

Supporting information for:

Nitrogen-embedded molecular bowls as electron donors in photoinduced electron transfer reactions

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Abstract

In recent years, the chemistry of curved π -conjugated molecules has experienced a sharp rise. The inclusion of a heteroatom in the carbon network significantly affects its semiconducting properties. In this work, we computationally study the photoinduced electron transfer in a series of C60 fullerene complexes with experimentally established nitrogen-doped molecular bowls. Our results demonstrate that introducing nitrogen into pentagonal rings of the bowl-shaped π -conjugated molecules and extending the π -conjugation can modulate their electron-transfer properties. Among the studied complexes, the hub-NCor \supset C60 complex exhibits the most desirable combination of ultrafast charge separation and slow charge recombination, suggesting its potential use in photovoltaics.

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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 using the Becke–Johnson damping.^{6,7} Vertical excitation energies were calculated using TDA formalism⁸ with the range-separated functional from Handy and coworkers' CAM-B3LYP⁹ and Ahlrichs' 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} Löwdin,¹³ Hirshfeld,¹⁴ CM5,¹⁵ and iterative Hirshfeld¹⁶ charges. The formation energy of the complexes was computed using B3LYP functional coupled with def2-TZVP basis¹⁷ (B3LYP(D3BJ)/def2-TZVP//B3LYP(D3BJ)/def2-SVP). Canonical energy decomposition analysis (EDA) was performed using the Amsterdam Density Functional (ADF) program.¹⁸ The excited states have been analyzed in terms of the natural transition orbitals (NTO) concept introduced by Luzanov *et al.*¹⁹ and implemented within modern many-body codes by Head-Gordon *et al.*²⁰ Molecular structures and frontier molecular orbitals were visualized by Chemcraft 1.8. program.²¹

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)²²⁻²⁴ 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:

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} \quad (1)$$

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 (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.^{25,26}

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.²⁷⁻²⁹ 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^* constructed as a superposition of singly excited configurations (where an occupied MO ψ_i is replaced a virtual MO ψ_a) is computed,

$$T_{\alpha\beta}^{0i} = \sum_{ia} A_{i \rightarrow a} {}^{\lambda}C_{\alpha i} {}^{\lambda}C_{\beta a} \quad (2)$$

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

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

$$\Omega(D, A) = \sum_{\alpha \in D, \beta \in A} (T_{\alpha\beta}^{0i})^2 \quad (3)$$

The weights of local excitations on D and A are $\Omega(D, D)$ and $\Omega(A, A)$. The weight of electron transfer configurations $D \rightarrow A$ and $A \rightarrow D$ is 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

$$\Delta q(CS) = \sum \Omega(D, A) - \Omega(A, D) \quad (4)$$

$$\Delta q(CT) = \sum \Omega(D, A) + \Omega(A, D) \quad (5)$$

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 model³⁰⁻³³ in the monopole approximation:

$$E_s^{eq}(Q, \epsilon) = -\frac{1}{2} f(\epsilon) Q^+ D Q \quad (6)$$

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.^{30,34} The GEPOL93 scheme³⁵ 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:

$$q_X^i = q_X^0 + \Delta_X^i, \quad \Delta_X^i = \sum_{Y \neq X} \sum_{\alpha \in X, \beta \in Y} (T_{\alpha\beta}^{0i} T_{\alpha\beta}^{0i} - T_{\beta\alpha}^{0i} T_{\beta\alpha}^{0i}), \quad (7)$$

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:³⁶

$$E_s^{neq}(Q^0, \Delta, \epsilon, n^2) = f(\epsilon)\Delta^+ D Q^0 - \frac{1}{2} f(n^2)\Delta^+ D \Delta, \quad (8)$$

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. (7). By definition, the external (solvent) reorganization energy is the difference of the non-equilibrium (Eq. 8) and equilibrium (Eq. 6) 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):

$$k_{ET} = \frac{2\pi}{\hbar} V^2 (FCWD) \quad (9)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:³⁷

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (10)$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD)^{38,39} 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^{40,41} 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,

$$k = \sum_{n=0}^{\infty} k_{0 \rightarrow n}, \text{ where } k_{0 \rightarrow n} = \frac{2\pi}{\hbar} V_{0 \rightarrow n}^2 \frac{1}{\sqrt{4\pi\lambda_s kT}} \exp\left[-\frac{(\Delta G + n\hbar\omega_i + \lambda_s)^2}{4\lambda_s kT}\right] \quad (11)$$

with

$$V_{0 \rightarrow n}^2 = V^2 \frac{S^n}{n!} \exp(-S) \quad (12)$$

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 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.

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

$$\begin{aligned}\lambda_i^1(C_{60}^* \rightarrow C_{60}^-) &= \frac{1}{2} \left[\left((C_{60}^*)_- - (C_{60}^*)_+ \right) + \left((C_{60}^-)_+ - (C_{60}^-)_- \right) \right] \\ \lambda_i^2(Bowl^0 \rightarrow Bowl^+) &= \frac{1}{2} \left[\left((Bowl^0)_+ - (Bowl^0)_0 \right) + \left((Bowl^+)_0 - (Bowl^+)_+ \right) \right]\end{aligned}$$

Activation energy

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

$$\Delta G^* = (\lambda + \Delta G^0)^2 / 4\lambda \quad (13)$$

Interaction energies

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

$$E_{int} = E_{Host \supset C_{60}} - (E_{Host} + E_{C_{60}}) \quad (14)$$

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.^{42,43} 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.⁴⁴⁻⁴⁶ The AIMALL suite of programs⁴⁷ 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 method⁴⁸⁻⁵⁰ relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s), defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \quad (15)$$

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.⁵¹

Table S1. HOMO/LUMO energies and HOMO-LUMO (HL) gap (in eV) for isolated bowls in equilibrium geometry and their complexes with fullerene computed at CAM-B3LYP-D3(BJ)/def2-SVP//B3LYP-D3(BJ)/def2-SVP level of theory.

System	Energy		
	HOMO	LUMO	HL gap ^[a]
Bowl			
Cor	-7.57	-0.77	6.80
<i>rim</i> -NCor	-7.24	-1.10	6.13
<i>hub</i> -NCor	-6.16	-0.81	5.34
PP-bowl	-5.81	-0.69	5.12
Hyd-bowl	-5.98	-0.82	5.16
Cyc-bowl	-7.14	-0.32	6.82
<i>rim</i> -3NSum	-7.82	-0.69	7.13
Sum	-6.98	0.12	7.10
Bowl\supsetC₆₀			
Cor \supset C ₆₀	-7.31	-2.56	4.75
<i>rim</i> -NCor \supset C ₆₀	-7.28	-2.51	4.77
<i>hub</i> -NCor \supset C ₆₀	-6.29	-2.47	3.82
PP-bowl \supset C ₆₀	-5.97	-2.416	3.56
Hyd-bowl \supset C ₆₀	-6.14	-2.50	3.65
Cyc-bowl \supset C ₆₀	-7.13	-2.54	4.59
<i>rim</i> -3NSum \supset C ₆₀	-7.43	-2.63	4.80
Sum \supset C ₆₀	-7.04	-2.61	4.43

^[a] The HL= E_{LUMO}-E_{HOMO}

Table S2. Charge separation (units are electrons) between the fragments in electronic ground state for Cor \supset C₆₀, *rim*-NCor \supset C₆₀, *hub*-NCor \supset C₆₀, PP-bowl \supset C₆₀, Hyd-bowl \supset C₆₀, Cyc-bowl \supset C₆₀, *rim*-3NSum \supset C₆₀, and Sum \supset C₆₀ complexes. Q_{Bowl} - charge on host, and $Q_{C_{60}}$ - charge on fullerene moiety. Total charge of the complexes $Q_{Tot} = 0$.

	Mulliken	Löwdin	Hirshfeld	CM5	Hirshfeld-Iter
Cor\supsetC₆₀					
Q_{Bowl}	0.028	0.025	-0.001	0.002	-0.070
$Q_{C_{60}}$	-0.028	-0.025	0.001	-0.002	0.070
<i>rim</i>-NCor\supsetC₆₀					
Q_{Bowl}	0.026	0.026	-0.002	-0.001	-0.082
$Q_{C_{60}}$	-0.026	-0.026	0.001	0.000	0.081
<i>hub</i>-NCor\supsetC₆₀					
Q_{Bowl}	0.025	0.035	0.004	0.005	-0.088

$Q_{C_{60}}$	-0.025	-0.035	-0.004	-0.005	0.088
PP-bowl\supsetC₆₀					
Q_{Bowl}	0.025	0.037	0.007	0.004	-0.082
$Q_{C_{60}}$	-0.025	-0.037	-0.007	-0.004	0.082
Hyd-bowl\supsetC₆₀					
Q_{Bowl}	0.030	0.038	0.016	0.015	-0.059
$Q_{C_{60}}$	-0.030	-0.038	-0.015	-0.015	0.060
Cyc-bowl\supsetC₆₀					
Q_{Bowl}	0.034	0.034	0.006	0.009	-0.065
$Q_{C_{60}}$	-0.034	-0.034	-0.007	-0.009	0.065
rim-3NSum\supsetC₆₀					
Q_{Bowl}	0.020	0.000	-0.073	-0.071	-0.167
$Q_{C_{60}}$	-0.020	0.000	0.073	0.071	0.167
Sum\supsetC₆₀					
Q_{Bowl}	0.019	0.006	-0.061	-0.052	-0.141
$Q_{C_{60}}$	-0.019	-0.006	0.061	0.053	0.141

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 the non-covalent interactions between the fragments in **Cor \supset C₆₀**, **rim-NCor \supset C₆₀**, **hub-NCor \supset C₆₀**, **PP-bowl \supset C₆₀**, **Hyd-bowl \supset C₆₀**, **Cyc-bowl \supset C₆₀**, **rim-3NSum \supset C₆₀**, and **Sum \supset C₆₀** complexes computed in the gas phase.

Bond critical points	Interaction	$\rho(r)$, au	$\nabla^2\rho(r)$, au	$V(r)$, au	$G(r)$, au	$H(r)$, au
Cor\supsetC₆₀						
Cor\cdots C₆₀	$\pi\cdots\pi$ C \cdots C	7.54E-03	2.31E-02	-3.76E-03	4.77E-03	1.01E-03
		7.59E-03	2.37E-02	-3.85E-03	4.89E-03	1.04E-03
		8.11E-03	2.43E-02	-4.07E-03	5.07E-03	9.99E-04
		7.70E-03	2.29E-02	-3.75E-03	4.74E-03	9.91E-04
		8.11E-03	2.34E-02	-3.96E-03	4.90E-03	9.40E-04
		7.13E-03	2.08E-02	-3.35E-03	4.28E-03	9.25E-04
		7.84E-03	2.13E-02	-3.59E-03	4.46E-03	8.65E-04
rim-NCor\supsetC₆₀						
rim-NCor\cdots C₆₀	$\pi\cdots\pi$ C \cdots C	9.35E-03	2.80E-02	-4.37E-03	5.68E-03	1.31E-03
		7.39E-03	2.12E-02	-3.74E-03	4.52E-03	7.85E-04
		9.40E-03	2.88E-02	-4.41E-03	5.80E-03	1.39E-03
		7.84E-03	2.25E-02	-3.52E-03	4.57E-03	1.05E-03
		9.34E-03	2.82E-02	-4.45E-03	5.75E-03	1.30E-03
		8.66E-03	2.62E-02	-4.08E-03	5.31E-03	1.23E-03

		7.07E-03	2.13E-02	-3.27E-03	4.29E-03	1.02E-03
<i>hub-NCor</i> ⊃ C ₆₀						
<i>hub-NCor</i> … C ₆₀	π…π C…C	5.90E-03 7.31E-03 8.22E-03 7.79E-03 7.24E-03 6.87E-03 9.29E-03 7.71E-03 9.27E-03 6.59E-03 6.71E-03	1.54E-02 2.09E-02 2.40E-02 2.30E-02 2.01E-02 1.98E-02 2.83E-02 2.27E-02 2.81E-02 1.76E-02 1.83E-02	-2.53E-03 -3.35E-03 -3.85E-03 -3.61E-03 -3.18E-03 -3.46E-03 -4.41E-03 -3.62E-03 -4.31E-03 -2.83E-03 -2.93E-03	3.18E-03 4.28E-03 4.93E-03 4.68E-03 4.10E-03 4.21E-03 5.74E-03 4.65E-03 5.67E-03 3.61E-03 3.76E-03	6.58E-04 9.37E-04 1.08E-03 1.06E-03 9.19E-04 7.47E-04 1.33E-03 1.03E-03 1.36E-03 7.82E-04 8.26E-04
PP-bowl ⊃ C ₆₀						
<i>PP-bowl</i> … C ₆₀	π…π C…C	9.06E-03 1.12E-02 6.55E-03 8.46E-03 7.51E-03 8.72E-03 8.65E-03 4.77E-03	2.73E-02 3.37E-02 1.85E-02 2.63E-02 2.16E-02 2.55E-02 2.65E-02 1.23E-02	-4.31E-03 -5.49E-03 -2.92E-03 -4.31E-03 -3.38E-03 -4.02E-03 -4.24E-03 -2.10E-03	5.57E-03 6.96E-03 3.77E-03 5.44E-03 4.39E-03 5.20E-03 5.44E-03 2.59E-03	1.26E-03 1.47E-03 8.56E-04 1.13E-03 1.01E-03 1.18E-03 1.19E-03 4.92E-04
Hyd-bowl ⊃ C ₆₀						
<i>Hyd-bowl</i> … C ₆₀	π…π C…C	6.15E-03 8.10E-03 9.20E-03 7.58E-03 9.46E-03 8.52E-03 7.43E-03 6.18E-03	1.57E-02 2.36E-02 2.71E-02 2.20E-02 2.80E-02 2.39E-02 2.06E-02 1.64E-02	-2.60E-03 -3.73E-03 -4.30E-03 -3.50E-03 -4.39E-03 -3.93E-03 -3.22E-03 -2.65E-03	3.27E-03 4.81E-03 5.54E-03 4.50E-03 5.70E-03 4.96E-03 4.18E-03 3.38E-03	6.66E-04 1.08E-03 1.24E-03 9.99E-04 1.31E-03 1.03E-03 9.68E-04 7.32E-04
Cyc-bowl ⊃ C ₆₀						
<i>Cyc-bowl</i> … C ₆₀	π…π C…C	9.21E-03 7.50E-03 8.33E-03 6.59E-03 7.35E-03 7.86E-03	2.61E-02 2.06E-02 2.31E-02 1.84E-02 2.10E-02 2.24E-02	-4.06E-03 -3.33E-03 -3.55E-03 -3.05E-03 -3.22E-03 -3.48E-03	5.29E-03 4.24E-03 4.67E-03 3.82E-03 4.24E-03 4.54E-03	1.23E-03 9.10E-04 1.12E-03 7.72E-04 1.01E-03 1.06E-03
rim-3NSum ⊃ C ₆₀						
<i>rim-3NSum</i> … C ₆₀	π…π C…C	5.32E-03 8.00E-03	1.35E-02 2.39E-02	-2.38E-03 -3.49E-03	2.88E-03 4.73E-03	5.01E-04 1.24E-03
	π…π N…C	7.66E-03 9.07E-03 7.73E-03	2.20E-02 2.65E-02 2.22E-02	-3.87E-03 -4.62E-03 -3.84E-03	4.69E-03 5.62E-03 4.69E-03	8.18E-04 9.98E-04 8.49E-04

