

Supporting information for:

Photoinduced electron transfer in nanotube $\supset$ C₇₀ inclusion complexes. Phenine vs nanographene nanotubes

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Abstract: Even small structural defects can considerably affect electronic properties of nanomaterials. In this work, we computationally study photoinduced electron transfer in fullerene inclusion complexes of two phenine nanotubes **pre-pNT $\supset$ C₇₀** and **pNT $\supset$ C₇₀** and their nanographene analog **[4]CHBC $\supset$ C₇₀**. Charge separation is shown to efficiently occur in **[4]CHBC $\supset$ C₇₀**. In contrast, the electron transfer process between the host and guest units in the **pre-pNT $\supset$ C₇₀** and **pNT $\supset$ C₇₀** complexes is blocked by regular structural changes incorporated in the nanographene framework.

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Computational Methodology

Quantum-chemical calculations

Geometry optimizations were performed employing the DFT BLYP^{1,2} exchange–correlation functional with Ahlrichs' Def2-SVP basis set,^{3, 4} and using the resolution of identity approximation (RI, alternatively termed density fitting)^{5, 6} implemented in the ORCA 4.1.2 program.^{7,8} Canonical energy decomposition analysis (EDA) was calculated using the Amsterdam Density Functional (ADF) program.⁹ Electronic structures calculations and vertical excitation energies were calculated using TDA formalism¹⁰ with the range-separated functional from Handy and coworkers' CAM-B3LYP¹¹ and Ahlrichs' Def2-SVP basis set,^{3, 4} using Gaussian 16 (rev. A03)¹² The empirical dispersion D3 correction with Becke–Johnson damping,^{13,14} was employed. The population analysis performed within Mulliken,^{15,16} Lowdin,¹⁷ Hirshfeld,¹⁸ CM5,¹⁹ iterative Hirshfeld²⁰ and NPA²¹ schemes were carried out using code implemented in Gaussian 16.

Topological analyses of the electron distributions were conducted according to the “Quantum Theory of Atoms in Molecules” (QTAIM) proposed by Bader.^{22,23} The QTAIM calculations were performed using the AIMALL suite of programs²⁴ to evaluate bond critical point properties and the associated bond descriptors – such parameters as the electron density [$\rho(r)$] in bond critical points (BCPs), its Laplacian [$\nabla^2\rho(r)$], potential energy density [$V(r)$], kinetic energy density [$G(r)$], and total electron energy density [$H(r)$] were taken into account. The NCI technique was carried out through the analysis of the reduced density gradient (RDG) at the CAM-B3LYP/Def2-SVP level Multiwfn program.²⁵ To visualize molecular structures, NCI isosurfaces and natural transition orbitals, Chemcraft 1.8. program²⁶ was used.

Analysis of excited states

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out using a tool suggested recently by Plasser et al.^{27,28} A key quantity is the parameter Ω :

$$\Omega(A, B) = \frac{1}{2} \sum_{\alpha \in A, \beta \in B} \left[\left(SP^{0i} \right)_{\alpha\beta} \left(P^{0i} S \right)_{\alpha\beta} + P_{\alpha\beta}^{0i} \left(SP^{0i} S \right)_{\alpha\beta} \right] \quad (1)$$

$$X(F_i) = \sum_{A \in F_i} \Omega(A, A) \quad (2)$$

$$\Delta q(CT^{F_i \rightarrow F_j}) = \sum_{A \in F_i, B \in F_j} \Omega(A, B) + \Omega(B, A) \quad (3)$$

$$\Delta q(CS^{F_i \rightarrow F_j}) = \sum_{A \in F_i, B \in F_j} \Omega(A, B) - \Omega(B, A) \quad (4)$$

where A and B are atoms, F_i and F_j are fragments, α and β are atomic orbitals, **P**⁰ⁱ is the transition density matrix for the ψ₀ → ψ_i excitation, and S is the overlap matrix. X(F_i) is the extent of exciton localization on the fragment F_i. Δq(CT^{F_i→F_j}) is the total amount of the electron density transferred between fragments F_i and F_j in the ψ₀ → ψ_i excitation. Δq(CS^{F_i→F_j}) is a measure of the charge separation between fragments F_i and F_j. Note that in the situation when charge transfer (F_i → F_j) is equal to the back transfer (F_j → F_i) there is no charge separation between the fragments, CS^{F_i→F_j} is equal to zero.

Solvent Effects

The equilibrium solvation energy E_s^{eq} in a medium with dielectric constant ε was estimated using a COSMO-like polarizable continuum model (CPCM) in the monopole approximation.²⁹

$$E_s^{\text{eq}}(\mathbf{Q}, \epsilon) = -\frac{1}{2} f(\epsilon) \mathbf{Q}^+ \mathbf{D} \mathbf{Q}, \quad (5)$$

where f(ε) is the dielectric scaling factor, f(ε)=(ε-1)/ε, **Q** is the vector of *n* atomic charges in the molecular system, and **D** is the *n* × *n* symmetric matrix determined by the shape of the boundary surface between solute and solvent; **D**=**B**⁺**A**⁻¹**B**, where the *m* × *m* matrix **A** describes electrostatic interaction between *m* surface charges and the *m* × *n* **B** matrix describes the interaction of the surface charges with *n* atomic charges of the solute. Atomic charges in the excited state ψ_i, were calculated using Eqs. 1-4.

Electron transfer rates

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

$$k_{ET} = \frac{2\pi}{\hbar^2} V^2 (FCWD) \quad (6)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:³⁰

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (7)$$

where λ is the reorganization energy and ΔG⁰ is the standard Gibbs energy change of the process. The fragment charge difference (FCD)^{31,32} method was employed to calculate the electronic couplings in this work.

The Marcus expression is derived for the high-temperature condition, ħω_{*l*} << *kT*, for all vibrational modes *l*. The semi-classical description of electron transfer (ET)^{33,34} 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*}, ħω_{*i*} >> *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,

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

$$V_{0 \rightarrow n}^2 = V^2 \frac{S^n}{n!} \exp(-S) \quad (8)$$

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 an 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 can be set up as 1600 cm^{-1} . It was shown that changing the parameter ω_i within a reasonable range does not lead to significant changes of the computed ET rate.³⁵

Reorganization energy

The reorganization energy is usually divided into two parts, $\lambda = \lambda_i + \lambda_s$, including the internal and solvent terms. Solvent reorganization energy corresponds to the energy required to move solvent molecules from the position they occupy in the GS to the location they have in the CT state, but without charge transfer having occurred. The λ_s for particular CT states were computed as a difference between equilibrium and non-equilibrium solvation energies. The internal reorganization energy λ_i corresponds to the energy of structural change when denoted fragments going from initial-state geometries to final-state geometries.

Interaction energies

Interaction energies were calculated directly from electronic energies of particular complexes and the electronic energies of individual fragments from which this object consists. For **Host**⋯**C₇₀**, the interaction energy can be expressed as follows:

$$E_{\text{int}} = E_{\text{Host-C}_{70}} - (E_{\text{Host}} + E_{\text{C}_{70}}) \quad (9)$$

Energy decomposition analysis

The interaction energy in the gas phase is examined in the framework of the Kohn-Sham MO model using a quantitative energy decomposition analysis (EDA)³⁶⁻³⁸ 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:

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} \quad (10)$$

The term ΔV_{elstat} corresponds to the classical electrostatic interactions between the unperturbed charge distributions of the prepared (i.e. deformed) bases 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 interaction, ΔE_{oi} , accounts for electron-pair bonding, charge transfer (i.e., donor–acceptor interactions between occupied orbitals on one moiety and unoccupied orbitals on the other, including the 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.^{39,40}

Non-covalent interactions (NCI)

The NCI method⁴¹⁻⁴³ relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s), defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \quad (11)$$

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.

