13E-03
		7.81E-03	2.20E-02	-3.37E-03	4.43E-03	1.06E-03
		6.04E-03	1.72E-02	-2.73E-03	3.52E-03	7.85E-04
		5.47E-03	1.48E-02	-2.45E-03	3.07E-03	6.25E-04
		5.92E-03	1.58E-02	-2.57E-03	3.26E-03	6.93E-04
		6.84E-03	1.82E-02	-2.80E-03	3.68E-03	8.74E-04
		5.55E-03	1.44E-02	-2.39E-03	2.99E-03	5.99E-04
		5.64E-03	1.49E-02	-2.45E-03	3.09E-03	6.44E-04
		5.62E-03	1.57E-02	-2.55E-03	3.24E-03	6.91E-04
8.23E-03	2.36E-02	-3.62E-03	4.76E-03	1.14E-03		
7.78E-03	2.19E-02	-3.36E-03	4.42E-03	1.05E-03		

		6.01E-03	1.71E-02	-2.72E-03	3.50E-03	7.80E-04	
		5.48E-03	1.47E-02	-2.44E-03	3.06E-03	6.23E-04	
		5.96E-03	1.59E-02	-2.58E-03	3.27E-03	6.97E-04	
		[10]MCPD→C₆₀					
[10]MCPD ... C₆₀	C...C	8.52E-03	2.54E-02	-4.03E-03	5.19E-03	1.16E-03	
		7.00E-03	1.92E-02	-3.09E-03	3.95E-03	8.58E-04	
		7.12E-03	2.14E-02	-3.39E-03	4.38E-03	9.82E-04	
		7.14E-03	2.03E-02	-3.30E-03	4.19E-03	8.87E-04	
		7.08E-03	1.98E-02	-3.21E-03	4.09E-03	8.72E-04	
		7.76E-03	2.35E-02	-3.68E-03	4.78E-03	1.10E-03	
		7.98E-03	2.34E-02	-3.75E-03	4.79E-03	1.05E-03	
		8.40E-03	2.51E-02	-3.98E-03	5.12E-03	1.15E-03	
		8.36E-03	2.42E-02	-3.85E-03	4.94E-03	1.10E-03	
		8.56E-03	2.58E-02	-4.07E-03	5.25E-03	1.19E-03	
		8.54E-03	2.55E-02	-4.04E-03	5.20E-03	1.17E-03	
		7.11E-03	2.14E-02	-3.39E-03	4.37E-03	9.78E-04	
		7.13E-03	2.02E-02	-3.29E-03	4.18E-03	8.84E-04	
		7.76E-03	2.35E-02	-3.68E-03	4.77E-03	1.09E-03	
		7.97E-03	2.33E-02	-3.75E-03	4.79E-03	1.04E-03	
		8.40E-03	2.50E-02	-3.97E-03	5.12E-03	1.15E-03	
		4.95E-03	1.27E-02	-2.16E-03	2.67E-03	5.06E-04	
		6.99E-03	1.92E-02	-3.09E-03	3.95E-03	8.57E-04	
	7.05E-03	1.98E-02	-3.21E-03	4.07E-03	8.68E-04		
	8.55E-03	2.57E-02	-4.06E-03	5.25E-03	1.19E-03		
	4.95E-03	1.27E-02	-2.16E-03	2.67E-03	5.05E-04		
	8.36E-03	2.41E-02	-3.84E-03	4.94E-03	1.10E-03		
		H...C	3.98E-03	1.27E-02	-1.72E-03	2.45E-03	7.28E-04
			4.23E-03	1.35E-02	-1.85E-03	2.61E-03	7.57E-04
			4.88E-03	1.54E-02	-2.14E-03	2.99E-03	8.54E-04
			4.79E-03	1.57E-02	-2.11E-03	3.02E-03	9.04E-04
	3.95E-03		1.26E-02	-1.71E-03	2.43E-03	7.25E-04	
	4.25E-03		1.35E-02	-1.86E-03	2.62E-03	7.60E-04	
	4.86E-03		1.53E-02	-2.13E-03	2.98E-03	8.54E-04	
	4.77E-03		1.56E-02	-2.10E-03	3.00E-03	9.01E-04	
		[10]ECPP→C₆₀					
[10]ECPP ... C₆₀	C...C	5.99E-03	1.67E-02	-2.67E-03	3.42E-03	7.57E-04	
		5.64E-03	1.55E-02	-2.52E-03	3.20E-03	6.80E-04	
		5.44E-03	1.47E-02	-2.45E-03	3.06E-03	6.07E-04	
		6.07E-03	1.69E-02	-2.73E-03	3.47E-03	7.44E-04	
		5.96E-03	1.76E-02	-2.74E-03	3.57E-03	8.28E-04	
		5.10E-03	1.30E-02	-2.19E-03	2.72E-03	5.33E-04	
		3.56E-03	9.80E-03	-1.69E-03	2.07E-03	3.82E-04	
		6.04E-03	1.67E-02	-2.67E-03	3.41E-03	7.48E-04	
		5.85E-03	1.61E-02	-2.61E-03	3.32E-03	7.07E-04	
		5.73E-03	1.56E-02	-2.52E-03	3.21E-03	6.88E-04	

		6.32E-03	1.79E-02	-2.86E-03	3.67E-03	8.09E-04
		5.82E-03	1.51E-02	-2.57E-03	3.18E-03	6.08E-04
		6.01E-03	1.68E-02	-2.68E-03	3.44E-03	7.62E-04
		5.66E-03	1.56E-02	-2.53E-03	3.22E-03	6.89E-04
		5.46E-03	1.47E-02	-2.46E-03	3.07E-03	6.09E-04
		6.07E-03	1.69E-02	-2.73E-03	3.47E-03	7.44E-04
		5.96E-03	1.76E-02	-2.74E-03	3.57E-03	8.29E-04
		5.10E-03	1.30E-02	-2.19E-03	2.72E-03	5.33E-04
		3.56E-03	9.79E-03	-1.68E-03	2.07E-03	3.82E-04
		6.04E-03	1.67E-02	-2.67E-03	3.42E-03	7.49E-04
		5.84E-03	1.61E-02	-2.61E-03	3.32E-03	7.06E-04
		5.73E-03	1.56E-02	-2.53E-03	3.22E-03	6.89E-04
		6.32E-03	1.79E-02	-2.86E-03	3.67E-03	8.07E-04
		5.81E-03	1.51E-02	-2.56E-03	3.17E-03	6.06E-04

Table S4. EDA results for [10]MCPD>C₆₀, [10]NCPD>C₆₀, [10]OCPD>C₆₀, and [10]SCPD>C₆₀ complexes.

Complex	Energy terms, kcal/mol ^[a]				
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}
[10]MCPD>C ₆₀	107.24	-54.54 (31%)	-23.00 (13%)	-96.63 (55%)	-66.94
[10]NCPD>C ₆₀	118.48	-61.10 (33%)	-26.77 (14%)	-97.40 (53%)	-66.79
[10]OCPD>C ₆₀	129.31	-63.90 (35%)	-25.29 (14%)	-95.97 (52%)	-55.85
[10]SCPD>C ₆₀	93.81	-46.21 (29%)	-18.33 (11%)	-97.34 (60%)	-68.07

^[a] The percentage contributions to the sum of all attractive energy terms ($\Delta E_{\text{elstat}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}}$) are listed in parentheses.

Table S5. Excitation energies (E_x , eV) and dipole moments in the ground state (μ_0 , D), change in dipole moments between the GS and state of interest ($\Delta\mu = \mu_i - \mu_0$, D), as well as solvation energies (E_{solv} , eV) in DCM calculated for [10]CPD>C₆₀, [10]ECPD>C₆₀, [10]MCPD>C₆₀, [10]NCPD>C₆₀, [10]OCPD>C₆₀ and [10]SCPD>C₆₀ complexes.

	Supramolecular host-guest system					
	[10]CPD>C ₆₀	[10]ECPD>C ₆₀	[10]MCPD>C ₆₀	[10]NCPD>C ₆₀	[10]OCPD>C ₆₀	[10]SCPD>C ₆₀
	Ground state (GS)					
E_x	0.000	0.000	0.000	0.000	0.000	0.000
μ_0	0.006	0.004	0.007	0.004	0.004	0.004
E_{solv}	-0.394	-0.522	-0.389	-0.979	-0.437	-0.515
	$LE^{\text{Guest}}(\text{C}_{60})$					
E_x	2.545	2.564	2.530	2.559	2.532	2.537
$\Delta\mu$	0.03	0.02	0.05	0.02	0.05	0.01
E_{solv}	-0.395	-0.520	-0.382	-0.934	-0.431	-0.517
	$LE^{\text{Host}}([\mathbf{10}]\mathbf{XCPD})$					

E_x	3.501	3.271	3.016	3.121	3.056	2.915
$\Delta\mu$	0.04	0.02	0.02	0.05	0.02	0.03
E_{solv}	-0.386	-0.525	-0.382	-1.032	-0.418	-0.754
CT ([10]XCPP \rightarrow C₆₀)						
E_x	2.685	2.675	2.160	2.215	2.642	2.776
$\Delta\mu$	0.09	0.03	0.06	0.03	0.15	0.03
E_{solv}	-0.468	-0.663	-0.412	-0.865	-0.479	-0.598

Table S6. Computed semi-classical rates (k_x in s^{-1}) and characteristic times (τ in ns) for the ET process in [10]MCP \supset C₆₀ and [10]NCP \supset C₆₀ complexes in DCM solution using different effective Huang-Rhys (S_{eff}) factors.

$\hbar\omega_{\text{eff}}$	ΔG^0 , eV	$ V_{ij} $, eV	λ_{solv} , eV	λ_{intr} , eV	S_{eff}	k_x , s^{-1}	τ , ns
[10]MCP\supsetC₆₀							
1400	-0.370	$2.87 \cdot 10^{-4}$	0.128	0.215	1.239	$1.36 \cdot 10^9$	0.74
1500					1.156	$1.35 \cdot 10^9$	0.74
1600					1.084	$1.37 \cdot 10^9$	0.73
1700					1.020	$1.40 \cdot 10^9$	0.71
1800					0.963	$1.43 \cdot 10^9$	0.70
[10]NCP\supsetC₆₀							
1400	-0.344	$3.14 \cdot 10^{-4}$	0.143	0.220	1.267	$1.80 \cdot 10^9$	0.56
1500					1.183	$1.78 \cdot 10^9$	0.56
1600					1.109	$1.76 \cdot 10^9$	0.57
1700					1.044	$1.73 \cdot 10^9$	0.58
1800					0.986	$1.68 \cdot 10^9$	0.60

Cartesian coordinates

[10]CPP

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.768804000	7.207530000	1.080658000
6	2.064207000	6.233073000	1.220951000
6	6.619252000	2.958236000	1.081159000
6	6.568762000	-0.036753000	1.220953000
6	4.859550000	-5.379852000	1.081205000
6	1.994819000	-6.255907000	1.220960000
6	-3.615434000	-6.282622000	1.080610000
6	-5.336215000	-3.830517000	1.220766000
6	-7.095029000	1.496844000	1.080559000
6	-5.293286000	3.890428000	1.220830000
6	-4.048477000	5.626472000	0.044031000
6	-2.760773000	6.357245000	-0.044675000
6	-1.994819000	6.255907000	-1.220960000
6	0.032452000	6.929668000	-0.044327000
6	1.503824000	6.764586000	0.044499000
6	3.615434000	6.282622000	-1.080610000
6	4.100731000	5.587411000	0.044555000
6	5.194541000	4.589498000	-0.044138000
6	5.336215000	3.830517000	-1.220766000
6	6.603691000	2.110788000	-0.044199000
6	6.901402000	0.660415000	0.044541000
6	7.095029000	-1.496844000	-1.080559000
6	6.583306000	-2.173077000	0.044470000
6	5.971611000	-3.521423000	-0.044248000
6	5.293286000	-3.890428000	-1.220830000
6	4.048477000	-5.626472000	-0.044031000
6	2.760773000	-6.357245000	0.044675000
6	0.768804000	-7.207530000	-1.080658000
6	-0.032452000	-6.929668000	0.044327000
6	-1.503824000	-6.764586000	-0.044499000
6	-2.064207000	-6.233073000	-1.220951000
6	-4.100731000	-5.587411000	-0.044555000
6	-5.194541000	-4.589498000	0.044138000
6	-6.619252000	-2.958236000	-1.081159000
6	-6.603691000	-2.110788000	0.044199000
6	-6.901402000	-0.660415000	-0.044541000
6	-6.568762000	0.036753000	-1.220953000
6	-6.413542000	1.419523000	-1.220908000
1	-6.025595000	1.903512000	-2.119000000
6	-7.250477000	0.112448000	1.080507000
1	-7.591840000	-0.384198000	1.991572000
6	-5.799149000	4.351342000	-1.081091000
1	-6.366783000	4.149882000	-1.992360000
6	-4.354792000	4.917758000	1.220723000
1	-3.756886000	5.081708000	2.119039000
6	-5.930741000	-4.169293000	-1.081178000
1	-5.914191000	-4.771371000	-1.992460000