	CH···π H···C	7.83E-03 7.99E-03 5.02E-03	2.45E-02 2.61E-02 1.84E-02	-3.84E-03 -3.94E-03 -2.40E-03	4.98E-03 5.23E-03 3.50E-03	1.14E-03 1.29E-03 1.10E-03
		Sum ΣC_{60}				
Sum ... C_{60}	$\pi^{...}\pi$ $C^{...}C$	9.06E-03 5.48E-03 8.41E-03 9.08E-03 8.61E-03	2.56E-02 1.82E-02 2.40E-02 2.53E-02 2.39E-02	-4.51E-03 -2.67E-03 -4.16E-03 -4.48E-03 -4.16E-03	5.46E-03 3.61E-03 5.07E-03 5.40E-03 5.07E-03	9.46E-04 9.40E-04 9.18E-04 9.16E-04 9.09E-04
		CH···π H···C	7.30E-03 7.79E-03	2.17E-02 2.32E-02	-3.64E-03 -3.90E-03	4.54E-03 4.85E-03
						8.98E-04 9.45E-04

Table S4. Main contributions of the Kohn-Sham molecular orbitals to the corresponding occupied (Occ) and vacant (Vac) natural transition orbitals.

	Supramolecular host-guest systems $Bowl \supset C_{60}$							
	Cor	rim-NCor	hub-NCor	PP-bowl	Hyd-bowl	Cyc-bowl	rim-NSum	Sum
LE ₁ (Fullerene C_{60})								
Occ	H(0.75) H-1(0.37)	H-1(0.54) H-2(0.62)	H-2(0.89) H-3(0.34)	H-3(0.76) H-4(0.58)	H-1(0.97) H-2(0.16)	H-1(0.65) H-2(0.51)	H(0.88) H-2(0.36)	H(0.49) H-4(0.64)
	Vac	L(0.58) L+1(0.81)	L(0.61) L+1(0.79)	L+1(0.58) L+2(0.71)	L(0.56) L+1(0.66)	L(0.66) L+1(0.55)	L(0.58) L+1(0.81)	L(0.95) L+2(0.29)
LE ₂ (Bowl)								
Occ	H-6(0.85) H-7(0.38)	H-3(0.37) H-5(0.74)	H(0.98) H-1(0.14)	H (0.98) H-1(0.15)	H(0.997)	H 0.89) H-5(0.43)	H-1(0.17) H-5(0.95)	H(0.94) H-1(0.26)
	Vac	L+6(0.72) L+7(0.58)	L+3(0.86) L+6(0.49)	L+6(0.84) L+7(0.37)	L+6(0.29) L+7(0.92)	L+3(0.20) L+7(0.97)	L+5(0.19) L+6(0.95)	L+6(0.97) L+7(0.17)
CT (Bowl → Fullerene C_{60})								
Occ	H-5(0.25) H-6(0.95)	H-3(0.34) H-5(0.86)	H(0.96) H-2(0.19)	H(0.999)	H(0.996)	H (0.64) H-5(0.74)	H-5(0.57) H-6(0.81)	H(0.38) H-1(0.85)
	Vac	L(0.93) L+1(0.30)	L+2(0.97) L+5(0.22)	L(0.20) L+1(0.95)	L(0.53) L+1(0.80)	L+1(0.21) L+2(0.94)	L+1(0.95) L+4(0.19)	L(0.95) L+2(0.31)

Table S5. Excitation energies (E_x , eV), main singly excited configuration (HOMO(H)-LUMO(L)) and its weight (W), oscillator strength (f), extent of charge transfer (CT, e) or localization of exciton (X) computed for **Cor \supset C₆₀**, **rim-NCor \supset C₆₀**, **hub-NCor \supset C₆₀**, **PP-bowl \supset C₆₀**, **Hyd-bowl \supset C₆₀**, **Cyc-bowl \supset C₆₀**, **rim-3NSum \supset C₆₀**, and **Sum \supset C₆₀** complexes in DCM.

	Supramolecular host-guest systems Bowl \supset C ₆₀							
	Cor	rim-NCor	hub-NCor	PP-bowl	Hyd-bowl	Cyc-bowl	rim-NSum	Sum
	LE ₁ (Fullerene C ₆₀)							
Ex	2.555	2.567	2.563	2.565	2.553	2.550	2.568	2.556
Trans. (W)	H-L (0.26)	H-L+2 (0.25)	H-2-L+2 (0.41)	H-3-L+2 (0.19)	H-1-L (0.28)	H-2-L (0.29)	H-L (0.42)	H-1-L (0.18)
f	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
X	0.976	0.977	0.923	0.958	0.967	0.973	0.980	0.953
	LE ₂ (Bowl)							
Ex	3.994	3.849	3.282	3.020	3.329	4.147 ^[a]	4.181	4.143
Trans. (W)	H-6-L+6 (0.35)	H-5-L+3 (0.30)	H-L+6 (0.47)	H-L+7 (0.74)	H-L+7 (0.90)	H-5-L+6 (0.32)	H-5-L+6 (0.41)	H-L+7 (0.24)
f	<0.001	0.029	0.187	0.003	0.001	0.030	0.025	0.038
X	0.799	0.796	0.924	0.920	0.955	0.508	0.831	0.633
	Most absorptive transition							
Ex	4.390	4.381	4.392	4.410	4.409	4.370	4.396	4.394
Trans. (W)	H-L+5 (0.24)	H-1-L+5 (0.18)	H-1-L+6 (0.23)	H-1-L+4 (0.18)	H-1-L+5 (0.17)	H-4-L+3 (0.18)	H-2-L+3 (0.23)	H-2-L+3 (0.20)
f	0.806	0.489	0.671	0.688	0.823	0.863	0.847	0.748
Localiz.	C₆₀	C₆₀	C₆₀	C₆₀	C₆₀	C₆₀	C₆₀	C₆₀
X	0.946	0.842	0.819	0.847	0.899	0.956	0.950	0.953
	CT (Bowl \rightarrow Fullerene C ₆₀)							
Ex	3.207	2.863	1.965	1.623	1.635	2.810	3.304	2.590
Trans. (W)	H-6-L (0.72)	H-5-L+2 (0.82)	H-L+2 (0.73)	H-L+1 (0.70)	H-L+2 (0.86)	H-5-L+1 (0.53)	H-6-L+2 (0.34)	H-L (0.29)
f	0.001	0.004	0.010	<0.001	0.023	<0.001	0.008	0.001
CT	0.889	0.962	0.831	0.965	0.908	0.801	0.823	0.896

^[a] LE₂ state is partially delocalized over C₆₀ unit

Table S6. 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 DCM solvation energies (E_{solv} , eV) calculated for **Cor \supset C₆₀**, **rim-NCor \supset C₆₀**, **hub-NCor \supset C₆₀**, **PP-bowl \supset C₆₀**, **Hyd-bowl \supset C₆₀**, **Cyc-bowl \supset C₆₀**, **rim-3NSum \supset C₆₀**, and **Sum \supset C₆₀** complexes.

	Supramolecular host-guest systems Bowl \supset C ₆₀							
	Cor	rim-NCor	hub-NCor	PP-bowl	Hyd-bowl	Cyc-bowl	rim-NSum	Sum
	Ground state (GS)							
E _x	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
μ_0	0.40	1.86	1.16	0.23	0.21	0.89	0.74	0.99
E _{solv}	-0.161	-0.225	-0.220	-0.276	-0.180	-0.156	-0.261	-0.155

	LE ₁ (Fullerene C ₆₀)							
E _x	2.555	2.567	2.563	2.565	2.553	2.550	2.568	2.556
Δμ	1.01	1.14	1.75	1.81	1.16	1.31	0.38	2.14
E _{solv}	-0.167	-0.228	-0.220	-0.271	-0.184	-0.157	-0.259	-0.151
	LE ₂ (Bowl)							
E _x	3.994	3.849	3.282	3.020	3.329	4.147	4.181	4.143
Δμ	3.89	1.11	3.1	3.06	1.19	2.49	1.56	1.61
E _{solv}	-0.143	-0.259	-0.183	-0.240	-0.135	-0.161	-0.251	-0.155
	Most absorptive transition							
E _x	4.390	4.381	4.392	4.410	4.409	4.370	4.396	4.394
Δμ	0.36	1.11	2.82	4.30	1.04	3.06	1.19	6.48
E _{solv}	-0.164	-0.235	-0.216	-0.265	-0.175	-0.155	-0.255	-0.150
	CT (Bowl → Fullerene C ₆₀)							
E _x	3.207	2.863	1.965	1.623	1.635	2.810	3.304	2.590
Δμ	24.81	23.26	21.36	26.36	25.05	21.35	25.1	24.93
E _{solv}	-0.789	-0.775	-0.565	-0.731	-0.665	-0.560	-0.870	-0.702

Table S7. Computed semi-classical rates (k_x in s⁻¹) and characteristic times (τ in ns/ps) for the charge separation processes in **Cor**⊸C₆₀, **Sum**⊸C₆₀ and **hub-N**Cor⊸C₆₀, complexes in DCM solution using different effective Huang-Rhys (S_{eff}) factors.

$\hbar\omega_{eff}$	ΔG^0 , eV	$ V $, eV	λ_s	λ_i	S_{eff}	k_x , s ⁻¹	τ
	Cor ⊸C ₆₀ (LE ₁ ^{Guest} → CT)						
1200	0.652	9.35·10 ⁻³	0.413	0.170	1.143	5.67·10 ⁰	n/a
1400					0.979	5.67·10 ⁰	
1600					0.857	5.67·10 ⁰	
1800					0.762	5.67·10 ⁰	
2000					0.686	5.67·10 ⁰	
Sum ⊸C ₆₀ (LE ₁ ^{Guest} → CT)							
1200	0.034	1.96·10 ⁻³	0.410	0.166	1.116	9.46·10 ⁸	1.06 ns
1400					0.956	9.41·10 ⁸	1.06 ns
1600					0.837	9.39·10 ⁸	1.07 ns
1800					0.744	9.38·10 ⁸	1.07 ns
2000					0.669	9.37·10 ⁸	1.07 ns
hub-N Cor⊸C ₆₀ (LE ₁ ^{Guest} → CT)							
1200	-0.598	1.98·10 ⁻³	0.246	0.165	1.109	4.31·10 ¹²	0.23 ps
1400					0.951	4.16·10 ¹²	0.24 ps
1600					0.832	3.99·10 ¹²	0.25 ps
1800					0.739	3.84·10 ¹²	0.26 ps
2000					0.665	3.80·10 ¹²	0.26 ps

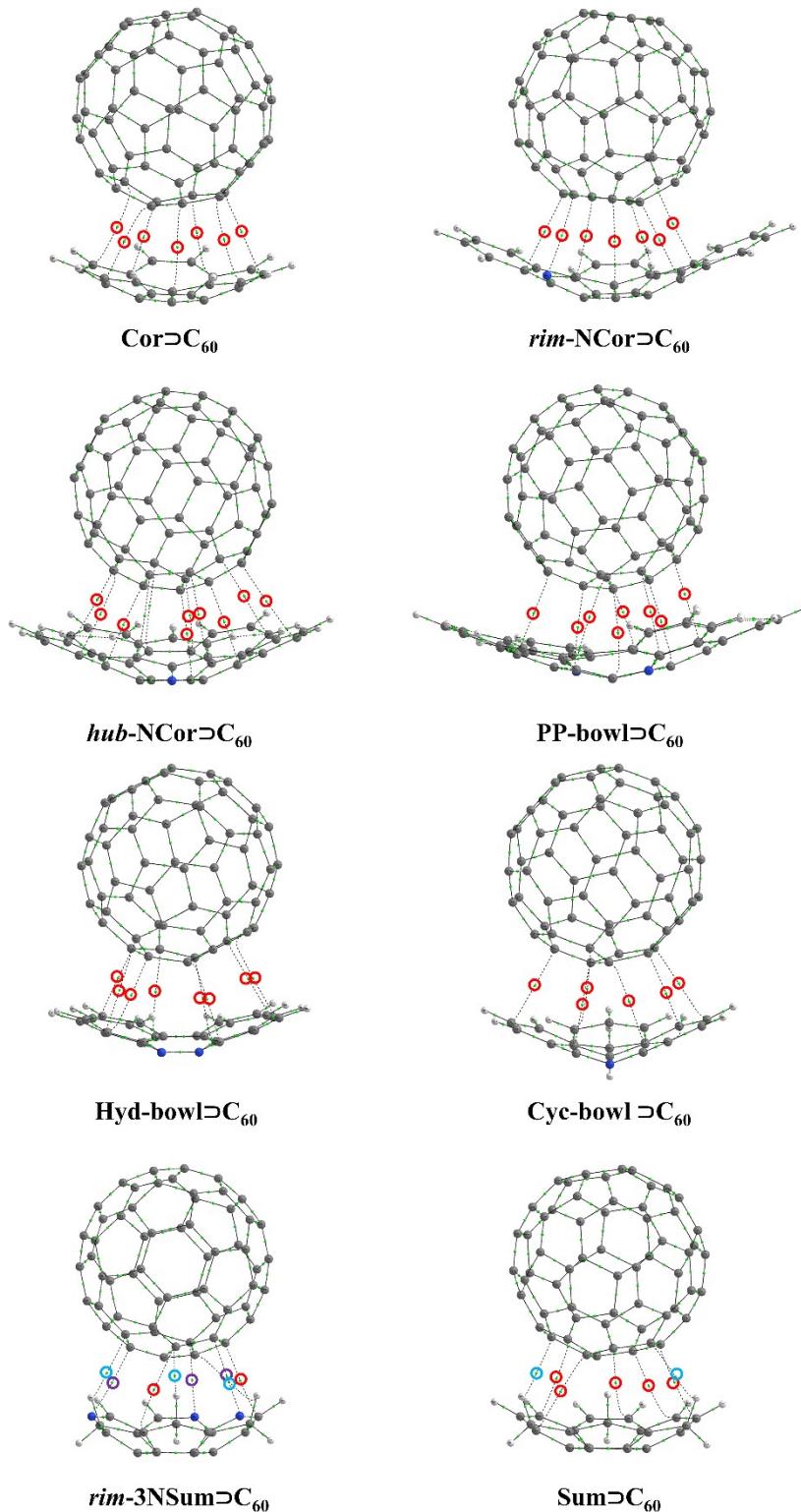


Figure S1. QTAIM molecular graph for **Cor>C₆₀**, **rim-NCor>C₆₀**, **hub-NCor>C₆₀**, **PP-bowl>C₆₀**, **Hyd-bowl>C₆₀**, **Cyc-bowl>C₆₀**, **rim-3NSum>C₆₀**, and **Sum>C₆₀** complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs. BCPs of interest are marked by red and blue circles. Red circles correspond to C···C contacts, blue to H···C, and purple to N···C contacts.

