Supporting information for:

Photoinduced electron transfer in non-covalent complexes of C_{60} and phosphangulene oxide derivatives.

A. J. Stasyuk,*[a,b] O. A. Stasyuk,[a] M. Solà*[a] and A. A. Voityuk*[a,c]

a. Institut de Química Computacional and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany 69, 17003 Girona, Spain

b. Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

c. Institució Catalana de Recerca i Estudis Avancats (ICREA), 08010 Barcelona, Spain

Abstract: Investigation of photoinduced electron transfer (PET) in a series of experimentally reported complexes of fullerene with phosphangulene oxides shows that the replacement of O atoms in the bridge of phosphangulene with S atoms promotes efficient and ultrafast ET from fullerene to phosphangulene oxide in **PGO^{OSS}⊃C$_{60}$** and **PGO^{SSS}⊃C$_{60}$** complexes. The results obtained can be useful in development of photovoltaic devices based on phosphangulenes.

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Computational Methodology

Quantum-chemical calculations

Geometry optimization of the complexes was performed employing the DFT B3LYP[1-3] exchange−correlation functional with Ahlrichs' Def2-SVP basis set,[4,5] and using the resolution of identity approximation (RI, alternatively termed density fitting)[6,7] implemented in the ORCA 4.2.1 program.[8,9] The host-guest interaction energy was computed using B3LYP functional coupled with triple-ξ Def2-TZVP basis.[10] Vertical excitation energies were calculated using TDA formalism[11] with the range-separated functional from Handy and coworkers' CAM-B3LYP[12] and Ahlrichs' Def2-SVP basis set.[4,5] 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] and CM5,[19] schemes were carried out using code implemented in Gaussian 16 (Rev. A03).[20] The excited states have been analyzed in terms of the natural transition orbitals (NTO) concept introduced by Luzanov *et al.*[21] and implemented within modern many-body codes by Head-Gordon *et al.*[22]

Topological analysys of the electron distributions was conducted using the "Quantum Theory of Atoms in Molecules" (QTAIM) approach proposed by Bader.[23,24] The AIMALL suite of programs[25] was applied to evaluate the bond critical point properties and the associated bond descriptors – 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 [$H(r)$]. The NCI technique was employed through the analysis of the reduced density gradient (RDG) at the CAM-B3LYP/Def2-SVP level Multiwfn program.[26] To visualize molecular structures, NCI isosurfaces, and natural transition orbitals, Chemcraft 1.8. program[27] was used.

Interaction energies

The interaction energies were calculated directly from the electronic energy of the complex and the electronic energies of the subsystems. For **PGO^{XXX}⊃C$_{60}$**, the interaction energy can be expressed as follows:

$$E_{\text{int}} = E_{PGO-C_{60}} - (E_{PGO} + E_{C_{60}}) \quad (1)$$

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)[28,29] into electrostatic interactions, Pauli repulsive orbital interactions, and attractive orbital interactions, to which a term ΔE_{disp} is added to account for the dispersion correction:

$$\Delta E_{\text{int}} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp} \quad (2)$$

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.[13,14] The analysis was performed using the ADF suite of programs.[30]

Non-covalent interactions (NCI)

The NCI method[31-33] relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s), defined as:

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

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.

Table S1. Energy decomposition analysis for **PG^{OOO}⊃PG^{OOO}, PG^{OOO}⊃C$_{60}$,** and **PGO^{OOO}⊃C$_{60}$** complexes.[a]

Complex	Energy terms				
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}
PG^{OOO}⊃PG^{OOO}	35.63	-17.96 (32.7%)	-6.65 (12.1%)	-30.38 (55.2%)	-19.36
PG^{OOO}⊃C$_{60}$	34.34	-16.46 (31.7%)	-7.75 (14.9%)	-27.67 (53.3%)	-17.54
PGO^{OOO}⊃C$_{60}$	34.38	-16.57 (31.4%)	-7.79 (14.8%)	-28.34 (53.8%)	-18.33

[a] The energy values are in kcal/mol. The percentage contributions of all attractive terms are given in parentheses.

Table S2. Charge separation between the fragments in electronic ground state for **PGO^{OOO}⊃C$_{60}$, PGO^{OOS}⊃C$_{60}$, PGO^{OSS}⊃C$_{60}$,** and **PGO^{SSS}⊃C$_{60}$** complexes. Q_{PGO} - charge on PGO^{XXX}, and $Q_{C_{60}}$ - charge on fullerene moiety. Total charge of the complexes Q_{Tot} equal to 0.

Charge	**PGO^{OOO}⊃C$_{60}$**		**PGO^{OOS}⊃C$_{60}$**		**PGO^{OSS}⊃C$_{60}$**		**PGO^{SSS}⊃C$_{60}$**	
	Q_{PGO}	$Q_{C_{60}}$	Q_{PGO}	$Q_{C_{60}}$	Q_{PGO}	$Q_{C_{60}}$	Q_{PGO}	$Q_{C_{60}}$
Mulliken	0.021	-0.021	0.018	-0.018	0.027	-0.027	0.027	-0.027
Löwdin	0.019	-0.019	0.023	-0.023	0.033	-0.033	0.036	-0.036
Hirshfeld	-0.010	0.010	-0.001	0.001	0.012	-0.012	0.018	-0.017
CM5	-0.009	0.009	0.000	0.000	0.012	-0.012	0.017	-0.017

Table S3. EDA results for **PGO^{OOO}⊃C$_{60}$, PGO^{OOS}⊃C$_{60}$, PGO^{OSS}⊃C$_{60}$,** and **PGO^{SSS}⊃C$_{60}$** complexes.[a]

Complex	Energy terms				
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}
PGO^{OOO}⊃C$_{60}$	34.38	-16.57 (31.4%)	-7.79 (14.8%)	-28.34 (53.8%)	-18.33
PGO^{OOS}⊃C$_{60}$	32.46	-15.42 (30.0%)	-7.03 (13.7%)	-28.95 (56.3%)	-18.94
PGO^{OSS}⊃C$_{60}$	34.36	-16.39 (30.0%)	-7.68 (14.1%)	-30.50 (55.9%)	-20.22
PGO^{SSS}⊃C$_{60}$	34.47	-16.27 (29.6%)	-7.57 (13.8%)	-31.20 (56.7%)	-20.58

[a] The energy values are in kcal/mol. The percentage contributions to the sum of all attractive energy terms are given in parentheses.

Table S4. 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 **PGO^{OOO}⊃C$_{60}$**, **PGO^{OOS}⊃C$_{60}$**, **PGO^{OSS}⊃C$_{60}$**, and **PGO^{SSS}⊃C$_{60}$** complexes 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
	PGO^{OOO}⊃C$_{60}$					
C$_{60}$ ··· PGO^{OOO}	π···π	7.60E-03	2.24E-02	-3.65E-03	4.62E-03	9.75E-04
		7.46E-03	2.21E-02	-3.66E-03	4.59E-03	9.30E-04
		6.99E-03	2.06E-02	-3.34E-03	4.24E-03	9.01E-04
		7.36E-03	2.15E-02	-3.59E-03	4.48E-03	8.93E-04
		7.39E-03	2.06E-02	-3.43E-03	4.28E-03	8.55E-04
		7.43E-03	2.14E-02	-3.54E-03	4.44E-03	9.00E-04
		7.63E-03	2.09E-02	-3.53E-03	4.38E-03	8.50E-04
	PGO^{OOS}⊃C$_{60}$					
C$_{60}$ ··· PGO^{OOS}	π···π	6.05E-03	1.80E-02	-2.75E-03	3.62E-03	8.71E-04
		7.13E-03	2.01E-02	-3.30E-03	4.16E-03	8.61E-04
		7.77E-03	2.20E-02	-3.74E-03	4.62E-03	8.84E-04
		6.96E-03	2.17E-02	-3.42E-03	4.43E-03	1.00E-03
		7.49E-03	2.13E-02	-3.58E-03	4.45E-03	8.65E-04
		8.04E-03	2.23E-02	-3.83E-03	4.70E-03	8.75E-04
	PGO^{OSS}⊃C$_{60}$					
C$_{60}$ ··· PGO^{OSS}	π···π	7.18E-03	2.07E-02	-3.36E-03	4.26E-03	9.01E-04
		6.02E-03	1.80E-02	-2.75E-03	3.62E-03	8.74E-04
		9.12E-03	2.50E-02	-4.45E-03	5.35E-03	9.06E-04
		8.33E-03	2.28E-02	-3.91E-03	4.81E-03	8.93E-04
		8.05E-03	2.29E-02	-3.95E-03	4.84E-03	8.90E-04
		7.28E-03	2.07E-02	-3.41E-03	4.30E-03	8.81E-04
	PGO^{SSS}⊃C$_{60}$					
C$_{60}$ ··· PGO^{SSS}	π···π	6.60E-03	1.91E-02	-3.00E-03	3.88E-03	8.86E-04
		9.66E-03	2.64E-02	-4.76E-03	5.68E-03	9.15E-04
		7.28E-03	2.12E-02	-3.47E-03	4.38E-03	9.11E-04
		8.40E-03	2.33E-02	-3.98E-03	4.90E-03	9.21E-04
		8.24E-03	2.37E-02	-4.04E-03	4.97E-03	9.39E-04
		4.34E-03	1.40E-02	-1.80E-03	2.65E-03	8.45E-04

Table S5. The Gibbs energy for photoinduced ET reaction in **PGO^{SSS}⊃C$_{60}$** complexes obtained using the Rehm-Weller equation.

	E_D^{ox}	E_A^{red}	$\Delta E_{Coulombic}$**	$E_{PGO^{SSS}\rightarrow C_{60}}^{CS}$	E_{C60}^{S}	ΔG_{ET}
Rehm-Weller	7.266	2.360	2.415	2.491	1.980	0.511

* The Rehm–Weller equation estimates the Gibbs energy for a photoinduced ET reaction between the donor and acceptor subunits in a DA complex as: $\Delta G_{ET} = E_D^{ox} - E_A^{red} - \Delta E_{Coulombic} - E_{S/T}^{*}$, where E_A^{red} and E_D^{ox} is the reduction and oxidation potentials of the donor and acceptor molecules, respectively, ΔE^* is the energy of the singlet or triplet excited state, and $\Delta E_{Coulombic}$ is the electrostatic work required to separate D^+ and A^- at infinite distance.