Charge delocalization index

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

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

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

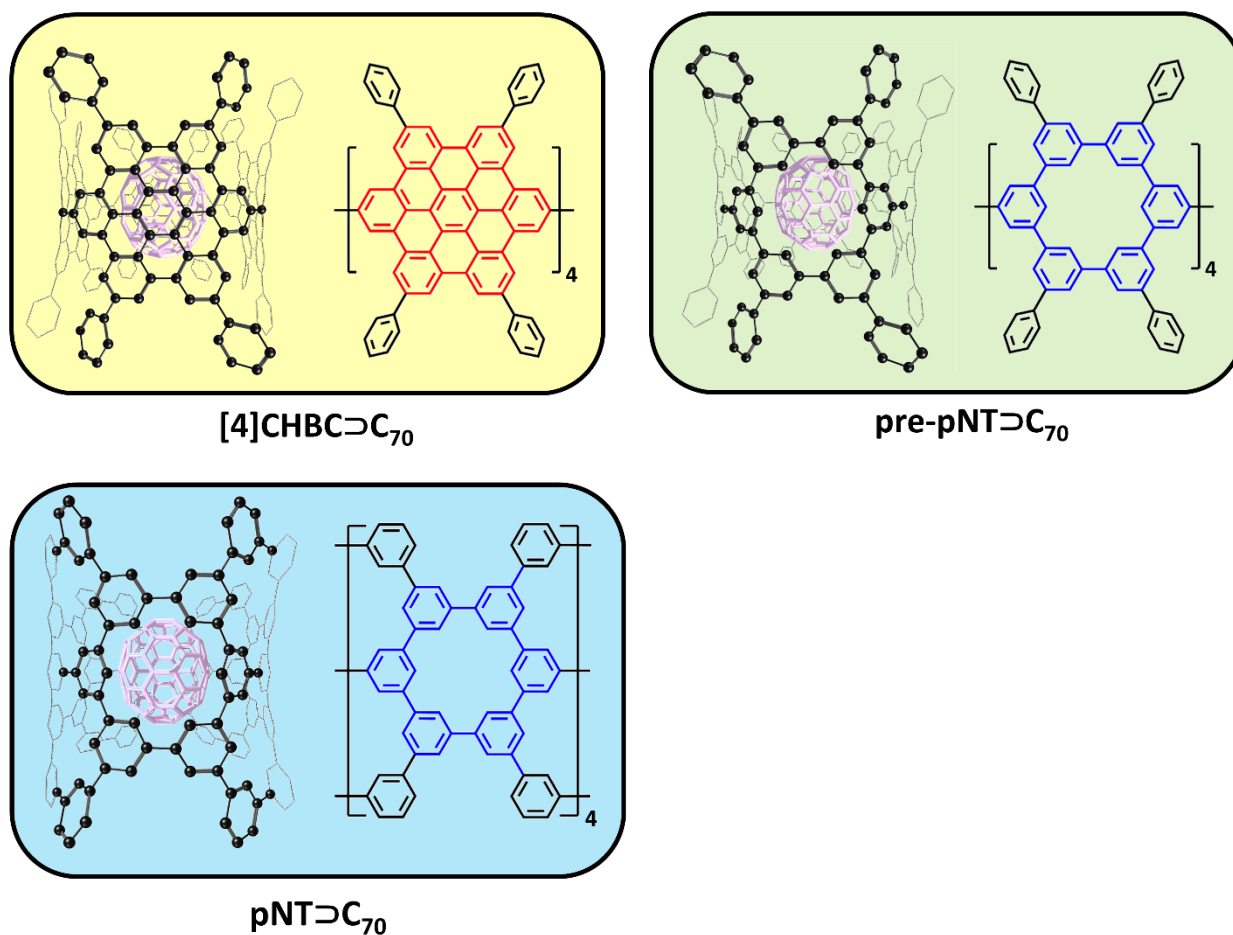


Figure S1. Graphical representation for **[4]CHBC $\supset$ C₇₀**, **pre-pNT $\supset$ C₇₀** and **pNT $\supset$ C₇₀** complexes.

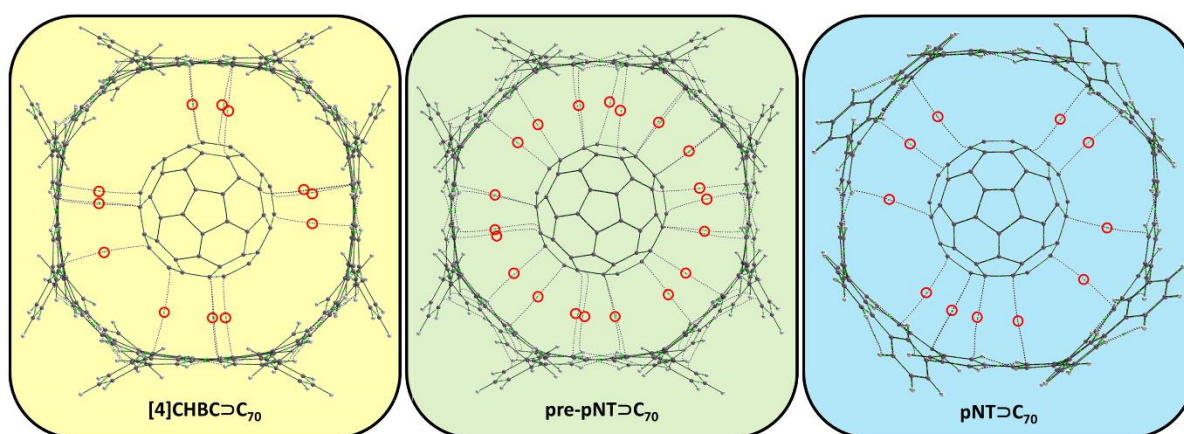


Figure S2. QTAIM molecular graph for **[4]CHBC $\supset$ C₇₀**, **pre-pNT $\supset$ C₇₀** and **pNT $\supset$ C₇₀** complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs. BCPs of interest marked by red circles.

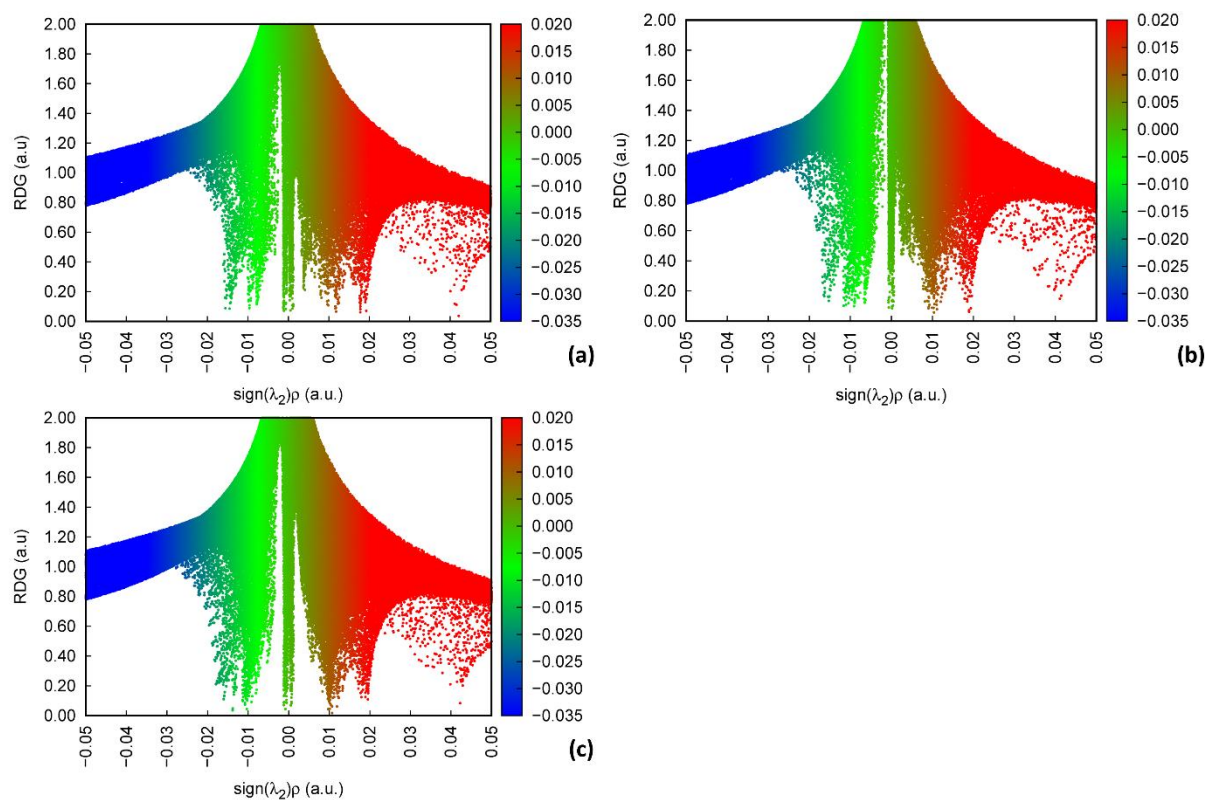


Figure S3. Plot of RDG vs. $\text{sign}(\lambda_2)\rho$ for (a) [4]CHBC $\supset$ C₇₀ (b) pre-pNT $\supset$ C₇₀ and (c) pNT $\supset$ C₇₀ complexes.

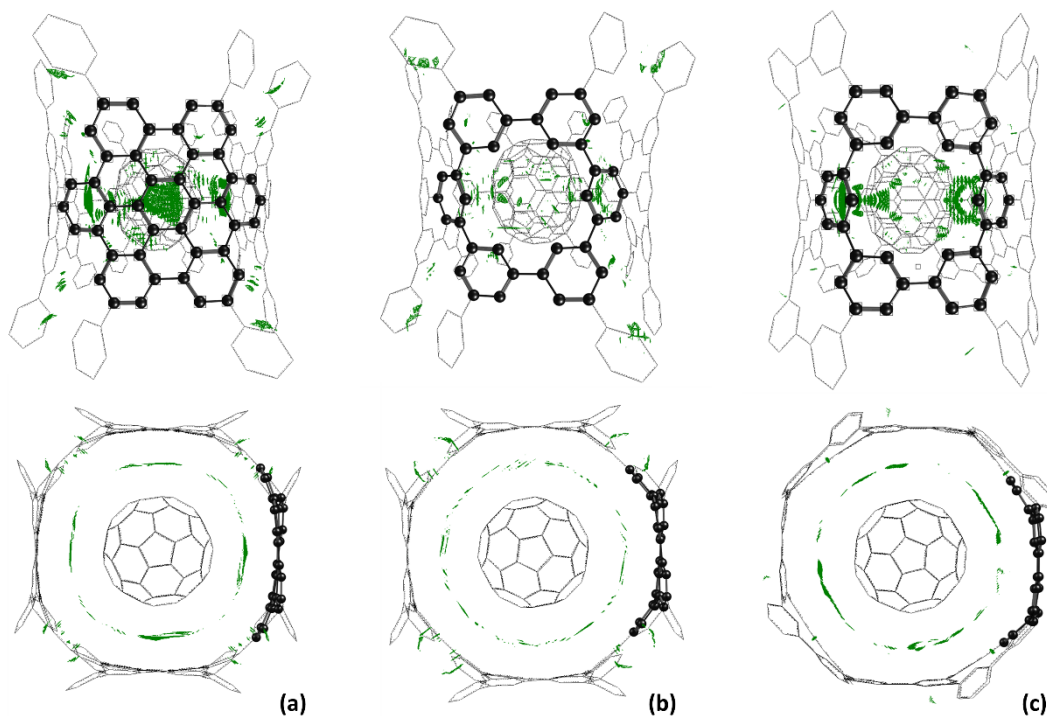


Figure S4. NCI isosurfaces of van der Waals interactions ($-0.005 < \text{sign}(\lambda_2)\rho < 0.005$ a.u.) for (a) [4]CHBC $\supset$ C₇₀, (b) pre-pNT $\supset$ C₇₀, and (c) pNT $\supset$ C₇₀ complexes. Isosurfaces were generated for RDG = 0.6 a.u.