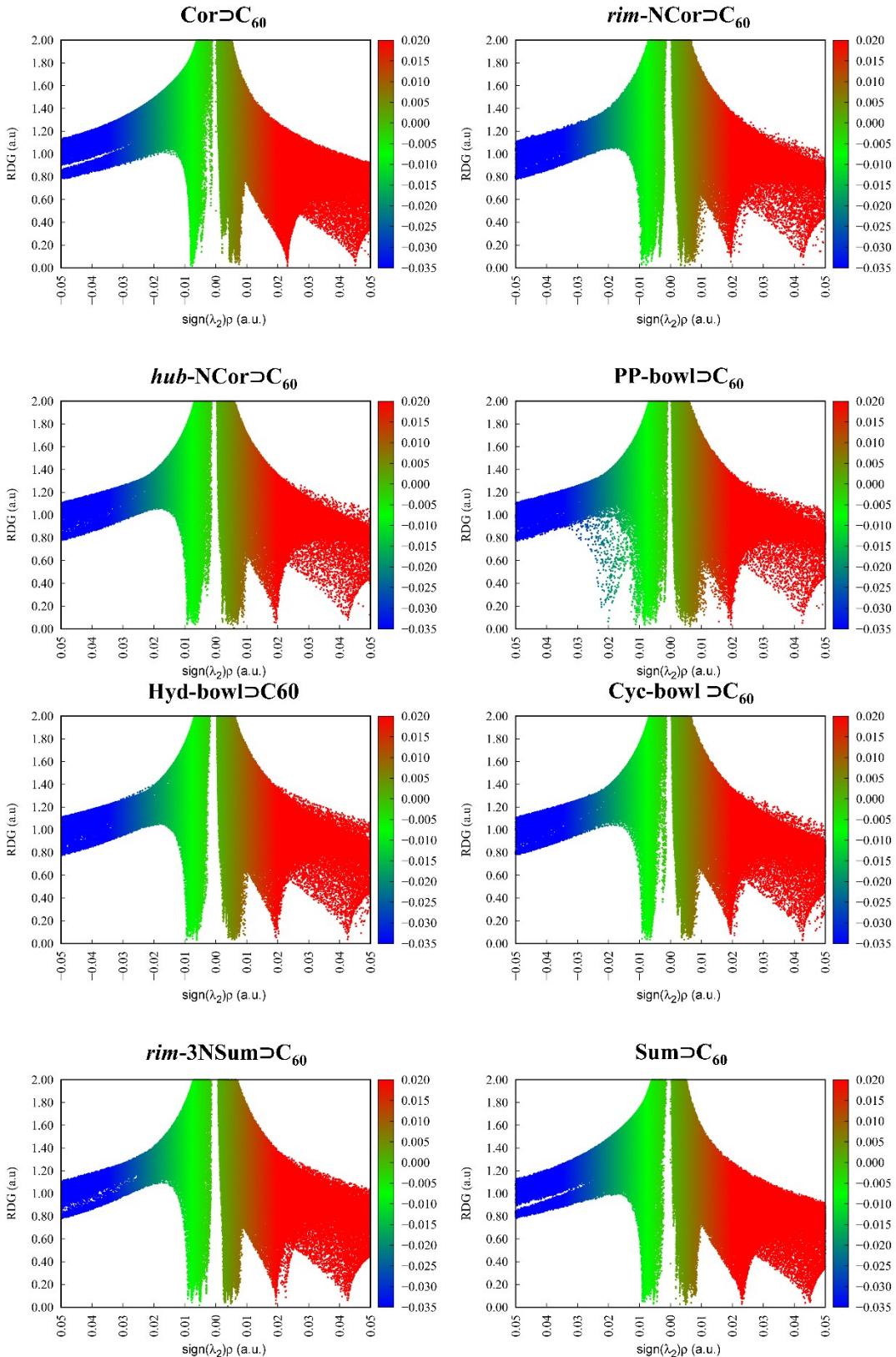


Figure S2. Plot of RDG vs. $\text{sign}(\lambda_2)\rho$ for **Cor-C₆₀**, **rim-NCor-C₆₀**, **hub-NCor-C₆₀**, **PP-bowl-C₆₀**, **Hyd-bowl-C₆₀**, **Cyc-bowl-C₆₀**, **rim-3NSum-C₆₀**, and **Sum-C₆₀** complexes.

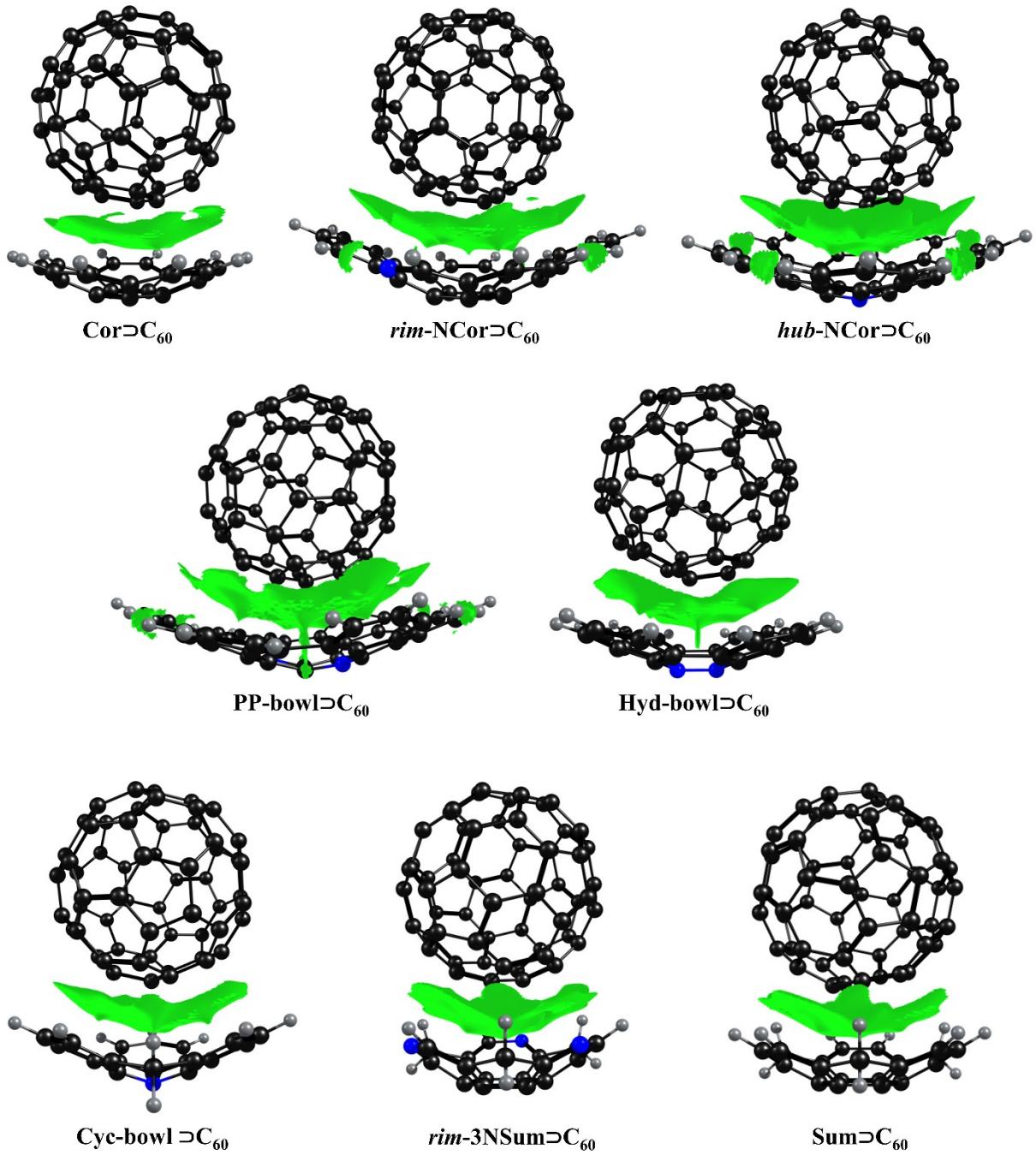


Figure S3. NCI isosurfaces of van der Waals interactions ($-0.015 < \text{sign}(\lambda_2) \times p < 0.010$ a.u.) for **Cor \supset C₆₀**, **rim-NCor \supset C₆₀**, **hub-NCor \supset C₆₀**, **PP-bowl \supset C₆₀**, **Hyd-bowl \supset C₆₀**, **Cyc-bowl \supset C₆₀**, **rim-3NSum \supset C₆₀**, and **Sum \supset C₆₀** complexes. Isosurfaces were generated for RDG = 0.65 a.u.

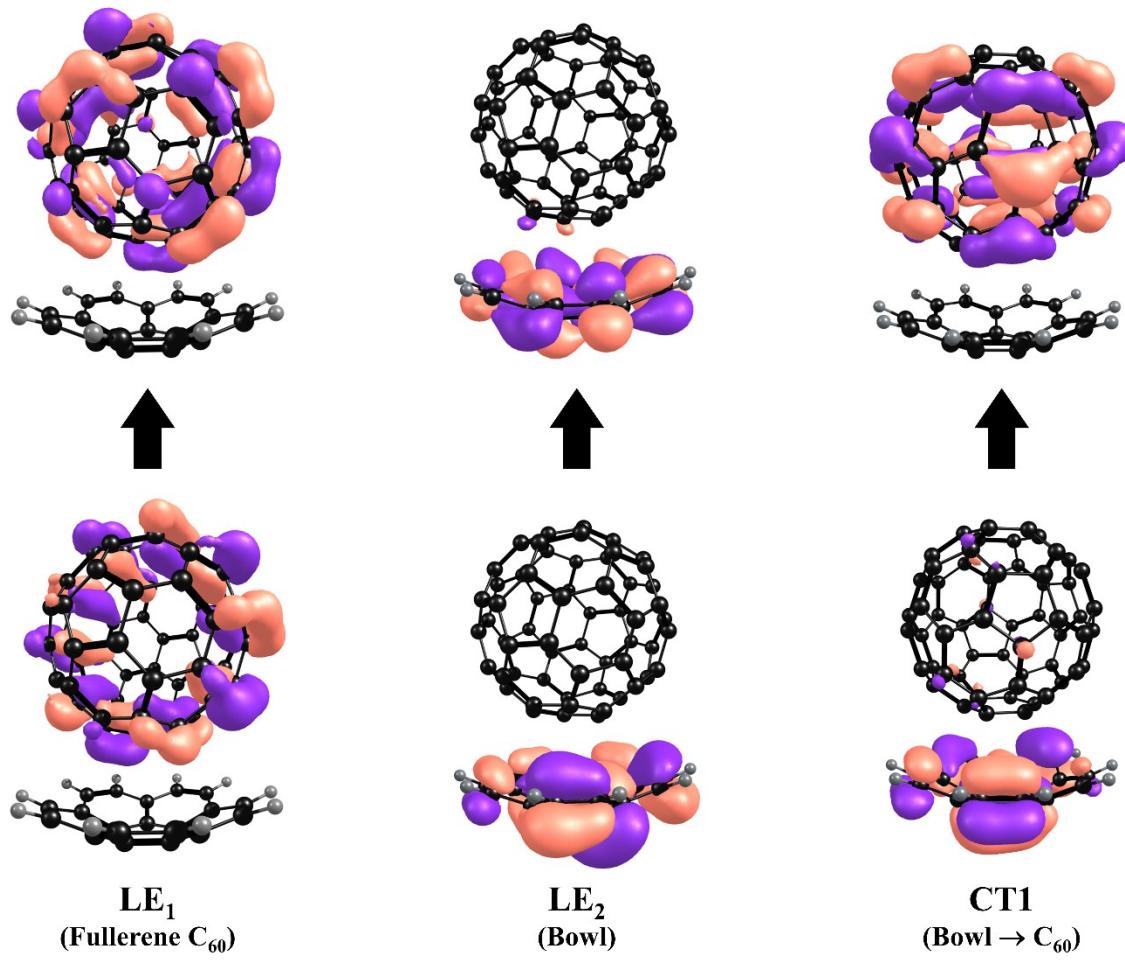


Figure S4. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **Cor>C₆₀** complex.