** $\Delta E_{Coulombic}$ computed for the distance d = 5.963Å between centers of C_{60} and PGO^{SSS} units.

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 solvation energies (E_{solv}, eV) in DCM calculated for **PGO^{OOO}⊃C$_{60}$**, **PGO^{OOS}⊃C$_{60}$**, **PGO^{OSS}⊃C$_{60}$**, and **PGO^{SSS}⊃C$_{60}$** complexes.

	Supramolecular host-guest systems			
	PGO^{OOO}⊃C$_{60}$	**PGO^{OOS}⊃C$_{60}$**	**PGO^{OSS}⊃C$_{60}$**	**PGO^{SSS}⊃C$_{60}$**
	Ground state (GS)			
E_x	0.000	0.000	0.000	0.000
μ_0	5.16	4.73	4.30	4.00
E_{solv}	-0.181	-0.163	-0.143	-0.135
	LE_1 (Fullerene C_{60})			
E_x	2.553	2.542	2.552	2.554
Δμ	1.03	0.88	0.66	0.75
E_{solv}	-0.190	-0.172	-0.150	-0.142
	LE_2 (Host PGO)			
E_x	4.812	4.470	4.532	4.270
Δμ	1.47	2.87	1.36	3.88
E_{solv}	-0.187	-0.274	-0.183	-0.209
	Most absorptive transition			
E_x	4.401	4.376	4.369	4.372
Δμ	0.13	0.80	1.08	2.59
E_{solv}	-0.184	-0.169	-0.146	-0.147
	CT (Host PGO → Fullerene C_{60})			
E_x	4.045	2.778	2.631	2.543
Δμ	23.92	20.22	22.71	23.92
E_{solv}	-0.990	-0.834	-0.910	-0.943

Table S7. ET parameters and the rate for charge separation reactions of **PGO^{OOO}⊃C$_{60}$** and **PGO^{SSS}⊃C$_{60}$** complexes in toluene (TOL) and dichloromethane (DCM).

Reaction	Solvent	ΔG^{0a}, eV	|V|, eV	λ, eV	E_a, eV	k_{ET},s^{-1}
	PGO^{OOO}⊃C$_{60}$					
$LE_1 \rightarrow CS$	TOL	1.836	$1.16\cdot10^{-2}$	0.205	5.080	$[2.57\cdot10^{-39}]$
	DCM	1.492	$1.16\cdot10^{-2}$	0.584	1.845	$[1.93\cdot10^{-19}]$
$MA \rightarrow CS$	TOL	-0.009	$9.64\cdot10^{-4}$	0.205	0.047	$5.57\cdot10^{9}$
	DCM	-0.356	$9.64\cdot10^{-4}$	0.584	0.022	$8.59\cdot10^{9}$
	PGO^{SSS}⊃C$_{60}$					
$LE_1 \rightarrow CS$	TOL	0.335	$1.61\cdot10^{-2}$	0.237	0.345	$1.31\cdot10^{7}$
	DCM	-0.011	$1.61\cdot10^{-2}$	0.603	0.145	$1.96\cdot10^{11}$
$MA \rightarrow CS$	TOL	-1.485	$1.54\cdot10^{-2}$	0.237	1.643	$[1.39\cdot10^{-15}]$
	DCM	-1.829	$1.54\cdot10^{-2}$	0.603	0.623	$[1.50\cdot10^{2}]$

Table S8. 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 **TBSubP⊃C$_{60}$**, **SubPc⊃C$_{60}$**, **Suma⊃C$_{60}$**, and **Cora⊃C$_{60}$** complexes in the gas-phase (VAC) and dichloromethane (DCM).

	Supramolecular host-guest systems					
	TBSubP⊃C$_{60}$		**Suma⊃C$_{60}$**		**Cora⊃C$_{60}$**	
	VAC	DCM	VAC	DCM	VAC	DCM
	LE_1 (Fullerene C_{60})					
E_x	2.549	2.540	2.552	2.549	2.561	2.553
Transition (W)	H-2 – L (0.46)		H-4 – L+1 (0.21)		H – L (0.27)	
f	<0.001		<0.001		<0.001	
X	0.972		0.928		0.974	
	LE_2 (Host)					
E_x	2.841	2.842	4.143	4.142	3.976	3.978
Transition (W)	H – L+3 (0.63)		H – L+6 (0.21)		H-6 – L+6 (0.36)	
f	0.160		<0.001		<0.001	
X	0.917		Suma/C_{60} (0.67/0.23)		0.856	
	CT (Host $\rightarrow$ Fullerene C_{60})					
E_x	2.140	1.600	3.137	2.516	3.835	3.158
Transition (W)	H – L (0.92)		H-1 – L (0.58)		H-6 – L (0.62)	
f	0.003		0.008		0.001	
CT	0.98		0.87		0.86	

Table S9. Computed semi-classical rates (k_X in s^{-1}) and characteristic times (τ in ps) for the CS process in **PGO^{SSS}⊃C$_{60}$** complex in DCM solution using different effective Huang-Rhys (S_{eff}) factors.

$h\omega_{eff}$	ΔG^0, eV	$\lvert V_{ij} \rvert$, eV	λ_s, eV	λ_i, eV	S_{eff}	k_X, s^{-1}	τ, ps
	$LE_1 \rightarrow CS$						
1200	-0.011	$1.61 \cdot 10^{-2}$	0.389	0.214	1.438	$1.981 \cdot 10^{11}$	5.05
1400					1.233	$1.970 \cdot 10^{11}$	5.08
1600					1.079	$1.964 \cdot 10^{11}$	5.09
1800					0.959	$1.961 \cdot 10^{11}$	5.10
2000					0.863	$1.959 \cdot 10^{11}$	5.10

Table S10. Semi-classical rates (k_X in s^{-1}) and characteristic times (τ in ps) computed for the $LE_1 \rightarrow CS$ and $LE_2 \rightarrow CS$ processes in the **TBSubP⊃C$_{60}$** complex

Reaction	LE	CT	ΔG^0	$\lvert V_{ij} \rvert$	Reorg. Energy		k_{ET}	τ, ns
					λ_i^d	λ_s		
$LE_1 \rightarrow CS$	2.540	1.600	-0.940	$1.75 \cdot 10^{-3}$	0.154	0.333	$7.05 \cdot 10^{9}$	0.14
$LE_2 \rightarrow CS$	2.842	1.600	-1.242	$2.49 \cdot 10^{-3}$	0.154	0.333	$1.39 \cdot 10^{9}$	0.72

Table S11. Semi-classical rates (k_X in s^{-1}) computed for the $LE_1 \rightarrow CS$ process for **PGO^{SSS}⊃C$_{60}$** in DCM using the Frank-Condon and relaxed LE_1 geometries

PGO^{SSS}⊃C$_{60}$	LE	CT	ΔG^0	$\lvert V_{ij} \rvert$	Reorg. Energy		k_{ET}
					λ_i^d	λ_s	
Frank-Condon geometry	2.554	2.543	-0.011	$1.61 \cdot 10^{-2}$	0.214	0.389	$1.964 \cdot 10^{11}$
Relaxed geometry	2.424	2.369	-0.055				$4.308 \cdot 10^{11}$

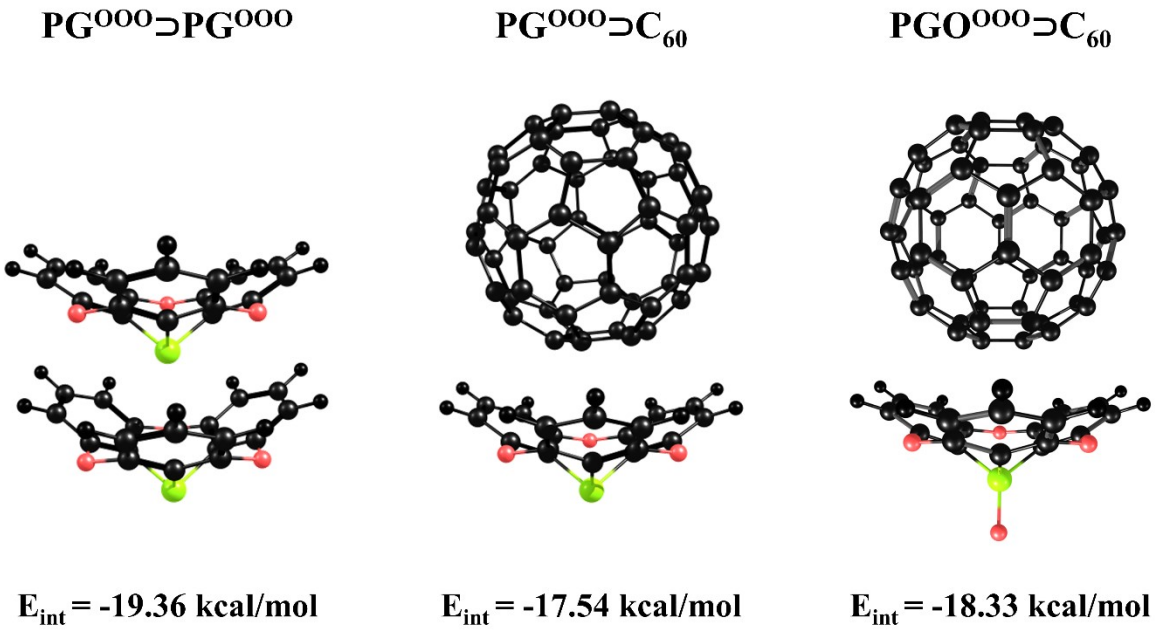

Figure S1. Structure and binding energies of **PG^{OOO}⊃PG^{OOO}, PG^{OOO}⊃C$_{60}$,** and **PGO^{OOO}⊃C$_{60}$** complexes.