[10]ECPP

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.658940000	6.867081000	1.201505000
6	2.164162000	6.550387000	1.201461000
6	6.329213000	2.749134000	1.201377000
6	6.900264000	-0.033661000	1.201487000
6	4.570462000	-5.169118000	1.201536000
6	2.100117000	-6.571879000	1.201422000
6	-3.503998000	-5.943095000	1.201483000
6	-5.602457000	-4.028188000	1.201540000
6	-6.736299000	1.495725000	1.201324000
6	-5.562457000	4.082658000	1.201315000
6	-4.028960000	5.609968000	0.050412000
6	-2.756175000	6.332620000	0.050481000
6	-2.100117000	6.571879000	-1.201422000
6	0.038289000	6.905712000	-0.050427000
6	1.492777000	6.742544000	-0.050448000
6	3.503998000	5.943095000	-1.201483000
6	4.090840000	5.564572000	0.050409000
6	5.172055000	4.578094000	0.050374000
6	5.602457000	4.028188000	-1.201540000
6	6.581251000	2.097885000	-0.050531000
6	6.875539000	0.664151000	-0.050468000
6	6.736299000	-1.495725000	-1.201324000
6	6.557226000	-2.170666000	0.050617000
6	5.952498000	-3.503499000	0.050625000
6	5.562457000	-4.082658000	-1.201315000
6	4.028960000	-5.609968000	-0.050412000
6	2.756175000	-6.332620000	-0.050481000
6	0.658940000	-6.867081000	-1.201505000
6	-0.038289000	-6.905712000	0.050427000
6	-1.492777000	-6.742544000	0.050448000
6	-2.164162000	-6.550387000	-1.201461000
6	-4.090840000	-5.564572000	-0.050409000
6	-5.172055000	-4.578094000	-0.050374000
6	-6.329213000	-2.749134000	-1.201377000
6	-6.581251000	-2.097885000	0.050531000
6	-6.875539000	-0.664151000	0.050468000
6	-6.900264000	0.033661000	-1.201487000
6	6.622255000	2.052933000	2.431274000
1	6.540177000	2.603821000	3.371681000
6	6.895384000	0.721771000	2.431328000
1	7.036854000	0.183154000	3.371786000
6	3.998784000	-5.663071000	2.431349000
1	4.497325000	-5.414968000	3.371821000
6	2.817098000	-6.334073000	2.431286000
1	2.348532000	-6.635138000	3.371704000
6	-4.150429000	-5.552259000	2.431360000
1	-3.760083000	-5.949511000	3.371789000

6	-6.023943000	-2.620896000	1.220803000	6	-5.154234000	-4.636301000	2.431391000
1	-5.995465000	-2.001518000	2.119090000	1	-5.585434000	-4.283890000	3.371847000
6	-2.346601000	-6.857761000	1.080627000	6	-6.564061000	2.231249000	2.431184000
1	-1.979648000	-7.335578000	1.991801000	1	-6.821460000	1.737393000	3.371628000
6	-3.331567000	-5.658638000	-1.220981000	6	-6.002521000	3.468689000	2.431172000
1	-3.672317000	-5.140327000	-2.119084000	1	-5.800324000	3.987615000	3.371605000
6	0.631717000	-6.535302000	1.220778000	6	0.093780000	6.930291000	2.431388000
1	0.051265000	-6.315775000	2.118683000	1	-0.455482000	7.022185000	3.371839000
6	2.133558000	-6.927876000	-1.080449000	6	1.444198000	6.778789000	2.431367000
1	2.711467000	-7.099190000	-1.991435000	1	2.000195000	6.746693000	3.371803000
6	4.354792000	-4.917758000	-1.220723000	6	5.154234000	4.636301000	-2.431391000
1	3.756886000	-5.081708000	-2.119039000	1	5.585434000	4.283890000	-3.371847000
6	5.799149000	-4.351342000	1.081091000	6	4.150429000	5.552259000	-2.431360000
1	6.366783000	-4.149882000	1.992360000	1	3.760083000	5.949511000	-3.371789000
6	6.413542000	-1.419523000	1.220908000	6	-2.817098000	6.334073000	-2.431286000
1	6.025595000	-1.903512000	2.119000000	1	-2.348532000	6.635138000	-3.371704000
6	7.250477000	-0.112448000	-1.080507000	6	-3.998784000	5.663071000	-2.431349000
1	7.591840000	0.384198000	-1.991572000	1	-4.497325000	5.414968000	-3.371821000
6	6.023943000	2.620896000	-1.220803000	6	-6.895384000	-0.721771000	-2.431328000
1	5.995465000	2.001518000	-2.119090000	1	-7.036854000	-0.183154000	-3.371786000
6	5.930741000	4.169293000	1.081178000	6	-6.622255000	-2.052933000	-2.431274000
1	5.914191000	4.771371000	1.992460000	1	-6.540177000	-2.603821000	-3.371681000
6	3.331567000	5.658638000	1.220981000	6	-1.444198000	-6.778789000	-2.431367000
1	3.672317000	5.140327000	2.119084000	1	-2.000195000	-6.746693000	-3.371803000
6	2.346601000	6.857761000	-1.080627000	6	-0.093780000	-6.930291000	-2.431388000
1	1.979648000	7.335578000	-1.991801000	1	0.455482000	-7.022185000	-3.371839000
6	-0.631717000	6.535302000	-1.220778000	6	6.002521000	-3.468689000	-2.431172000
6	-6.583306000	2.173077000	-0.044470000	6	-6.767617000	1.429614000	-1.220371000
6	-5.971611000	3.521423000	0.044248000	1	-6.699777000	1.915214000	-2.195018000
6	-4.859550000	5.379852000	-1.081205000	6	-6.916569000	0.105121000	1.220200000
1	-0.051265000	6.315775000	-2.118683000	1	-6.958304000	-0.383436000	2.194833000
6	-2.133558000	6.927876000	1.080449000	6	-5.533543000	4.149917000	-1.220395000
1	-2.711467000	7.099190000	1.991435000	1	-5.854440000	3.779082000	-2.195003000
1	-7.317780000	2.056557000	1.991769000	6	-4.634787000	5.134185000	1.220167000
1	-6.297818000	-0.520943000	-2.119215000	1	-4.294590000	5.487343000	2.194790000
1	-5.402494000	3.280421000	2.119322000	6	-5.657480000	-3.980008000	-1.220164000
1	-4.710354000	5.963237000	-1.992575000	1	-5.403888000	-4.399778000	-2.194760000
1	-0.305463000	7.592247000	1.991966000	6	-6.315966000	-2.821023000	1.220329000
1	-2.441468000	5.825864000	-2.119227000	1	-6.546798000	-2.388341000	2.194934000
1	1.449921000	6.147649000	2.119110000	6	-2.237001000	-6.543924000	1.220256000
1	4.216500000	6.321597000	-1.991863000	1	-1.785099000	-6.734472000	2.194840000
1	7.127941000	2.636315000	1.992630000	6	-3.450990000	-5.993308000	-1.220225000
1	4.789550000	4.122595000	-2.119192000	1	-3.892030000	-5.778782000	-2.194805000
1	6.297818000	0.520943000	2.119215000	6	0.731488000	-6.877093000	1.220207000
1	7.317780000	-2.056557000	-1.991769000	1	0.248674000	-6.962950000	2.194822000
1	5.402494000	-3.280421000	-2.119322000	6	2.037215000	-6.608910000	-1.220290000
1	4.710354000	-5.963237000	1.992575000	1	2.514797000	-6.497405000	-2.194884000
1	0.305463000	-7.592247000	-1.991966000	6	4.634787000	-5.134185000	-1.220167000
1	2.441468000	-5.825864000	2.119227000	1	4.294590000	-5.487343000	-2.194790000
1	-4.216500000	-6.321597000	1.991863000	6	5.533543000	-4.149917000	1.220395000
1	-1.449921000	-6.147649000	-2.119110000	1	5.854440000	-3.779082000	2.195003000
1	-4.789550000	-4.122595000	2.119192000	6	6.767617000	-1.429614000	1.220371000
1	-7.127941000	-2.636315000	-1.992630000	1	6.699777000	-1.915214000	2.195018000

6	6.916569000	-0.105121000	-1.220200000
1	6.958304000	0.383436000	-2.194833000
6	6.315966000	2.821023000	-1.220329000
1	6.546798000	2.388341000	-2.194934000
6	5.657480000	3.980008000	1.220164000
1	5.403888000	4.399778000	2.194760000
6	3.450990000	5.993308000	1.220225000
1	3.892030000	5.778782000	2.194805000
6	2.237001000	6.543924000	-1.220256000
1	1.785099000	6.734472000	-2.194840000
6	-0.731488000	6.877093000	-1.220207000
6	-6.557226000	2.170666000	-0.050617000
6	-5.952498000	3.503499000	-0.050625000
6	-4.570462000	5.169118000	-1.201536000
1	5.800324000	-3.987615000	-3.371605000
6	6.564061000	-2.231249000	-2.431184000
1	6.821460000	-1.737393000	-3.371628000
1	-0.248674000	6.962950000	-2.194822000
6	-2.037215000	6.608910000	1.220290000
1	-2.514797000	6.497405000	2.194884000

[10]MCP

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	6.476587000	1.646089000	1.054910000
6	6.644821000	-0.710331000	1.054841000
6	3.566937000	-5.649878000	1.054919000
6	1.377595000	-6.537503000	1.055009000
6	-4.271744000	-5.137916000	1.054988000
6	-5.793022000	-3.330509000	1.054939000
6	-6.207379000	2.474718000	1.054930000
6	-4.957963000	4.479680000	1.054906000
6	0.435610000	6.667123000	1.054960000
6	2.728734000	6.099043000	1.055013000
6	4.626743000	4.852735000	0.288454000
6	5.572507000	3.729004000	0.288444000
6	5.792995000	3.330563000	-1.054887000
6	6.596057000	1.206683000	-0.288423000
6	6.700623000	-0.258325000	-0.288469000
6	6.207337000	-2.474696000	-1.055051000
6	6.045848000	-2.900531000	0.288267000
6	5.269000000	-4.147025000	0.288276000
6	4.957954000	-4.479738000	-1.055026000
6	3.185800000	-5.899249000	-0.288384000
6	1.824701000	-6.451166000	-0.288319000
6	-0.435630000	-6.667201000	-1.054853000
6	-0.890488000	-6.644927000	0.288474000
6	-2.316117000	-6.291707000	0.288457000
6	-2.728747000	-6.099051000	-1.054882000
6	-4.626757000	-4.852721000	-0.288348000
6	-5.572530000	-3.729002000	-0.288379000
6	-6.476619000	-1.646119000	-1.054922000