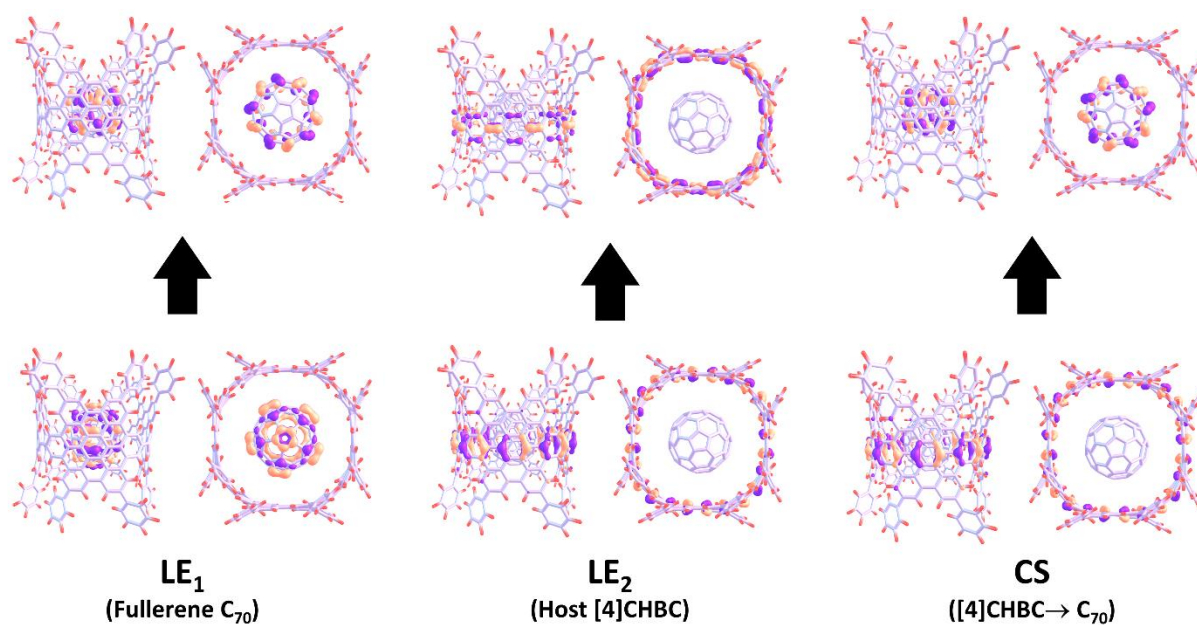


Figure S5. Natural transition molecular orbitals representing the LE1, LE2, and CS states in [4]CHBC⊃C₇₀ complex.

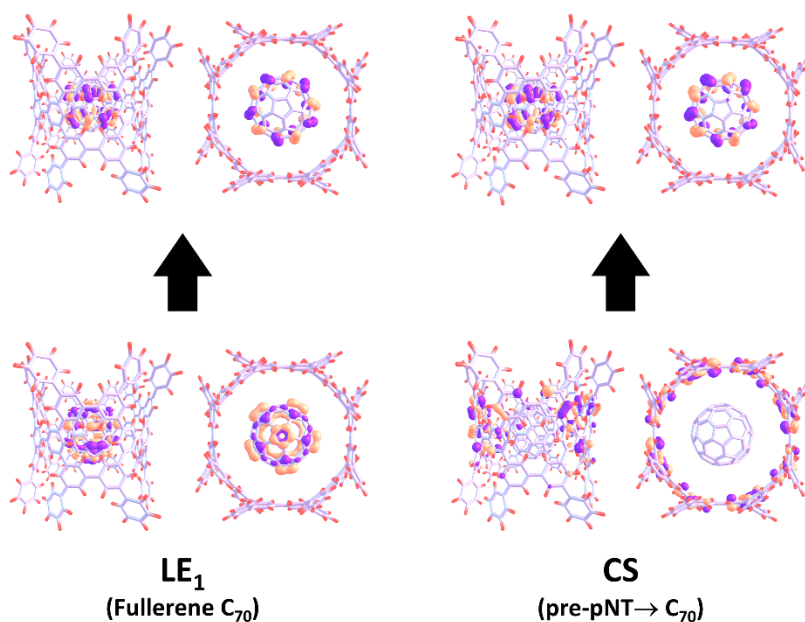


Figure S6. Natural transition molecular orbitals representing the LE1 and CS states in pre-pNT⊃C₇₀ complex.

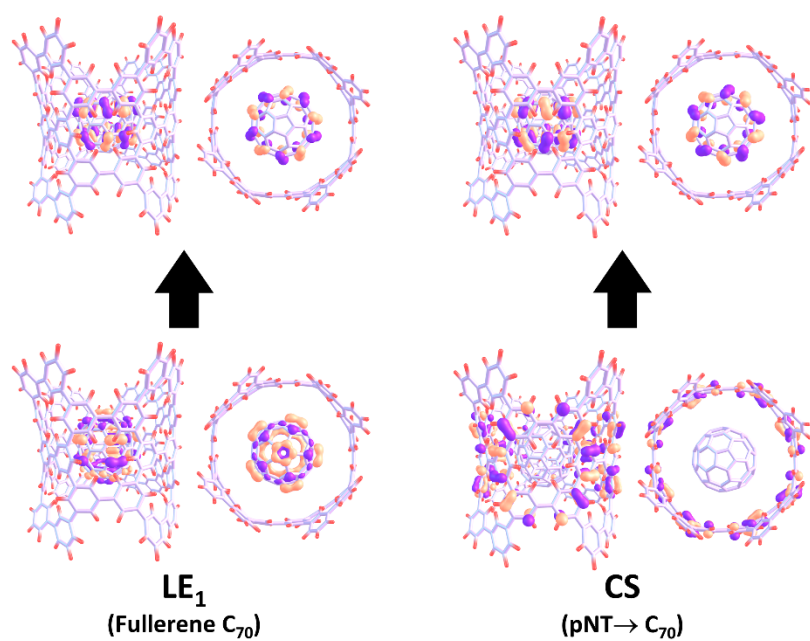


Figure S7. Natural transition molecular orbitals representing the LE1 and CS states in **pNT⊃C₇₀** complex.

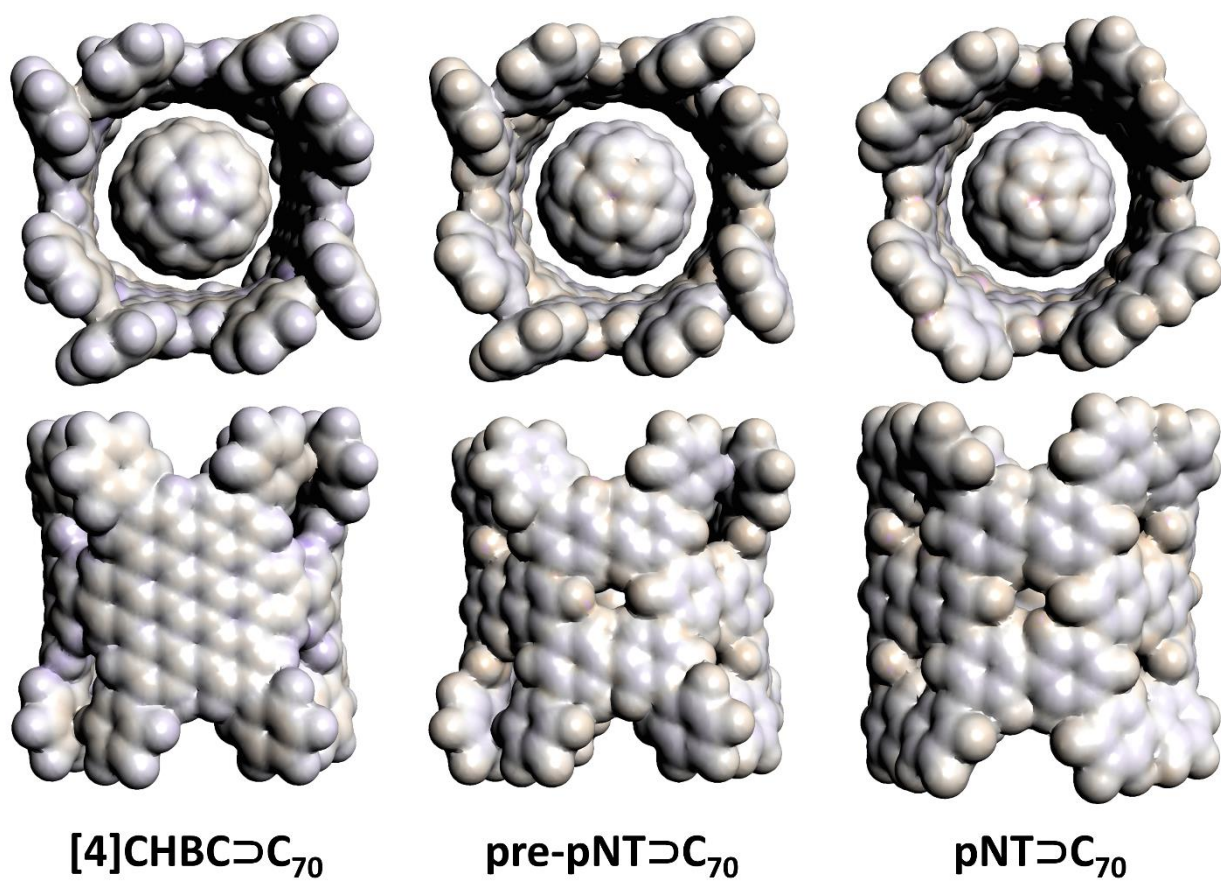


Figure S8. Solvent-excluded surface for **[4]CHBC⊃C₇₀**, **pre-pNT⊃C₇₀** and **pNT⊃C₇₀** complexes.