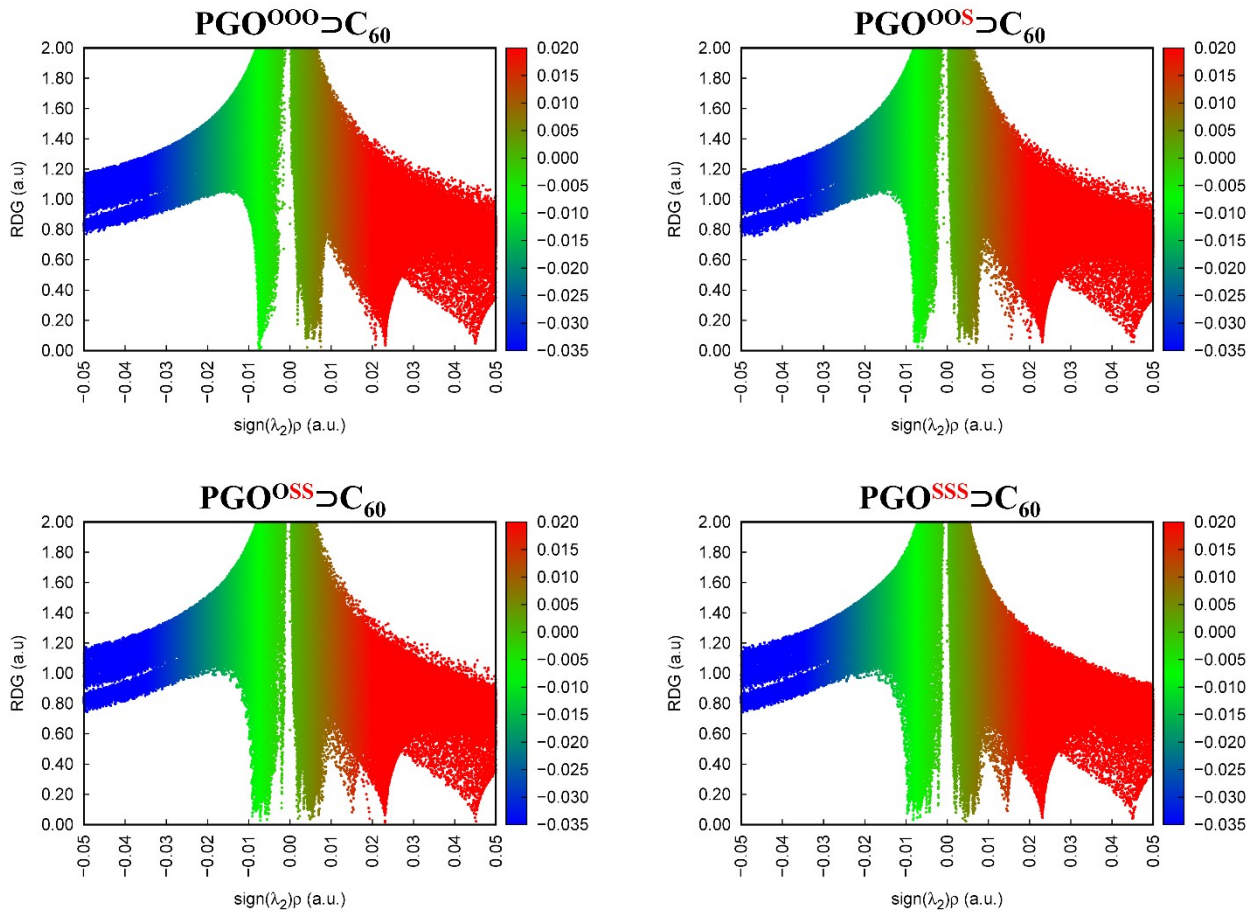

Figure S2. Plot of RDG *vs.* sign(λ2)×ρ for (a) **PGO^{OOO}⊃C$_{60}$**, (b) **PGO^{OOS}⊃C$_{60}$**, (c) **PGO^{OSS}⊃C$_{60}$**, and (d) **PGO^{SSS}⊃C$_{60}$** complexes.

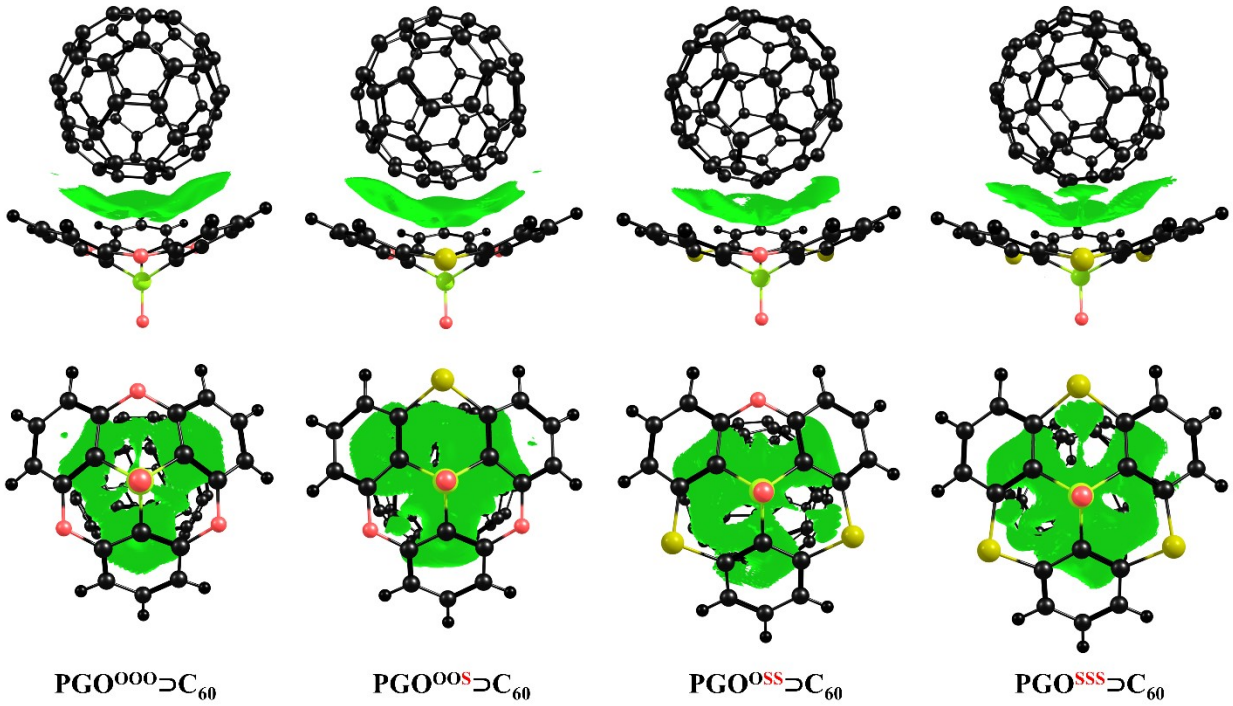

Figure S3. NCI isosurfaces of van der Waals interactions (−0.005 < sign(λ2)×ρ < 0.005 a.u.) for **PGO^{OOO}⊃C$_{60}$**, **PGO^{OOS}⊃C$_{60}$**, **PGO^{OSS}⊃C$_{60}$**, and **PGO^{SSS}⊃C$_{60}$** complexes. Isosurfaces were generated for RDG = 0.5 a.u.

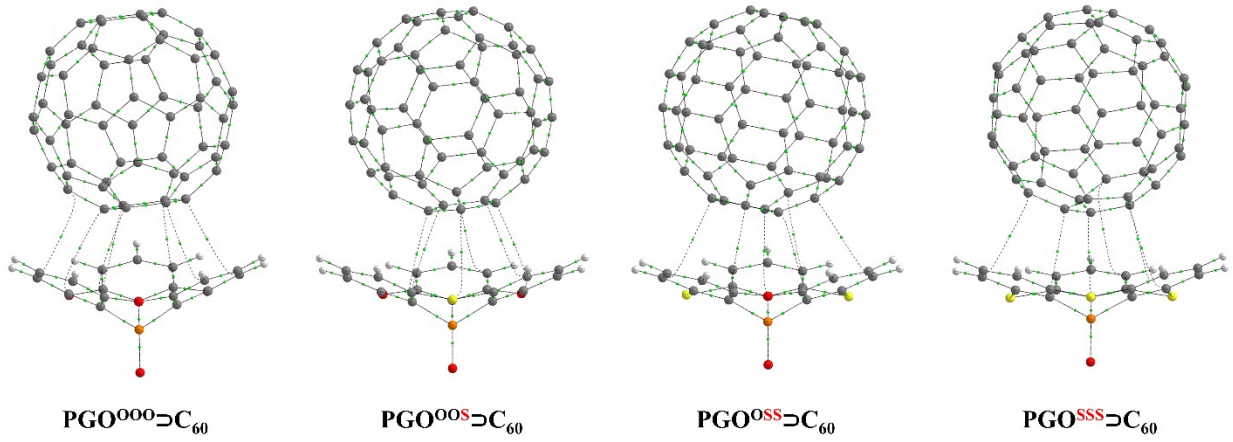

Figure S4. QTAIM molecular graph for **PGO^{OOO}⊃C$_{60}$**, **PGO^{OOS}⊃C$_{60}$**, **PGO^{OSS}⊃C$_{60}$**, and **PGO^{SSS}⊃C$_{60}$** complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs.