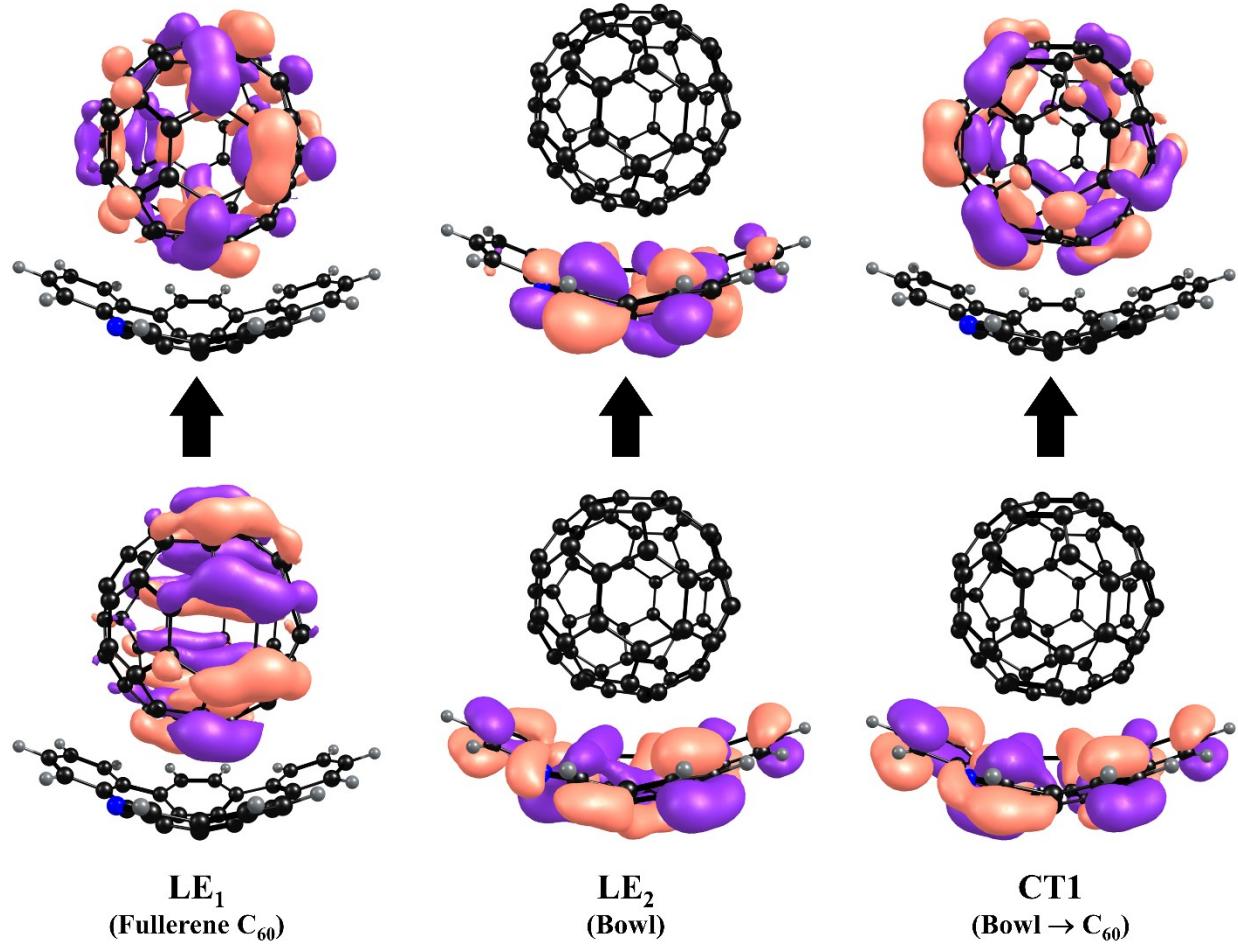


Figure S5. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in *rim*-NCor \supset C₆₀ complex.

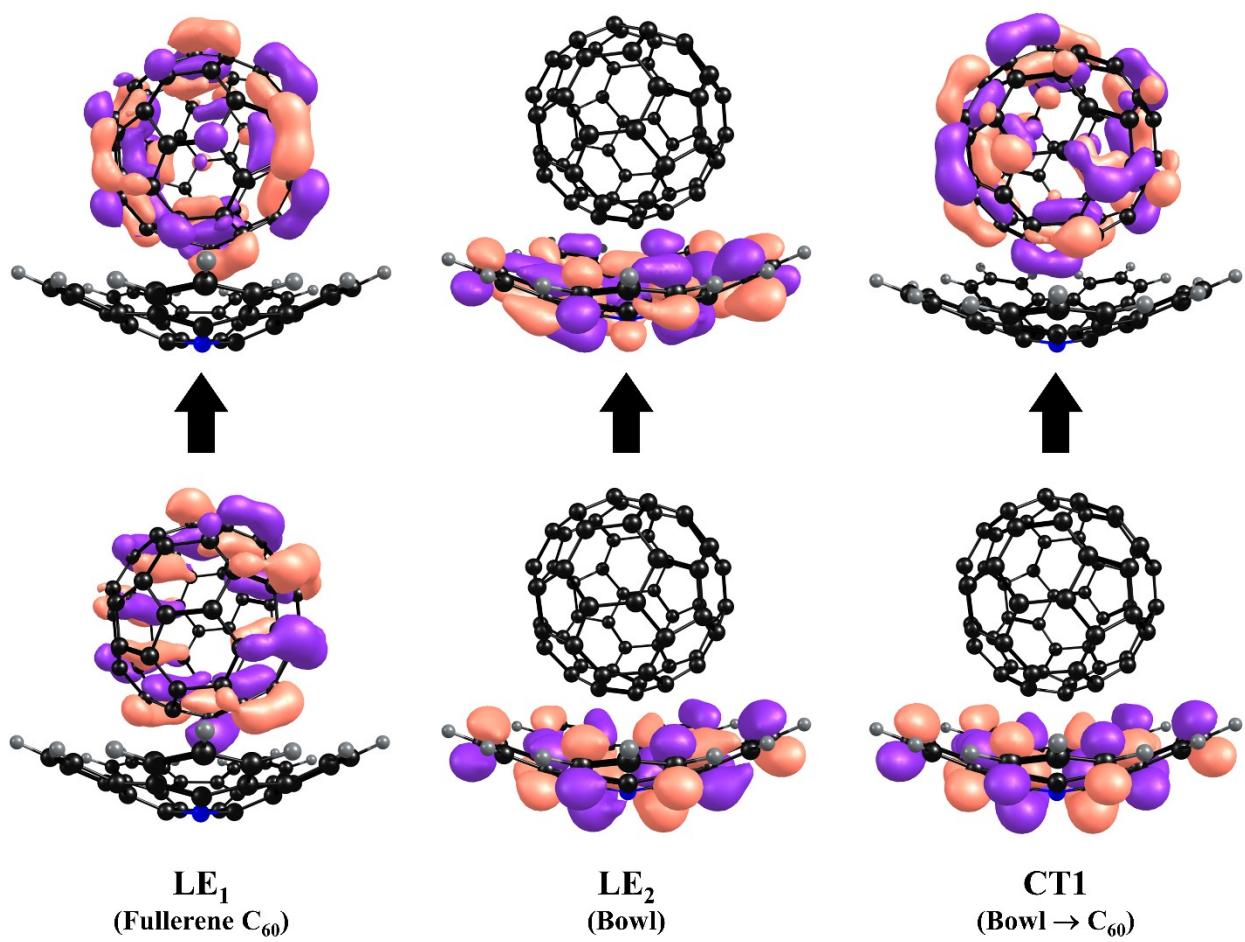


Figure S6. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **hub-NCor>C₆₀**, complex.

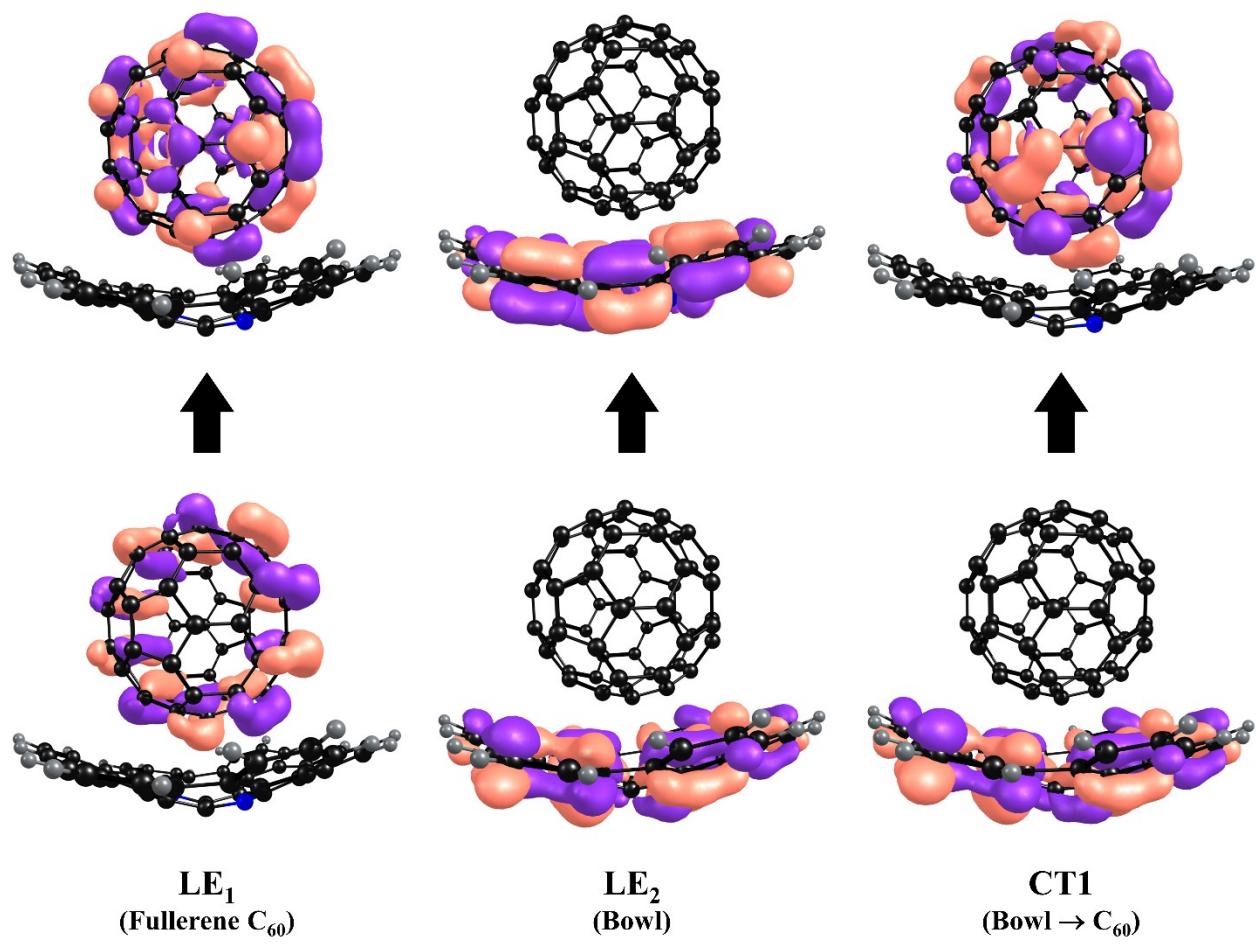


Figure S7. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **PP-bowl**–C₆₀ complex.

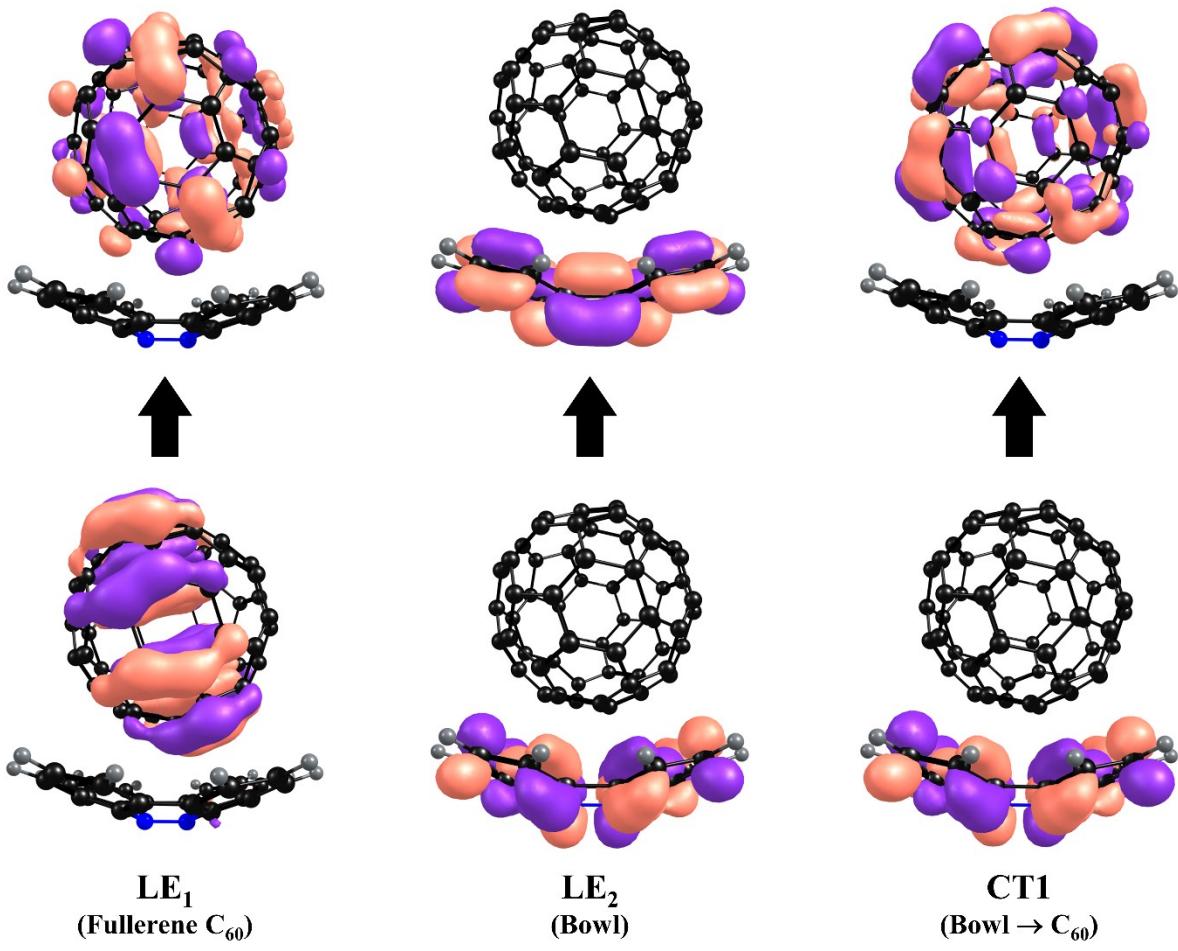


Figure S8. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **Hyd-bowl** \supset **C₆₀** complex.