Table S1. EDA Results for [4]CHBC $\supset$ C₇₀, pre-pNT $\supset$ C₇₀ and pNT $\supset$ C₇₀ investigated complexes.^[a]

Complex	Energy terms				
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}
[4]CHBC $\supset$ C ₇₀	9.09	-6.22 (10.1)	-8.19 (13.2)	-47.46 (76.7)	-61.87
pre-pNT $\supset$ C ₇₀	7.40	-3.31 (7.4)	-5.81 (13.0)	-35.45 (79.6)	-44.57
pNT $\supset$ C ₇₀	8.55	-4.46 (8.7)	-6.89 (13.5)	-39.64 (77.6)	-50.99

^[a] The energy values are listed in kilocalories per mole. The relative values (in parentheses) are listed in percent and express the contribution to the sum of all attractive energy terms: $\Delta E_{\text{elstat}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}}$.

Table S2. Charge separation between the fragments in electronic ground state for [4]CHBC $\supset$ C₇₀, pre-pNT $\supset$ C₇₀ and pNT $\supset$ C₇₀ complexes. Q_{Tot} - total charge of the complex, Q_{Cage} - charge on the cage, and $Q_{\text{C}_{70}}$ - charge on C₇₀.

Charge Scheme	[4]CHBC $\supset$ C ₇₀			pre-pNT $\supset$ C ₇₀			pNT $\supset$ C ₇₀		
	Q_{Tot}	Q_{Cage}	$Q_{\text{C}_{70}}$	Q_{Tot}	Q_{Cage}	$Q_{\text{C}_{70}}$	Q_{Tot}	Q_{Cage}	$Q_{\text{C}_{70}}$
Mulliken	0.000	0.002	-0.002	0.000	0.005	-0.005	0.000	0.005	-0.005
Lowdin	0.000	0.002	-0.002	0.000	0.003	-0.003	0.000	0.003	-0.003
Hirsh.	-0.001	0.033	-0.034	-0.001	0.029	-0.029	-0.001	0.029	-0.029
CM5	-0.001	0.033	-0.034	-0.001	0.028	-0.029	-0.001	0.028	-0.029
Hirsh.-I	-0.001	0.077	-0.078	-0.001	0.120	-0.121	-0.001	0.012	-0.012
NPA	0.000	-0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000

Table S3. Selected bond critical points 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 $[H(r)]$ related to the non-covalent interactions of the fragments for studied [4]CHBC $\supset$ C₇₀ and pre-pNT $\supset$ C₇₀ complexes in the gas phase.

Bond critical points	Interacting atoms	$\rho(r)$, au	$\nabla^2\rho(r)$, au	$V(r)$, au	$G(r)$, au	$H(r)$, au
[4]CHBC $\supset$ C ₇₀						
C ₇₀ ...[4]CHBC	C...C	3.91E-04	1.73E-03	-1.71E-04	3.01E-04	1.30E-04
		1.10E-03	3.42E-03	-4.78E-04	6.67E-04	1.89E-04
		1.24E-03	3.72E-03	-5.31E-04	7.31E-04	2.00E-04
		1.24E-03	3.70E-03	-5.33E-04	7.29E-04	1.96E-04
		1.12E-03	3.48E-03	-4.78E-04	6.73E-04	1.95E-04
		1.17E-03	3.50E-03	-4.86E-04	6.80E-04	1.94E-04
		1.11E-03	3.40E-03	-4.63E-04	6.56E-04	1.93E-04
		6.20E-04	2.42E-03	-2.74E-04	4.40E-04	1.66E-04
		6.05E-04	2.38E-03	-2.67E-04	4.31E-04	1.64E-04
		1.13E-03	3.42E-03	-4.70E-04	6.63E-04	1.93E-04
		1.12E-03	3.40E-03	-4.64E-04	6.57E-04	1.93E-04
		1.11E-03	3.44E-03	-4.70E-04	6.65E-04	1.95E-04
		1.26E-03	3.73E-03	-5.37E-04	7.34E-04	1.97E-04

		3.86E-04	1.70E-03	-1.68E-04	2.96E-04	1.28E-04
		1.09E-03	3.39E-03	-4.72E-04	6.60E-04	1.88E-04
		2.93E-04	1.44E-03	-1.35E-04	2.47E-04	1.12E-04
	pre-pNT$\supset$C₇₀					
C₇₀...pre-pNT	C...C	6.39E-04	2.24E-03	-2.53E-04	4.07E-04	1.54E-04
		7.06E-04	2.52E-03	-2.93E-04	4.61E-04	1.68E-04
		3.33E-04	1.39E-03	-1.29E-04	2.37E-04	1.08E-04
		3.63E-04	1.34E-03	-1.23E-04	2.30E-04	1.07E-04
		3.02E-04	1.34E-03	-1.21E-04	2.28E-04	1.07E-04
		6.14E-04	2.27E-03	-2.57E-04	4.13E-04	1.56E-04
		6.27E-04	2.30E-03	-2.60E-04	4.17E-04	1.57E-04
		3.24E-04	1.41E-03	-1.29E-04	2.40E-04	1.11E-04
		3.02E-04	1.29E-03	-1.17E-04	2.20E-04	1.03E-04
		6.91E-04	2.49E-03	-2.88E-04	4.55E-04	1.67E-04
		6.22E-04	2.20E-03	-2.46E-04	3.97E-04	1.51E-04
		3.77E-04	1.54E-03	-1.48E-04	2.66E-04	1.18E-04
		1.96E-04	9.82E-04	-8.20E-05	1.64E-04	8.20E-05
		6.87E-04	2.35E-03	-2.69E-04	4.28E-04	1.59E-04
		5.39E-04	2.05E-03	-2.18E-04	3.65E-04	1.47E-04
		5.48E-04	2.08E-03	-2.23E-04	3.71E-04	1.48E-04
		6.87E-04	2.35E-03	-2.69E-04	4.28E-04	1.59E-04
		1.96E-04	9.71E-04	-8.10E-05	1.62E-04	8.10E-05
		4.21E-04	1.52E-03	-1.50E-04	2.65E-04	1.15E-04
		3.54E-04	1.47E-03	-1.39E-04	2.53E-04	1.14E-04
	C...H	3.70E-04	1.40E-03	-1.31E-04	2.40E-04	1.09E-04
		3.45E-04	1.32E-03	-1.20E-04	2.25E-04	1.05E-04
		3.79E-04	1.39E-03	-1.30E-04	2.39E-04	1.09E-04
		3.90E-04	1.43E-03	-1.38E-04	2.48E-04	1.10E-04
		2.14E-04	8.93E-04	-7.10E-05	1.47E-04	7.60E-05
		1.95E-04	8.29E-04	-6.50E-05	1.36E-04	7.10E-05
	pNT$\supset$C₇₀					
C₇₀...pNT	C...C	5.23E-04	2.00E-03	-2.13E-04	3.56E-04	1.43E-04
		5.23E-04	2.00E-03	-2.13E-04	3.56E-04	1.43E-04
		1.18E-03	3.46E-03	-4.80E-04	6.72E-04	1.92E-04
		1.18E-03	3.45E-03	-4.80E-04	6.72E-04	1.92E-04
		1.08E-03	3.36E-03	-4.51E-04	6.46E-04	1.95E-04
		7.88E-04	2.82E-03	-3.48E-04	5.26E-04	1.78E-04
		7.92E-04	2.83E-03	-3.50E-04	5.29E-04	1.79E-04
		6.14E-04	2.07E-03	-2.32E-04	3.75E-04	1.43E-04
		6.16E-04	2.07E-03	-2.33E-04	3.76E-04	1.43E-04
		2.33E-04	1.07E-03	-9.00E-05	1.79E-04	8.90E-05
		2.33E-04	1.07E-03	-9.00E-05	1.79E-04	8.90E-05
		1.19E-03	3.62E-03	-4.99E-04	7.02E-04	2.03E-04
		5.84E-04	1.98E-03	-2.16E-04	3.55E-04	1.39E-04
		5.84E-04	1.98E-03	-2.16E-04	3.55E-04	1.39E-04
		7.32E-04	2.67E-03	-3.13E-04	4.90E-04	1.77E-04

		9.15E-04	2.86E-03	-3.64E-04	5.40E-04	1.76E-04
		9.12E-04	2.86E-03	-3.63E-04	5.39E-04	1.76E-04
	C...H	4.04E-04	1.51E-03	-1.45E-04	2.61E-04	1.16E-04
		4.03E-04	1.51E-03	-1.45E-04	2.61E-04	1.16E-04

Table S4. Excitation energies (E_x , eV) and dipole moments in ground state (μ_0 , D), change in dipole moments between ground state and state of interest ($\Delta\mu = \mu_i - \mu_0$, D) and solvation energies (E_{solv} , eV) calculated for DCM.

	Supramolecular host-guest systems		
	[4]CHBC $\supset$ C ₇₀	pre-pNT $\supset$ C ₇₀	pNT $\supset$ C ₇₀
	Ground state (GS)		
E _x	0.000	0.000	0.000
μ ₀	0.07	0.01	0.14
E _{solv}	-0.233	-0.241	-0.217
	LE ₁ (Fullerene C ₇₀)		
E _x	2.289	2.298	2.300
Δμ	0.02	0.09	0.09
E _{solv}	-0.240	-0.249	-0.225
	LE ₂ (Host)		
E _x	2.946	n/f*	n/f*
Δμ	0.03		
E _{solv}	-0.233		
	Most absorptive transition		
E _x	3.140	3.372	3.372
Δμ	0.06	0.56	0.35
E _{solv}	-0.246	-0.275	-0.250
	CS (Host → Fullerene C ₇₀)		
E _x	2.182	3.659	3.641
Δμ	0.46	2.17	1.24
E _{solv}	-0.629	-0.816	-0.768

* n/f – states of interest are not found within considered number of excited states.