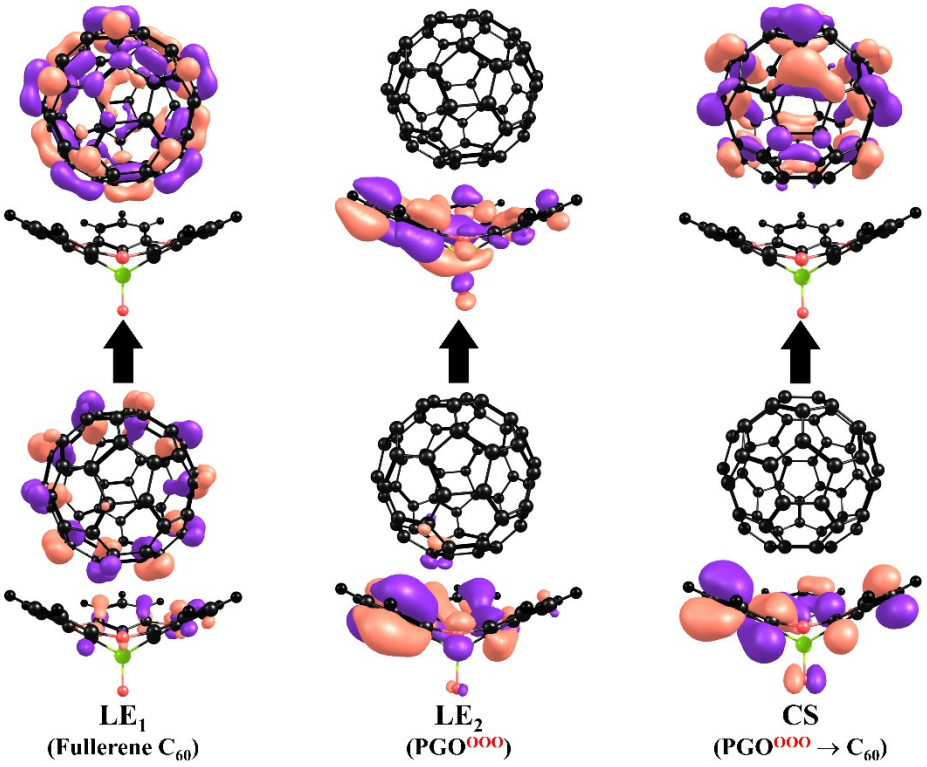

Figure S5. Natural transition molecular orbitals representing the LE_1, LE_2, and CT states in **$PGO^{OOO}\supset C_{60}$**

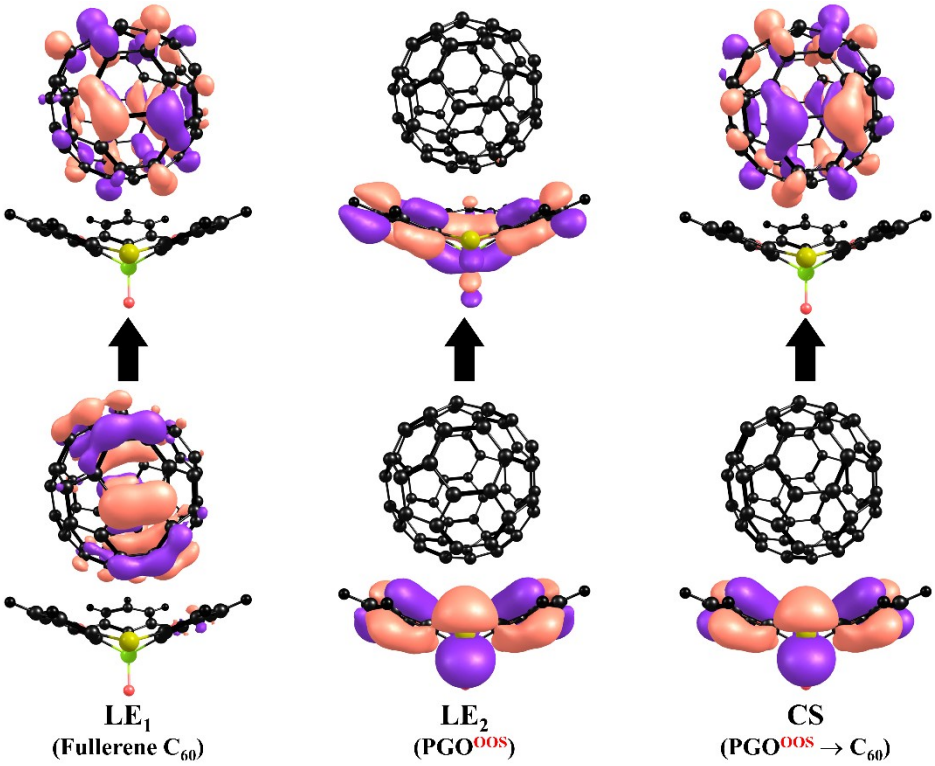

Figure S6. Natural transition molecular orbitals representing the LE_1, LE_2, and CT states in **$PGO^{OOS}\supset C_{60}$**

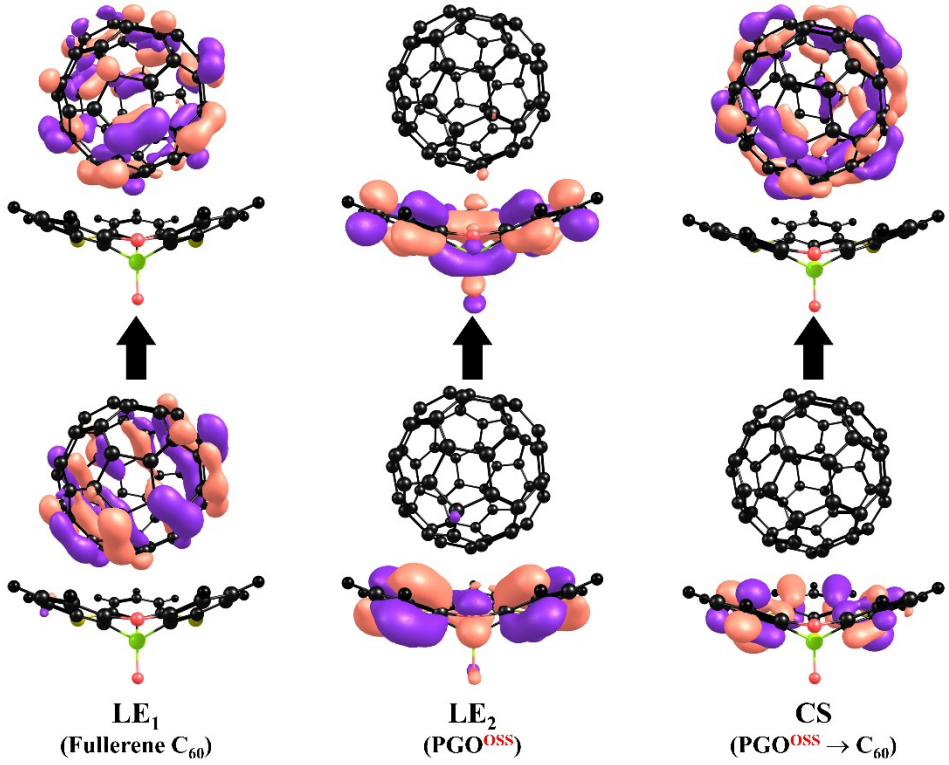

Figure S7. Natural transition molecular orbitals representing the LE_1, LE_2, and CT states in **$PGO^{OSS}\supset C_{60}$**

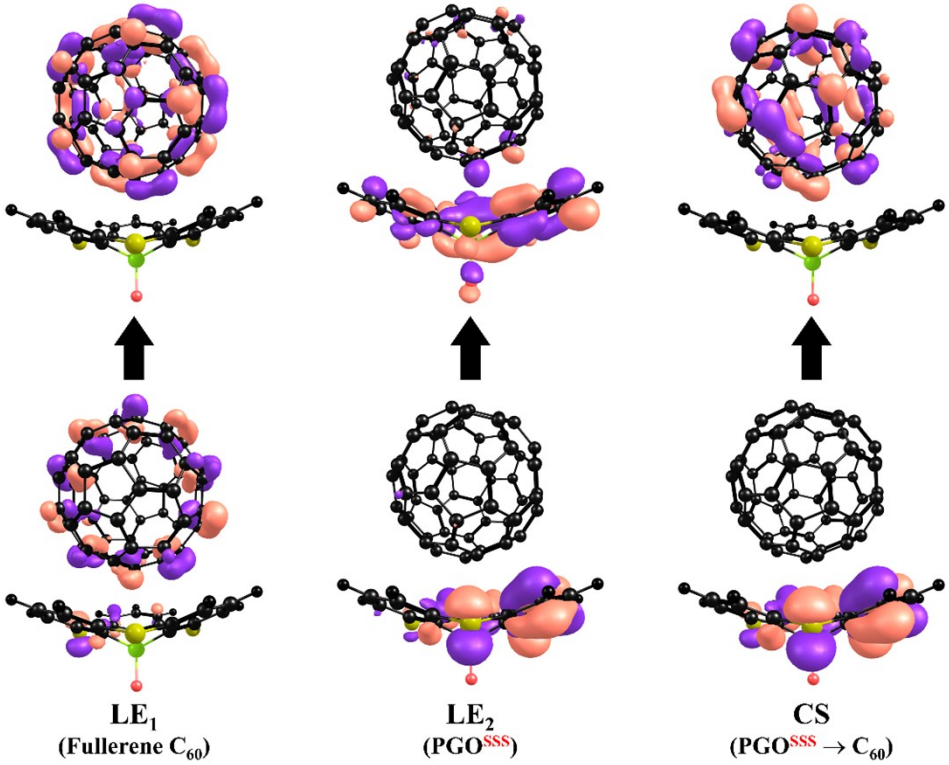

Figure S8. Natural transition molecular orbitals representing the LE_1, LE_2, and CT states in **$PGO^{SSS}\supset C_{60}$**

