Supporting information for:

Rational design of perylene diimide macrocycles with diverse electron transfer properties in complexes with fullerene

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Abstract

Perylene diimide (PDI)-based macrocycles offer a versatile platform for creating host-guest complexes with fullerenes. About 100 bay- and ortho-substituted PDIs, as well as their □-extended derivatives have been tested to select the best electron donor and electron acceptor systems. This work presents a computational study of macrocycles consisting of two PDI units linked by flexible spacers as hosts for C_{60} fullerene. The results provide insight into their ground and excited state electronic properties and help to rationally design complexes with tailored photoinduced electron transfer behavior, thereby advancing the development of artificial photosystems. The results revealed that in the ground state, there is almost no electronic communication between macrocycle and fullerene. However, upon photoexcitation, the electron transfer from macrocycle to fullerene or vice versa was predicted, demonstrating a tunable directionality unprecedented in similar systems. The direction of electron transfer is determined by the electronic nature of the macrocycle. For electron-donating macrocyles, the electron is transferred from the macrocycle to fullerene, whereas for electron-accepting hosts, it occurs in the opposite direction. The electron transfer occurs within the normal Marcus region, with optimal electron transfer rates observed in specific complexes, making them interesting systems for photovoltaic technology. Based on the structure-electronic properties relationship, design principles for novel PDI-based macrocycles were formulated to guide chemists in developing advanced organic materials for photovoltaic applications.

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Computational Methodology

Energy decomposition analysis

The interaction energy between MC-PDI macrocycle and fullerene in the gas phase was examined in the framework of the Kohn-Sham MO model using a quantitative energy decomposition into electrostatic interactions, Pauli repulsive orbital interactions and attractive orbital interactions, to which a term ΔE_{disp} was added to account for the dispersion correction:[1-3]

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

The term ΔV_{elstat} corresponds to the classical electrostatic interactions between the unperturbed charge distributions of the prepared (i.e. deformed) fragments and is usually attractive. The Pauli repulsion, ΔE_{Pauli}, comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interactions, ΔE_{oi}, account for electron-pair bonding, charge transfer (*i.e.*, donor–acceptor interactions between occupied orbitals on one moiety and unoccupied orbitals on the other, including HOMO-LUMO interactions) and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). The term ΔE_{disp} accounts for the dispersion corrections.[4,5]

Analysis of excited states

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out in terms of the transition density.[6-8] The analysis was done in the Löwdin orthogonalized basis. The matrix ${}^{\lambda}\mathbf{C}$ of orthogonalized MO coefficients was obtained from the coefficients **C** in the original basis ${}^{\lambda}\mathbf{C} = \mathbf{S}^{1/2}\,\mathbf{C}$, where **S** is the atomic orbital overlap matrix. The transition density matrix T^{0i} for an excited state Φ_i^* constructed as a superposition of singly excited configurations (where an occupied MO ψ_j is replaced a virtual MO ψ_a) is computed as,

$$T_{\alpha\beta}^{0i} = \sum_{ja} A_{j\to a}\, {}^{\lambda}C_{\alpha j}\, {}^{\lambda}C_{\beta a} \quad (2)$$

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

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

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

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

$$\Delta q(CS) = \sum \Omega(D,A) - \Omega(A,D) \tag{4}$$

$$\Delta q(CT) = \sum \Omega(D,A) + \Omega(A,D) \tag{5}$$

Solvent Effects

The equilibrium solvation energy E_S^{eq} of a molecule (in the ground or excited state) in the medium with the dielectric constant ε was estimated using a COSMO-like polarizable continuum model[9-12] in the monopole approximation:

$$E_S^{eq}(Q,\varepsilon) = -\frac{1}{2} f(\varepsilon) Q^{+} D Q \tag{6}$$

where the $f(\varepsilon)$ is the dielectric scaling factor, $f(\varepsilon) = \frac{\varepsilon - 1}{\varepsilon}$, **Q** – the vector of *n* atomic charges in the molecular system, **D** is the *n* x *n* symmetric matrix determined by the shape of the boundary surface between solute and solvent. $\mathbf{D=B^{+}A^{-1}B}$, where the *m* x *m* matrix **A** describes electrostatic interaction between *m* surface charges and the *m* x *n* **B** matrix describes the interaction of the surface charges with *n* atomic charges of the solute.[9,13] The GEPOL93 scheme[14] was used to construct the molecular boundary surface.