[10]CPP=C₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.873172000	7.052805000	-1.187295000
6	0.517687000	7.085805000	-1.180681000
6	1.250407000	6.769794000	-0.018723000
6	0.518963000	6.613570000	1.172789000
6	-0.872085000	6.577335000	1.165594000
6	-1.600554000	6.700142000	-0.032667000
1	-1.402536000	7.249337000	-2.121979000
1	1.045856000	7.305508000	-2.110766000
1	1.040491000	6.372666000	2.100279000
1	-1.389288000	6.311217000	2.088264000
6	2.667452000	6.341165000	-0.074313000
6	3.155934000	5.720850000	-1.239463000
6	3.485828000	6.288700000	1.071399000
6	4.310276000	4.946685000	-1.213487000
1	2.558774000	5.734722000	-2.151938000
6	4.646215000	5.519047000	1.095992000
1	3.180688000	6.817539000	1.976635000
6	5.039379000	4.761186000	-0.024039000
1	4.572848000	4.370412000	-2.101723000
1	5.226938000	5.461083000	2.019264000
6	-2.991209000	6.194888000	-0.103132000
6	-3.805609000	6.069790000	1.040229000
6	-3.440190000	5.563722000	-1.278560000
6	-4.907021000	5.218853000	1.052656000
1	-3.539534000	6.604648000	1.954200000
6	-4.538053000	4.709452000	-1.265779000
1	-2.845385000	5.629218000	-2.190290000
1	-5.482204000	5.107001000	1.974395000
1	-4.756203000	4.126025000	-2.161788000
6	5.972291000	3.615370000	0.074126000

6	-6.596106000	-1.206669000	0.288394000	6	6.014922000	2.861209000	1.260756000
6	-6.700686000	0.258340000	0.288387000	6	6.618451000	3.072818000	-1.055410000
6	-6.644802000	0.710287000	-1.054934000	6	6.502026000	1.557540000	1.268744000
6	-6.045751000	2.900464000	-0.288404000	1	5.524809000	3.241973000	2.158396000
6	-5.268985000	4.146994000	-0.288411000	6	7.100283000	1.767260000	-1.048900000
6	-3.566875000	5.649801000	-1.055006000	1	6.687728000	3.660365000	-1.973493000
6	-3.185776000	5.899160000	0.288306000	6	6.959590000	0.945507000	0.087597000
6	-1.824686000	6.451088000	0.288333000	1	6.385014000	0.960716000	2.174638000
6	-1.377528000	6.537565000	-1.054957000	1	7.536892000	1.355499000	-1.961453000
6	-0.023816000	6.654677000	-1.353611000	6	6.974363000	-0.533122000	0.000914000
1	0.323339000	6.617066000	-2.389535000	6	6.524829000	-1.152799000	-1.180576000
6	-0.921017000	6.590659000	1.353583000	6	7.143057000	-1.353438000	1.133514000
1	-1.259300000	6.504131000	2.389519000	6	6.094388000	-2.475742000	-1.180665000
6	3.129282000	5.873519000	-1.353547000	1	6.380148000	-0.554854000	-2.081581000
1	2.804714000	6.002253000	-2.389483000	6	6.716942000	-2.678524000	1.132163000
6	3.892732000	5.398068000	1.353670000	1	7.564033000	-0.930660000	2.048274000
1	4.151448000	5.163566000	2.389598000	6	6.098536000	-3.242733000	-0.001135000
6	-4.619777000	4.790935000	-1.353656000	1	5.619244000	-2.872773000	-2.079033000
1	-4.842666000	4.522195000	-2.389598000	1	6.815473000	-3.270105000	2.044993000
6	-3.931375000	5.369823000	1.353538000	6	5.246330000	-4.450488000	0.083846000
1	-3.628356000	5.543353000	2.389466000	6	4.534905000	-4.707176000	1.269615000
6	-6.554054000	1.160932000	1.353600000	6	4.910663000	-5.221494000	-1.046747000
1	-6.576207000	0.812463000	2.389534000	6	3.437896000	-5.562312000	1.281395000
6	-6.337670000	2.033883000	-1.353619000	1	4.750558000	-4.121777000	2.164884000
1	-6.194565000	2.352362000	-2.389558000	6	3.809547000	-6.073047000	-1.035512000
6	-6.322757000	-2.079267000	1.353609000	1	5.487825000	-5.110374000	-1.967347000
1	-6.394227000	-1.737497000	2.389544000	6	2.992830000	-6.196810000	0.106193000
6	-5.984589000	-2.912683000	-1.353607000	1	2.840698000	-5.626607000	2.191641000
1	-5.797791000	-3.207636000	-2.389556000	1	3.545562000	-6.609000000	-1.949456000
6	-3.892748000	-5.398085000	-1.353549000	6	1.602420000	-6.702778000	0.034237000
1	-4.151490000	-5.163646000	-2.389485000	6	0.874910000	-6.580115000	-1.164598000
6	-3.129226000	-5.873357000	1.353675000	6	0.874260000	-7.055168000	1.188449000
1	-2.804625000	-6.002022000	2.389611000	6	-0.516223000	-6.614504000	-1.172440000
6	0.023877000	-6.654483000	1.353701000	1	1.393244000	-6.314993000	-2.086932000
1	-0.323245000	-6.616789000	2.389636000	6	-0.516590000	-7.087225000	1.181019000
6	0.920990000	-6.590792000	-1.353525000	1	1.403138000	-7.252042000	2.123344000
1	1.259241000	-6.504349000	-2.389475000	6	-1.248306000	-6.769851000	0.018800000
6	3.931322000	-5.369860000	-1.353636000	1	-1.037155000	-6.372715000	-2.100062000
1	3.628251000	-5.543358000	-2.389552000	1	-1.045574000	-7.306967000	2.110636000
6	4.619811000	-4.790955000	1.353543000	6	-2.664598000	-6.338812000	0.074653000
1	4.842760000	-4.522238000	2.389479000	6	-3.151092000	-5.717293000	1.240012000
6	6.337765000	-2.033955000	1.353493000	6	-3.484164000	-6.286062000	-1.070169000
1	6.194692000	-2.352466000	2.389426000	6	-4.305310000	-4.943006000	1.215221000
6	6.553939000	-1.160876000	-1.353706000	1	-2.552758000	-5.731113000	2.151708000
1	6.576029000	-0.812375000	-2.389630000	6	-4.644838000	-5.516681000	-1.093380000
6	6.322707000	2.079319000	-1.353602000	1	-3.180139000	-6.815172000	-1.975636000
6	0.890513000	6.645019000	-0.288356000	6	-5.036870000	-4.758807000	0.027082000
6	2.316144000	6.291794000	-0.288324000	1	-4.566408000	-4.366218000	2.103529000
6	4.271765000	5.138013000	-1.054874000	1	-5.226956000	-5.459506000	-2.015818000
1	6.394154000	1.737584000	-2.389551000	6	-5.971986000	-3.614548000	-0.069090000
6	5.984578000	2.912648000	1.353642000	6	-6.020671000	-2.861245000	-1.256030000
1	5.797786000	3.207572000	2.389600000	6	-6.614985000	-3.072511000	1.062515000
6	-2.525464000	6.225205000	-1.994345000	6	-6.509323000	-1.558085000	-1.262623000
				1	-5.534177000	-3.241975000	-2.155639000
				6	-7.097875000	-1.767356000	1.057494000
				1	-6.680368000	-3.659855000	1.980995000

6	-5.703127000	3.552276000	1.994245000	6	-6.961888000	-0.945822000	-0.079707000
6	-6.702573000	-0.478054000	-1.994254000	1	-6.396877000	-0.961527000	-2.169293000
6	-5.140966000	-4.325589000	1.994299000	1	-7.531146000	-1.355695000	1.971678000
6	-1.616335000	-6.520997000	-1.994189000	6	-6.975096000	0.532829000	0.007389000
6	2.525627000	-6.225198000	1.994315000	6	-6.518227000	1.150832000	1.186939000
6	5.703044000	-3.552280000	-1.994365000	6	-7.148720000	1.354291000	-1.123624000
6	6.702515000	0.477973000	1.994200000	6	-6.087333000	2.473541000	1.186308000
6	5.140965000	4.325690000	-1.994210000	1	-6.368568000	0.551735000	2.086347000
6	1.616294000	6.520924000	1.994318000	6	-6.721250000	2.679066000	-1.123298000
1	-2.895962000	7.139226000	-2.495138000	1	-7.574785000	0.932711000	-2.036604000
1	-2.239503000	5.520023000	-2.791182000	6	-6.097375000	3.241853000	0.007675000
1	1.853507000	7.478388000	2.494820000	1	-5.607089000	2.869103000	2.082582000
1	1.433317000	5.782511000	2.791361000	1	-6.823592000	3.271624000	-2.035092000
1	5.895609000	4.960856000	-2.494802000	6	-5.245758000	4.449857000	-0.078550000
1	4.558875000	3.835775000	-2.791177000	6	-1.710100000	2.662110000	-1.629062000
1	7.686487000	0.548203000	2.494571000	6	-2.644429000	1.560179000	-1.812531000
1	5.943783000	0.423814000	2.791316000	6	-0.490856000	2.671349000	-2.312364000
1	6.540102000	-4.073884000	-2.495126000	6	-2.317022000	0.503314000	-2.668920000
1	5.057235000	-3.149767000	-2.791188000	6	-2.609258000	-0.870315000	-2.275875000
1	2.896251000	-7.139267000	2.494941000	6	-3.275730000	1.288153000	-0.526982000
1	2.239779000	-5.520067000	2.791234000	6	-3.554450000	-0.028105000	-0.150500000
1	-1.853584000	-7.478509000	-2.494582000	6	-3.211114000	-1.128881000	-1.041222000
1	-1.433372000	-5.782644000	-2.791287000	6	0.669652000	3.483129000	-0.285992000
1	-4.558892000	-3.835633000	2.791251000	6	-0.602526000	3.474909000	0.423238000
1	-5.895614000	-4.960770000	2.494858000	6	0.725564000	3.091131000	-1.626033000
1	-7.686606000	-0.548283000	-2.494513000	6	-1.766601000	3.072900000	-0.232578000
1	-5.943902000	-0.423937000	-2.791423000	6	-2.735529000	2.225673000	0.447603000
1	-5.057390000	3.149878000	2.791180000	6	-0.354125000	3.044836000	1.792946000
1	-6.540265000	4.073918000	2.494836000	6	-1.282782000	2.228739000	2.447720000
				6	-2.500875000	1.812229000	1.761969000
				6	2.812347000	1.833746000	-1.199181000
				6	2.753427000	2.245845000	0.197155000
				6	1.818079000	2.247785000	-2.092079000
				6	1.705737000	3.055474000	0.643973000
				6	1.073116000	2.784775000	1.930240000
				6	3.211216000	1.129407000	1.014076000
				6	2.609439000	0.870774000	2.248755000
				6	1.514529000	1.713592000	2.714359000
				6	1.753450000	-0.007443000	-3.110193000
				6	2.791362000	-0.438453000	-2.181323000
				6	1.277353000	1.307029000	-3.065816000
				6	3.307637000	0.463488000	-1.244751000
				6	3.554461000	0.028565000	0.123441000
				6	2.501083000	-1.811684000	-1.789102000
				6	2.735680000	-2.225174000	-0.474706000
				6	3.275896000	-1.287707000	0.499880000
				6	-1.044163000	0.508158000	-3.377163000
				6	-0.548472000	-0.861051000	-3.422609000
				6	-0.149236000	1.569924000	-3.202056000
				6	0.821613000	-1.113051000	-3.290307000
				6	1.283014000	-2.228172000	-2.474908000
				6	-1.514380000	-1.713084000	-2.741523000
				6	-1.072884000	-2.784113000	-1.957308000
				6	0.354340000	-3.044141000	-1.820057000
				6	1.710341000	-2.661782000	1.601949000
				6	1.766911000	-3.072647000	0.205390000

6	0.602617000	-3.474195000	-0.450353000
6	0.491117000	-2.670922000	2.285275000
6	1.044350000	-0.507664000	3.350006000
6	2.317221000	-0.502849000	2.641696000
6	2.644736000	-1.559887000	1.785485000
6	0.149437000	-1.569411000	3.174875000
6	-1.753319000	0.007982000	3.082959000
6	-0.821432000	1.113550000	3.263078000
6	0.548653000	0.861557000	3.395442000
6	-1.277180000	-1.306492000	3.038580000
6	-2.812211000	-1.833184000	1.172024000
6	-3.307760000	-0.463027000	1.217699000
6	-2.791389000	0.439011000	2.154246000
6	-1.817900000	-2.247242000	2.064861000
6	-0.669485000	-3.482479000	0.258904000
6	-1.705573000	-3.054958000	-0.671067000
6	-2.753372000	-2.245428000	-0.224306000
6	-0.725336000	-3.090582000	1.598891000