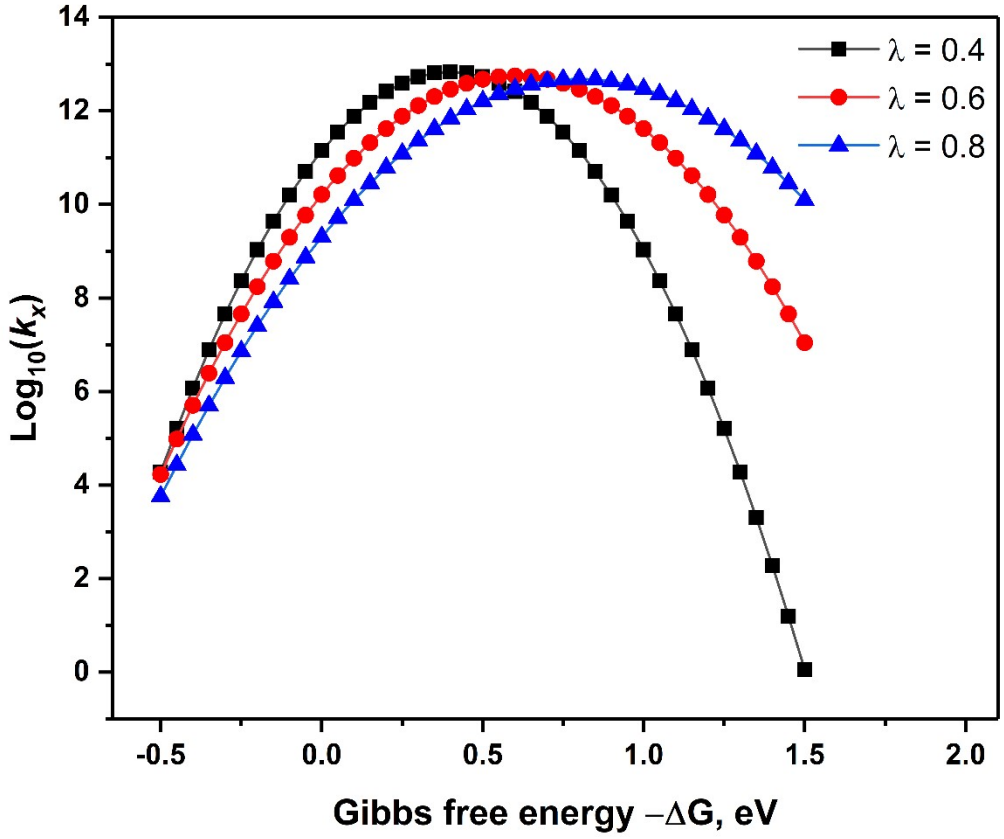

Figure S9. Dependence of the electron transfer rate on Gibbs free energy for **PGO^{SSS}⊃C$_{60}$** complex in DCM. The electronic coupling |Vij| is equal to $1.61 \cdot 10^{-2}$ eV.

Cartesian coordinates

PGO^{OOO}⊃C$_{60}$

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

Atom	X	Y	Z
6	8.195669000	26.741591000	-4.346985000
6	8.392159000	25.299818000	-4.287369000
6	7.573118000	24.517772000	-3.470122000
6	6.519643000	25.143938000	-2.682070000
6	6.329397000	26.528133000	-2.740892000
6	7.184702000	27.344243000	-3.592172000
6	9.505204000	27.370126000	-4.443542000
6	10.511544000	26.317150000	-4.441819000
6	9.825007000	25.037166000	-4.344841000
6	10.379931000	24.001365000	-3.588006000
6	8.151132000	23.439402000	-2.678138000
6	6.449897000	24.454522000	-1.401543000
6	6.189774000	25.174094000	-0.232777000
6	5.990908000	26.616096000	-0.293761000
6	6.058378000	27.280224000	-1.522322000
6	6.746805000	28.560242000	-1.620586000
6	7.442993000	28.599630000	-2.899874000
6	8.700391000	29.203749000	-2.993353000
6	9.752050000	28.575412000	-3.780709000
6	11.725750000	26.511395000	-3.777728000
6	11.981676000	27.766811000	-3.085960000
6	11.016463000	28.776806000	-3.087421000
6	10.747302000	29.529198000	-1.870537000
6	9.315994000	29.793685000	-1.811986000
6	8.648164000	29.756637000	-0.584335000
6	7.337772000	29.127077000	-0.486582000
6	7.265766000	28.435277000	0.793154000
6	6.604960000	27.206480000	0.888042000
6	7.457813000	23.403174000	-1.400409000
6	9.404564000	25.270757000	2.345769000
6	9.157995000	24.066289000	1.682031000
6	10.209721000	23.438818000	0.893512000
6	11.466942000	24.040616000	0.800812000
6	11.724379000	25.297175000	1.491966000
6	10.517031000	27.340717000	2.187057000
6	9.085316000	27.602549000	2.245010000
6	8.397705000	26.323352000	2.344364000
6	7.184457000	26.129050000	1.678163000
6	6.927314000	24.873516000	0.987096000
6	7.894925000	23.867594000	0.986277000
6	9.593243000	22.850214000	-0.288956000
6	10.260585000	22.884804000	-1.515710000
6	11.572421000	23.512988000	-1.613525000
6	12.163301000	24.079774000	-0.479922000
6	12.849742000	25.360730000	-0.578442000
6	12.578960000	26.112915000	0.640161000

PGO^{OOS}⊃C$_{60}$

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

Atom	X	Y	Z
6	8.977430000	27.482643000	-4.667886000
6	9.154944000	26.050082000	-4.862469000
6	8.158404000	25.158528000	-4.454710000
6	6.942661000	25.665007000	-3.830976000
6	6.772610000	27.040626000	-3.643413000
6	7.811055000	27.969050000	-4.071297000
6	10.269247000	28.051378000	-4.309493000
6	11.243818000	26.970544000	-4.282028000
6	10.555674000	25.733812000	-4.623475000
6	10.906055000	24.538718000	-3.989152000
6	8.521779000	23.912492000	-3.791997000
6	6.554641000	24.732390000	-2.781467000
6	6.011655000	25.214129000	-1.586374000
6	5.836967000	26.646650000	-1.391042000
6	6.206924000	27.542503000	-2.399048000
6	6.895315000	28.780713000	-2.057101000
6	7.887354000	29.044103000	-3.091192000
6	9.128116000	29.590122000	-2.747128000
6	10.343183000	29.082172000	-3.368954000
6	12.254027000	26.964211000	-3.317730000
6	12.332473000	28.038273000	-2.338055000
6	11.396498000	29.075995000	-2.362945000
6	10.832518000	29.579657000	-1.118061000
6	9.430446000	29.896995000	-1.355571000
6	8.479042000	29.643086000	-0.363131000
6	7.186241000	29.073840000	-0.721229000
6	6.800316000	28.140599000	0.328759000
6	6.140996000	26.952512000	0.000548000
6	7.530389000	23.650437000	-2.756663000
6	8.490459000	24.622258000	1.656136000
6	8.417524000	23.594711000	0.713076000
6	9.632245000	23.086285000	0.091369000
6	10.873119000	23.628375000	0.437136000
6	10.949506000	24.702181000	1.418461000
6	9.604540000	26.622020000	2.208628000
6	8.203250000	26.938833000	1.969650000
6	7.514885000	25.702295000	1.629473000
6	6.503963000	25.708675000	0.664852000
6	6.425670000	24.635056000	-0.315029000
6	7.365040000	23.602398000	-0.291590000
6	9.329555000	22.779005000	-1.300431000
6	10.280194000	23.031398000	-2.291924000
6	11.574124000	23.597652000	-1.933691000
6	11.865462000	23.890888000	-0.597321000
6	12.553085000	25.129579000	-0.255367000
6	11.987065000	25.631501000	0.989829000

6	12.388475000	27.496890000	0.581254000
6	11.337040000	28.123874000	1.370359000
6	8.530527000	28.638012000	1.487192000
6	9.385315000	29.454743000	0.635723000
6	10.759600000	29.202034000	0.579059000
6	11.454867000	29.240988000	-0.699764000
6	12.460724000	28.187889000	-0.698601000
6	12.718780000	27.466268000	-1.867477000
6	12.918911000	26.024399000	-1.807004000
6	12.305529000	25.433608000	-2.988547000
6	11.645803000	24.203237000	-2.894633000
6	8.164460000	23.116090000	-0.230837000
6	9.524570000	23.184867000	-2.735092000
6	10.714452000	25.899398000	2.248738000
15	7.490292000	18.975170000	-1.504547000
8	5.481337000	20.633968000	-0.001297000
8	7.787504000	20.287169000	-4.204939000
8	10.126571000	19.378530000	-0.107326000
8	7.100402000	17.534692000	-1.583576000
6	10.187013000	20.353679000	-4.181879000
1	10.184162000	20.733992000	-5.204152000
6	8.980830000	20.039342000	-3.553676000
6	9.000201000	19.537497000	-2.245716000
6	7.733415000	19.735861000	0.076450000
6	6.666256000	20.416147000	0.680282000
6	6.832470000	20.946505000	1.960586000
1	6.008972000	21.472792000	2.444434000
6	8.094249000	20.847987000	2.564454000
1	8.237400000	21.285017000	3.555334000
6	5.486957000	20.847224000	-1.368651000
6	6.437280000	20.224959000	-2.190402000
6	6.664284000	20.674755000	-3.498265000
6	10.171109000	19.573317000	-1.475502000
6	9.022575000	19.778247000	0.624094000
6	9.203835000	20.303327000	1.904467000
1	10.200782000	20.328166000	2.345912000
6	11.387181000	19.873660000	-2.092363000
1	12.309075000	19.878897000	-1.509574000
6	11.375389000	20.222861000	-3.450499000
1	12.319458000	20.478028000	-3.937414000
6	5.779281000	21.590726000	-4.069368000
1	5.947073000	21.945174000	-5.087192000
6	4.726000000	22.081030000	-3.285804000
1	4.038631000	22.807278000	-3.725113000
6	4.583701000	21.751595000	-1.930241000
1	3.829911000	22.229876000	-1.304305000