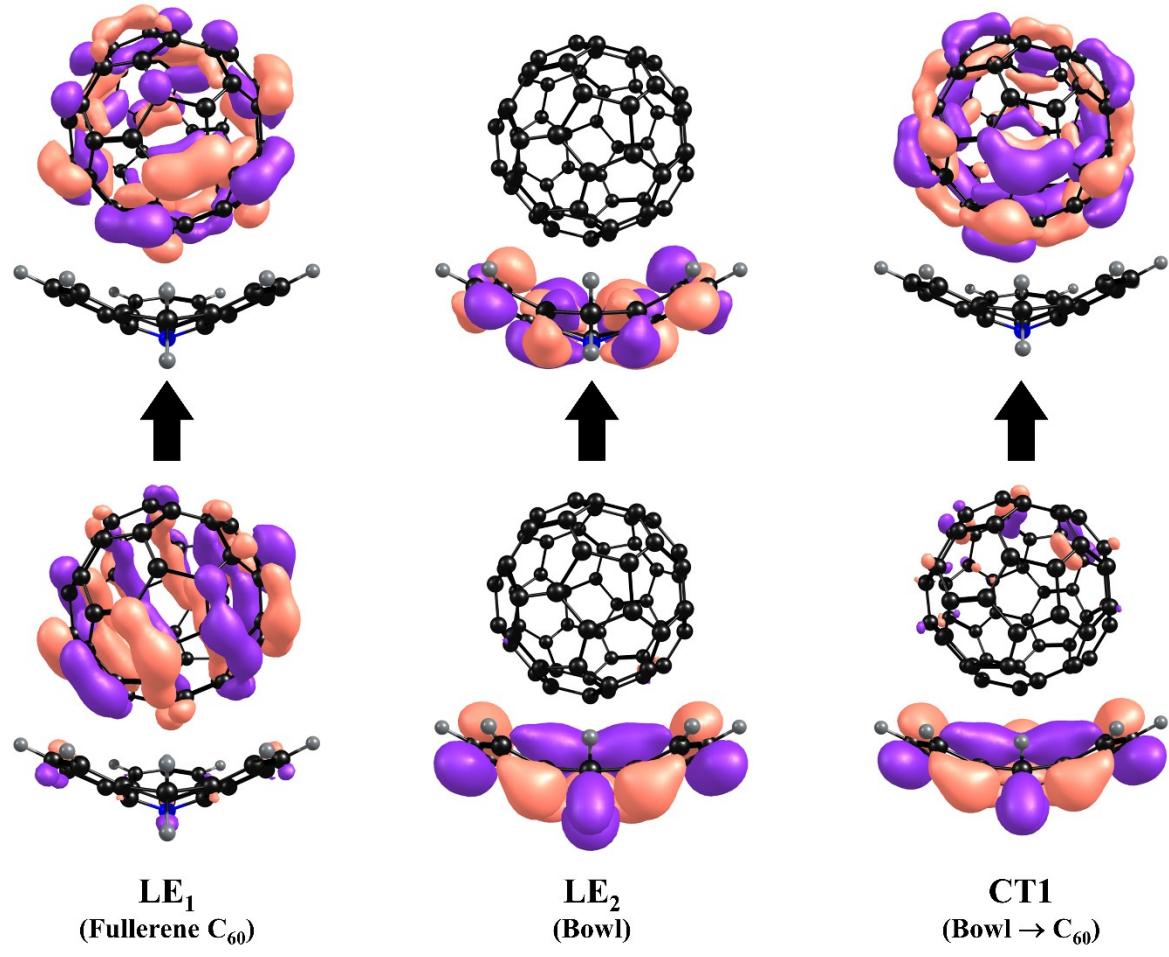


Figure S9. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **Cyc-bowl**–C₆₀ complex.

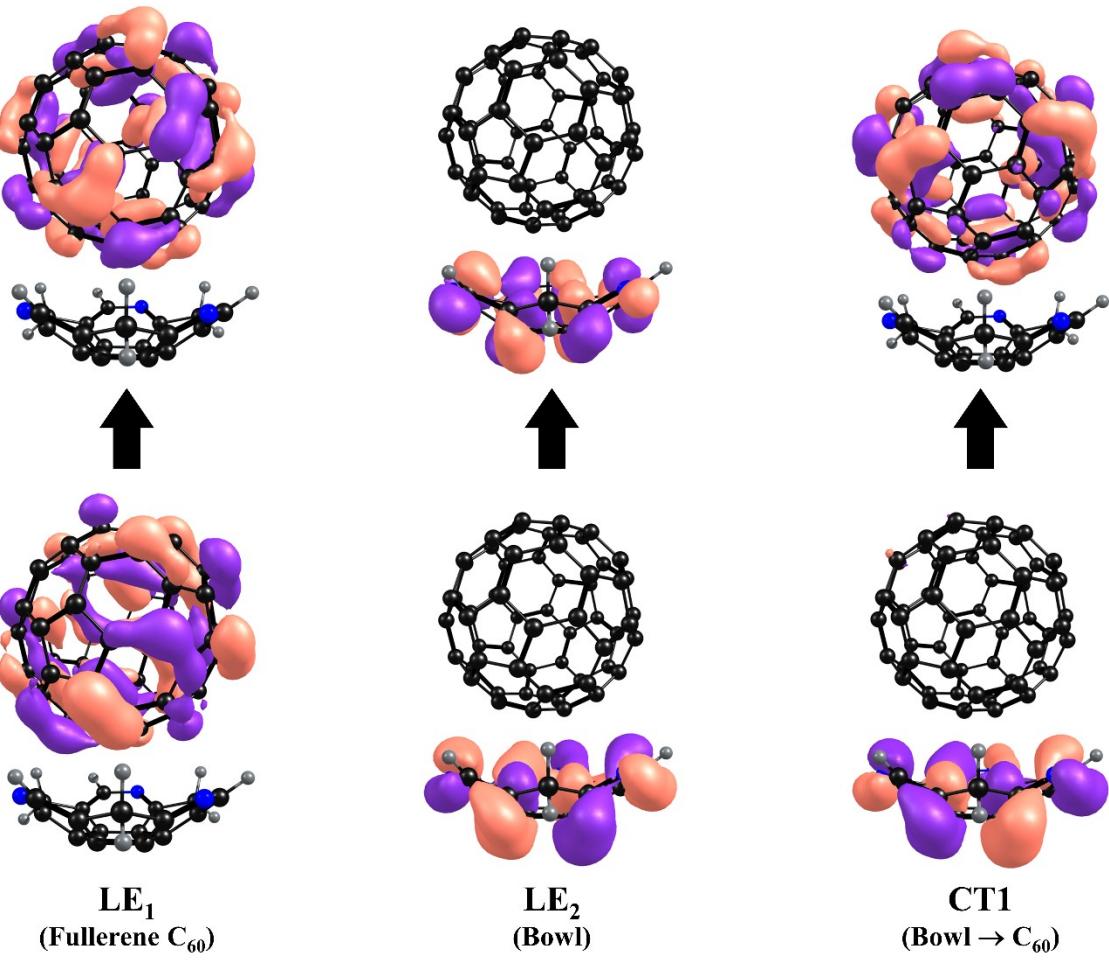


Figure S10. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in *rim*-3NSum- \supset C₆₀ complex.

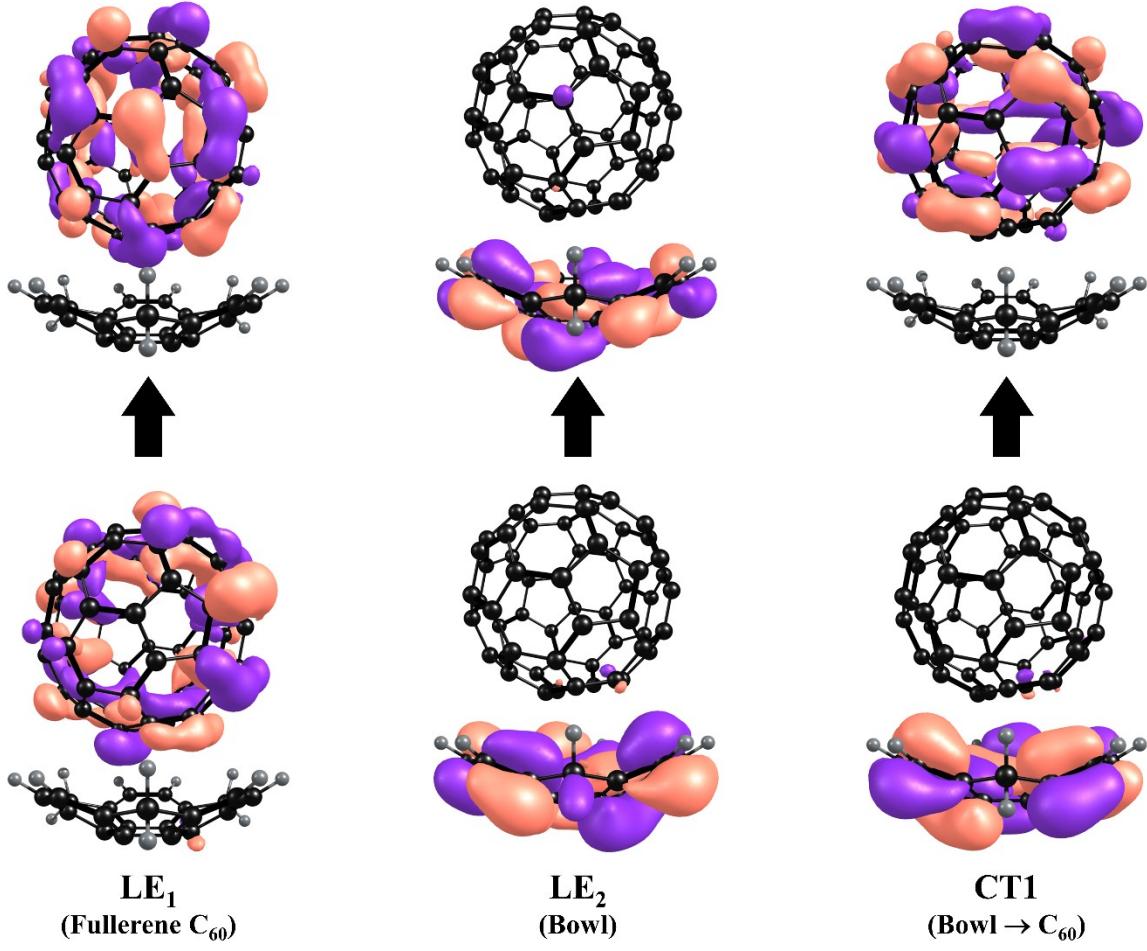
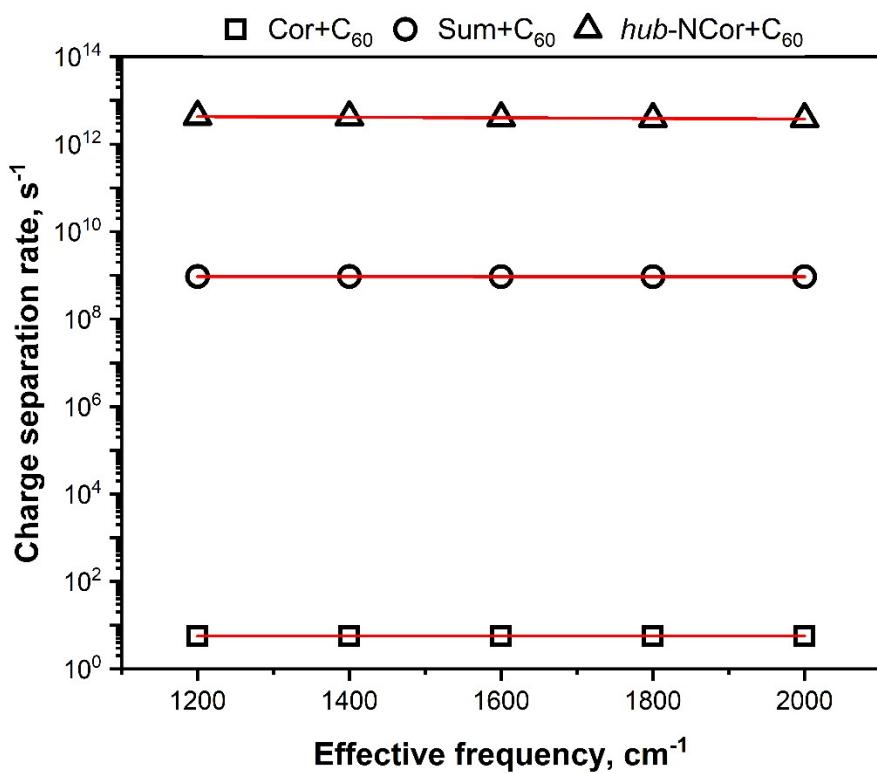


Figure S11. Natural transition molecular orbitals representing the LE₁, LE₂ and CT states in **Sum>C₆₀** complex.

Figure S12. Dependence of the charge separation rate for the Cor \supset C₆₀, Sum \supset C₆₀ and hub-NCor \supset C₆₀, complexes on the effective frequency computed using Marcus-Levich-Jortner approach.