[10]ECPD₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.653241000	6.797229000	1.282979000
6	2.154444000	6.455063000	1.345535000
6	6.299041000	2.693383000	1.396589000
6	6.842132000	-0.084194000	1.376579000
6	4.493629000	-5.173091000	1.248969000
6	2.028849000	-6.575919000	1.169353000
6	-3.545636000	-5.906533000	1.047643000
6	-5.644572000	-3.991540000	1.023035000
6	-6.740120000	1.497054000	1.061502000
6	-5.523986000	4.055705000	1.129166000
6	-3.985149000	5.600886000	0.020542000
6	-2.717471000	6.320608000	0.061645000
6	-2.028459000	6.574731000	-1.167364000
6	0.073781000	6.872038000	0.050685000
6	1.523276000	6.698905000	0.082576000
6	3.546315000	5.906734000	-1.044527000
6	4.101923000	5.505298000	0.212041000
6	5.183155000	4.527195000	0.224448000
6	5.645336000	3.991874000	-1.020162000
6	6.600496000	2.064176000	0.145871000
6	6.881079000	0.631750000	0.136249000
6	6.739449000	-1.496948000	-1.059607000
6	6.524463000	-2.190417000	0.175083000
6	5.906598000	-3.511139000	0.140213000
6	5.522978000	-4.055469000	-1.127556000
6	3.984963000	-5.601439000	-0.018876000
6	2.717439000	-6.321403000	-0.059823000
6	0.652980000	-6.798266000	-1.280643000
6	-0.073690000	-6.873152000	-0.048165000
6	-1.523148000	-6.699712000	-0.079691000
6	-2.154667000	-6.456449000	-1.342577000
6	-4.101466000	-5.505474000	-0.208953000
6	-5.182494000	-4.527159000	-0.221489000

[10]MCPD₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	6.460461000	1.622541000	1.277565000
6	6.624119000	-0.730113000	1.267321000
6	3.533256000	-5.634684000	1.129997000
6	1.338560000	-6.506680000	1.060104000
6	-4.319477000	-5.108454000	0.904410000
6	-5.873900000	-3.318243000	0.858286000
6	-6.280125000	2.474124000	0.880004000
6	-4.992910000	4.463105000	0.941347000
6	0.408359000	6.613966000	1.109198000
6	2.697826000	6.028649000	1.176866000
6	4.631702000	4.815610000	0.450459000
6	5.588630000	3.705378000	0.478789000
6	5.873768000	3.318579000	-0.854766000
6	6.669978000	1.197970000	-0.060995000
6	6.772093000	-0.269512000	-0.067515000
6	6.280042000	-2.474224000	-0.876681000
6	6.056695000	-2.909820000	0.454028000
6	5.270573000	-4.147344000	0.415921000
6	4.992891000	-4.463334000	-0.937899000
6	3.196903000	-5.888209000	-0.224939000
6	1.832013000	-6.431509000	-0.268282000
6	-0.408570000	-6.614392000	-1.105279000
6	-0.907233000	-6.600422000	0.223069000
6	-2.332680000	-6.244637000	0.181794000
6	-2.698024000	-6.028859000	-1.172957000
6	-4.631686000	-4.815314000	-0.446757000
6	-5.588649000	-3.705095000	-0.475229000
6	-6.460911000	-1.622512000	-1.274208000
6	-6.670489000	-1.197911000	0.064323000
6	-6.772571000	0.269552000	0.070786000
6	-6.624688000	0.730151000	-1.264054000
6	-6.056765000	2.909733000	-0.450707000
6	-5.270575000	4.147247000	-0.412521000

6	-6.298494000	-2.693603000	-1.393948000	6	-3.533382000	5.634850000	-1.126427000
6	-6.600125000	-2.064249000	-0.143350000	6	-3.197021000	5.888110000	0.228546000
6	-6.881026000	-0.631893000	-0.133964000	6	-1.832147000	6.431365000	0.272031000
6	-6.842449000	0.083849000	-1.374406000	6	-1.338658000	6.506950000	-1.056304000
6	6.524990000	1.978283000	2.629143000	6	0.025805000	6.612953000	-1.311513000
1	6.396637000	2.515480000	3.572269000	1	0.404964000	6.564173000	-2.335639000
6	6.781697000	0.644899000	2.619473000	6	-0.958843000	6.555275000	1.364254000
1	6.868045000	0.085443000	3.554446000	1	-1.328432000	6.462608000	2.388930000
6	3.881161000	-5.661631000	2.460706000	6	3.182744000	5.847363000	-1.223212000
1	4.345752000	-5.398449000	3.414893000	1	2.886283000	5.996639000	-2.265015000
6	2.703611000	-6.339259000	2.422661000	6	3.858318000	5.334381000	1.500882000
1	2.201660000	-6.642222000	3.345551000	1	4.088698000	5.075836000	2.538025000
6	-4.200496000	-5.509089000	2.270821000	6	-4.585916000	4.788229000	-1.456654000
1	-3.817064000	-5.905705000	3.214795000	1	-4.782717000	4.518588000	-2.497564000
6	-5.203583000	-4.591549000	2.259032000	6	-3.972774000	5.353960000	1.270804000
1	-5.643922000	-4.231957000	3.193017000	1	-3.692080000	5.522866000	2.313917000
6	-6.558226000	2.194109000	2.311118000	6	-6.668620000	1.163308000	1.148503000
1	-6.827845000	1.677347000	3.235974000	1	-6.746508000	0.805833000	2.178916000
6	-5.966456000	3.416197000	2.343774000	6	-6.290317000	2.051360000	-1.535701000
1	-5.737717000	3.902750000	3.295685000	1	-6.070968000	2.370885000	-2.557882000
6	0.059798000	6.798020000	2.536031000	6	-6.444620000	-2.077631000	1.135470000
1	-0.517544000	6.852935000	3.462364000	1	-6.575066000	-1.741214000	2.167773000
6	1.407168000	6.634182000	2.566070000	6	-5.941441000	-2.881554000	-1.554722000
1	1.939477000	6.554389000	3.517196000	1	-5.674899000	-3.160301000	-2.577852000
6	5.204584000	4.592307000	-2.256055000	6	-3.858418000	-5.334463000	-1.497080000
1	5.645366000	4.233223000	-3.190025000	1	-4.088730000	-5.076033000	-2.534267000
6	4.201492000	5.509831000	-2.267721000	6	-3.182698000	-5.846747000	1.227111000
1	3.818266000	5.906863000	-3.211602000	1	-2.886078000	-5.995618000	2.268929000
6	-2.702735000	6.337591000	-2.420852000	6	-0.025882000	-6.612511000	1.315420000
1	-2.200370000	6.640130000	-3.343652000	1	-0.404989000	-6.563324000	2.339545000
6	-3.880278000	5.659970000	-2.459038000	6	0.958645000	-6.555883000	-1.360416000
1	-4.344597000	5.396484000	-3.413275000	1	1.328161000	-6.463377000	-2.385134000
6	-6.781912000	-0.645450000	-2.617173000	6	3.972711000	-5.354214000	-1.267248000
1	-6.868590000	-0.086265000	-3.552276000	1	3.691967000	-5.523145000	-2.310343000
6	-6.524541000	-1.978714000	-2.626596000	6	4.585851000	-4.788132000	1.460125000
1	-6.396043000	-2.515967000	-3.569671000	1	4.782805000	-4.518549000	2.501021000
6	-1.407787000	-6.636101000	-2.563285000	6	6.289981000	-2.051364000	1.539001000
1	-1.940424000	-6.557027000	-3.514285000	1	6.070707000	-2.370903000	2.561194000
6	-0.060359000	-6.799462000	-2.533528000	6	6.668383000	-1.163349000	-1.145205000
1	0.516784000	-6.854557000	-3.459975000	1	6.746039000	-0.805864000	-2.175631000
6	5.964925000	-3.415566000	-2.342144000	6	6.444190000	2.077842000	-1.132053000
6	-6.699529000	1.475715000	-1.363536000	6	0.907118000	6.600600000	-0.219128000
1	-6.582464000	1.975986000	-2.325665000	6	2.332599000	6.244859000	-0.177851000
6	-6.947812000	0.112656000	1.048425000	6	4.319631000	5.109140000	-0.900642000
1	-7.023692000	-0.393662000	2.011505000	1	6.574363000	1.741448000	-2.164397000
6	-5.465509000	4.165555000	-1.294402000	6	5.941302000	2.881679000	1.558200000
1	-5.778352000	3.809096000	-2.276789000	1	5.674885000	3.160405000	2.581372000
6	-4.600985000	5.106497000	1.175531000	6	-2.448984000	6.181004000	-2.034302000
1	-4.273047000	5.447310000	2.158330000	6	-5.763167000	3.520572000	1.850421000
6	-5.627733000	-3.921403000	-1.401370000	6	-6.614221000	-0.447190000	-2.215893000
1	-5.333457000	-4.327450000	-2.369731000	6	-5.211608000	-4.287393000	1.820440000
6	-6.373576000	-2.795158000	1.029048000	6	-1.552276000	-6.427734000	-2.081921000
1	-6.640813000	-2.370297000	1.997749000	6	2.448939000	-6.180707000	2.038003000
6	-2.289845000	-6.527254000	1.078845000	6	5.762988000	-3.520715000	-1.847037000
1	-1.860510000	-6.750345000	2.056788000	6	6.613552000	0.447165000	2.219193000
6	-3.434609000	-5.893643000	-1.375541000	6	5.211565000	4.287942000	-1.816761000