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

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

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

The non-equilibrium solvation energy for excited state Φ_i*can be estimated as:[15]

$$E_S^{neq}(Q^0, \Delta, \varepsilon, n^2) = f(\varepsilon) \Delta^{+} D Q^0 - \frac{1}{2} f(n^2) \Delta^{+} D \Delta, \tag{8}$$

In Eq. (8), n^2 (the refraction index squared) is the optical dielectric constant of the medium and the vector Δ describes the change of atomic charges in the molecule by excitation in terms of atomic charges, see Eq. (7). By definition, the external (solvent) reorganization energy is the difference of the non-equilibrium (Eq. 8) and equilibrium (Eq. 6) solvation energies of the excited state.

Reorganization energy

The reorganization energy is usually divided into two parts, $\lambda = \lambda_i + \lambda_s$, including the internal and solvent terms. The solvent reorganization energy corresponds to the energy required to move solvent molecules

from the position they occupy in the initial state to the location they have in the CT state, but without charge transfer having occurred. The λ_s for a particular CT state was computed as a difference between the equilibrium (E_s^{eq}, see eq. 6) and non-equilibrium (E_s^{neq}, see eq. 8) solvation energies. The internal reorganization energy λ_i corresponds to the energy of structural changes when donor/acceptor fragments going from initial-state geometries to final-state geometries.

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

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

$$\lambda_i^2(MC^* \rightarrow MC^+) = \frac{1}{2}\left[\left((MC^*)_+ - (MC^*)_*\right) + \left((MC^+)_* - (MC^+)_+\right)\right], \text{ or for CT2} \quad (9)$$

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

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

Electron transfer rates

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

$$k_{ET} = \frac{2\pi}{\hbar} V^2 \, (FCWD) \quad (10)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:[16]

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (11)$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD)[17,18] method was employed to calculate the electronic couplings in this work.

The Marcus expression is derived for the high-temperature condition, $\hbar\omega_l \ll kT$, for all vibrational modes *l*. The semi-classical description of ET[19,20] includes the effect of the quantum vibrational modes in an effective way, the solvent (low frequency) modes are treated classically, while a single high-frequency intramolecular mode ω_i, $\hbar\omega_i \gg kT$, is described quantum mechanically. Because ET occurs normally from the lowest vibrational level of the initial state, the rate *k* can be expressed as a sum over all channels connecting the initial state with the vibrational quantum number n = 0 to manifold vibrational levels of the final state,

$$k = \sum_{n=0}^{\infty} k_{0\rightarrow n}, \text{ where } k_{0\rightarrow n} = \frac{2\pi}{\mathsf{h}} V_{0\rightarrow n}^2 \frac{1}{\sqrt{4\pi\lambda_s kT}} \exp\left[-\frac{(\Delta G + n\mathsf{h}\omega_i + \lambda_s)^2}{4\lambda_s kT}\right] \quad (12)$$

with

$$V_{0\to n}^2 = V^2 \frac{S^n}{n!}\exp(-S) \tag{13}$$

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 (compared to the Marcus equation) enters the semi-classical expression - the frequency ω_i of a vibrational mode that effectively describes the nuclear intramolecular relaxation following the ET. Typically, in organic systems (including fullerene and other carbon nanostructures) the main contribution to the internal reorganization energy is due to stretching of C=C bonds. The corresponding frequencies are found to be in the range of 1400-1800 cm^{-1}.