Cartesian coordinates

CorrC₆₀				rim-NCorrC₆₀			
Gas-phase. B3LYP-D3(BJ)/def2-SVP				Gas-phase. B3LYP-D3(BJ)/def2-SVP			
Atom	X	Y	Z	Atom	X	Y	Z
6	0.934401000	1.329324000	-3.103006000	6	4.831420000	-0.703307000	-0.579113000
6	0.948428000	-0.100654000	-3.384666000	6	4.797642000	-1.150796000	0.781693000
6	0.002510000	-0.938640000	-2.785815000	6	4.751943000	-0.014352000	1.623871000
6	-0.994469000	-0.382560000	-1.882089000	6	4.756665000	1.146320000	0.807435000
6	-1.007847000	0.987465000	-1.613578000	6	4.809359000	0.717376000	-0.562473000
6	-0.025122000	1.861821000	-2.236396000	6	4.318628000	-1.450752000	-1.626307000
6	2.315749000	1.786029000	-3.027079000	6	4.209632000	-2.329151000	1.180738000
6	3.183784000	0.640053000	-3.262594000	6	4.169179000	-0.065256000	2.883602000
6	2.338611000	-0.526260000	-3.482272000	6	4.169184000	2.327305000	1.217246000
6	2.725568000	-1.772919000	-2.980861000	6	4.297263000	1.469496000	-1.605016000
6	0.404891000	-2.238642000	-2.264537000	6	3.898746000	2.842772000	-1.254114000
6	-1.209130000	-1.335732000	-0.804526000	6	3.827562000	3.262993000	0.134056000
6	-1.426838000	-0.880884000	0.496033000	6	3.757533000	2.354202000	2.604163000
6	-1.443915000	0.545353000	0.775762000	6	3.754877000	1.215105000	3.403221000
6	-1.238931000	1.461488000	-0.256756000	6	3.804775000	-1.410765000	3.291946000
6	-0.396341000	2.629651000	-0.037610000	6	3.845972000	-3.255465000	0.101122000
6	0.354852000	2.876806000	-1.260903000	6	3.912749000	-2.826761000	-1.283958000
6	1.680625000	3.314691000	-1.189897000	6	3.992805000	-0.680691000	-2.797545000
6	2.681150000	2.758612000	-2.091245000	6	3.986122000	0.713985000	-2.788674000
6	4.381106000	0.512011000	-2.551249000	1	3.328925000	3.268062000	3.020249000
6	4.761530000	1.525377000	-1.576014000	1	3.328031000	1.281914000	4.407333000
6	3.927650000	2.624355000	-1.350352000	1	3.414749000	-1.577553000	4.304431000
6	3.697745000	3.098072000	0.007804000	1	3.622349000	-1.183293000	-3.693188000
6	2.308867000	3.524770000	0.107165000	1	3.613222000	1.224793000	-3.678673000
6	1.586749000	3.288073000	1.281061000	6	3.440351000	-3.715878000	-2.269046000
6	0.204676000	2.834736000	1.208156000	6	2.923413000	-4.962530000	-1.938942000
6	-0.010666000	1.877386000	2.287174000	1	3.474373000	-3.410629000	-3.316512000
6	-0.815217000	0.756349000	2.072990000	1	2.562277000	-5.625291000	-2.728603000
6	-0.346419000	-2.484691000	-1.040041000	6	3.308001000	-4.519110000	0.404809000
6	1.649114000	-1.818062000	3.074137000	6	2.854191000	-5.366486000	-0.596159000
6	1.283263000	-2.790160000	2.137118000	1	3.240735000	-4.798753000	1.457535000
6	2.283619000	-3.344609000	1.235129000	1	2.436874000	-6.342701000	-0.339410000
6	3.609041000	-2.905700000	1.305775000	6	3.466340000	3.745353000	-2.245378000
6	3.989946000	-1.892812000	2.280862000	6	2.983381000	5.007258000	-1.926790000
6	3.015296000	0.070019000	3.427963000	1	3.510454000	3.437359000	-3.291451000
6	1.626252000	0.496109000	3.529879000	1	2.655721000	5.681374000	-2.721229000
6	0.781791000	-0.671405000	3.310096000	6	3.327019000	4.548687000	0.419048000
6	-0.412979000	-0.542446000	2.596360000	6	2.912317000	5.411892000	-0.585740000
6	-0.790837000	-1.554449000	1.619180000	1	3.263574000	4.869565000	1.460264000
6	0.035728000	-2.658223000	1.397227000	1	2.528863000	6.402071000	-0.330344000
6	1.654415000	-3.555704000	-0.062019000	7	3.807390000	-2.462917000	2.490754000
6	2.376173000	-3.319255000	-1.236151000	6	-0.176054000	2.453791000	1.904714000
6	3.757036000	-2.862092000	-1.162121000	6	-0.419947000	1.424528000	2.908198000
6	4.360447000	-2.659473000	0.082680000	6	0.241280000	0.195389000	2.825162000
6	5.207313000	-1.493994000	0.301375000	6	1.170930000	-0.057210000	1.732959000
6	4.976302000	-1.019726000	1.659896000	6	1.401976000	0.927745000	0.771788000

6	4.962599000	0.352073000	1.929379000	6	0.715024000	2.208516000	0.857721000
6	3.962059000	0.907828000	2.830695000	6	-1.438369000	3.130564000	1.637219000
6	1.238529000	1.742320000	3.026844000	6	-2.461349000	2.520485000	2.474938000
6	2.224925000	2.614515000	2.405046000	6	-1.832671000	1.466405000	3.259603000
6	3.558572000	2.205565000	2.308841000	6	-2.525327000	0.279471000	3.517041000
6	4.310232000	2.452655000	1.085696000	6	-0.480146000	-1.042068000	3.093914000
6	5.178799000	1.307396000	0.851332000	6	1.025253000	-1.447266000	1.329966000
6	5.400685000	0.852979000	-0.452456000	6	1.119960000	-1.796189000	-0.017508000
6	5.415183000	-0.576421000	-0.733069000	6	1.362487000	-0.768939000	-1.017399000
6	4.785468000	-0.786941000	-2.030589000	6	1.500537000	0.563961000	-0.631662000
6	3.972810000	-1.905375000	-2.239573000	6	0.876045000	1.618946000	-1.416660000
6	0.264331000	-3.132612000	0.037849000	6	0.390588000	2.636919000	-0.496019000
6	1.738704000	-2.646589000	-2.360331000	6	-0.817268000	3.289678000	-0.751724000
6	3.029535000	-1.359844000	3.146382000	6	-1.751856000	3.540739000	0.337587000
6	-4.779752000	-0.686940000	0.932634000	6	-3.756909000	2.345197000	1.979994000
6	-4.793919000	-1.109196000	-0.425527000	6	-4.083263000	2.771627000	0.626654000
6	-4.787502000	0.052702000	-1.245337000	6	-3.100945000	3.356126000	-0.177836000
6	-4.772540000	1.193060000	-0.395538000	6	-3.000214000	2.991535000	-1.584743000
6	-4.766525000	0.736513000	0.950729000	6	-1.588898000	2.951036000	-1.940157000
6	-4.238912000	-1.457206000	1.953414000	6	-1.119191000	1.974815000	-2.824794000
6	-4.272059000	-2.326605000	-0.842667000	6	0.142917000	1.297247000	-2.560706000
6	-4.267391000	0.065533000	-2.532059000	6	-0.000994000	-0.097075000	-2.963792000
6	-4.230936000	2.412010000	-0.781743000	6	0.599030000	-1.109205000	-2.209483000
6	-4.214674000	1.471801000	1.991873000	6	0.008328000	-2.058629000	2.171000000
6	-3.840064000	2.825507000	1.636918000	6	-2.439564000	-3.129547000	-1.596876000
6	-3.847409000	3.271738000	0.319058000	6	-2.126132000	-3.538413000	-0.297230000
6	-3.891463000	2.497716000	-2.188436000	6	-3.060639000	-3.285216000	0.790732000
6	-3.905749000	1.381743000	-3.017680000	6	-4.270950000	-2.634188000	0.535808000
6	-3.925710000	-2.379489000	-2.248714000	6	-4.597012000	-2.207837000	-0.817639000
6	-3.921368000	-1.242138000	-3.049769000	6	-3.455460000	-1.421985000	-2.864139000
6	-3.906247000	-3.222676000	0.234888000	6	-2.044002000	-1.465940000	-3.219300000
6	-3.889586000	-2.809070000	1.562933000	6	-1.416101000	-2.521716000	-2.436683000
6	-3.865990000	-0.706548000	3.135946000	6	-0.120640000	-2.347425000	-1.941801000
6	-3.856625000	0.684596000	3.154838000	6	0.204822000	-2.773754000	-0.586713000
1	-3.438596000	3.489103000	2.407656000	6	-0.775654000	-3.358804000	0.218475000
1	-3.448955000	4.267364000	0.104176000	6	-2.288308000	-2.947870000	1.978615000
1	-3.509646000	3.439608000	-2.592827000	6	-2.758013000	-1.973220000	2.864067000
1	-3.528780000	1.490140000	-4.038828000	6	-4.018199000	-1.294437000	2.597060000
1	-3.552981000	-3.315458000	-2.674687000	6	-4.759704000	-1.618520000	1.457679000
1	-3.541939000	-1.330430000	-4.071859000	6	-5.388110000	-0.564317000	0.673843000
1	-3.527908000	-4.220523000	-0.004923000	6	-5.287378000	-0.928543000	-0.732368000
1	-3.501044000	-3.499078000	2.316759000	6	-5.052991000	0.057555000	-1.694492000
1	-3.480691000	-1.240281000	4.009196000	6	-4.118335000	-0.194251000	-2.782357000
1	-3.463382000	1.189500000	4.041492000	6	-1.351498000	-0.278872000	-3.477485000
				6	-2.042075000	1.000833000	-3.391369000
				6	-3.397226000	1.041971000	-3.050960000
				6	-3.886220000	2.057823000	-2.129676000
				6	-4.909536000	1.449281000	-1.291032000
				6	-5.006257000	1.798962000	0.058647000
				6	-5.250543000	0.771486000	1.061223000
				6	-4.478199000	1.109080000	2.248759000
				6	-3.874670000	0.097479000	3.000791000
				6	-0.876231000	-2.993551000	1.625682000

6	-1.835477000	-1.000332000	3.432977000
6	-3.699705000	-2.449731000	-1.861521000

hub-NCor ⊃ C₆₀

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

Atom	X	Y	Z
6	-3.480975000	-2.203411000	2.570163000
6	-3.823472000	-2.387025000	1.194720000
6	-3.345115000	-3.463980000	0.370759000
6	-2.819445000	-3.271208000	3.187093000
6	-2.698646000	-4.503788000	1.065874000
6	-3.632604000	-0.838840000	3.159333000
6	-3.159917000	-0.481248000	4.432948000
6	-3.353343000	1.897232000	3.920041000
6	-4.059748000	0.245303000	2.335625000
6	-3.836243000	1.623945000	2.628969000
6	-4.448622000	-1.325741000	0.534608000
7	-4.558847000	-0.064475000	1.090904000
6	-4.626933000	0.860028000	0.065998000
6	-4.476725000	-1.196068000	-0.847016000
6	-4.584979000	0.177064000	-1.140397000
6	-3.333114000	-3.313298000	-1.112408000
6	-3.826297000	-2.101898000	-1.699487000
6	-3.453864000	-1.617680000	-3.000684000
6	-2.771886000	-2.536651000	-3.809941000
6	-3.228976000	2.693832000	-3.458328000
6	-3.019658000	0.456979000	-4.450222000
6	-3.570379000	-0.151878000	-3.313230000
6	-3.789083000	2.160384000	-2.280437000
6	-4.051458000	0.751346000	-2.304961000
6	-3.485559000	4.231793000	-0.801146000
6	-3.898772000	2.900034000	-0.991751000
6	-4.212034000	2.185002000	0.215470000
6	-3.459884000	3.961016000	1.640960000
6	-3.897833000	2.636523000	1.533763000
6	-2.659207000	-4.182004000	-1.991569000
6	-2.428538000	-3.806797000	-3.318182000
6	-2.898220000	1.855036000	-4.526123000
6	-3.307014000	4.746856000	0.486805000
6	-3.057646000	0.861586000	4.810963000
6	-2.478942000	-4.414153000	2.444884000
1	-2.509682000	-3.210529000	4.232011000
1	-2.310470000	-5.369709000	0.526880000
1	-2.821904000	-1.255251000	5.123212000
1	-3.159512000	2.927632000	4.222108000
1	-2.447115000	-2.258341000	-4.814383000
1	-2.996732000	3.758183000	-3.533488000
1	-2.628951000	-0.148232000	-5.270058000
1	-3.244542000	4.863465000	-1.658093000
1	-3.184771000	4.385649000	2.607880000
1	-2.257138000	-5.131839000	-1.634471000
1	-1.892348000	-4.496143000	-3.974649000