1	-3.842960000	-5.633612000	-2.352741000	6	1.551943000	6.426956000	2.085874000
6	0.660623000	-6.876285000	1.143371000	1	-2.789792000	7.079342000	-2.582599000
1	0.149701000	-6.979024000	2.101617000	1	-2.131311000	5.444645000	-2.789800000
6	2.030565000	-6.555799000	-1.255480000	1	1.776928000	7.357998000	2.638858000
1	2.530430000	-6.408166000	-2.213473000	1	1.330013000	5.651751000	2.837100000
6	4.600124000	-5.106371000	-1.173927000	1	5.949281000	4.915888000	-2.349803000
1	4.271736000	-5.446785000	-2.156711000	1	4.627159000	3.755882000	-2.586019000
6	5.465273000	-4.166025000	1.295980000	1	7.552888000	0.509420000	2.799872000
1	5.778547000	-3.810113000	2.278435000	1	5.787753000	0.384831000	2.946531000
6	6.698896000	-1.476017000	1.365447000	1	6.584423000	-4.041312000	-2.373887000
1	6.581853000	-1.976523000	2.327455000	1	5.119124000	-3.072063000	-2.621439000
6	6.947657000	-0.112620000	-1.046246000	1	2.789773000	-7.079068000	2.586253000
1	7.023476000	0.393857000	-2.009250000	1	2.131409000	-5.444331000	2.793543000
6	6.374159000	2.795379000	-1.026394000	1	-1.777445000	-7.359050000	-2.634368000
1	6.641483000	2.370733000	-1.995166000	1	-1.330346000	-5.652968000	-2.833586000
6	5.628457000	3.921279000	1.404224000	1	-4.627330000	-3.755136000	2.589644000
1	5.334541000	4.327390000	2.372673000	1	-5.949328000	-4.915523000	2.353243000
6	3.434537000	5.892603000	1.378622000	1	-7.553646000	-0.509558000	-2.796413000
1	3.842663000	5.632200000	2.355817000	1	-5.788545000	-0.384854000	-2.943362000
6	2.290386000	6.527166000	-1.075786000	1	-5.119472000	3.072002000	2.625003000
1	1.861302000	6.750629000	-2.053757000	1	-6.584742000	4.041281000	2.376949000
6	-0.660216000	6.875032000	-1.141035000	6	0.495485000	-3.151356000	1.570713000
6	-6.525098000	2.190324000	-0.173304000	6	-0.954408000	-3.014877000	1.629683000
6	-5.907286000	3.511082000	-0.138575000	6	1.312077000	-2.328398000	2.354292000
6	-4.493410000	5.172165000	-1.247343000	6	-1.531912000	-2.055826000	2.468012000
1	5.735623000	-3.901770000	-3.294098000	6	-2.663566000	-1.264580000	1.998541000
6	6.556907000	-2.193582000	-2.309348000	6	-1.478431000	-3.214365000	0.284657000
1	6.826131000	-1.676545000	-3.234164000	6	-2.560768000	-2.457894000	-0.166054000
1	-0.149021000	6.977338000	-2.099177000	6	-3.162273000	-1.459754000	0.706457000
6	-2.030869000	6.555028000	1.257471000	6	2.874021000	-2.035035000	0.461393000
1	-2.531066000	6.407600000	2.215317000	6	2.025882000	-2.894144000	-0.351182000
6	0.583206000	-3.035981000	1.762285000	6	2.528940000	-1.759260000	1.787055000
6	-0.872388000	-2.948260000	1.791671000	6	0.862241000	-3.439732000	0.190899000
6	1.355759000	-2.134751000	2.504215000	6	-0.357529000	-3.482091000	-0.602491000
6	-1.498352000	-1.960538000	2.560234000	6	2.024024000	-2.374105000	-1.711910000
6	-2.650247000	-1.240596000	2.029173000	6	0.852581000	-2.417234000	-2.475827000
6	-1.369402000	-3.252911000	0.455771000	6	-0.364027000	-2.986609000	-1.909706000
6	-2.472707000	-2.561606000	-0.054002000	6	3.173127000	0.609513000	1.486161000
6	-3.126704000	-1.534118000	0.747354000	6	3.539125000	0.316177000	0.107006000
6	2.946883000	-1.901817000	0.625199000	6	2.678907000	-0.407246000	2.309832000
6	2.141516000	-2.840495000	-0.146964000	6	3.392606000	-0.978698000	-0.393908000
6	2.562818000	-1.555878000	1.924303000	6	2.869709000	-1.187555000	-1.738555000
6	0.985265000	-3.397109000	0.408732000	6	3.162529000	1.459609000	-0.713022000
6	-0.221958000	-3.534756000	-0.398074000	6	2.663901000	1.264536000	-2.005143000
6	2.140722000	-2.396579000	-1.534827000	6	2.510107000	-0.088716000	-2.526238000
6	0.981588000	-2.526314000	-2.308442000	6	0.973534000	1.133420000	3.229454000
6	-0.223547000	-3.108733000	-1.729681000	6	1.493324000	2.193578000	2.373757000
6	3.130046000	0.816435000	1.493957000	6	1.554950000	-0.139477000	3.199830000
6	3.532923000	0.454659000	0.140298000	6	2.569016000	1.934451000	1.518693000
6	2.654717000	-0.168771000	2.366011000	6	2.561055000	2.457762000	0.159495000
6	3.442494000	-0.875542000	-0.284322000	6	0.364382000	2.986553000	1.903108000
6	2.944505000	-1.182290000	-1.620088000	6	0.357916000	3.482182000	0.595937000
6	3.126638000	1.534981000	-0.751972000	6	1.478759000	3.214253000	-0.291223000
6	2.650240000	1.241496000	-2.033809000	6	-0.682592000	-1.193204000	3.280253000
6	2.555031000	-0.145403000	-2.474873000	6	-1.286939000	0.131139000	3.311333000
6	0.877807000	1.358563000	3.165257000	6	0.710028000	-1.326395000	3.225639000

6	1.373232000	2.386832000	2.257395000	6	-0.475537000	1.271726000	3.287253000
6	1.505543000	0.108868000	3.219745000	6	-0.852237000	2.417238000	2.469266000
6	2.475057000	2.118517000	1.437621000	6	-2.509747000	0.088672000	2.519662000
6	2.472647000	2.562461000	0.049436000	6	-2.869334000	1.187496000	1.731966000
6	0.223599000	3.109606000	1.725026000	6	-2.023672000	2.374094000	1.705330000
6	0.221953000	3.535745000	0.393447000	6	-0.495114000	3.151319000	-1.577314000
6	1.369332000	3.253690000	-0.460452000	6	-0.861860000	3.439786000	-0.197483000
6	-0.694026000	-1.020576000	3.330769000	6	-2.025453000	2.894085000	0.344603000
6	-1.346728000	0.280622000	3.274561000	6	-1.311702000	2.328316000	-2.360861000
6	0.702931000	-1.105056000	3.303381000	6	0.682942000	1.193163000	-3.286863000
6	-0.576538000	1.446004000	3.193678000	6	1.532245000	2.055775000	-2.474626000
6	-0.981591000	2.527216000	2.303802000	6	0.954753000	3.014816000	-1.636266000
6	-2.555048000	0.146287000	2.470222000	6	-0.709682000	1.326332000	-3.232229000
6	-2.944528000	1.183212000	1.615462000	6	-0.973175000	-1.133452000	-3.235984000
6	-2.140740000	2.397528000	1.530216000	6	0.475888000	-1.271750000	-3.293806000
6	-0.583252000	3.036829000	-1.766929000	6	1.287307000	-0.131182000	-3.317906000
6	-0.985261000	3.398035000	-0.413394000	6	-1.554633000	0.139421000	-3.206448000
6	-2.141422000	2.841316000	0.142284000	6	-3.172748000	-0.609596000	-1.492724000
6	-1.355775000	2.135594000	-2.508868000	6	-2.568686000	-1.934558000	-1.525264000
6	0.694007000	1.021428000	-3.335429000	6	-1.492991000	-2.193630000	-2.380363000
6	1.498337000	1.961353000	-2.564874000	6	-2.678564000	0.407161000	-2.316428000
6	0.872331000	2.949070000	-1.796340000	6	-2.873514000	2.034886000	-0.467955000
6	-0.702948000	1.105918000	-3.308033000	6	-3.392176000	0.978611000	0.387347000
6	-0.877828000	-1.357712000	-3.169883000	6	-3.538768000	-0.316263000	-0.113562000
6	0.576523000	-1.445136000	-3.198312000	6	-2.528575000	1.759169000	-1.793645000
6	1.346711000	-0.279753000	-3.279214000				
6	-1.505550000	-0.108020000	-3.224383000				
6	-3.130008000	-0.815593000	-1.498571000				
6	-2.475166000	-2.117767000	-1.442279000				
6	-1.373262000	-2.385994000	-2.261999000				
6	-2.654698000	0.169615000	-2.370633000				
6	-2.946911000	1.902710000	-0.629830000				
6	-3.442464000	0.876449000	0.279688000				
6	-3.532764000	-0.453746000	-0.144919000				
6	-2.562818000	1.556704000	-1.928921000				

[10]CPP \supset C₆₀ from [10]ECP \supset C₆₀
Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.653241000	6.797229000	1.282979000
6	2.154444000	6.455063000	1.345535000
6	6.299041000	2.693383000	1.396589000
6	6.842132000	-0.084194000	1.376579000
6	4.493629000	-5.173091000	1.248969000
6	2.028849000	-6.575919000	1.169353000
6	-3.545636000	-5.906533000	1.047643000
6	-5.644572000	-3.991540000	1.023035000
6	-6.740120000	1.497054000	1.061502000
6	-5.523986000	4.055705000	1.129166000
6	-3.985149000	5.600886000	0.020542000
6	-2.717471000	6.320608000	0.061645000
6	-2.028459000	6.574731000	-1.167364000
6	0.073781000	6.872038000	0.050685000
6	1.523276000	6.698905000	0.082576000
6	3.546315000	5.906734000	-1.044527000

[10]CPP \supset C₆₀ from [10]MCP \supset C₆₀
Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	6.460461000	1.622541000	1.277565000
6	6.624119000	-0.730113000	1.267321000
6	3.533256000	-5.634684000	1.129997000
6	1.338560000	-6.506680000	1.060104000
6	-4.319477000	-5.108454000	0.904410000
6	-5.873900000	-3.318243000	0.858286000
6	-6.280125000	2.474124000	0.880004000
6	-4.992910000	4.463105000	0.941347000
6	0.408359000	6.613966000	1.109198000
6	2.697826000	6.028649000	1.176866000
6	4.631702000	4.815610000	0.450459000
6	5.588630000	3.705378000	0.478789000
6	5.873768000	3.318579000	-0.854766000
6	6.669978000	1.197970000	-0.060995000
6	6.772093000	-0.269512000	-0.067515000
6	6.280042000	-2.474224000	-0.876681000

6	4.101923000	5.505298000	0.212041000	6	6.056695000	-2.909820000	0.454028000
6	5.183155000	4.527195000	0.224448000	6	5.270573000	-4.147344000	0.415921000
6	5.645336000	3.991874000	-1.020162000	6	4.992891000	-4.463334000	-0.937899000
6	6.600496000	2.064176000	0.145871000	6	3.196903000	-5.888209000	-0.224939000
6	6.881079000	0.631750000	0.136249000	6	1.832013000	-6.431509000	-0.268282000
6	6.739449000	-1.496948000	-1.059607000	6	-0.408570000	-6.614392000	-1.105279000
6	6.524463000	-2.190417000	0.175083000	6	-0.907233000	-6.600422000	0.223069000
6	5.906598000	-3.511139000	0.140213000	6	-2.332680000	-6.244637000	0.181794000
6	5.522978000	-4.055469000	-1.127556000	6	-2.698024000	-6.028859000	-1.172957000
6	3.984963000	-5.601439000	-0.018876000	6	-4.631686000	-4.815314000	-0.446757000
6	2.717439000	-6.321403000	-0.059823000	6	-5.588649000	-3.705095000	-0.475229000
6	0.652980000	-6.798266000	-1.280643000	6	-6.460911000	-1.622512000	-1.274208000
6	-0.073690000	-6.873152000	-0.048165000	6	-6.670489000	-1.197911000	0.064323000
6	-1.523148000	-6.699712000	-0.079691000	6	-6.772571000	0.269552000	0.070786000
6	-2.154667000	-6.456449000	-1.342577000	6	-6.624688000	0.730151000	-1.264054000
6	-4.101466000	-5.505474000	-0.208953000	6	-6.056765000	2.909733000	-0.450707000
6	-5.182494000	-4.527159000	-0.221489000	6	-5.270575000	4.147247000	-4.142521000
6	-6.298494000	-2.693603000	-1.393948000	6	-3.533382000	5.634850000	-1.126427000
6	-6.600125000	-2.064249000	-0.143350000	6	-3.197021000	5.888110000	0.228546000
6	-6.881026000	-0.631893000	-0.133964000	6	-1.832147000	6.431365000	0.272031000
6	-6.842449000	0.083849000	-1.374406000	6	-1.338658000	6.506950000	-1.056304000
6	-6.699529000	1.475715000	-1.363536000	6	0.025805000	6.612953000	-1.311513000
1	-6.582464000	1.975986000	-2.325665000	1	0.404964000	6.564173000	-2.335639000
6	-6.947812000	0.112656000	1.048425000	6	-0.958843000	6.555275000	1.364254000
1	-7.023692000	-0.393662000	2.011505000	1	-1.328432000	6.462608000	2.388930000
6	-5.465509000	4.165555000	-1.294402000	6	3.182744000	5.847363000	-1.223212000
1	-5.778352000	3.809096000	-2.276789000	1	2.886283000	5.996639000	-2.265015000
6	-4.600985000	5.106497000	1.175531000	6	3.858318000	5.334381000	1.500882000
1	-4.273047000	5.447310000	2.158330000	1	4.088698000	5.075836000	2.538025000
6	-5.627733000	-3.921403000	-1.401370000	6	-4.585916000	4.788229000	-1.456654000
1	-5.333457000	-4.327450000	-2.369731000	1	-4.782717000	4.518588000	-2.497564000
6	-6.373576000	-2.795158000	1.029048000	6	-3.972774000	5.353960000	1.270804000
1	-6.640813000	-2.370297000	1.997749000	1	-3.692080000	5.522866000	2.313917000
6	-2.289845000	-6.527254000	1.078845000	6	-6.668620000	1.163308000	1.148503000
1	-1.860510000	-6.750345000	2.056788000	1	-6.746508000	0.805833000	2.178916000
6	-3.434609000	-5.893643000	-1.375541000	6	-6.290317000	2.051360000	-1.535701000
1	-3.842960000	-5.633612000	-2.352741000	1	-6.070968000	2.370885000	-2.557882000
6	0.660623000	-6.876285000	1.143371000	6	-6.444620000	-2.077631000	1.135470000
1	0.149701000	-6.979024000	2.101617000	1	-6.575066000	-1.741214000	2.167773000
6	2.030565000	-6.555799000	-1.255480000	6	-5.941441000	-2.881554000	-1.554722000
1	2.530430000	-6.408166000	-2.213473000	1	-5.674899000	-3.160301000	-2.577852000
6	4.600124000	-5.106371000	-1.173927000	6	-3.858418000	-5.334463000	-1.497080000
1	4.271736000	-5.446785000	-2.156711000	1	-4.088730000	-5.076033000	-2.534267000
6	5.465273000	-4.166025000	1.295980000	6	-3.182698000	-5.846747000	1.227111000
1	5.778547000	-3.810113000	2.278435000	1	-2.886078000	-5.995618000	2.268929000
6	6.698896000	-1.476017000	1.365447000	6	-0.025882000	-6.612511000	1.315420000
1	6.581853000	-1.976523000	2.327455000	1	-0.404989000	-6.563324000	2.339545000
6	6.947657000	-0.112620000	-1.046246000	6	0.958645000	-6.555883000	-1.360416000
1	7.023476000	0.393857000	-2.009250000	1	1.328161000	-6.463377000	-2.385134000
6	6.374159000	2.795379000	-1.026394000	6	3.972711000	-5.354214000	-1.267248000
1	6.641483000	2.370733000	-1.995166000	1	3.691967000	-5.523145000	-2.310343000
6	5.628457000	3.921279000	1.404224000	6	4.585851000	-4.788132000	1.460125000
1	5.334541000	4.327390000	2.372673000	1	4.782805000	-4.518549000	2.501021000
6	3.434537000	5.892603000	1.378622000	6	6.289981000	-2.051364000	1.539001000
1	3.842663000	5.632200000	2.355817000	1	6.070707000	-2.370903000	2.561194000
6	2.290386000	6.527166000	-1.075786000	6	6.668383000	-1.163349000	-1.145205000