6	11.816091000	27.006971000	1.176929000
6	10.600772000	27.513077000	1.799841000
6	7.853300000	28.133458000	1.334168000
6	8.891331000	29.061839000	0.907642000
6	10.237011000	28.758282000	1.136292000
6	11.228484000	29.022527000	0.102024000
6	12.203936000	27.940053000	0.127203000
6	12.745980000	27.458153000	-1.067713000
6	12.922393000	26.025520000	-1.263353000
6	12.618238000	25.720212000	-2.654233000
6	11.959681000	24.531611000	-2.983158000
6	7.927996000	23.098452000	-1.536315000
6	9.868103000	23.609567000	-3.563250000
6	9.782239000	25.189063000	2.015704000
15	7.616935000	19.117580000	-0.688730000
16	5.631024000	20.851368000	1.281498000
8	7.363695000	19.988081000	-3.572429000
8	10.530112000	19.527398000	0.027859000
8	7.216827000	17.684935000	-0.529388000
6	9.703063000	20.038520000	-4.040005000
1	9.478666000	20.273299000	-5.081067000
6	8.660137000	19.834145000	-3.136557000
6	8.943968000	19.523836000	-1.799941000
6	8.241732000	19.984915000	0.740933000
6	7.379542000	20.656509000	1.623933000
6	7.897014000	21.209624000	2.801533000
1	7.244216000	21.750800000	3.488794000
6	9.266426000	21.094771000	3.069580000
1	9.668592000	21.529491000	3.987845000
6	5.509917000	20.929847000	-0.505154000
6	6.403671000	20.245839000	-1.345373000
6	6.374821000	20.456783000	-2.734542000
6	10.258984000	19.592423000	-1.319939000
6	9.630179000	19.990519000	0.963583000
6	10.144751000	20.509482000	2.154417000
1	11.221193000	20.482957000	2.329831000
6	11.315349000	19.785752000	-2.210480000
1	12.338713000	19.826421000	-1.835220000
6	11.019337000	19.979859000	-3.564685000
1	11.840629000	20.149154000	-4.264688000
6	5.345552000	21.207902000	-3.305346000
1	5.318503000	21.350135000	-4.386600000
6	4.408254000	21.814737000	-2.465114000
1	3.621983000	22.431457000	-2.906373000
6	4.499916000	21.717128000	-1.071352000
1	3.811887000	22.274009000	-0.432976000

$PGO^{OSS}\supset C_{60}$

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

Atom	X	Y	Z
6	8.762500000	27.500321000	-4.625063000
6	8.872958000	26.062908000	-4.831909000

$PGO^{SSS}\supset C_{60}$

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

Atom	X	Y	Z
6	8.712443000	27.549542000	-4.598288000
6	8.765739000	26.110419000	-4.816582000

6	7.872832000	25.208412000	-4.358350000	6	7.743575000	25.290624000	-4.328384000
6	6.719843000	25.757921000	-3.656023000	6	6.624745000	25.877177000	-3.600828000
6	6.614098000	27.138365000	-3.457183000	6	6.574025000	27.259171000	-3.391045000
6	7.656623000	28.028013000	-3.952778000	6	7.639689000	28.112718000	-3.901034000
6	10.096185000	28.019712000	-4.354783000	6	10.069386000	28.017491000	-4.349901000
6	11.030256000	26.903417000	-4.393447000	6	10.960960000	26.867657000	-4.413734000
6	10.274383000	25.694343000	-4.688419000	6	10.155413000	25.689382000	-4.702236000
6	10.621129000	24.485676000	-4.078298000	6	10.468977000	24.464244000	-4.106238000
6	8.232270000	23.948215000	-3.721500000	6	8.068356000	24.014334000	-3.705740000
6	6.367161000	24.837669000	-2.582854000	6	6.258135000	24.962991000	-2.526785000
6	5.920343000	25.335089000	-1.354104000	6	5.853567000	25.467779000	-1.286073000
6	5.813331000	26.773109000	-1.147153000	6	5.803943000	26.907454000	-1.067933000
6	6.150481000	27.657369000	-2.177569000	6	6.154551000	27.785668000	-2.099106000
6	6.907566000	28.867188000	-1.881954000	6	6.962198000	28.963999000	-1.810387000
6	7.838531000	29.095696000	-2.978923000	6	7.879683000	29.165997000	-2.923724000
6	9.119010000	29.594334000	-2.718823000	6	9.182217000	29.615692000	-2.685227000
6	10.270678000	29.043735000	-3.419997000	6	10.299413000	29.028124000	-3.412072000
6	12.103297000	26.857509000	-3.499177000	6	12.048065000	26.775806000	-3.539775000
6	12.285534000	27.924936000	-2.525094000	6	12.287808000	27.828955000	-2.562439000
6	11.388489000	28.997003000	-2.487238000	6	11.431643000	28.933067000	-2.500683000
6	10.926972000	29.517156000	-1.207389000	6	11.013849000	29.460340000	-1.208829000
6	9.524285000	29.885951000	-1.350540000	6	9.623563000	29.881994000	-1.322808000
6	8.631746000	29.664906000	-0.297619000	6	8.743700000	29.686457000	-0.254267000
6	7.296913000	29.146124000	-0.568232000	6	7.385817000	29.219371000	-0.502523000
6	6.946608000	28.224739000	0.504514000	6	7.021615000	28.304351000	0.570984000
6	6.220525000	27.063469000	0.221944000	6	6.246996000	27.173136000	0.295296000
6	7.302378000	23.720959000	-2.622948000	6	7.150639000	23.812599000	-2.592038000
6	8.589615000	24.643223000	1.716762000	6	8.553538000	24.656813000	1.730267000
6	8.415694000	23.622580000	0.779932000	6	8.324523000	23.650726000	0.789671000
6	9.567529000	23.072892000	0.078526000	6	9.441950000	23.064988000	0.062514000
6	10.849053000	23.565532000	0.340396000	6	10.745836000	23.505312000	0.303590000
6	11.030461000	24.632566000	1.315188000	6	10.984844000	24.558434000	1.281983000
6	9.812648000	26.598386000	2.192125000	6	9.857144000	26.561995000	2.194831000
6	8.410760000	26.967660000	2.048216000	6	8.467032000	26.983738000	2.079720000
6	7.654447000	25.759038000	1.755484000	6	7.660735000	25.806190000	1.793544000
6	6.580589000	25.804977000	0.861048000	6	6.572179000	25.897881000	0.919935000
6	6.397198000	24.737217000	-0.112969000	6	6.330971000	24.844447000	-0.057613000
6	7.298374000	23.670514000	-0.152499000	6	7.191653000	23.745502000	-0.120799000
6	9.162362000	22.783288000	-1.290454000	6	9.000975000	22.803416000	-1.299828000
6	10.053338000	23.002100000	-2.342408000	6	9.879007000	22.993454000	-2.367330000
6	11.388988000	23.516146000	-2.071692000	6	11.238432000	23.452778000	-2.119630000
6	11.779758000	23.793410000	-0.757331000	6	11.662776000	23.706684000	-0.810664000
6	12.535436000	25.004050000	-0.462013000	6	12.468361000	24.886408000	-0.522408000
6	12.071814000	25.523244000	0.818573000	6	12.049023000	25.413289000	0.770614000
6	11.964920000	26.903746000	1.016472000	6	11.996569000	26.795545000	0.978994000
6	10.812151000	27.452456000	1.717711000	6	10.878451000	27.381513000	1.705760000
6	8.064153000	28.175724000	1.436944000	6	8.153741000	28.208024000	1.482361000
6	9.105922000	29.065029000	0.941920000	6	9.218430000	29.061099000	0.972413000
6	10.451751000	28.711501000	1.079728000	6	10.552610000	28.657314000	1.082173000
6	11.382392000	28.942196000	-0.016861000	6	11.469843000	28.860859000	-0.030744000
6	12.317568000	27.824510000	-0.056390000	6	12.362189000	27.709918000	-0.095051000
6	12.761910000	27.326317000	-1.285106000	6	12.764550000	27.204591000	-1.335287000
6	12.872059000	25.888382000	-1.492521000	6	12.818024000	25.764966000	-1.553719000

6	12.464900000	25.598599000	-2.861076000
6	11.739719000	24.436871000	-3.144702000
6	7.759564000	23.151327000	-1.432430000
6	9.578921000	23.596415000	-3.583240000
6	9.923624000	25.160634000	1.988068000
15	7.726269000	19.212680000	-0.851037000
16	5.502004000	20.792025000	1.038120000
16	7.628655000	19.814595000	-4.092168000
8	10.537221000	19.664857000	0.240946000
8	7.346227000	17.766760000	-0.764184000
6	10.341319000	20.009771000	-3.902292000
1	10.300523000	20.185506000	-4.978997000
6	9.158420000	19.808876000	-3.182813000
6	9.201579000	19.611133000	-1.792298000
6	8.172986000	20.047069000	0.675442000
6	7.211059000	20.642167000	1.511269000
6	7.582882000	21.155672000	2.759350000
1	6.839157000	21.640175000	3.394384000
6	8.918855000	21.078060000	3.165583000
1	9.210055000	21.487206000	4.135908000
6	5.518964000	20.917778000	-0.741852000
6	6.478667000	20.294733000	-1.563609000
6	6.425529000	20.484757000	-2.957866000
6	10.434320000	19.710936000	-1.124993000
6	9.523447000	20.073304000	1.066000000
6	9.898411000	20.555029000	2.323108000
1	10.953310000	20.545278000	2.601069000
6	11.623774000	19.881373000	-1.838542000
1	12.565707000	19.941832000	-1.291964000
6	11.565512000	20.014373000	-3.225860000
1	12.487655000	20.172866000	-3.789657000
6	5.381489000	21.224379000	-3.527193000
1	5.351578000	21.382332000	-4.607161000
6	4.407788000	21.793132000	-2.704140000
1	3.607228000	22.387487000	-3.150518000
6	4.479262000	21.663203000	-1.316730000
1	3.747217000	22.158726000	-0.676191000