PP-bowl ⊃ C₆₀

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

Atom	X	Y	Z
6	1.826085000	0.071032000	6.615282000
6	0.964582000	-1.020354000	6.769160000
6	-0.292870000	-0.441069000	6.969354000
6	-0.176096000	0.945998000	6.892063000
6	-2.262400000	0.380906000	6.422556000
6	-1.408016000	1.478901000	6.499979000
7	-1.579275000	-0.801781000	6.668852000
7	1.134545000	1.285871000	6.681555000
6	3.124066000	-0.035588000	6.133957000
6	3.792552000	1.166001000	5.777294000
6	3.609267000	-1.353401000	5.871163000
6	5.108556000	1.021987000	5.323107000
6	4.938048000	-1.422995000	5.410436000
6	5.669259000	-0.257537000	5.179331000
1	5.708018000	1.886991000	5.038576000
1	5.405504000	-2.384663000	5.196758000
1	6.696304000	-0.342791000	4.816213000
6	1.305722000	-2.326495000	6.328545000
6	0.297550000	-3.340650000	6.126409000
6	2.680012000	-2.501686000	5.931396000
6	0.775318000	-4.540059000	5.579686000
6	3.071952000	-3.770351000	5.457847000
6	2.130514000	-4.768910000	5.294232000
1	0.083763000	-5.334622000	5.311670000
1	4.104459000	-3.955624000	5.160594000
1	2.429936000	-5.733927000	4.878638000
6	-3.548363000	0.424827000	5.904614000
6	-4.210118000	-0.815786000	5.693205000
6	-4.031279000	1.708544000	5.504868000
6	-5.485409000	-0.736822000	5.125122000
6	-5.326057000	1.711166000	4.950126000
6	-6.025514000	0.514685000	4.779528000
1	-6.062391000	-1.635995000	4.904528000
1	-5.785224000	2.639908000	4.608516000
1	-7.016683000	0.547371000	4.320697000
6	-1.766109000	2.746738000	5.992901000
6	-0.780555000	3.783225000	5.842899000
6	-3.141269000	2.888847000	5.589447000
6	-1.324924000	5.045805000	5.563691000
6	-3.575993000	4.180508000	5.232837000
6	-2.688734000	5.243260000	5.284279000
1	-0.696423000	5.932716000	5.537202000
1	-4.609824000	4.354563000	4.930775000
1	-3.039577000	6.253558000	5.060849000
6	1.610413000	2.468762000	6.104425000
6	3.003868000	2.428137000	5.745405000
6	0.757482000	3.601017000	5.794532000
6	3.584336000	3.580237000	5.195205000
6	1.444957000	4.680656000	5.204269000

1	-2.454706000	2.297204000	-5.421741000	6	2.814202000	4.700520000	4.942380000
1	-2.963050000	5.777974000	0.598542000	1	4.637044000	3.576986000	4.913842000
1	-2.674821000	1.108949000	5.803753000	1	0.884693000	5.549967000	4.876453000
1	-1.959490000	-5.231646000	2.950494000	1	3.261917000	5.585043000	4.484388000
6	5.237993000	-0.821382000	-1.517860000	6	-2.068889000	-2.050665000	6.318197000
6	5.636483000	-0.689556000	-0.123068000	6	-3.462198000	-2.072917000	5.970032000
6	5.168608000	-1.603373000	0.826711000	6	-1.232664000	-3.223857000	6.286255000
6	4.283305000	-2.687128000	0.421421000	6	-4.075988000	-3.326515000	5.829325000
6	3.900559000	-2.812894000	-0.917759000	6	-1.963357000	-4.427490000	6.227812000
6	4.387338000	-1.860670000	-1.906917000	1	-5.136499000	-3.385579000	5.581821000
6	5.046237000	0.517315000	-2.058869000	1	-1.435915000	-5.372862000	6.330175000
6	5.327849000	1.477126000	-1.000143000	1	-3.836963000	-5.462227000	5.982607000
6	5.691917000	0.730770000	0.196966000	6	1.851445000	-3.065219000	0.282049000
6	5.274789000	1.180555000	1.453013000	6	0.525595000	-3.600078000	0.562730000
6	4.734791000	-1.134060000	2.135311000	6	2.507793000	-2.284700000	1.239242000
6	3.303481000	-2.889426000	1.481113000	6	-0.091079000	-3.337079000	1.790076000
6	1.981026000	-3.210704000	1.158811000	6	-1.512362000	-3.009649000	1.837669000
6	1.582982000	-3.341127000	-0.237893000	6	-0.251781000	-3.547210000	-0.667991000
6	2.523493000	-3.147728000	-1.255041000	6	-1.613636000	-3.232845000	-0.622536000
6	2.159368000	-2.399821000	-2.451957000	6	-2.257953000	-2.959127000	0.655324000
6	3.312004000	-1.605927000	-2.855568000	6	3.273688000	-0.720199000	-0.518207000
6	3.127641000	-0.320099000	-3.373902000	6	2.588268000	-1.533203000	-1.514542000
6	4.012960000	0.762691000	-2.967942000	6	3.232817000	-1.087415000	0.830633000
6	4.562929000	2.643108000	-0.892211000	6	1.892513000	-2.680870000	-1.122985000
6	3.487036000	2.900212000	-1.840337000	6	0.592937000	-2.979602000	-1.709622000
6	3.216804000	1.977659000	-2.855923000	6	2.015418000	-0.637837000	-2.510636000
6	1.839434000	1.645982000	-3.194374000	6	0.768278000	-0.925648000	-3.074502000
6	1.784019000	0.225255000	-3.515415000	6	0.043017000	-2.121182000	-2.666192000
6	0.677154000	-0.536003000	-3.127594000	6	2.896607000	1.271908000	1.493906000
6	0.869489000	-1.876378000	-2.584443000	6	2.936439000	1.653397000	0.087742000
6	-0.107208000	-2.074982000	-1.523853000	6	3.042194000	-0.071881000	1.857951000
6	0.240272000	-2.792428000	-0.375887000	6	3.121650000	0.678095000	-0.897254000
6	3.582812000	-1.928393000	2.540157000	6	2.345122000	0.729319000	-2.129446000
6	-0.669106000	-0.196989000	2.098468000	6	1.964973000	2.720553000	-0.118069000
6	0.355844000	-0.443939000	3.013958000	6	1.219399000	2.770095000	-1.300496000
6	1.240518000	0.640382000	3.417923000	6	1.412800000	1.753009000	-2.326137000
6	1.056354000	1.927098000	2.898821000	6	1.236186000	0.156150000	3.523146000
6	-0.019689000	2.184518000	1.951486000	6	1.085217000	1.554638000	3.146567000
6	-1.260438000	1.009479000	0.163892000	6	2.195195000	-0.641379000	2.896979000
6	-1.315430000	-0.409585000	-0.156482000	6	1.901434000	2.105345000	2.155967000
6	-0.948901000	-1.156198000	1.039625000	6	1.324664000	2.999507000	1.160247000
6	-0.190434000	-2.323688000	0.933286000	6	-0.333754000	1.881325000	3.190035000
6	0.883151000	-2.581212000	1.882562000	6	-0.885711000	2.747762000	2.246069000
6	1.151926000	-1.660111000	2.900764000	6	-0.038453000	3.313918000	1.204834000
6	2.584198000	0.095135000	3.554594000	6	0.593028000	-2.522056000	2.783997000
6	3.690594000	0.856365000	3.166122000	6	-0.403891000	-1.689895000	3.440466000
6	3.499629000	2.195114000	2.624683000	6	1.867064000	-2.009834000	2.518590000
6	2.209794000	2.718407000	2.492459000	6	-0.088554000	-0.379846000	3.800346000
6	1.846146000	3.466780000	1.295558000	6	-1.058105000	0.686542000	3.595509000
6	0.467816000	3.135842000	0.960273000	6	-1.706243000	-1.991728000	2.861277000
6	0.086170000	3.009345000	-0.379401000	6	-2.638214000	-0.966887000	2.664488000
6	-0.794896000	1.922882000	-0.785056000	6	-2.306937000	0.400786000	3.040903000
6	-0.900320000	-0.859099000	-1.411171000	6	-2.142236000	2.827914000	0.255181000
6	-2.187155000	-0.785056000	-2.187155000	6	-2.882160000	1.298450000	1.660922000
6	-0.900320000	-0.859099000	-1.411171000	6	-2.882160000	1.298450000	2.050265000

6	-0.418690000	0.092330000	-2.401878000	6	-2.798184000	2.046759000	-0.701668000
6	-0.365492000	1.454886000	-2.093628000	6	-0.882491000	2.282885000	-2.249202000
6	0.786441000	2.248521000	-2.499166000	6	-0.199042000	3.097451000	-1.253417000
6	1.066858000	3.210841000	-1.439110000	6	-0.815107000	3.362216000	-0.026189000
6	2.389696000	3.530722000	-1.116882000	6	-2.154222000	1.768740000	-1.978979000
6	2.787453000	3.660943000	0.278833000	6	-1.527097000	-0.395083000	-2.997444000
6	4.130375000	3.112637000	0.416957000	6	-0.202263000	0.140919000	-3.278903000
6	4.478887000	2.395744000	1.565688000	6	0.113304000	1.452646000	-2.912592000
6	2.529170000	-1.325902000	3.234695000	6	-2.482546000	0.402006000	-2.360340000
6	4.787761000	0.228983000	2.442394000	6	-3.182933000	-1.507150000	-0.955123000
6	-0.862057000	1.141138000	1.559001000	6	-2.186464000	-2.337217000	-1.617724000
				6	-1.375543000	-1.792909000	-2.618298000
				6	-3.328370000	-0.165034000	-1.319210000
				6	-3.567480000	0.484610000	1.054632000
				6	-3.415887000	-0.915707000	1.433952000
				6	-3.228560000	-1.891602000	0.449819000
				6	-3.523557000	0.851401000	-0.294001000

Hyd-bowl \supset C₆₀

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

Atom	X	Y	Z
6	-3.739281000	-3.028091000	2.907804000
6	-3.846426000	-3.498931000	1.593734000
1	-3.580146000	-4.531151000	1.356294000
6	-4.232939000	-2.597297000	0.584716000
6	-4.568794000	-1.291479000	1.024094000
6	-4.347387000	-0.735036000	2.299103000
6	-3.939304000	-1.671395000	3.257301000
1	-3.712244000	-1.347591000	4.275239000
7	-4.893496000	-0.548474000	-0.080946000
6	-4.205335000	-2.536220000	-0.889061000
6	-3.763706000	-3.346006000	-1.950932000
6	-4.536688000	-1.199914000	-1.232526000
6	-3.611709000	-2.767120000	-3.216688000
1	-3.482457000	-4.388620000	-1.786863000
6	-4.288021000	-0.540531000	-2.453092000
6	-3.831885000	-1.391147000	-3.467169000
1	-3.577449000	-0.985147000	-4.448481000
6	-4.273597000	0.760543000	2.356617000
6	-4.454289000	1.437616000	1.133323000
6	-3.765231000	1.571077000	3.379432000
6	-4.010855000	2.742008000	0.796422000
7	-4.847187000	0.817142000	-0.024527000
6	-3.438460000	2.925227000	3.135469000
1	-3.551523000	1.143948000	4.361622000
6	-3.523558000	3.513631000	1.866791000
6	-4.449027000	1.532336000	-1.124916000
1	-3.159172000	4.531109000	1.708987000
6	-4.008380000	2.804126000	-0.677987000
6	-4.249799000	0.957497000	-2.396248000
6	-3.521809000	3.666858000	-1.678069000
6	-3.745950000	1.854325000	-3.345688000
6	-3.431650000	3.187898000	-2.990469000
1	-3.161476000	4.668457000	-1.433387000
1	-3.524708000	1.511118000	-4.358553000

Cyc-bowl \supset C₆₀

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

Atom	X	Y	Z
6	-4.303945000	2.976575000	0.874091000
6	-4.819872000	1.673273000	0.823066000
6	-5.062301000	1.178260000	-0.488592000
6	-4.645753000	1.710873000	-1.704140000
6	-4.104417000	2.998376000	-1.599898000
6	-3.983692000	3.618205000	-0.336103000
6	-4.535450000	-0.713793000	-2.549088000
6	-4.957149000	-1.086759000	-1.278678000
6	-4.633131000	-2.265353000	-0.552910000
6	-4.014973000	-3.273881000	-1.308616000
6	-3.686082000	-3.000142000	-2.647902000
6	-3.887396000	-1.738736000	-3.251682000
1	-4.079181000	3.467799000	1.823221000
1	-3.721381000	3.514605000	-2.484162000
1	-3.547389000	4.619067000	-0.292617000
1	-3.720904000	-4.226099000	-0.861809000
1	-3.177433000	-3.774263000	-3.226986000
1	-3.485860000	-1.557352000	-4.252371000
6	-4.710378000	0.772889000	-2.929908000
6	-5.256912000	-0.575829000	0.867804000
6	-4.930382000	0.485699000	1.730905000
6	-4.804027000	-1.908159000	0.891932000
6	-4.442668000	0.052790000	2.977001000
6	-4.304635000	-2.300568000	2.147135000
6	-4.204965000	-1.328684000	3.169249000
1	-4.145120000	0.755155000	3.758398000
1	-3.901660000	-3.300272000	2.325764000
1	-3.798448000	-1.647545000	4.132396000
7	-5.454109000	-0.138994000	-0.411478000
1	-5.687599000	0.904469000	-3.431808000
1	-3.944679000	1.061685000	-3.665098000
6	-0.287629000	-2.260753000	2.044545000
6	1.059732000	-2.789436000	2.209825000
6	1.998592000	-2.086398000	2.971444000