1	1.861302000	6.750629000	-2.053757000	1	6.746039000	-0.805864000	-2.175631000
6	-0.660216000	6.875032000	-1.141035000	6	6.444190000	2.077842000	-1.132053000
6	-6.525098000	2.190324000	-0.173304000	6	0.907118000	6.600600000	-0.219128000
6	-5.907286000	3.511082000	-0.138575000	6	2.332599000	6.244859000	-0.177851000
6	-4.493410000	5.172165000	-1.247343000	6	4.319631000	5.109140000	-0.900642000
1	-0.149021000	6.977338000	-2.099177000	1	6.574363000	1.741448000	-2.164397000
6	-2.030869000	6.555028000	1.257471000	6	5.941302000	2.881679000	1.558200000
1	-2.531066000	6.407600000	2.215317000	1	5.674885000	3.160405000	2.581372000
1	-6.742028922	2.043835531	2.005257592	1	-2.041753437	6.481511953	-1.893282657
1	-5.947850670	3.654912657	2.050769246	1	-2.956314581	6.112554613	-1.922865985
1	-0.136235882	6.928200841	2.234399196	1	-6.776531619	0.033187982	-2.092733448
1	1.640479570	6.706196111	2.274201264	1	-6.712039611	-0.948601346	-2.097799168
1	6.923566081	0.451941729	2.322927390	1	-2.058597721	-6.413724142	-1.972041737
1	6.589695988	2.219468092	2.334977322	1	-1.109753920	-6.672063400	-1.942260888
1	2.565086686	-6.536301443	2.118314483	1	5.585815838	-4.002908455	-1.732865675
1	4.127367415	-5.627389517	2.170442609	1	6.145654250	-3.176801721	-1.703632050
1	-5.430966906	-4.510303721	1.958398763	1	5.643212099	4.002408630	-1.676194375
1	-4.095094958	-5.730409721	1.973236727	1	4.977649470	4.752692373	-1.697812209
1	-1.641095695	-6.708282228	-2.271271161	1	6.775712148	-0.033085738	2.095992270
1	0.135757595	-6.929382433	-2.231925171	1	6.711400904	0.948498698	2.101105952
1	-6.923917725	-0.452464126	-2.320650885	1	2.058218587	6.413082030	1.976013773
1	-6.589156417	-2.219867725	-2.332424719	1	1.109494739	6.671311757	1.946242622
1	5.946496584	-3.654360356	-2.049180744	1	-5.585832666	4.002579176	1.736257207
1	6.740933705	-2.043508594	-2.003491324	1	-6.145619669	3.176661377	1.706970208
1	4.096046808	5.731119469	-1.970055379	1	-5.643189353	-4.001947877	1.679774770
1	5.431953841	4.510938874	-1.955409569	1	-4.977338289	-4.751625170	1.701539393
1	-4.126469084	5.625855138	-2.168846080	1	2.041696064	-6.481053005	1.897042763
1	-2.564388985	6.534868877	-2.116489053	1	2.956096096	-6.112156853	1.926507941
6	0.583206000	-3.035981000	1.762285000	6	0.495485000	-3.151356000	1.570713000
6	-0.872388000	-2.948260000	1.791671000	6	-0.954408000	-3.014877000	1.629683000
6	1.355759000	-2.134751000	2.504215000	6	1.312077000	-2.328398000	2.354292000
6	-1.498352000	-1.960538000	2.560234000	6	-1.531912000	-2.055826000	2.468012000
6	-2.650247000	-1.240596000	2.029173000	6	-2.663566000	-1.264580000	1.998541000
6	-1.369402000	-3.252911000	0.455771000	6	-1.478431000	-3.214365000	0.284657000
6	-2.472707000	-2.561606000	-0.054002000	6	-2.560768000	-2.457894000	-0.166054000
6	-3.126704000	-1.534118000	0.747354000	6	-3.162273000	-1.459754000	0.706457000
6	2.946883000	-1.901817000	0.625199000	6	2.874021000	-2.035035000	0.461393000
6	2.141516000	-2.840495000	-0.146964000	6	2.025882000	-2.894144000	-0.351182000
6	2.562818000	-1.555878000	1.924303000	6	2.528940000	-1.759260000	1.787055000
6	0.985265000	-3.397109000	0.408732000	6	0.862241000	-3.439732000	0.190899000
6	-0.221958000	-3.534756000	-0.398074000	6	-0.357529000	-3.482091000	-0.602491000
6	2.140722000	-2.396579000	-1.534827000	6	2.024024000	-2.374105000	-1.711910000
6	0.981588000	-2.526314000	-2.308442000	6	0.852581000	-2.417234000	-2.475827000
6	-0.223547000	-3.108733000	-1.729681000	6	-0.364027000	-2.986609000	-1.909706000
6	3.130046000	0.816435000	1.493957000	6	3.173127000	0.609513000	1.486161000
6	3.532923000	0.454659000	0.140298000	6	3.539125000	0.316177000	0.107006000
6	2.654717000	-0.168771000	2.366011000	6	2.678907000	-0.407246000	2.309832000
6	3.442494000	-0.875542000	-0.284322000	6	3.392606000	-0.978698000	-0.393908000
6	2.944505000	-1.182290000	-1.620088000	6	2.869709000	-1.187555000	-1.738555000
6	3.126638000	1.534981000	-0.751972000	6	3.162529000	1.459609000	-0.713022000
6	2.650240000	1.241496000	-2.033809000	6	2.663901000	1.264536000	-2.005143000
6	2.555031000	-0.145403000	-2.474873000	6	2.510107000	-0.088716000	-2.526238000
6	0.877807000	1.358563000	3.165257000	6	0.973534000	1.133420000	3.229454000
6	1.373232000	2.386832000	2.257395000	6	1.493324000	2.193578000	2.373757000
6	1.505543000	0.108868000	3.219745000	6	1.554950000	-0.139477000	3.199830000
6	2.475057000	2.118517000	1.437621000	6	2.569016000	1.934451000	1.518693000

6	2.472647000	2.562461000	0.049436000	6	2.561055000	2.457762000	0.159495000
6	0.223599000	3.109606000	1.725026000	6	0.364382000	2.986553000	1.903108000
6	0.221953000	3.535745000	0.393447000	6	0.357916000	3.482182000	0.595937000
6	1.369332000	3.253690000	-0.460452000	6	1.478759000	3.214253000	-0.291223000
6	-0.694026000	-1.020576000	3.330769000	6	-0.682592000	-1.193204000	3.280253000
6	-1.346728000	0.280622000	3.274561000	6	-1.286939000	0.131139000	3.311333000
6	0.702931000	-1.105056000	3.303381000	6	0.710028000	-1.326395000	3.225639000
6	-0.576538000	1.446004000	3.193678000	6	-0.475537000	1.271726000	3.287253000
6	-0.981591000	2.527216000	2.303802000	6	-0.852237000	2.417238000	2.469266000
6	-2.555048000	0.146287000	2.470222000	6	-2.509747000	0.088672000	2.519662000
6	-2.944528000	1.183212000	1.615462000	6	-2.869334000	1.187496000	1.731966000
6	-2.140740000	2.397528000	1.530216000	6	-2.023672000	2.374094000	1.705330000
6	-0.583252000	3.036829000	-1.766929000	6	-0.495114000	3.151319000	-1.577314000
6	-0.985261000	3.398035000	-0.413394000	6	-0.861860000	3.439786000	-0.197483000
6	-2.141422000	2.841316000	0.142284000	6	-2.025453000	2.894085000	0.344603000
6	-1.355775000	2.135594000	-2.508868000	6	-1.311702000	2.328316000	-2.360861000
6	0.694007000	1.021428000	-3.335429000	6	0.682942000	1.193163000	-3.286863000
6	1.498337000	1.961353000	-2.564874000	6	1.532245000	2.055775000	-2.474626000
6	0.872331000	2.949070000	-1.796340000	6	0.954753000	3.014816000	-1.636266000
6	-0.702948000	1.105918000	-3.308033000	6	-0.709682000	1.326332000	-3.232229000
6	-0.877828000	-1.357712000	-3.169883000	6	-0.973175000	-1.133452000	-3.235984000
6	0.576523000	-1.445136000	-3.198312000	6	0.475888000	-1.271750000	-3.293806000
6	1.346711000	-0.279753000	-3.279214000	6	1.287307000	-0.131182000	-3.317906000
6	-1.505550000	-0.108020000	-3.224383000	6	-1.554633000	0.139421000	-3.206448000
6	-3.130008000	-0.815593000	-1.498571000	6	-3.172748000	-0.609596000	-1.492724000
6	-2.475166000	-2.117767000	-1.442279000	6	-2.568686000	-1.934558000	-1.525264000
6	-1.373262000	-2.385994000	-2.261999000	6	-1.492991000	-2.193630000	-2.380363000
6	-2.654698000	0.169615000	-2.370633000	6	-2.678564000	0.407161000	-2.316428000
6	-2.946911000	1.902710000	-0.629830000	6	-2.873514000	2.034886000	-0.467955000
6	-3.442464000	0.876449000	0.279688000	6	-3.392176000	0.978611000	0.387347000
6	-3.532764000	-0.453746000	-0.144919000	6	-3.538768000	-0.316263000	-0.113562000
6	-2.562818000	1.556704000	-1.928921000	6	-2.528575000	1.759169000	-1.793645000