Table S5. Charge delocalization over the fragment index (IPR) in the CS states for [4]CHBC $\supset$ C₇₀, pre-pNT $\supset$ C₇₀ and pNT $\supset$ C₇₀ complexes. Δq - indicates charge difference on the fragment, while Δq_i^2 - corresponds to square of particular atom charge difference in CS state as compared to GS.

	[4]CHBC $\supset$ C ₇₀		pre-pNT $\supset$ C ₇₀		pNT $\supset$ C ₇₀	
	C ₇₀	[4]CHBC	C ₇₀	pre-pNT	C ₇₀	pNT
Δq	0.995	-0.995	0.991	-0.991	0.992	-0.992
$\sum_i^n q_i^2$	0.0213	0.0091	0.0187	0.0147	0.018	0.011
IPR	47	109	53	67	54	92

Table S6. Semi-classical rates (k_x in s^{-1}) and characteristic times (τ in ps) computed for the CS process in **[4]CHBC**→**C₇₀** complex in DCM using different values of the effective Huang-Rhys (S_{eff}) factor.

$\hbar\omega_{eff}$	ΔG^0 , eV	$ V $, eV	λ_s	λ_i	S_{eff}	k_x , s^{-1}	τ , ps
	LE ₁ → CS						
1200	-0.107	$2.05 \cdot 10^{-4}$	0.148	0.177	0.995	$1.33 \cdot 10^{11}$	7.54
1400					0.853	$1.31 \cdot 10^{11}$	7.66
1600					0.746	$1.29 \cdot 10^{11}$	7.73
1800					0.663	$1.29 \cdot 10^{11}$	7.77
2000					0.597	$1.28 \cdot 10^{11}$	7.79

Table S7. Semi-classical rates (k_x in s^{-1}) computed for the CS process in **[4]CHBC**→**C₇₀** in DCM using different values of the internal (λ_i) and solvent (λ_s) reorganization energy.

		Solvent reorg. energy (λ_s)			
Internal reorg. energy (λ_i)		150	200	250	300
	150	$1.633 \cdot 10^{11}$	$1.045 \cdot 10^{11}$	$6.425 \cdot 10^{10}$	$3.883 \cdot 10^{10}$
	200	$1.632 \cdot 10^{11}$	$1.046 \cdot 10^{11}$	$6.427 \cdot 10^{10}$	$3.884 \cdot 10^{10}$
	250	$1.631 \cdot 10^{11}$	$1.046 \cdot 10^{11}$	$6.425 \cdot 10^{10}$	$3.883 \cdot 10^{10}$
	300	$1.629 \cdot 10^{11}$	$1.045 \cdot 10^{11}$	$6.421 \cdot 10^{10}$	$3.881 \cdot 10^{10}$

Cartesian coordinates

[4]CHBC $\supset$ C₇₀

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

Atom	X	Y	Z
6	-1.238948000	1.431343000	-8.277443000
6	-0.027085000	0.756420000	-8.530552000
6	1.192724000	2.793047000	-7.870591000
6	1.167400000	1.506295000	-8.440181000
6	2.462335000	3.477818000	-7.585477000
6	3.673286000	3.083194000	-8.189426000
6	4.911032000	4.647478000	-6.818889000
6	4.907729000	3.669746000	-7.835895000
6	-3.777976000	2.825886000	-7.762909000
6	-2.541779000	3.352376000	-7.342894000
6	-1.272696000	2.728014000	-7.734578000
6	-0.024252000	4.505669000	-6.520156000
6	-0.036078000	3.374484000	-7.413928000
6	1.227230000	5.023492000	-6.056441000
6	2.471210000	4.528558000	-6.608011000
6	3.752211000	6.027957000	-5.058914000
6	3.728121000	5.073298000	-6.178503000
6	4.964576000	6.461118000	-4.478275000
6	-4.976794000	4.461970000	-6.444568000
6	-5.005660000	3.350319000	-7.312079000
6	-3.764996000	5.046219000	-6.014796000
6	-2.522000000	4.487092000	-6.467844000
6	-1.240064000	6.048098000	-5.015251000
6	-1.258407000	5.026629000	-6.012497000
6	0.011594000	6.512645000	-4.498632000
6	1.245698000	6.013439000	-5.027914000
6	2.530227000	7.339200000	-3.350853000
6	2.509566000	6.471076000	-4.490976000
6	3.766777000	7.762544000	-2.827880000
6	4.994272000	7.321738000	-3.361265000
6	-4.925062000	6.795190000	-4.621931000
6	-3.741475000	6.160774000	-5.054463000
6	-2.475084000	7.563323000	-3.455840000
6	-2.484158000	6.591757000	-4.511986000
6	-1.203934000	7.849985000	-2.774625000
6	0.024315000	7.399700000	-3.362149000
6	1.231344000	8.260611000	-1.420138000
6	1.262179000	7.722036000	-2.718812000
6	-4.921973000	7.807159000	-3.639015000
6	-3.686829000	8.161213000	-3.054242000
6	-1.175682000	8.416692000	-1.486726000
6	0.021048000	8.509775000	-0.740864000
1	-2.180568000	0.883382000	-8.357589000
1	2.120933000	1.027470000	-8.680488000
1	3.663031000	2.292657000	-8.948721000
1	5.865196000	5.109825000	-6.545908000
1	-3.798211000	1.991458000	-8.472183000
1	5.917495000	6.081722000	-4.862949000
1	-5.929439000	4.839366000	-6.057249000
1	3.787427000	8.466300000	-1.988799000

pre-pNT $\supset$ C₇₀

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

Atom	X	Y	Z
6	-3.299223000	-2.465246000	0.001599000
6	-2.516496000	-2.841677000	-1.174901000
6	-4.047891000	-1.269131000	0.000239000
6	-2.516184000	-2.017296000	-2.313883000
6	-1.272005000	-1.782667000	-3.040220000
6	-0.055529000	-2.446839000	-2.671928000
6	1.162108000	-1.785465000	-3.041475000
6	-3.296420000	-0.775077000	2.321233000
6	-2.514275000	-2.010698000	2.315359000
6	-4.046398000	-0.406552000	1.184012000
6	-2.515381000	-2.838074000	1.178509000
6	-1.272020000	-3.456299000	0.729061000
6	-0.054734000	-3.311902000	1.473079000
6	1.161595000	-3.459161000	0.728043000
6	-0.056052000	-3.316013000	-1.470171000
6	-1.272729000	-3.458561000	-0.724780000
6	1.160909000	-3.461119000	-0.725792000
6	-3.293570000	1.953158000	1.430391000
6	-2.510129000	1.565717000	2.602780000
6	-4.044520000	0.985721000	0.729326000
6	-2.511101000	0.228712000	3.038185000
6	-1.267552000	-0.390478000	3.486017000
6	-0.049772000	0.361395000	3.575251000
6	1.166236000	-0.393099000	3.484713000
6	-0.053326000	-2.439158000	2.672225000
6	-1.269487000	-1.774086000	3.039937000
6	1.164617000	-1.776752000	3.038711000
6	-3.294816000	1.949042000	-1.439751000
6	-2.509681000	2.943214000	-0.709421000
6	-4.045196000	0.983630000	-0.735282000
6	-2.509139000	2.945335000	0.696698000
6	-1.264665000	3.179930000	1.422397000
6	-0.047492000	3.496383000	0.733444000
6	1.169544000	3.176995000	1.421333000
6	-0.048391000	1.771755000	3.116489000
6	-1.265217000	2.328041000	2.600213000
6	1.169291000	2.325168000	2.599230000
6	-3.298448000	-0.781722000	-2.322782000
6	-2.513764000	0.220083000	-3.043240000
6	-4.047488000	-0.409927000	-1.185981000
6	-2.512461000	1.558358000	-2.611822000
6	-1.267490000	2.320563000	-2.612348000
6	-0.051042000	1.762967000	-3.128001000
6	1.167005000	2.317949000	-2.613247000
6	-0.048070000	3.494236000	-0.749804000
6	-1.265816000	3.175716000	-1.436857000
6	1.168415000	3.173241000	-1.437886000
6	-0.052800000	0.351280000	-3.582774000
6	-1.270487000	-0.400255000	-3.490109000
6	1.163275000	-0.403085000	-3.491453000