6	12.375372000	25.499807000	-2.916567000
6	11.602299000	24.367746000	-3.193526000
6	7.610890000	23.222207000	-1.413009000
6	9.403636000	23.611449000	-3.596488000
6	9.911189000	25.122448000	1.979614000
15	7.927097000	19.277528000	-0.837089000
16	5.480376000	20.705036000	0.926810000
16	7.809465000	19.818629000	-4.118024000
16	10.970680000	19.507185000	0.531175000
8	7.598799000	17.817724000	-0.748224000
6	10.480321000	20.027860000	-3.975758000
1	10.385576000	20.188005000	-5.051714000
6	9.326046000	19.847528000	-3.201907000
6	9.409374000	19.668263000	-1.807003000
6	8.229706000	20.112311000	0.747452000
6	7.163284000	20.667255000	1.485147000
6	7.377074000	21.206287000	2.761649000
1	6.541445000	21.651344000	3.304902000
6	8.657742000	21.210501000	3.310463000
1	8.827250000	21.657652000	4.292761000
6	5.581414000	20.832211000	-0.838380000
6	6.628238000	20.282921000	-1.607441000
6	6.579570000	20.444341000	-3.006412000
6	10.684565000	19.715238000	-1.205882000
6	9.520421000	20.154586000	1.314174000
6	9.732523000	20.698588000	2.588811000
1	10.745818000	20.743173000	2.993884000
6	11.839616000	19.886141000	-1.982579000
1	12.815972000	19.928288000	-1.495633000
6	11.732008000	20.029479000	-3.364102000
1	12.630539000	20.179668000	-3.966821000
6	5.504258000	21.102682000	-3.617769000
1	5.497734000	21.232169000	-4.701835000
6	4.467992000	21.614301000	-2.838357000
1	3.641015000	22.143910000	-3.316816000
6	4.507212000	21.494431000	-1.450745000
1	3.720998000	21.931538000	-0.832055000

TBSubP⊃C_{60}

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

Atom	X	Y	Z
6	2.181490000	0.997384000	1.265213000
6	1.809774000	1.330999000	-0.103379000
6	0.462892000	1.484901000	-0.438255000
6	-0.565895000	1.323352000	0.577707000
6	-0.210502000	1.011626000	1.891172000
6	1.192463000	0.840360000	2.240788000
6	3.305033000	0.072067000	1.211570000
6	3.627372000	-0.166145000	-0.190218000
6	2.704132000	0.615127000	-1.003767000
6	2.212238000	0.086520000	-2.202099000
6	-0.046842000	0.936238000	-1.684599000

SubPc⊃C_{60}

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

Atom	X	Y	Z
6	-0.079941000	1.161676000	0.727827000
6	-0.079947000	1.161663000	-0.727809000
6	-1.175036000	0.646156000	-1.425388000
6	-2.316121000	0.108759000	-0.698611000
6	-2.316115000	0.108755000	0.698634000
6	-1.175025000	0.646158000	1.425404000
6	1.275474000	0.874455000	1.178364000
6	2.114425000	0.698806000	-0.000008000
6	1.275456000	0.874448000	-1.178361000
6	1.479795000	0.080864000	-2.309477000
6	-0.963085000	-0.178218000	-2.606122000

6	-1.713190000	0.674608000	-0.041140000	6	-2.810695000	-1.050763000	-1.426725000
6	-2.464602000	-0.258839000	0.674863000	6	-3.286836000	-2.165148000	-0.728918000
6	-2.091202000	-0.590206000	2.043692000	6	-3.286832000	-2.165149000	0.728951000
6	-0.988328000	0.033094000	2.639589000	6	-2.810675000	-1.050768000	1.426753000
6	-0.062255000	-0.746657000	3.450592000	6	-1.972648000	-1.229668000	2.605604000
6	1.284932000	-0.246351000	3.203928000	6	-0.963059000	-0.178216000	2.606140000
6	2.363701000	-1.134557000	3.153481000	6	0.337754000	-0.457468000	3.035257000
6	3.394163000	-0.972841000	2.137120000	6	1.479833000	0.080896000	2.309494000
6	4.027083000	-1.439552000	-0.609028000	6	3.125161000	-0.267587000	-0.000013000
6	4.118471000	-2.528124000	0.355893000	6	3.337131000	-1.098044000	1.179128000
6	3.809131000	-2.299358000	1.700096000	6	2.531197000	-0.926131000	2.309891000
6	3.033827000	-3.281017000	2.447035000	6	2.037513000	-2.089396000	3.035809000
6	2.140929000	-2.561379000	3.345398000	6	0.682309000	-1.799002000	3.484196000
6	0.849198000	-3.041707000	3.580432000	6	-0.286300000	-2.807233000	3.483970000
6	-0.275098000	-2.116104000	3.633944000	6	-1.641707000	-2.517323000	3.037071000
6	-1.422899000	-2.764977000	3.013758000	6	-2.134530000	-3.679255000	2.309444000
6	-2.311907000	-2.017617000	2.234241000	6	-2.939546000	-3.506858000	1.178623000
6	-1.392586000	0.436959000	-1.440670000	6	-1.972678000	-1.229669000	-2.605583000
6	-2.102550000	-4.078625000	-0.834428000	6	-0.878353000	-5.484248000	-1.178005000
6	-2.191613000	-3.033494000	-1.759610000	6	-1.083159000	-4.687410000	-2.308347000
6	-1.160483000	-2.871475000	-2.776709000	6	0.058647000	-4.148296000	-3.034722000
6	-0.081174000	-3.758728000	-2.826033000	6	1.358582000	-4.427408000	-2.603523000
6	0.011135000	-4.846513000	-1.862750000	6	1.572115000	-5.257417000	-1.426193000
6	-0.605389000	-5.339265000	0.480371000	6	0.476704000	-5.775643000	0.728318000
6	-1.498787000	-4.619164000	1.378530000	6	-0.878341000	-5.484250000	1.178016000
6	-2.424252000	-3.840080000	0.565561000	6	-1.716013000	-5.304582000	0.000010000
6	-2.824471000	-2.566864000	0.984636000	6	-2.725516000	-4.336219000	0.000016000
6	-2.919648000	-1.478735000	0.020240000	6	-2.939556000	-3.506855000	-1.178591000
6	-2.610180000	-1.707938000	-1.324801000	6	-2.134552000	-3.679251000	-2.309421000
6	-0.938940000	-1.445636000	-2.971511000	6	-0.286334000	-2.807236000	-3.483975000
6	0.354155000	-0.965051000	-3.206374000	6	0.682275000	-1.799006000	-3.484205000
6	1.478204000	-1.890093000	-3.258093000	6	2.037489000	-2.089399000	-3.035843000
6	1.264650000	-3.259190000	-3.072701000	6	2.368232000	-3.376883000	-2.603857000
6	2.189571000	-4.037805000	-2.260197000	6	3.206115000	-3.556379000	-1.426393000
6	1.414280000	-5.018582000	-1.512347000	6	2.713664000	-4.718289000	-0.698985000
6	1.772669000	-5.340685000	-0.200279000	6	2.713672000	-4.718288000	0.698959000
6	0.741881000	-5.503613000	0.816906000	6	1.572132000	-5.257420000	1.426181000
6	-1.007111000	-4.090809000	2.575956000	6	-1.083134000	-4.687413000	2.308361000
6	0.396222000	-4.261623000	2.926166000	6	0.058678000	-4.148294000	3.034723000
6	1.252956000	-4.953658000	2.064892000	6	1.358606000	-4.427408000	2.603508000
6	2.599013000	-4.452873000	1.820016000	6	2.368257000	-3.376881000	2.603830000
6	2.920207000	-4.691151000	0.419893000	6	3.206132000	-3.556378000	1.426366000
6	3.664613000	-3.749070000	-0.297454000	6	3.680188000	-2.440628000	0.728544000
6	3.291390000	-3.414931000	-1.665117000	6	3.680171000	-2.440629000	-0.728572000
6	3.514749000	-1.988227000	-1.857580000	6	3.337109000	-1.098051000	-1.179152000
6	2.626806000	-1.240154000	-2.638015000	6	2.531170000	-0.926142000	-2.309908000
6	-1.834110000	-0.727083000	-2.073082000	6	-1.641737000	-2.517321000	-3.037062000
6	0.808885000	0.253987000	-2.551344000	6	0.337721000	-0.457475000	-3.035255000
6	-0.977843000	-5.002874000	-0.887050000	6	0.476696000	-5.775640000	-0.728319000
5	-1.162896000	4.959414000	-0.393384000	6	-3.553400000	3.121157000	-0.716404000
7	-2.348894000	4.024924000	-0.500211000	6	-3.553410000	3.121170000	0.716391000
7	-0.155796000	4.463883000	-1.427404000	6	-4.532370000	2.417743000	1.425760000
7	-0.517943000	4.645143000	0.955323000	6	-5.513697000	1.737366000	0.704837000