[10]NCPD>C₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-5.979540000	-2.873297000	0.914389000
6	-6.611602000	-0.696836000	0.931019000
6	-4.618876000	4.763175000	1.013351000
6	-2.719891000	6.000007000	1.049346000
6	3.121501000	5.801295000	1.120940000
6	4.911228000	4.406990000	1.126998000
6	6.563587000	-1.201459000	1.081181000
6	5.784422000	-3.333139000	1.052018000
6	0.890037000	-6.530319000	0.953295000
6	-1.376938000	-6.452959000	0.926346000
6	-3.516175000	-5.638675000	0.244993000
6	-4.662477000	-4.746246000	0.241522000
6	-4.911515000	-4.407291000	-1.127858000
6	-6.172338000	-2.494555000	-0.454190000
6	-6.583674000	-1.098888000	-0.443909000
6	-6.563868000	1.201758000	-1.081802000
6	-6.514698000	1.599813000	0.292504000
6	-6.021212000	2.965575000	0.310948000
6	-5.785056000	3.333635000	-1.052661000

[10]OCPD>C₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-6.394762000	-1.843212000	0.703914000
6	-6.640703000	0.352742000	0.688732000
6	-3.738921000	5.441669000	0.809292000
6	-1.733255000	6.366674000	0.888798000
6	3.979784000	5.184167000	1.130723000
6	5.484531000	3.572026000	1.203066000
6	6.131467000	-2.214141000	1.243930000
6	5.046305000	-4.133034000	1.198516000
6	-0.245693000	-6.560730000	0.987604000
6	-2.405428000	-6.111096000	0.895541000
6	-4.367442000	-4.969609000	0.223335000
6	-5.365121000	-3.910691000	0.174736000
6	-5.484915000	-3.572185000	-1.201437000
6	-6.457754000	-1.479997000	-0.669340000
6	-6.616157000	-0.034350000	-0.679261000
6	-6.131892000	2.214361000	-1.241278000
6	-6.101500000	2.593605000	0.130094000
6	-5.381144000	3.860106000	0.160043000
6	-5.046827000	4.133351000	-1.195960000

6	-4.317931000	5.082561000	-0.349817000	6	-3.375142000	5.677363000	-0.545444000
6	-3.097835000	5.873920000	-0.327446000	6	-2.056271000	6.287055000	-0.493242000
6	-0.889945000	6.530351000	-0.954215000	6	0.245395000	6.560677000	-0.985869000
6	-0.495112000	6.595850000	0.422049000	6	0.574677000	6.589176000	0.397752000
6	0.958440000	6.550585000	0.438941000	6	1.998104000	6.289107000	0.458077000
6	1.377078000	6.453287000	-0.927317000	6	2.405154000	6.110945000	-0.894099000
6	3.516335000	5.638854000	-0.245919000	6	4.367155000	4.969268000	-0.221990000
6	4.662488000	4.746185000	-0.242394000	6	5.364804000	3.910273000	-0.173196000
6	5.979812000	2.873384000	-0.915207000	6	6.395131000	1.843010000	-0.701853000
6	6.172337000	2.494577000	0.453380000	6	6.457548000	1.479950000	0.671442000
6	6.583958000	1.099052000	0.443143000	6	6.616086000	0.034363000	0.681635000
6	6.612333000	0.696997000	-0.931766000	6	6.641480000	-0.352935000	-0.686286000
6	6.515054000	-1.599673000	-0.293112000	6	6.101750000	-2.593629000	-0.127399000
6	6.021200000	-2.965353000	-0.311577000	6	5.381075000	-3.859996000	-0.157424000
6	4.619123000	-4.763154000	-1.014132000	6	3.739093000	-5.441814000	-0.806799000
6	4.317799000	-5.082273000	0.349008000	6	3.374983000	-5.677381000	0.547873000
6	3.097703000	-5.873503000	0.326538000	6	2.056077000	-6.286970000	0.495467000
6	2.720137000	-6.000178000	-1.050282000	6	1.733225000	-6.366415000	-0.886628000
6	1.438495000	-6.385612000	-1.439040000	6	0.441085000	-6.547341000	-1.365730000
1	1.138153000	-6.373473000	-2.489441000	1	0.222629000	-6.482103000	-2.432323000
6	2.188426000	-6.202775000	1.341756000	6	1.052006000	-6.435480000	1.467038000
1	2.438327000	-6.038000000	2.392701000	1	1.247197000	-6.295587000	2.530857000
6	-1.864416000	-6.285322000	-1.478703000	6	-2.826720000	-5.860935000	-1.505607000
1	-1.539109000	-6.298125000	-2.521613000	1	-2.514313000	-5.908571000	-2.549579000
6	-2.655153000	-6.026069000	1.282744000	6	-3.589488000	-5.487432000	1.271191000
1	-2.917627000	-5.837949000	2.326527000	1	-3.805573000	-5.267301000	2.317706000
6	5.491612000	-3.732296000	-1.359270000	6	4.749470000	-4.567515000	-1.194122000
1	5.631577000	-3.429400000	-2.399615000	1	4.915441000	-4.322112000	-2.244090000
6	4.963727000	-4.407502000	1.396717000	6	4.073002000	-5.044620000	1.587405000
1	4.696165000	-4.608220000	2.436906000	1	3.764346000	-5.133341000	2.629893000
6	6.632030000	0.137676000	1.464280000	6	6.402560000	-0.925402000	1.683619000
1	6.555549000	0.429769000	2.514160000	1	6.294835000	-0.655825000	2.734957000
6	6.602500000	-0.642268000	-1.314293000	6	6.415138000	-1.653357000	-1.123697000
1	6.507743000	-0.929426000	-2.363978000	1	6.318114000	-1.879445000	-2.186462000
6	5.692451000	3.309206000	1.489694000	6	6.038330000	2.383820000	1.660690000
1	5.793432000	3.002685000	2.533512000	1	5.987315000	2.108881000	2.714860000
6	5.258183000	4.010017000	-1.277062000	6	5.878211000	3.050073000	-1.157764000
1	5.024701000	4.226253000	-2.322473000	1	5.721850000	3.230602000	-2.222148000
6	2.655296000	6.026342000	-1.283669000	6	3.589025000	5.486960000	-1.269823000
1	2.917804000	5.838211000	-2.327445000	1	3.804970000	5.266831000	-2.316367000
6	1.864353000	6.285148000	1.477737000	6	2.826578000	5.861006000	1.507019000
1	1.538774000	6.297169000	2.520571000	1	2.514562000	5.909158000	2.551083000
6	-1.438235000	6.385295000	1.438119000	6	-0.441000000	6.547554000	1.367641000
1	-1.137886000	6.372749000	2.488509000	1	-0.222276000	6.482747000	2.434204000
6	-2.188404000	6.202990000	-1.342638000	6	-1.052407000	6.435510000	-1.465015000
1	-2.438420000	6.038561000	-2.393612000	1	-1.247833000	6.295085000	-2.528720000
6	-4.964349000	4.408022000	-1.397417000	6	-4.073412000	5.044815000	-1.584911000
1	-4.697310000	4.609086000	-2.437677000	1	-3.764851000	5.133536000	-2.627430000
6	-5.490999000	3.732103000	1.358578000	6	-4.749246000	4.567405000	1.196730000
1	-5.630028000	3.428638000	2.398880000	1	-4.915227000	4.322103000	2.246717000
6	-6.601633000	0.642383000	1.313642000	6	-6.414250000	1.653071000	1.126323000
1	-6.506388000	0.929413000	2.363317000	1	-6.317014000	1.878991000	2.189103000
6	-6.632348000	-0.137382000	-1.464960000	6	-6.403228000	0.925711000	-1.681113000
1	-6.556774000	-0.429379000	-2.514933000	1	-6.295871000	0.656254000	-2.732524000
6	-5.692662000	-3.309401000	-1.490476000	6	-6.038575000	-2.383782000	-1.658751000
6	0.495249000	-6.595950000	-0.422995000	6	-0.574790000	-6.589135000	-0.396068000

6	-0.958351000	-6.550504000	-0.439919000	6	-1.998220000	-6.289027000	-0.456614000
6	-3.121578000	-5.801427000	-1.121883000	6	-3.980154000	-5.184435000	-1.129378000
1	-5.793696000	-3.002901000	-2.534301000	1	-5.987910000	-2.108792000	-2.712926000
6	-5.257811000	-4.009858000	1.276209000	6	-5.877724000	-3.050314000	1.159508000
1	-5.023521000	-4.225551000	2.321554000	1	-5.720442000	-3.230635000	2.223797000
7	3.734068000	-5.458736000	-1.840062000	8	2.793634000	-5.958669000	-1.663237000
7	6.269174000	-2.312571000	1.871951000	8	5.600001000	-3.199500000	2.041016000
7	6.403995000	1.822220000	-1.728320000	8	6.622424000	0.751809000	-1.507643000
7	4.069368000	5.175835000	1.934259000	8	4.735453000	4.418420000	1.986622000
7	0.256980000	6.601903000	-1.746075000	8	1.372101000	6.390438000	-1.758147000
7	-3.733676000	5.458569000	1.839240000	8	-2.793521000	5.958829000	1.665586000
7	-6.270240000	2.313165000	-1.872545000	8	-5.600757000	3.199893000	-2.038404000
7	-6.403237000	-1.822020000	1.727562000	8	-6.621315000	-0.752077000	1.509952000
7	-4.069756000	-5.176278000	-1.935160000	8	-4.735976000	-4.418599000	-1.985180000
7	-0.256891000	-6.601393000	1.745121000	8	-1.372552000	-6.390574000	1.759697000
1	-0.256679000	-6.275655000	2.703114000	6	0.727415000	-3.159528000	1.451910000
1	3.550851000	-5.153286000	-2.787595000	6	-0.726657000	-3.129311000	1.517275000
1	5.972816000	-2.216950000	2.834516000	6	1.485304000	-2.313639000	2.266948000
1	6.091597000	1.738222000	-2.687211000	6	-1.369467000	-2.251442000	2.393412000
1	3.839236000	4.884644000	2.876151000	6	-2.554568000	-1.525589000	1.954203000
1	0.256816000	6.276262000	-2.704105000	6	-1.238913000	-3.315766000	0.166452000
1	-3.550436000	5.153044000	2.786742000	6	-2.373002000	-2.623514000	-0.255978000
1	-5.974304000	2.217769000	-2.835265000	6	-3.037920000	-1.705226000	0.655172000
1	-6.090573000	-1.738040000	2.686368000	6	3.012076000	-1.836885000	0.383270000
1	-3.839692000	-4.885071000	-2.877068000	6	2.225524000	-2.721082000	-0.463058000
6	0.098669000	-3.129261000	1.691525000	6	2.654044000	-1.637160000	1.719520000
6	-1.335660000	-2.900033000	1.567870000	6	1.106887000	-3.364395000	0.060705000
6	0.864559000	-2.332319000	2.549265000	6	-0.107113000	-3.464621000	-0.732734000
6	-1.952598000	-1.886327000	2.308683000	6	2.184350000	-2.154807000	-1.805067000
6	-2.966190000	-1.042015000	1.687291000	6	1.016243000	-2.253033000	-2.568713000
6	-1.701829000	-3.105268000	0.173429000	6	-0.154232000	-2.927546000	-2.021560000
6	-2.671598000	-2.300860000	-0.422259000	6	3.123237000	0.778431000	1.508643000
6	-3.313333000	-1.245215000	0.347443000	6	3.497366000	0.564083000	0.117079000
6	2.662950000	-2.189132000	0.858625000	6	2.710046000	-0.300475000	2.295712000
6	1.868838000	-3.022660000	-0.033791000	6	3.444671000	-0.714627000	-0.433635000
6	2.176118000	-1.854906000	2.125789000	6	2.941358000	-0.910937000	-1.787143000
6	0.613001000	-3.475890000	0.372633000	6	3.038064000	1.705320000	-0.658129000
6	-0.500065000	-3.463892000	-0.562219000	6	2.554709000	1.525733000	-1.957156000
6	2.065432000	-2.540791000	-1.394991000	6	2.499653000	0.188020000	-2.531558000
6	0.995018000	-2.536288000	-2.295825000	6	0.901181000	1.076985000	3.275263000
6	-0.315241000	-3.013574000	-1.871468000	6	1.339048000	2.201983000	2.458260000
6	3.002793000	0.461904000	1.856864000	6	1.572919000	-0.148386000	3.196539000
6	3.509512000	0.106771000	0.536869000	6	2.425284000	2.053210000	1.592118000
6	2.345289000	-0.498538000	2.633315000	6	2.373212000	2.623655000	0.253036000
6	3.348482000	-1.191346000	0.050622000	6	0.154310000	2.927636000	2.018482000
6	2.981420000	-1.408067000	-1.342665000	6	0.107270000	3.464704000	0.729602000
6	3.313187000	1.245026000	-0.346086000	6	1.239028000	3.315737000	-0.169585000
6	2.966006000	1.041836000	-1.685898000	6	-0.582215000	-1.362585000	3.238868000
6	2.792244000	-0.314002000	-2.193376000	6	-1.281246000	-0.087389000	3.321405000
6	0.640630000	1.167299000	3.303004000	6	0.815654000	-1.392903000	3.177893000
6	1.326792000	2.168985000	2.496063000	6	-0.554102000	1.108362000	3.339223000
6	1.139665000	-0.138997000	3.369809000	6	-1.016133000	2.253160000	2.565570000
6	2.482813000	1.821651000	1.786600000	6	-2.499535000	-0.187961000	2.528568000
6	2.671515000	2.300698000	0.423624000	6	-2.941320000	0.911035000	1.784181000
6	0.315084000	3.013423000	1.872863000	6	-2.184396000	2.155008000	1.802018000
6	0.499907000	3.463756000	0.563620000	6	-0.727318000	3.159455000	-1.454989000