1	-5.879606000	6.521722000	-5.083192000	6	3.194505000	1.941800000	-1.442436000
1	2.174651000	8.342806000	-0.875268000	6	2.410207000	1.552860000	-2.613775000
1	-3.676685000	8.915962000	-2.259390000	6	2.408207000	0.214586000	-3.045331000
1	-2.128178000	8.653843000	-1.004371000	6	3.943295000	0.974690000	-0.738639000
6	6.175831000	3.266756000	-8.508688000	6	3.195792000	1.945834000	1.427716000
6	-6.285642000	2.703431000	-7.711562000	6	2.412902000	2.939689000	0.694572000
6	6.275203000	7.724748000	-2.718343000	6	2.412365000	2.937860000	-0.711550000
6	-6.190481000	8.476867000	-3.232211000	6	3.943972000	0.976738000	0.725968000
6	6.187107000	2.863854000	-9.868173000	6	3.193306000	-0.782459000	2.318450000
6	7.385546000	2.508868000	-10.509507000	6	2.410873000	0.223145000	3.036035000
6	8.605583000	2.550937000	-9.809013000	6	2.412514000	1.560165000	2.600828000
6	8.611822000	2.940749000	-8.456366000	6	3.943162000	-0.415544000	1.180606000
6	7.412015000	3.289091000	-7.813716000	6	3.190356000	-2.472568000	-0.001142000
1	5.248048000	2.858996000	-10.438413000	6	2.406754000	-2.843887000	1.176437000
1	7.367442000	2.206167000	-11.566440000	6	2.408262000	-2.016288000	2.313079000
1	9.543508000	2.274478000	-10.311457000	6	3.941664000	-1.278110000	-0.003170000
1	9.555640000	2.959828000	-7.892387000	6	3.191257000	-0.788935000	-2.325547000
1	7.429774000	3.560811000	-6.749538000	6	2.406341000	-2.022792000	-2.316191000
6	7.443188000	7.972807000	-3.480382000	6	2.405642000	-2.846939000	-1.176990000
6	8.643614000	8.351451000	-2.854660000	6	3.942057000	-0.418866000	-1.189370000
6	8.702075000	8.487335000	-1.454477000	6	-2.589185544	4.675379377	-6.677642891
6	7.551656000	8.238897000	-0.682414000	1	-1.636923764	5.097508880	-6.343712470
6	6.353829000	7.861594000	-1.309101000	6	-2.553398581	3.542250528	-7.516020234
1	7.400349000	7.894994000	-4.576088000	6	-3.779941606	2.990260628	-7.944955764
1	9.536386000	8.550172000	-3.465800000	1	-3.778318039	2.144567098	-8.643260228
1	9.640229000	8.784661000	-0.963671000	6	-5.016154915	3.510599064	-7.502538236
1	7.589991000	8.329660000	0.409694000	6	-5.011070383	4.626209616	-6.631801816
1	5.471639000	7.639231000	-0.692935000	1	-5.969690906	4.982774911	-6.235942897
6	-6.358333000	1.294623000	-7.855550000	6	-3.802686774	5.229503345	-6.206420011
6	-7.555320000	0.664313000	-8.229397000	6	-2.573801431	6.708600958	-4.570366948
6	-8.710745000	1.432179000	-8.467290000	1	-1.659503645	6.143786712	-4.776111066
6	-8.658198000	2.831867000	-8.324113000	6	-3.781319861	6.351843095	-5.213621889
6	-7.458608000	3.461238000	-7.948890000	6	-4.951656391	7.050857937	-4.834594455
1	-5.472141000	0.681397000	-7.641126000	1	-5.903874269	6.828044965	-5.330605394
1	-7.588959000	-0.427378000	-8.325571000	6	-4.931653695	8.052101968	-3.833962093
1	-9.648282000	0.938402000	-8.761619000	6	-3.698814862	8.385020454	-3.225288755
1	-9.554886000	3.439863000	-8.514684000	1	-3.672097890	9.151736082	-2.439887880
1	-7.420500000	4.556708000	-7.865494000	6	-2.508624790	7.718180695	-3.587324857
6	-7.426133000	7.781006000	-3.257378000	6	0.016118798	7.830208976	-3.566624924
6	-8.626529000	8.421344000	-2.906771000	1	0.010234384	7.723778621	-4.658815182
6	-8.621463000	9.772415000	-2.511551000	6	-1.214068831	7.943591055	-2.879242668
6	-7.401943000	10.473606000	-2.466259000	6	-1.198388007	8.127676633	-1.480405959
6	-6.202940000	9.834605000	-2.823462000	1	-2.160423196	8.185839550	-0.960170855
1	-7.443056000	6.717886000	-3.533232000	6	0.009482089	8.131718588	-0.743970196
1	-9.569886000	7.856680000	-2.928211000	6	1.215533290	7.988474490	-1.464621311
1	-9.559864000	10.273093000	-2.233533000	1	2.161571508	7.905143618	-0.921758478
1	-7.384650000	11.529176000	-2.158813000	6	1.243882483	7.835251994	-2.867963660
1	-5.264370000	10.405614000	-2.816111000	6	2.576575132	6.693963041	-4.673446781
6	-1.149475000	1.497288000	8.441534000	1	1.624097189	6.357318074	-5.092925828
6	0.045566000	0.748237000	8.531604000	6	2.541668153	7.531776308	-3.539872090
6	1.290171000	2.722991000	7.742040000	6	3.768570892	7.964153509	-2.991388774
6	1.257238000	1.424985000	8.282051000	1	3.767404573	8.662053231	-2.145366462
6	2.558972000	3.350967000	7.355063000	6	5.004548409	7.525758936	-3.515676554
6	3.795042000	2.827549000	7.779223000	6	4.998746698	6.655494899	-4.631643564
6	4.994071000	4.467736000	6.465972000	1	5.957466479	6.262678029	-4.991291491
6	5.022896000	3.355714000	7.333060000	6	3.789831627	6.226661820	-5.231412723
6	-3.656894000	3.072362000	8.190478000	6	2.561421496	4.587863221	-6.707771310

6	-2.445554000	3.468550000	7.588272000	1	1.648243101	4.790518769	-6.140031594
6	-1.175539000	2.784850000	7.874076000	6	3.768100976	5.234456680	-6.354253508
6	0.041407000	4.500449000	6.527531000	6	4.937458187	4.859334595	-7.057008311
6	0.053245000	3.368227000	7.419970000	1	5.888869047	5.358027621	-6.836746158
6	1.275693000	5.023613000	6.022507000	6	4.917430361	3.859111743	-8.058654198
6	2.539219000	4.486315000	6.480686000	6	3.685405767	3.246983594	-8.388227895
6	3.758883000	6.162083000	5.069761000	1	3.658688911	2.461968634	-9.155337849
6	3.782250000	5.048546000	6.031509000	6	2.496137640	3.605191358	-7.717694286
6	4.942538000	6.796545000	4.637206000	6	-0.028824915	3.576846223	-7.821808742
6	-4.894217000	4.637077000	6.820213000	1	-0.025918838	4.668984373	-7.714704757
6	-4.891412000	3.658705000	7.836605000	6	1.203083795	2.893267737	-7.939462535
6	-3.711035000	5.063650000	6.180988000	6	1.191124284	1.494484810	-8.124209772
6	-2.454125000	4.520175000	6.611817000	1	2.154581217	0.977245610	-8.185550320
6	-1.228161000	6.008564000	5.035366000	6	-0.014503725	0.754396343	-8.125032466
6	-1.209994000	5.017350000	6.062681000	6	-1.222307914	1.471310518	-7.977817247
6	0.006119000	6.509647000	4.508230000	1	-2.166447357	0.925546279	-7.891980160
6	1.257601000	6.045926000	5.026113000	6	-1.254481415	2.874470750	-7.823754294
6	2.493019000	7.562612000	3.468542000	6	2.607955655	4.668738585	6.682881334
6	2.501835000	6.591365000	4.525065000	1	1.655652885	5.090221229	6.348269844
6	3.704730000	8.160955000	3.067657000	6	2.572099512	3.535113454	7.520585043
6	4.939586000	7.807502000	3.653241000	6	3.798549073	2.983502157	7.950255845
6	-4.946810000	6.448325000	4.478058000	1	3.796736107	2.137369679	8.648029361
6	-3.734714000	6.018165000	5.061419000	6	5.034841611	3.504973497	7.509384699
6	-2.512011000	7.332812000	3.356676000	6	5.029862298	4.621261896	6.639514066
6	-2.491850000	6.464287000	4.496402000	1	5.988692364	4.978799418	6.245054695
6	-1.243475000	7.718343000	2.727335000	6	3.821532431	5.224078376	6.213299975
6	-0.006075000	7.397210000	3.372097000	6	2.593035523	6.704826756	4.578366139
6	1.195220000	8.415218000	1.497798000	1	1.678489693	6.140310968	4.783770642
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6	-2.528650000	-7.329373000	-3.337464000	1	-7.395600057	3.638248134	6.953595397
6	-1.256763000	-7.717066000	-2.716468000	1	-5.237981508	3.069664785	10.677683068
6	-0.016821000	-6.499419000	-4.497772000	1	-9.500633057	2.896864053	8.058960854
6	-0.022816000	-7.392076000	-3.365732000	1	-7.333262222	2.285479780	11.771922041
6	1.231806000	-6.032393000	-5.019483000	1	-9.484409427	2.205416301	10.475982656
6	2.478855000	-6.579093000	-4.526811000	6	-6.244166498	-2.842000544	7.945446262
6	3.750882000	-5.028247000	-6.031970000	6	-6.298566199	-1.432963161	8.100470046
6	3.732995000	-6.145794000	-5.074906000	6	-7.423285342	-3.585779098	8.195383036
6	4.960185000	-4.444727000	-6.469790000	6	-7.481512628	-0.789366395	8.498284108
6	-4.969546000	-6.440747000	-4.441976000	6	-8.609500526	-2.943910809	8.592041565
6	-4.992648000	-7.306359000	-3.328715000	6	-8.642973614	-1.544932013	8.747002172
6	-3.760666000	-6.008190000	-5.030190000	1	-5.407564741	-0.829326474	7.879416997
6	-2.514709000	-6.456198000	-4.473647000	1	-7.400528188	-4.681071838	8.104687611
6	-1.241598000	-5.002824000	-6.041195000	1	-7.500207020	0.303327993	8.606589346
6	-1.254026000	-5.997453000	-5.017119000	1	-9.510926391	-3.542141662	8.790985192
6	0.007139000	-4.483388000	-6.510362000	1	-9.570264320	-1.042896918	9.059366036
6	1.244273000	-5.006445000	-6.012141000	6	-6.174520564	-8.713915432	3.427633802
6	2.519845000	-3.330295000	-7.347542000	6	-7.394735568	-7.993573228	3.379135089
6	2.505201000	-4.466549000	-6.474396000	6	-6.188699308	-10.073515499	3.026933362
6	3.753531000	-2.804615000	-7.775827000	6	-8.583327448	-8.609823536	2.952333526
6	4.983964000	-3.331388000	-7.335324000	6	-7.375941883	-10.689330891	2.596656101
6	-4.929943000	-4.623501000	-6.779327000	6	-8.580025786	-9.961267197	2.558607666
6	-3.743194000	-5.050450000	-6.147019000	1	-7.404200838	-6.929185756	3.651394652
6	-2.485711000	-3.453087000	-7.558864000	1	-5.261246171	-10.660683379	3.075997200
6	-2.488794000	-4.505497000	-6.583272000	1	-9.514669733	-8.026355317	2.913387339
6	-1.217487000	-2.769375000	-7.852128000	1	-7.361919146	-11.746640017	2.294815634
6	0.013819000	-3.350763000	-7.402280000	1	-9.508549561	-10.442895862	2.220022017
6	1.212355000	-1.409635000	-8.276830000	6	-6.270715984	-7.935049409	-2.828442690
6	1.248704000	-2.704969000	-7.730870000	6	-7.452624137	-8.181263157	-3.569023620
6	-4.932710000	-3.644377000	-7.794924000	6	-6.321468305	-8.091098679	-1.419381523
6	-3.700357000	-3.057361000	-8.154807000	6	-8.637989019	-8.575466944	-2.924072314
6	-1.194858000	-1.484420000	-8.425604000	6	-7.503537532	-8.486543082	-0.772724619