6	-3.089646000	3.632145000	0.580379000
6	-4.167867000	2.814476000	0.050143000
6	-5.221307000	2.128072000	0.668936000
1	-5.414015000	2.248452000	1.737886000
6	-6.015646000	1.286770000	-0.105488000
1	-6.839623000	0.741379000	0.360718000
6	-5.761519000	1.114199000	-1.482971000
1	-6.389821000	0.433270000	-2.061488000
6	-4.723741000	1.795591000	-2.113980000
1	-4.519125000	1.638012000	-3.175662000
6	-3.930295000	2.666811000	-1.354442000
6	-2.732809000	3.430207000	-1.670475000
6	-1.858539000	3.439715000	-2.772360000
6	-0.533701000	3.887555000	-2.612118000
6	0.697763000	3.618705000	-3.335969000
6	0.953752000	3.004240000	-4.569953000
1	0.133431000	2.701072000	-5.224361000
6	2.275579000	2.768621000	-4.938287000
1	2.493258000	2.283737000	-5.892993000
6	3.343715000	3.130441000	-4.090772000
1	4.368961000	2.922845000	-4.407430000
6	3.107691000	3.729110000	-2.856385000
1	3.938302000	3.991605000	-2.197452000
6	1.782816000	3.981343000	-2.472038000
6	1.199164000	4.475814000	-1.236174000
6	1.710357000	4.652385000	0.063470000
6	0.836640000	4.630113000	1.164871000
6	1.023522000	4.288844000	2.565682000
6	2.172338000	4.075573000	3.340643000
1	3.165947000	4.268011000	2.929053000
6	2.021965000	3.594900000	4.638208000
1	2.905569000	3.411603000	5.253919000
6	0.743534000	3.315054000	5.166739000
1	0.659110000	2.914420000	6.179918000
6	-0.407292000	3.525508000	4.413479000
1	-1.391199000	3.287164000	4.824751000
6	-0.274636000	4.023738000	3.109702000
6	-1.237555000	4.221695000	2.040834000
6	-2.570311000	3.804768000	1.875387000
1	2.786535000	4.608452000	0.229926000
1	-2.146284000	2.929397000	-3.691148000
1	-3.126969000	3.428932000	2.733614000
8	-1.590603000	6.304089000	-0.568053000
6	-0.655223000	7.344977000	-0.552756000
1	0.116749000	7.226849000	-1.338992000
1	-1.181873000	8.296537000	-0.731530000
1	-0.126141000	7.421334000	0.418560000
6	-5.513677000	1.737339000	-0.704852000
6	-4.532337000	2.417700000	-1.425773000
6	-2.331520000	3.793995000	-1.147581000
6	-2.331538000	3.794014000	1.147571000
1	-4.513267000	2.395386000	2.517013000
1	-6.288265000	1.184595000	1.241135000
1	-6.288227000	1.184541000	-1.241148000
1	-4.513202000	2.395307000	-2.517024000
6	1.951146000	3.663811000	-2.457715000
6	0.713991000	3.502076000	-3.163557000
6	0.679295000	2.826408000	-4.386606000
6	1.878378000	2.342747000	-4.908071000
6	3.097988000	2.518631000	-4.222245000
6	3.146004000	3.172232000	-2.992030000
6	1.626930000	4.214908000	-1.146851000
6	-0.350803000	3.979890000	-2.287605000
1	-0.269932000	2.666677000	-4.901017000
1	1.874904000	1.805836000	-5.859423000
1	4.015652000	2.118726000	-4.660576000
1	4.081261000	3.286401000	-2.440822000
6	0.713971000	3.502059000	3.163546000
6	1.951131000	3.663783000	2.457706000
6	3.145980000	3.172198000	2.992036000
6	3.097948000	2.518614000	4.222260000
6	1.878334000	2.342744000	4.908079000
6	0.679257000	2.826403000	4.386601000
6	-0.350816000	3.979870000	2.287587000
6	1.626919000	4.214892000	1.146846000
1	4.081245000	3.286349000	2.440837000
1	4.015609000	2.118712000	4.660602000
1	1.874850000	1.805845000	5.859440000
1	-0.269977000	2.666686000	4.901003000
7	0.284149000	4.493176000	1.186643000
7	-1.755180000	4.273677000	-0.000005000
7	0.284157000	4.493201000	-1.186658000
7	-1.661734000	3.714126000	2.301098000
7	-1.661716000	3.714117000	-2.301107000
7	2.311242000	4.155689000	0.000000000
5	-0.459513000	5.015731000	-0.000005000
17	-0.658694000	6.863475000	0.000034000

Suma⊃C_{60}

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

Atom	X	Y	Z
6	5.739719000	-2.805671000	1.762324000

Cora⊃C_{60}

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

Atom	X	Y	Z
6	0.934401000	1.329324000	-3.103006000

6	5.779913000	-1.784644000	2.800652000	6	0.948428000	-0.100654000	-3.384666000
6	4.837267000	-0.752416000	2.800862000	6	0.002510000	-0.938640000	-2.785815000
6	3.818651000	-0.699537000	1.763664000	6	-0.994469000	-0.382560000	-1.882089000
6	3.777473000	-1.678991000	0.770269000	6	-1.007847000	0.987465000	-1.613578000
6	4.757106000	-2.755004000	0.768824000	6	-0.025122000	1.861821000	-2.236396000
6	7.112020000	-3.145797000	1.411395000	6	2.315749000	1.786029000	-3.027079000
6	7.999799000	-2.332572000	2.232255000	6	3.183784000	0.640053000	-3.262594000
6	7.176382000	-1.491376000	3.091089000	6	2.338611000	-0.526260000	-3.482272000
6	7.571659000	-0.179978000	3.373660000	6	2.725568000	-1.772919000	-2.980861000
6	5.246537000	0.614413000	3.097671000	6	0.404891000	-2.238642000	-2.264537000
6	3.595519000	0.694541000	1.419380000	6	-1.209130000	-1.335732000	-0.804526000
6	3.338244000	1.055003000	0.096634000	6	-1.426838000	-0.880884000	0.496033000
6	3.301976000	0.033756000	-0.939812000	6	-1.443915000	0.545353000	0.775762000
6	3.515998000	-1.303618000	-0.610259000	6	-1.238931000	1.461488000	-0.256756000
6	4.334510000	-2.148265000	-1.469483000	6	-0.396341000	2.629651000	-0.037610000
6	5.103347000	-3.045188000	-0.616766000	6	0.354852000	2.876806000	-1.260903000
6	6.420588000	-3.371908000	-0.953595000	6	1.680625000	3.314691000	-1.189897000
6	7.445404000	-3.422520000	0.081837000	6	2.681150000	2.758612000	-2.091245000
6	9.184222000	-1.826465000	1.688609000	6	4.381106000	0.512011000	-2.551249000
6	9.531600000	-2.114084000	0.304245000	6	4.761530000	1.525377000	-1.576014000
6	8.680157000	-2.895424000	-0.483027000	6	3.927650000	2.624355000	-1.350352000
6	8.418936000	-2.519602000	-1.865874000	6	3.697745000	3.098072000	0.007804000
6	7.022862000	-2.813684000	-2.156962000	6	2.308867000	3.524770000	0.107165000
6	6.283781000	-1.953420000	-2.976383000	6	1.586749000	3.288073000	1.281061000
6	4.911905000	-1.614607000	-2.625714000	6	0.204676000	2.834736000	1.208156000
6	4.690475000	-0.215358000	-2.970966000	6	-0.010666000	1.877386000	2.287174000
6	3.906517000	0.589775000	-2.141796000	6	-0.815217000	0.756349000	2.072990000
6	4.476577000	1.509278000	2.243509000	6	-0.346419000	-2.484691000	-1.040041000
6	6.384763000	3.277220000	-1.573504000	6	1.649114000	-1.818062000	3.074137000
6	6.050726000	3.553377000	-0.243675000	6	1.283263000	-2.790160000	2.137118000
6	7.075684000	3.500887000	0.791097000	6	2.283619000	-3.344609000	1.235129000
6	8.392373000	3.173408000	0.454081000	6	3.609041000	-2.905700000	1.305775000
6	8.739409000	2.885051000	-0.930402000	6	3.989946000	-1.892812000	2.280862000
6	7.716727000	1.913377000	-2.960457000	6	3.015296000	0.070019000	3.427963000
6	6.321184000	1.622298000	-3.254423000	6	1.626252000	0.496109000	3.529879000
6	5.497686000	2.463347000	-2.394670000	6	0.781791000	-0.671405000	3.310096000
6	4.314963000	1.956195000	-1.849965000	6	-0.412979000	-0.542446000	2.596360000
6	3.967694000	2.242535000	-0.465091000	6	-0.790837000	-1.554449000	1.619180000
6	4.814897000	3.028585000	0.321950000	6	0.035728000	-2.658223000	1.397227000
6	6.473405000	2.943565000	1.995213000	6	1.654415000	-3.555704000	-0.062019000
6	7.213204000	2.083524000	2.814110000	6	2.376173000	-3.319255000	-1.236151000
6	8.584507000	1.743392000	2.461845000	6	3.757036000	-2.862092000	-1.162121000
6	9.163170000	2.278636000	1.307032000	6	4.360447000	-2.659473000	0.082680000
6	9.986284000	1.437157000	0.448611000	6	5.207313000	-1.493994000	0.301375000
6	9.722572000	1.811652000	-0.933551000	6	4.976302000	-1.019726000	1.659896000
6	9.684141000	0.831475000	-1.928794000	6	4.962599000	0.352073000	1.929379000
6	8.661241000	0.882757000	-2.962716000	6	3.962059000	0.907828000	2.830695000
6	5.925922000	0.310460000	-3.535675000	6	1.238529000	1.742320000	3.026844000
6	6.910468000	-0.763885000	-3.538563000	6	2.224925000	2.614515000	2.405046000
6	8.250682000	-0.482721000	-3.257862000	6	3.558572000	2.205565000	2.308841000
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6	9.907173000	-0.565548000	-1.584436000	6	5.178799000	1.307396000	0.851332000
6	10.159250000	-0.926058000	-0.257931000	6	5.400685000	0.852979000	-0.452456000

6	10.199486000	0.096031000	0.779804000
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6	6.586921000	0.894803000	3.377429000
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6	-0.073239000	0.030514000	-1.442099000
6	0.559950000	-0.089045000	-2.687236000
6	1.049274000	1.101223000	-3.245296000
6	1.025467000	2.333698000	-2.513442000
6	0.513386000	2.396117000	-1.208706000
6	0.736197000	3.320282000	0.021734000
1	1.590611000	1.089306000	-4.195161000
1	1.544718000	3.189831000	-2.953503000
1	1.750498000	3.746136000	0.036189000
1	0.032849000	4.172258000	0.025879000
6	-0.060068000	-1.222140000	-0.741162000
6	-0.067885000	-1.239502000	0.648032000
6	0.558548000	-2.250564000	1.389998000
6	1.080689000	-3.325029000	0.652800000
6	1.093767000	-3.305557000	-0.779986000
6	0.584325000	-2.211641000	-1.496818000
6	0.856995000	-1.599868000	-2.898238000
1	1.617120000	-4.135641000	1.153860000
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1	1.899057000	-1.766909000	-3.213902000
1	0.215596000	-2.046309000	-3.678500000
6	-0.089811000	-0.006100000	1.381716000
6	-0.103420000	1.206584000	0.704017000
6	0.492962000	2.364718000	1.223611000
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6	1.005787000	1.014273000	3.229539000
6	0.523367000	-0.160430000	2.633132000
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6	-3.865990000	-0.706548000	3.135946000
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1	-3.552981000	-3.315458000	-2.674687000
1	-3.541939000	-1.330430000	-4.071859000
1	-3.527908000	-4.220523000	-0.004923000
1	-3.501044000	-3.499078000	2.316759000
1	-3.480691000	-1.240281000	4.009196000
1	-3.463382000	1.189500000	4.041492000

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