6	1.701679000	3.105061000	-0.172009000	6	-1.106786000	3.364438000	-0.063754000
6	-1.153116000	-1.052785000	3.198143000	6	-2.225452000	2.721055000	0.459895000
6	-1.672104000	0.305880000	3.128791000	6	-1.485286000	2.313688000	-2.270087000
6	0.225019000	-1.271254000	3.316580000	6	0.582341000	1.362580000	-3.241949000
6	-0.793593000	1.394429000	3.181126000	6	1.369552000	2.251405000	-2.396487000
6	-0.995199000	2.536232000	2.297268000	6	0.726688000	3.129250000	-1.520368000
6	-2.792412000	0.313861000	2.194809000	6	-0.815564000	1.392970000	-3.181036000
6	-2.981590000	1.407921000	1.344081000	6	-0.901090000	-1.076950000	-3.278403000
6	-2.065568000	2.540680000	1.396360000	6	0.554156000	-1.108295000	-3.342334000
6	-0.098777000	3.129047000	-1.690166000	6	1.281372000	0.087455000	-3.324447000
6	-0.613108000	3.475744000	-0.371291000	6	-1.572808000	0.148438000	-3.199700000
6	-1.868958000	3.022498000	0.035137000	6	-3.122921000	-0.778429000	-1.511748000
6	-0.864633000	2.332099000	-2.547873000	6	-2.425269000	-2.053394000	-1.595214000
6	1.153057000	1.052669000	-3.196837000	6	-1.338942000	-2.201902000	-2.461328000
6	1.952544000	1.886254000	-2.307359000	6	-2.709961000	0.300474000	-2.298897000
6	1.335555000	2.899892000	-1.566456000	6	-3.011912000	1.836786000	-0.386379000
6	-0.225080000	1.271087000	-3.315244000	6	-3.444206000	0.714480000	0.430562000
6	-0.640740000	-1.167454000	-3.301659000	6	-3.497170000	-0.564152000	-0.120238000
6	0.793470000	-1.394541000	-3.179723000	6	-2.653951000	1.637107000	-1.722648000
6	1.672024000	-0.306022000	-3.127442000				
6	-1.139744000	0.138845000	-3.368455000				
6	-3.002803000	-0.462041000	-1.855462000				
6	-2.482910000	-1.821796000	-1.785216000				
6	-1.326899000	-2.169122000	-2.494703000				
6	-2.345333000	0.498384000	-2.631914000				
6	-2.663028000	2.188898000	-0.857229000				
6	-3.348564000	1.191159000	-0.049210000				
6	-3.509576000	-0.106935000	-0.535496000				
6	-2.176176000	1.854733000	-2.124396000				

[10]SCPP \supset C₆₀

Gas-phase. B3LYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	5.642581000	3.680330000	1.102075000
6	6.607641000	1.357603000	1.097349000
6	5.266429000	-4.225090000	1.108235000
6	3.334811000	-5.840108000	1.107223000
6	-2.401353000	-6.287504000	1.086573000
6	-4.539351000	-4.973704000	1.086366000
6	-6.712929000	0.333493000	1.091094000
6	-6.133271000	2.771899000	1.089190000
6	-1.758637000	6.463167000	1.090158000
6	0.740430000	6.672139000	1.096503000
6	2.909896000	6.109595000	0.235394000
6	4.153422000	5.351703000	0.235450000
6	4.539152000	4.973821000	-1.082534000
6	5.953733000	3.239488000	-0.214575000
6	6.507332000	1.893261000	-0.217355000
6	6.712697000	-0.333637000	-1.087764000
6	6.731919000	-0.877102000	0.228549000
6	6.394692000	-2.294864000	0.230387000
6	6.133168000	-2.772114000	-1.085856000
6	4.920207000	-4.642671000	-0.208021000
6	3.804898000	-5.573916000	-0.209278000
6	1.758395000	-6.463617000	-1.086226000

6	1.244507000	-6.636200000	0.231186000
6	-0.207840000	-6.751091000	0.226573000
6	-0.740694000	-6.672718000	-1.092420000
6	-2.910137000	-6.109791000	-0.231392000
6	-4.153531000	-5.351681000	-0.231567000
6	-5.642851000	-3.680583000	-1.098437000
6	-5.954102000	-3.239645000	0.218145000
6	-6.507775000	-1.893464000	0.220788000
6	-6.607977000	-1.357863000	-1.093944000
6	-6.731998000	0.876903000	-0.225244000
6	-6.394585000	2.294610000	-0.227084000
6	-5.266495000	4.225036000	-1.104808000
6	-4.920436000	4.642588000	0.211491000
6	-3.805062000	5.573712000	0.212885000
6	-3.335137000	5.840513000	-1.103535000
6	-2.076861000	6.393684000	-1.330327000
1	-1.691386000	6.501214000	-2.346015000
6	-3.032617000	5.955156000	1.318290000
1	-3.359535000	5.711066000	2.330944000
6	1.070913000	6.622603000	-1.319060000
1	0.678817000	6.639813000	-2.337554000
6	2.078855000	6.375155000	1.333118000
1	2.432039000	6.195577000	2.350494000
6	-6.026253000	3.079440000	-1.330686000
1	-6.199004000	2.717648000	-2.346215000
6	-5.428339000	3.949115000	1.316818000
1	-5.142829000	4.241142000	2.329203000
6	-6.633600000	-1.035849000	1.322485000
1	-6.521984000	-1.418501000	2.338377000
6	-6.752716000	0.007685000	-1.324673000
1	-6.725899000	0.402128000	-2.342129000
6	-5.452280000	-3.949033000	1.318829000
1	-5.658285000	-3.609186000	2.335305000
6	-4.777314000	-4.746408000	-1.331513000
1	-4.476930000	-5.004750000	-2.348702000
6	-2.079105000	-6.375675000	-1.329056000
1	-2.432281000	-6.196266000	-2.346466000
6	-1.071066000	-6.622282000	1.323112000
1	-0.679060000	-6.639390000	2.341646000
6	2.076597000	-6.393266000	1.334218000
1	1.691104000	-6.500311000	2.349951000
6	3.032356000	-5.955605000	-1.314538000
1	3.359252000	-5.711826000	-2.327276000
6	5.428048000	-3.949250000	-1.313407000
1	5.142218000	-4.241150000	-2.325738000
6	6.026409000	-3.079637000	1.334034000
1	6.199403000	-2.717899000	2.349540000
6	6.752549000	-0.007939000	1.328016000
1	6.725893000	-0.402421000	2.345461000
6	6.633207000	1.035717000	-1.319111000
1	6.521380000	1.418394000	-2.334966000
6	5.451983000	3.949091000	-1.315158000
6	-1.244727000	6.636105000	-0.227210000
6	0.207645000	6.750958000	-0.222495000
6	2.401182000	6.287711000	-1.082536000
1	5.657878000	3.609316000	-2.331677000

6	4.777168000	4.746216000	1.335307000
1	4.477011000	5.004628000	2.352547000
16	-4.367422000	5.112329000	-2.344831000
16	-6.493136000	1.571401000	2.331962000
16	-6.198304000	-2.546717000	-2.337083000
16	-3.522253000	-5.717085000	2.327098000
16	0.520525000	-6.664694000	-2.330671000
16	4.367291000	-5.112094000	2.348387000
16	6.493027000	-1.571599000	-2.328645000
16	6.198182000	2.546391000	2.340585000
16	3.522101000	5.717471000	-2.323142000
16	-0.520806000	6.663633000	2.334706000
6	0.153501000	-3.209181000	1.528650000
6	-1.281584000	-3.034445000	1.340333000
6	0.836803000	-2.425702000	2.463682000
6	-1.979065000	-2.088012000	2.096328000
6	-2.994816000	-1.254489000	1.464922000
6	-1.570102000	-3.187400000	-0.078795000
6	-2.542859000	-2.389006000	-0.685545000
6	-3.267075000	-1.401487000	0.101159000
6	2.714163000	-2.120386000	0.884209000
6	2.003979000	-2.937063000	-0.089993000
6	2.145339000	-1.872257000	2.137071000
6	0.750226000	-3.466106000	0.223819000
6	-0.315248000	-3.454485000	-0.767609000
6	2.247694000	-2.374514000	-1.412868000
6	1.223861000	-2.365064000	-2.365441000
6	-0.083686000	-2.919690000	-2.037898000
6	2.880746000	0.488758000	2.033015000
6	3.473251000	0.226420000	0.727436000
6	2.228406000	-0.539311000	2.721868000
6	3.394015000	-1.051031000	0.165512000
6	3.106874000	-1.207246000	-1.254084000
6	3.267419000	1.401725000	-0.106660000
6	2.995089000	1.254663000	-1.470411000
6	2.910576000	-0.077920000	-2.055077000
6	0.417879000	1.014699000	3.381027000
6	1.098834000	2.086027000	2.664306000
6	0.970767000	-0.270143000	3.408374000
6	2.304865000	1.827736000	2.003688000
6	2.543305000	2.389351000	0.680090000
6	0.084010000	2.919928000	2.032415000
6	0.315584000	3.454622000	0.762090000
6	1.570460000	3.187636000	0.073287000
6	-1.265993000	-1.269831000	3.068782000
6	-1.842300000	0.068045000	3.041667000
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6	-1.223559000	2.365294000	2.359955000
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6	-0.153176000	3.209414000	-1.534160000
6	-0.749904000	3.466297000	-0.229322000
6	-2.003605000	2.937158000	0.084526000
6	-0.836439000	2.425912000	-2.469229000

6	1.266313000	1.270061000	-3.074345000
6	1.979328000	2.088189000	-2.101831000
6	1.281916000	3.034660000	-1.345835000
6	-0.111172000	1.435919000	-3.254910000
6	-0.417556000	-1.014522000	-3.386614000
6	1.017091000	-1.187402000	-3.199391000
6	1.842574000	-0.067835000	-3.047181000
6	-0.970426000	0.270330000	-3.413968000
6	-2.880400000	-0.488548000	-2.038549000
6	-2.304506000	-1.827494000	-2.009186000
6	-1.098518000	-2.085848000	-2.669887000
6	-2.228036000	0.539501000	-2.727388000
6	-2.713661000	2.120419000	-0.889677000
6	-3.393701000	1.051195000	-0.171036000
6	-3.473043000	-0.226239000	-0.733015000
6	-2.144878000	1.872382000	-2.142544000

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