6	-0.000690000	-0.735533000	-8.526370000	6	-8.667796772	-8.731663962	-1.525148646
1	-2.158008000	-8.347068000	-0.870985000	1	-7.432882614	-8.089376557	-4.664277119
1	2.143809000	-8.656777000	-1.026480000	1	-5.428265919	-7.872547291	-0.818094123
1	3.684182000	-8.914641000	-2.292703000	1	-9.541627769	-8.771624524	-3.519879087
1	5.871399000	-6.505376000	-5.115682000	1	-7.519341349	-8.595783380	0.319918878
1	-3.777945000	-8.459742000	-1.970858000	1	-9.594389400	-9.042192731	-1.020695129
1	5.915277000	-4.824404000	-6.090857000	6	-6.205459268	-3.415723257	-8.700246765
1	-5.924427000	-6.057333000	-4.817677000	6	-6.221104291	-3.015873908	-10.060080331
1	3.769570000	-1.968847000	-8.483593000	6	-7.424410536	-3.364781172	-7.977963167
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1	2.153604000	-0.862184000	-8.364670000	6	-8.613207106	-2.936095294	-8.592514436
1	-3.694784000	-2.265604000	-8.912849000	6	-8.611354290	-2.543108751	-9.944182214
1	-2.149478000	-1.006106000	-8.662323000	1	-5.294670991	-3.067071864	-10.648674957
6	6.192648000	-8.467836000	-3.274369000	1	-7.432597744	-3.636758745	-6.913489645
6	-6.269507000	-7.709457000	-2.677907000	1	-7.395772506	-2.282709544	-11.731757881
6	6.261681000	-2.686398000	-7.745220000	1	-9.543581187	-2.895216490	-8.007634781
6	-6.204435000	-3.243961000	-8.462383000	1	-9.539990913	-2.202836616	-10.424406991
6	6.209007000	-9.828539000	-2.875783000	6	-6.287437437	2.847135416	-7.913168850
6	7.410267000	-10.467307000	-2.525723000	6	-7.467610627	3.591260615	-8.157014277
6	8.627992000	-9.762816000	-2.568250000	6	-6.343104023	1.438092796	-8.067717329
6	8.629075000	-8.408762000	-2.953219000	6	-8.656058382	2.949727721	-8.547486711
6	7.426504000	-7.768789000	-3.296948000	6	-7.528308381	0.794824784	-8.459290767
1	5.271673000	-10.401622000	-2.870555000	6	-8.690801006	1.550736508	-8.702063730
1	7.396199000	-11.525314000	-2.226585000	1	-7.444061067	4.686556138	-8.066551718
1	9.568115000	-10.263214000	-2.295566000	1	-5.451216006	0.834194905	-7.850998849
1	9.571105000	-7.841814000	-2.972645000	1	-9.558352121	3.548206324	-8.741694127
1	7.440134000	-6.703577000	-3.564872000	1	-7.547931508	-0.297887713	-8.567320169
6	7.431770000	-3.445960000	-7.991040000	1	-9.619845822	1.049009092	-9.009677850
6	8.629066000	-2.818634000	-8.376831000	6	-6.192480754	8.720832333	-3.397589026
6	8.682245000	-1.419226000	-8.522443000	6	-6.203632568	10.081091463	-2.999033316
6	7.529707000	-0.649555000	-8.276431000	6	-7.413089270	8.001658519	-3.342415798
6	6.335075000	-1.277832000	-7.891705000	6	-7.388319838	10.698610118	-2.564182980
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1	9.523479000	-3.427995000	-8.573629000	6	-8.592859882	9.971677597	-2.519515710
1	9.617912000	-0.927172000	-8.825484000	1	-5.275919979	10.667378522	-3.053421277
1	7.563950000	0.442029000	-8.374667000	1	-7.424782542	6.936921333	-3.613224470
1	5.451361000	-0.663182000	-7.671239000	1	-7.372043424	11.756435969	-2.264272970
6	-7.437685000	-3.268887000	-7.762299000	1	-9.530837493	8.037065505	-2.866983389
6	-8.641134000	-2.924934000	-8.400490000	1	-9.519345122	10.454575402	-2.177173064
6	-8.641603000	-2.536901000	-9.753659000	6	6.212121537	8.717394264	3.407555966
6	-7.424536000	-2.491990000	-10.459149000	6	6.223435701	10.078040031	3.010328170
6	-6.222426000	-2.842409000	-9.822206000	6	7.432669703	7.998158104	3.351861529
1	-7.450284000	-3.539274000	-6.697711000	6	7.408258755	10.695898299	2.576322524
1	-9.582564000	-2.945926000	-7.832605000	6	8.618862084	8.616450023	2.921350023
1	-9.582448000	-2.264340000	-10.252751000	6	8.612735306	9.968893850	2.531109333
1	-7.411582000	-2.190089000	-11.516381000	1	5.295746347	10.664328947	3.065134658
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6	-7.531585000	-8.230876000	-0.634958000	1	9.550503611	8.033864072	2.876797254
6	-8.688484000	-8.472657000	-1.399376000	1	9.539335532	10.452079976	2.189485769
6	-8.640466000	-8.329667000	-2.799246000	6	6.306195135	2.842089976	7.920741835
6	-7.443952000	-7.950655000	-3.432197000	6	7.485603193	3.586864359	8.166312074
1	-5.450545000	-7.635443000	-0.658168000	6	6.362686605	1.432978831	8.074352727
1	-7.561736000	-8.326777000	0.456862000	6	8.674122423	2.945877098	8.557448817
1	-9.623458000	-8.770432000	-0.902820000	6	7.547963413	0.790246685	8.466602838
1	-9.538384000	-8.522953000	-3.404563000	6	8.709692681	1.546795557	8.711036765
1	-7.409423000	-7.867169000	-4.527775000	1	7.461366519	4.682214620	8.076714733

6	-3.299223000	-2.465246000	0.001599000	1	5.471384849	0.828640014	7.856452865
6	-2.516496000	-2.841677000	-1.174901000	1	9.575797480	3.544844165	8.753013327
6	-4.047891000	-1.269131000	0.000239000	1	7.568248534	-0.302535624	8.573873426
6	-2.516184000	-2.017296000	-2.313883000	1	9.638823690	1.045518866	9.019124680
6	-1.272005000	-1.782667000	-3.040220000	6	6.276586951	7.940028374	-2.855955087
6	-0.055529000	-2.446839000	-2.671928000	6	7.453729222	8.187767123	-3.603588967
6	1.162108000	-1.785465000	-3.041475000	6	6.336130272	8.094015337	-1.447017211
6	-3.296420000	-0.775077000	2.321233000	6	8.642960782	8.581521086	-2.965522207
6	-2.514275000	-2.010698000	2.315359000	6	7.522125610	8.488827301	-0.807204590
6	-4.046398000	-0.406552000	1.184012000	6	8.681532211	8.735531456	-1.566567846
6	-2.515381000	-2.838074000	1.178509000	1	7.427108663	8.097602964	-4.698838038
6	-1.272020000	-3.456299000	0.729061000	1	5.446817592	7.874199818	-0.840451201
6	-0.054734000	-3.311902000	1.473079000	1	9.542797835	8.778800834	-3.566688619
6	1.161595000	-3.459161000	0.728043000	1	7.544771894	8.596366092	0.285478268
6	-0.056052000	-3.316013000	-1.470171000	1	9.611170904	9.045720131	-1.067532614
6	-1.272729000	-3.458561000	-0.724780000	6	6.177511251	3.426714265	-8.731354371
6	1.160909000	-3.461119000	-0.725792000	6	7.400326070	3.374464148	-8.015713041
6	-3.293570000	1.953158000	1.430391000	6	6.185820582	3.028880742	-10.091846007
6	-2.510129000	1.565717000	2.602780000	6	8.585773433	2.946660666	-8.637302256
6	-4.044520000	0.985721000	0.729326000	6	7.369899894	2.597537889	-10.712983254
6	-2.511101000	0.228712000	3.038185000	6	8.576633531	2.555715966	-9.989523721
6	-1.267552000	-0.390478000	3.486017000	1	7.414355268	3.644845207	-6.950894276
6	-0.049772000	0.361395000	3.575251000	1	5.256265442	3.081005493	-10.675420966
6	1.166236000	-0.393099000	3.484713000	1	9.519225072	2.904676408	-8.057426821
6	-0.053326000	-2.439158000	2.672225000	1	7.351387897	2.298071629	-11.770899375
6	-1.269487000	-1.774086000	3.039937000	1	9.502667487	2.216225191	-10.475294361
6	1.164617000	-1.776752000	3.038711000	6	6.263381273	-2.834515950	-7.951372890
6	-3.294816000	1.949042000	-1.439751000	6	6.317849509	-1.425306499	-8.104800621
6	-2.509681000	2.943214000	-0.709421000	6	7.442280191	-3.578139229	-8.202796791
6	-4.045196000	0.983630000	-0.735282000	6	7.500657030	-0.781379267	-8.502493706
6	-2.509139000	2.945335000	0.696698000	6	8.628359380	-2.935940520	-8.599325012
6	-1.264665000	3.179930000	1.422397000	6	8.661900105	-1.536788482	-8.752700136
6	-0.047492000	3.496383000	0.733444000	1	5.427013469	-0.821843313	-7.882603421
6	1.169544000	3.176995000	1.421333000	1	7.419457274	-4.673531364	-8.113328610
6	-0.048391000	1.771755000	3.116489000	1	7.519407479	0.311437216	-8.609561439
6	-1.265217000	2.328041000	2.600213000	1	9.529605408	-3.534040532	-8.799472612
6	1.169291000	2.325168000	2.599230000	1	9.589103798	-1.034503582	-9.064923438
6	-3.298448000	-0.781722000	-2.322782000	6	6.195630682	-8.711891870	-3.440410041
6	-2.513764000	0.220083000	-3.043240000	6	6.209602046	-10.072387399	-3.042744829
6	-4.047488000	-0.409927000	-1.185981000	6	7.416254768	-7.992257968	-3.391711402
6	-2.512461000	1.558358000	-2.611822000	6	7.396995538	-10.689688558	-2.615020499
6	-1.267490000	2.320563000	-2.612348000	6	8.604996486	-8.609993209	-2.967476907
6	-0.051042000	1.762967000	-3.128001000	6	8.601478996	-9.962301156	-2.576730196
6	1.167005000	2.317949000	-2.613247000	1	5.281855313	-10.659052544	-3.092258379
6	-0.048070000	3.494236000	-0.749804000	1	7.425987524	-6.927334687	-3.661855263
6	-1.265816000	3.175716000	-1.436857000	1	7.382820229	-11.747690101	-2.315623441
6	1.168415000	3.173241000	-1.437886000	1	9.536679833	-8.027084343	-2.928356270
6	-0.052800000	0.351280000	-3.582774000	1	9.530094197	-10.445053170	-2.240003375
6	-1.270487000	-0.400255000	-3.490109000	6	6.292157577	-7.934575642	2.820489331
6	1.163275000	-0.403085000	-3.491453000	6	6.343196741	-8.088345280	1.411191579
6	3.194505000	1.941800000	-1.442436000	6	7.474058171	-8.181464875	3.560859522
6	2.410207000	1.552860000	-2.613775000	6	7.525514510	-8.482311775	0.764095334
6	2.408207000	0.214586000	-3.045331000	6	8.659677071	-8.574179986	2.915469216
6	3.943295000	0.974690000	-0.738639000	6	8.689768585	-8.728116875	1.516300963
6	3.195792000	1.945834000	1.427716000	1	5.449988731	-7.869246690	0.810113285
6	2.412902000	2.939689000	0.694572000	1	7.454124284	-8.091289534	4.656251067
6	2.412365000	2.937860000	-0.711550000	1	7.541583375	-8.589620398	-0.328723715