Quantum Theory of Atoms in Molecules (QTAIM)

Topological analysis of the electron density distributions was conducted using the "Quantum Theory of Atoms in Molecules" (QTAIM) proposed by Bader.[21,22] Electron density properties measured at the bond critical point (BCP) give information about the character of different chemical bonds.[23-25] The AIMALL suite of programs[26] was applied to evaluate BCP properties and associated bond descriptors – 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 [$H(r)$].

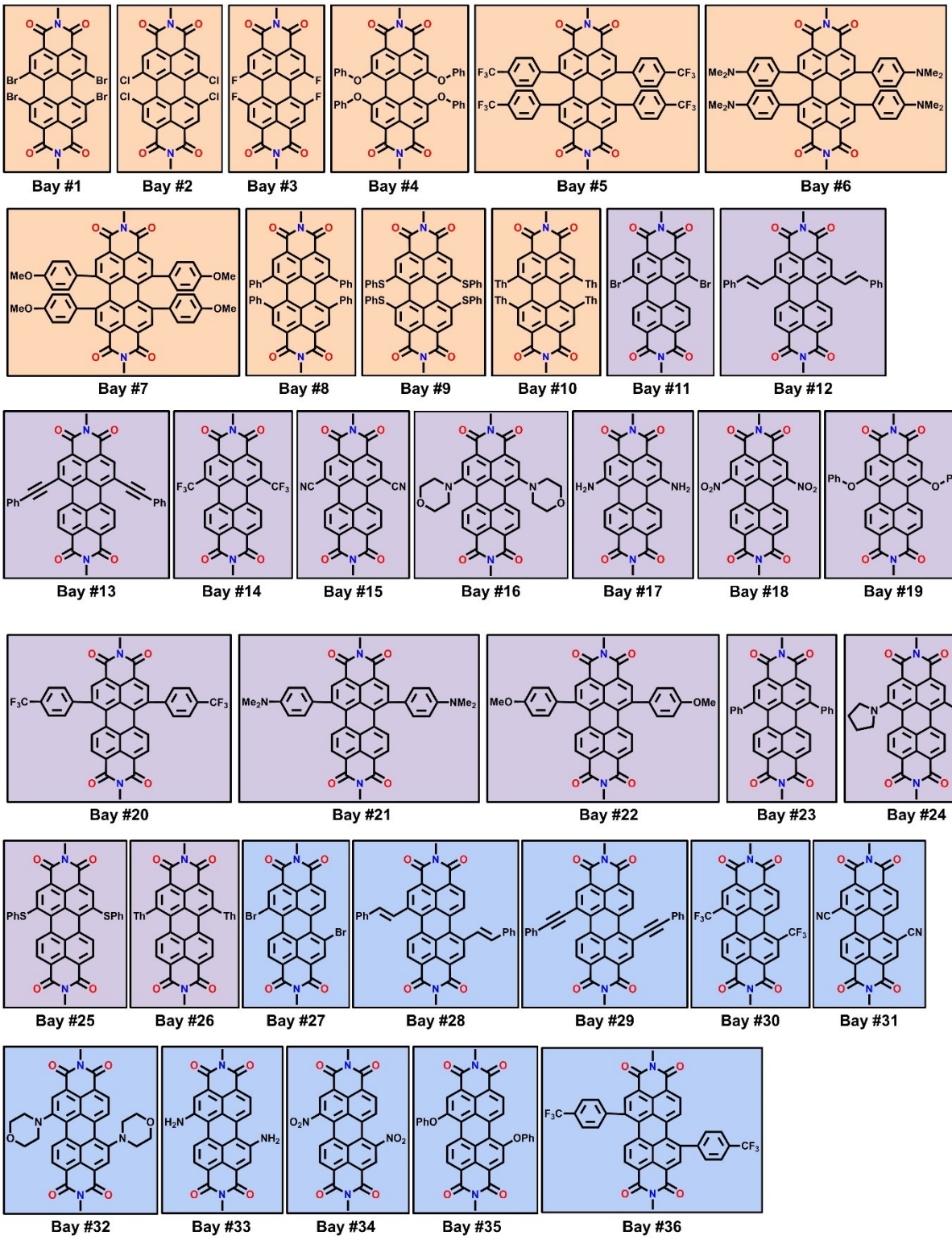
Non-covalent interaction (NCI) index

The NCI method[27-29] relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s) defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \tag{14}$$