1	-3.246865000	-3.388680000	-4.037332000	6	1.630741000	-0.823774000	3.596713000
1	-3.420395000	-3.721014000	3.689360000	6	0.338108000	-0.314665000	3.437617000
1	-3.037645000	3.516590000	3.961442000	6	-0.639534000	-1.046586000	2.643818000
1	-3.034059000	3.848337000	-3.764054000	6	-0.720175000	-2.552652000	0.683875000
6	-1.421987000	-1.118862000	-0.597356000	6	0.358942000	-3.262860000	0.009769000
6	-1.590203000	0.311454000	-0.394271000	6	1.458903000	-3.409577000	0.953107000
6	-1.111092000	1.214863000	-1.342303000	6	2.780912000	-3.302767000	0.508666000
6	-0.438607000	0.727065000	-2.535690000	6	3.375022000	-1.974405000	2.507818000
6	-0.272318000	-0.648737000	-2.729753000	6	2.780024000	0.068207000	3.520034000
6	-0.778742000	-1.592238000	-1.742484000	6	2.590612000	1.433229000	3.286854000
6	-1.158060000	-1.725770000	0.699221000	6	1.244403000	1.964470000	3.121710000
6	-1.168235000	-0.670499000	1.702322000	6	0.140129000	1.109146000	3.195548000
6	-1.436742000	0.590045000	1.026048000	6	-0.960292000	1.256313000	2.252294000
6	-0.803714000	1.761514000	1.442841000	6	-1.440529000	-0.076782000	1.910595000
6	-0.452472000	2.438104000	-0.910425000	6	-1.851688000	-0.355501000	0.606391000
6	0.649751000	1.646650000	-2.839916000	6	-1.481004000	-1.615772000	-0.019773000
6	1.864424000	1.150706000	-3.323814000	6	0.626497000	-3.012080000	-1.339831000
6	2.039439000	-0.282365000	-3.524098000	6	-0.173124000	-2.040498000	-2.072279000
6	0.993186000	-1.164504000	-3.234697000	6	-1.200753000	-1.354807000	-1.422521000
6	1.267385000	-2.427035000	-2.557488000	6	-1.404457000	0.064777000	-1.668353000
6	0.171437000	-2.690561000	-1.634286000	6	-1.805728000	0.684508000	-0.412362000
6	0.428799000	-3.273762000	-0.388454000	6	-1.342517000	1.960505000	-0.087035000
6	-0.253449000	-2.783368000	0.803449000	6	-0.910617000	2.252734000	1.272505000
6	-0.272179000	-0.710379000	2.772536000	6	0.238176000	3.144873000	1.196950000
6	0.678876000	-1.808894000	2.878764000	6	1.293693000	3.003348000	2.102768000
6	0.687419000	-2.823959000	1.914767000	6	3.858066000	-0.642621000	2.847396000
6	1.953295000	-3.338904000	1.409604000	6	4.014184000	2.652879000	-0.383429000
6	1.793323000	-3.616565000	-0.012834000	6	4.785053000	1.722541000	0.320225000
6	2.845776000	-3.363557000	-0.898803000	6	5.152669000	0.459921000	-0.306353000
6	2.577800000	-2.756681000	-2.196311000	6	4.736478000	0.179969000	-1.611320000
6	3.666733000	-1.836450000	-2.496748000	6	3.933740000	1.149841000	-2.344382000
6	3.403678000	-0.626012000	-3.145844000	6	2.234787000	2.893741000	-1.910542000
6	0.640622000	2.705415000	-1.835340000	6	1.836563000	3.513076000	-0.654430000
6	4.964632000	1.610770000	-0.643602000	6	2.936374000	3.364084000	0.289696000
6	4.052148000	2.664009000	-0.746384000	6	2.670319000	3.114196000	1.638716000
6	3.370641000	3.155568000	0.443369000	6	3.472369000	2.145052000	2.371993000
6	3.628327000	2.572865000	1.688447000	6	4.507430000	1.462393000	1.725856000
6	4.578223000	1.474194000	1.794640000	6	5.103754000	-0.579831000	0.713082000
6	5.405643000	-0.427938000	0.451046000	6	4.639688000	-1.857644000	0.386630000
6	5.245748000	-0.705440000	-0.969095000	6	4.207242000	-2.149887000	-0.973180000
6	4.973235000	0.554637000	-1.645703000	6	4.254238000	-1.151840000	-1.951623000
6	4.070628000	0.594026000	-2.711740000	6	3.155151000	-1.004477000	-2.896444000
6	3.119716000	1.692018000	-2.819940000	6	2.956762000	0.418086000	-3.138764000
6	3.111308000	2.706855000	-1.857523000	6	1.663926000	0.927631000	-3.297987000
6	2.006658000	3.502759000	0.068144000	6	1.295646000	2.191100000	-2.672547000
6	0.955121000	3.248768000	0.954507000	6	0.514904000	3.406011000	-0.209991000
6	1.223393000	2.641245000	2.253460000	6	-0.462547000	2.673247000	-1.003184000
6	2.533544000	2.310474000	2.613367000	6	-0.081708000	2.081180000	-2.211592000
6	2.807154000	1.048485000	3.289742000	6	-0.565121000	0.748125000	-2.552447000
6	4.071211000	0.531729000	2.783308000	6	0.514577000	0.036360000	-3.223719000
6	4.239096000	-0.842927000	2.589639000	6	0.705881000	-1.329288000	-2.988926000
6	4.920548000	-1.332661000	1.399330000	6	2.051675000	-1.859734000	-2.822182000
6	4.606674000	-1.876051000	-1.385343000	6	2.002664000	-2.899937000	-1.802671000
6	4.100137000	-2.819180000	-0.397440000	6	3.058128000	-3.042215000	-0.897218000
6	4.254009000	-2.553076000	0.966412000	6	4.705222000	0.040274000	1.969331000
6	3.159259000	-2.818728000	1.890283000	6	3.757914000	-2.569813000	1.302137000

6	3.150130000	-1.761544000	2.893570000	6	3.580861000	2.362101000	-1.743404000
6	1.935184000	-1.266166000	3.378188000				
6	1.760206000	0.167067000	3.579613000				
6	0.394967000	0.511240000	3.205785000				
6	0.133380000	1.722283000	2.554976000				
6	1.846345000	3.225385000	-1.353984000				
6	-0.299783000	2.704820000	0.453918000				
6	5.231610000	1.003258000	0.652701000				

rim-3NSum ⊃ C₆₀

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

Atom	X	Y	Z
6	-0.589393000	-1.492355000	-1.478279000
6	0.831552000	-1.282973000	-1.531711000
6	1.337358000	0.010463000	-1.571647000
6	0.443075000	1.134789000	-1.632509000
6	-0.930777000	0.929402000	-1.577158000
6	-1.456554000	-0.407101000	-1.531776000
6	0.999447000	2.217406000	-0.928846000
7	0.230229000	3.139972000	-0.364232000
6	-1.124235000	2.958107000	-0.355414000
6	-1.762936000	1.819381000	-0.872836000
6	-2.624137000	-0.430729000	-0.750643000
7	-3.002700000	-1.532246000	-0.115083000
6	-2.173937000	-2.617791000	-0.113074000
6	-0.900770000	-2.627397000	-0.707044000
6	1.480123000	-2.247972000	-0.741100000
7	2.650960000	-1.994879000	-0.168445000
6	3.166329000	-0.731469000	-0.247243000
6	2.512643000	0.342964000	-0.872209000
6	-3.047170000	1.041747000	-0.492232000
6	2.485581000	1.873582000	-0.638251000
6	0.436256000	-3.345616000	-0.395160000
1	-3.914610000	1.329717000	-1.111558000
1	-3.336914000	1.192630000	0.558051000
1	2.768368000	2.154354000	0.385148000
1	3.163318000	2.413040000	-1.322770000
1	0.582511000	-4.245646000	-1.018074000
1	0.516260000	-3.662278000	0.654027000
1	4.075366000	-0.568133000	0.342594000
1	-1.685160000	3.701348000	0.221492000
1	-2.510791000	-3.451091000	0.513035000
6	-1.025734000	1.570487000	2.469740000
6	-0.940618000	0.166510000	2.093708000
6	-1.857397000	-0.748952000	2.614698000
6	-2.903490000	-0.302654000	3.522912000
6	-2.986323000	1.046536000	3.881032000
6	-2.029385000	2.003765000	3.340668000
6	0.329969000	2.083726000	2.603397000
6	1.253307000	0.997692000	2.311753000
6	0.469202000	-0.188019000	1.991991000
6	0.904471000	-1.442200000	2.425421000
6	-1.405066000	-2.059056000	3.056740000
6	-3.095949000	-1.336656000	4.531700000
6	-3.363470000	-0.980554000	5.856970000

Sum ⊃ C₆₀

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

Atom	X	Y	Z
6	5.739719000	-2.805671000	1.762324000
6	5.779913000	-1.784644000	2.800652000
6	4.837267000	-0.752416000	2.800862000
6	3.818651000	-0.699537000	1.763664000
6	3.777473000	-1.678991000	0.770269000
6	4.757106000	-2.755004000	0.768824000
6	7.112020000	-3.145797000	1.411395000
6	7.999799000	-2.332572000	2.232255000
6	7.176382000	-1.491376000	3.091089000
6	7.571659000	-0.179978000	3.373660000
6	5.246537000	0.614413000	3.097671000
6	3.595519000	0.694541000	1.419380000
6	3.338244000	1.055003000	0.096634000
6	3.301976000	0.033756000	-0.939812000
6	3.515998000	-1.303618000	-0.610259000
6	4.334510000	-2.148265000	-1.469483000
6	5.103347000	-3.045188000	-0.616766000
6	6.420588000	-3.371908000	-0.953595000
6	7.445404000	-3.422520000	0.081837000
6	9.184222000	-1.826465000	1.688609000
6	9.531600000	-2.114084000	0.304245000
6	8.680157000	-2.895424000	-0.483027000
6	8.418936000	-2.519602000	-1.865874000
6	7.022862000	-2.813684000	-2.156962000
6	6.283781000	-1.953420000	-2.976383000
6	4.911905000	-1.614607000	-2.625714000
6	4.690475000	-0.215358000	-2.970966000
6	3.906517000	0.589775000	-2.141796000
6	4.476577000	1.509278000	2.243509000
6	6.384763000	3.277220000	-1.573504000
6	6.050726000	3.553377000	-0.243675000
6	7.075684000	3.500887000	0.791097000
6	8.392373000	3.173408000	0.454081000
6	8.739409000	2.885051000	-0.930402000
6	7.716727000	1.913377000	-2.960457000
6	6.321184000	1.622298000	-3.254423000
6	5.497686000	2.463347000	-2.394670000
6	4.314963000	1.956195000	-1.849965000
6	3.967694000	2.242535000	-0.465091000
6	4.814897000	3.028585000	0.321950000
6	6.473405000	2.943565000	1.995213000
6	7.213204000	2.083524000	2.814110000
6	8.584507000	1.743392000	2.461845000

6	-3.448707000	0.425621000	6.229896000	6	9.163170000	2.278636000	1.307032000
6	-3.264499000	1.418745000	5.261933000	6	9.986284000	1.437157000	0.448611000
6	-2.476345000	2.603990000	5.574320000	6	9.722572000	1.811652000	-0.933551000
6	-1.715121000	2.967398000	4.387179000	6	9.684141000	0.831475000	-1.928794000
6	-0.412063000	3.458348000	4.516177000	6	8.661241000	0.882757000	-2.962716000
6	0.631430000	3.009724000	3.603637000	6	5.925922000	0.310460000	-3.535675000
6	2.444760000	0.878094000	3.033593000	6	6.910468000	-0.763885000	-3.538563000
6	2.759905000	1.842168000	4.080141000	6	8.250682000	-0.482721000	-3.257862000
6	1.869550000	2.884215000	4.359900000	6	9.020914000	-1.378758000	-2.405842000
6	1.591619000	3.255767000	5.740142000	6	9.907173000	-0.565548000	-1.584436000
6	0.181631000	3.610439000	5.836931000	6	10.159250000	-0.926058000	-0.257931000
6	-0.549822000	3.263349000	6.976496000	6	10.199486000	0.096031000	0.779804000
6	-1.906121000	2.750096000	6.842614000	6	9.596592000	-0.461068000	1.982870000
6	-2.096858000	1.715624000	7.849369000	6	8.805873000	0.345593000	2.807088000
6	-2.852451000	0.577759000	7.550719000	6	5.076269000	2.652118000	1.705704000
6	-2.168742000	-2.423404000	4.242314000	6	6.586921000	0.894803000	3.377429000
6	-0.283320000	-1.939683000	8.430176000	6	7.756361000	2.935025000	-1.922980000
6	-0.585180000	-2.863779000	7.425790000	6	-0.093294000	1.225158000	-0.731002000
6	0.457832000	-3.311688000	6.512650000	6	-0.073239000	0.030514000	-1.442099000
6	1.760127000	-2.819468000	6.640812000	6	0.559950000	-0.089045000	-2.687236000
6	2.073989000	-1.856446000	7.686886000	6	1.049274000	1.101223000	-3.245296000
6	0.986766000	-0.021223000	8.937142000	6	1.025467000	2.333698000	-2.513442000
6	-0.423163000	0.333038000	9.033916000	6	0.513386000	2.396117000	-1.208706000
6	-1.209009000	-0.853261000	8.721598000	6	0.736197000	3.320282000	0.021734000
6	-2.397941000	-0.733137000	7.994697000	1	1.590611000	1.089306000	-4.195161000
6	-2.712873000	-1.696306000	6.947781000	1	1.544718000	3.189831000	-2.953503000
6	-1.823570000	-2.738605000	6.668945000	1	1.750498000	3.746136000	0.036189000
6	-0.135935000	-3.464718000	5.191791000	1	0.032849000	4.172258000	0.025879000
6	0.596158000	-3.117012000	4.053045000	6	-0.060068000	-1.222140000	-0.741162000
6	1.953531000	-2.604010000	4.185040000	6	-0.067885000	-1.239502000	0.648032000
6	2.522739000	-2.457785000	5.453348000	6	0.558548000	-2.250564000	1.389998000
6	3.310374000	-1.272626000	5.766008000	6	1.080689000	-3.325029000	0.652800000
6	3.030660000	-0.900243000	7.146346000	6	1.093767000	-3.305557000	-0.779986000
6	2.947800000	0.448698000	7.504514000	6	0.584325000	-2.211641000	-1.496818000
6	1.904782000	0.896892000	8.417941000	6	0.856995000	-1.599868000	-2.898238000
6	-0.858288000	1.590457000	8.606051000	1	1.617120000	-4.135641000	1.153860000
6	0.098178000	2.546831000	8.066499000	1	1.643995000	-4.099559000	-1.292896000
6	1.450910000	2.206766000	7.973437000	1	1.899057000	-1.766909000	-3.213902000
6	2.213472000	2.568444000	6.786095000	1	0.215596000	-2.046309000	-3.678500000
6	3.140014000	1.482154000	6.496138000	6	-0.089811000	-0.006100000	1.381716000
6	3.409087000	1.125873000	5.170680000	6	-0.103420000	1.206584000	0.704017000
6	3.495631000	-0.280427000	4.97333000	6	0.492962000	2.364718000	1.223611000
6	2.901038000	-0.433562000	3.475220000	6	0.986635000	2.267029000	2.532992000
6	2.143961000	-1.570335000	3.177180000	6	1.005787000	1.014273000	3.229539000
6	-1.545823000	-3.110035000	5.288370000	6	0.523367000	-0.160430000	2.633132000
6	-0.052222000	-2.398176000	2.964760000	6	0.792382000	-1.680604000	2.815541000
6	1.073301000	-1.426311000	8.563953000	1	1.501609000	3.110827000	3.001214000
				1	1.537433000	0.975812000	4.184836000
				1	1.816317000	-1.875235000	3.168675000
				1	0.109318000	-2.132733000	3.556404000

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