6	3.943972000	0.976738000	0.725968000	1	9.563318486	-8.770865389	3.511099926
6	3.193306000	-0.782459000	2.318450000	1	9.616533283	-9.037572031	1.011501731
6	2.410873000	0.223145000	3.036035000	6	6.224356577	-3.424076227	8.699144668
6	2.412514000	1.560165000	2.600828000	6	6.239476416	-3.026287766	10.059587230
6	3.943162000	-0.415544000	1.180606000	6	7.443473021	-3.371612343	7.977249477
6	3.190356000	-2.472568000	-0.001142000	6	7.426594799	-2.594642062	10.674672161
6	2.406754000	-2.843887000	1.176437000	6	8.631949345	-2.943417431	8.592761535
6	2.408262000	-2.016288000	2.313079000	6	8.629582023	-2.552476160	9.945024667
6	3.941664000	-1.278110000	-0.003170000	1	5.312876390	-3.078682782	10.647815449
6	3.191257000	-0.788935000	-2.325547000	1	7.451993556	-3.641972647	6.912367052
6	2.406341000	-2.022792000	-2.316191000	1	7.413460138	-2.295240476	11.732686637
6	2.405642000	-2.846939000	-1.176990000	1	9.562471762	-2.901302259	8.008205955
6	3.942057000	-0.418866000	-1.189370000	1	9.557972585	-2.212616460	10.426017328

pNTD_{C70}

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

Atom	X	Y	Z
6	-0.086034000	8.232745000	-6.302589000
1	0.355325000	7.618923000	-5.509059000
6	0.711713000	8.629344000	-7.399888000
6	0.075552000	9.362064000	-8.434038000
1	0.657677000	9.718967000	-9.293946000
6	-1.297009000	9.658210000	-8.365378000
6	-2.069491000	9.258308000	-7.259695000
1	-3.134648000	9.523529000	-7.200428000
6	-1.459216000	8.551118000	-6.199234000
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References

- 1 A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098-3100.
- 2 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789.
- 3 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297-3305.
- 4 F. Weigend, *Phys. Chem. Chem. Phys.* 2006, **8**, 1057-1065.
- 5 K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett.* 1995, **240**, 283-290.
- 6 K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor. Chem. Acc.* 1997, **97**, 119-124.
- 7 F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.* 2012, **2**, 73-78.
- 8 ORCA—an ab initio density functional, and semiempirical program package, version 4.1.2
- 9 ADF 2018, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, [d](#). E.J. Baerends, T. Ziegler, A.J. Atkins, J. Autschbach, O. Baseggio, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, C. Daul, D.P. Chong, D.V. Chulhai, L. Deng, R.M. Dickson, J.M. Dieterich, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, A. Förster, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A. Goetz, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, Z. Hu, C.R. Jacob, H. Jacobsen, L. Jensen, L. Joubert, J.W. Kaminski, G. van Kessel, C. König, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, C.A. Peebles, P.H.T. Philipsen, D. Post, C.C. Pye, H. Ramanantoanina, P. Ramos, W. Ravenek, J.I. Rodríguez, P. Ros, R. Rüger, P.R.T. Schipper, D. Schlüns, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Stener, M. Swart, D. Swerhone, V. Tognetti, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev
- 10 S. Hirata and M. Head-Gordon, *Chem. Phys. Lett.* 1999, **314**, 291-299.
- 11 T. Yanai, D. P. Tew and N. C. Handy, *Chem. Phys. Lett.* 2004, **393**, 51-57.
- 12 Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
- 13 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.
- 14 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456-1465.
- 15 R. S. Mulliken, *J. Chem. Phys.* **1955**, 23, 1833-1840.
- 16 R. S. Mulliken, *J. Chem. Phys.* **1955**, 23, 1841-1846.
- 17 P. O. Löwdin, *J. Chem. Phys.* **1950**, 18, 365-375.
- 18 F. L. Hirshfeld, *Theor. Chim. Acta* **1977**, 44, 129-138.
- 19 A. V. Marenich, S. V. Jerome, C. J. Cramer, D.G. Truhlar, *J. Chem. Theory Comput.* 2012, **8**, 527-541.

- 20 P. Bultinck, C. V. Alsenoy, P. W. Ayers, R. Carbó-Dorca, *J. Chem. Phys.* **2007**, *126*, 144111.
- 21 A. E. Reed, R. B. Weinstock, F. Weinhold, *J. Chem. Phys.* 1985, **83**, 735.
- 22 R. F. W. Bader, *Chem. Rev.* **1991**, *91*, 893–928.
- 23 R. F. W. Bader, *Atoms in Molecules: A Quantum Theory*; International Series of Monographs on Chemistry 22; Oxford University Press: Oxford, U.K., **1990**.
- 24 Keith, T. A. AIMAll, version 14.06.21; TK Gristmill Software: Overland Park, KS, **2014**.
- 25 T. Lu, F. Chen, *J. Comput. Chem.* 2012, **33**, 580-592.
- 26 G. A. Zhurko, Chemcraft 1.80 (build 523b) - graphical program for visualization of quantum chemistry computations. (<https://chemcraftprog.com>).
- 27 F. Plasser and H. Lischka, *J. Chem. Theory Comput.* 2012, **8**, 2777-2789.
- 28 F. Plasser, S. A. B  ppler, M. Wormit and A. Dreuw, *J. Chem. Phys.* 2014, **141**, 024107.
- 29 J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999-3093.
- 30 R. A. Marcus and N. Sutin, *Biochim. Biophys. Acta, Rev. Bioenerg.* 1985, **811**, 265-322.
- 31 A. A. Voityuk and N. R  sch, *J. Chem. Phys.* 2002, **117**, 5607-5616.
- 32 A. A. Voityuk, *Phys. Chem. Chem. Phys.* 2012, **14**, 13789-13793.
- 33 J. Ulstrup, J. Jortner, *J. Chem. Phys.* 1975, **63**, 4358-4368.
- 34 J. Jortner, *J. Chem. Phys.* 1976, **64**, 4860-4867.
- 35 T. Liu, A. Troisi, *J. Phys. Chem. C* 2011, **115**, 2406-2415.
- 36 T. Ziegler, A. Rauk, *Theor. Chim. Acta* 1977, **46**, 1-10.
- 37 T. Ziegler, A. Rauk, *Inorg. Chem.* 1979, **18**, 1558-1565.
- 38 T. Ziegler, A. Rauk, *Inorg. Chem.* 1979, **18**, 1755-1759.
- 39 S. Grimme, *J. Comput. Chem.* 2004, **25**, 1463-1473.
- 40 S. Grimme, *J. Comput. Chem.* 2006, **27**, 1787-1799.
- 41 E. Johnson, S. Keinan, P. Mori-S  nchez, J. Contreras-Garc  a, A. Cohen and W. Yang, *J. Am. Chem. Soc.* 2010, **132**, 6498–6506.
- 42 J. Contreras-Garc  a, E. Johnson, S. Keinan, R. Chaudret, J. Piquemal, D. Beratan and W. Yang, *J. Chem. Theory Comput.* 2011, **7**, 625–632.
- 43 J. Contreras-Garc  a, W. Yang and E. Johnson, *J. Phys. Chem. A*, 2011, **115**, 12983–12990.