The combination of s and ρ allows a rough partition of real space into bonding regions: high-s low-ρ region corresponds to non-interacting density tails, low-s high-ρ region to covalent bonds, and low-s low-ρ one to non-covalent interactions. The NCI analysis was carried out at the BLYP-D3(BJ)/def2-SVP level using Multiwfn.[30]

Molecular structures and frontier molecular orbitals were visualized by VMD software[31] and Chemcraft 1.8. program.[32]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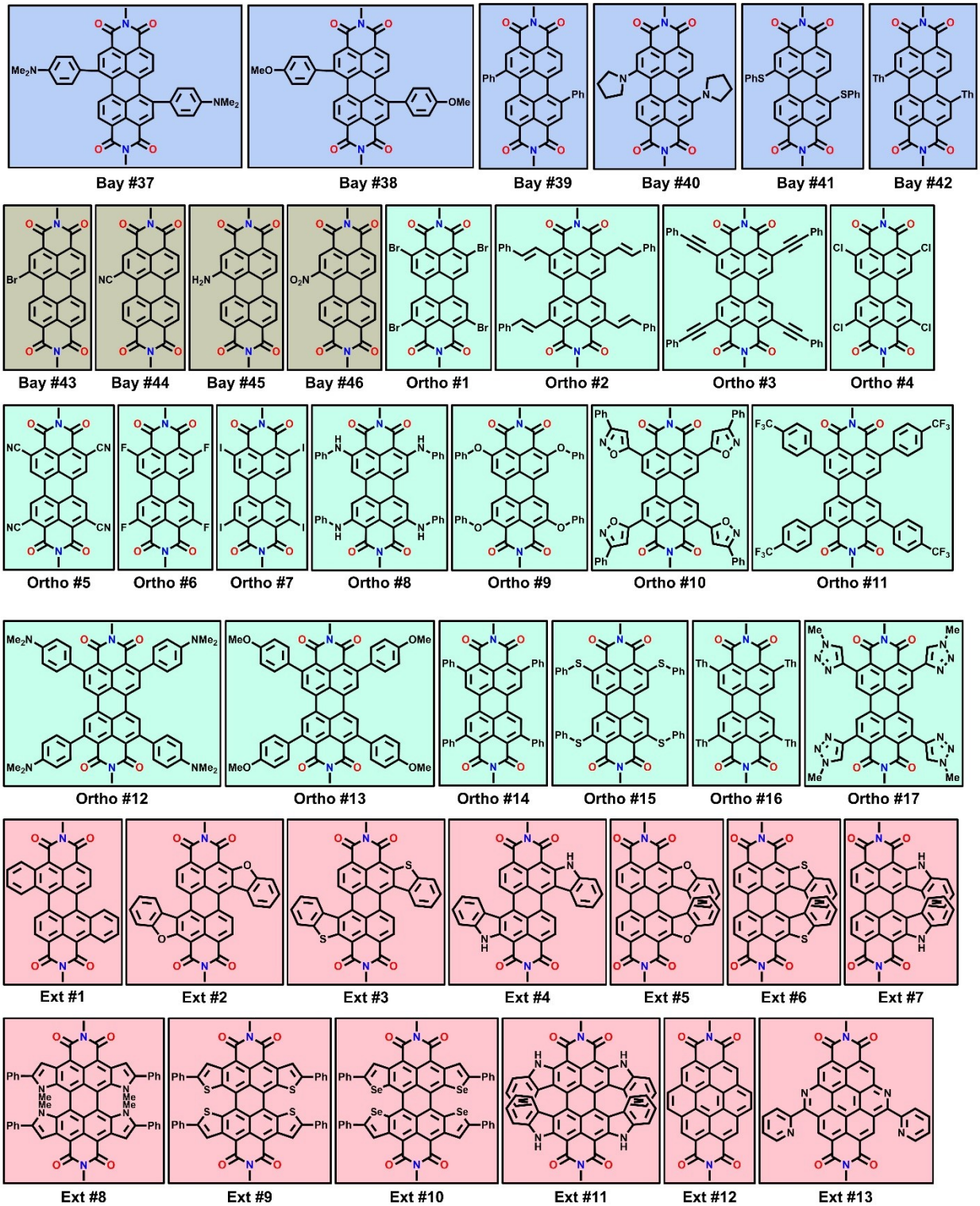
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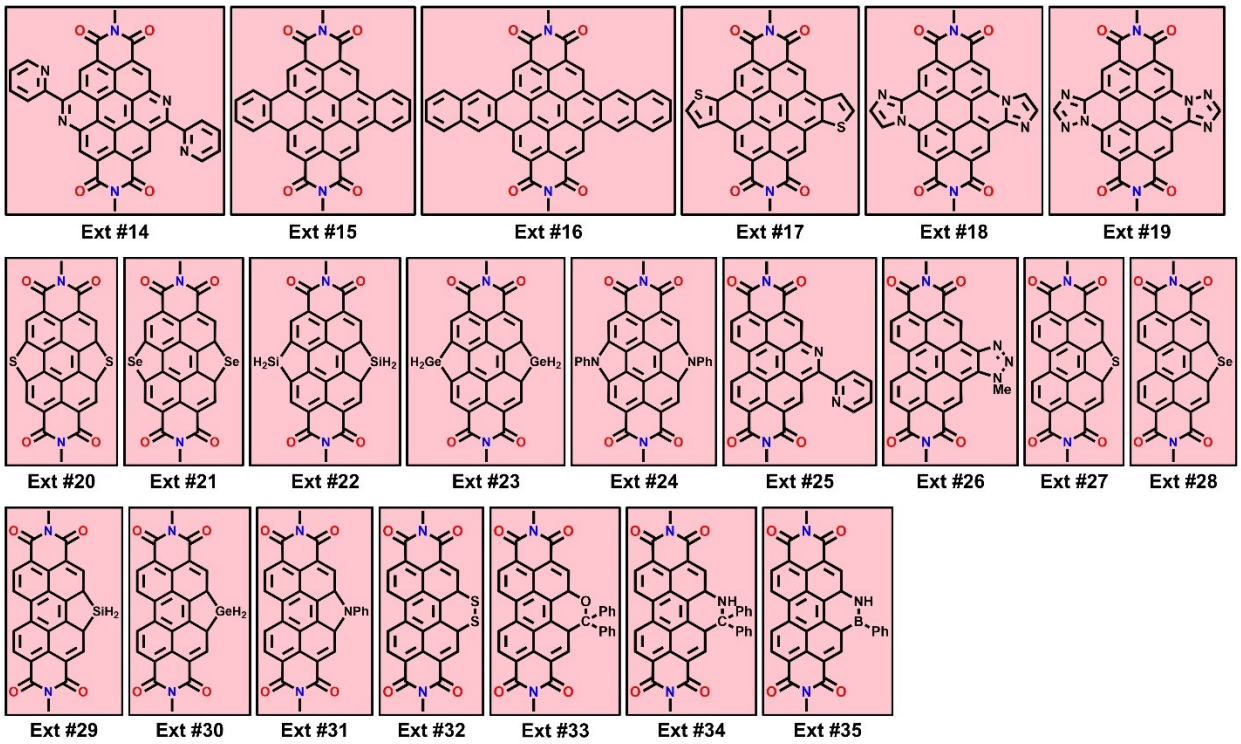

Figure S1. Structures of PDI molecules considered in this work. Colors of structures match the colors in Figure 1 in the main text.

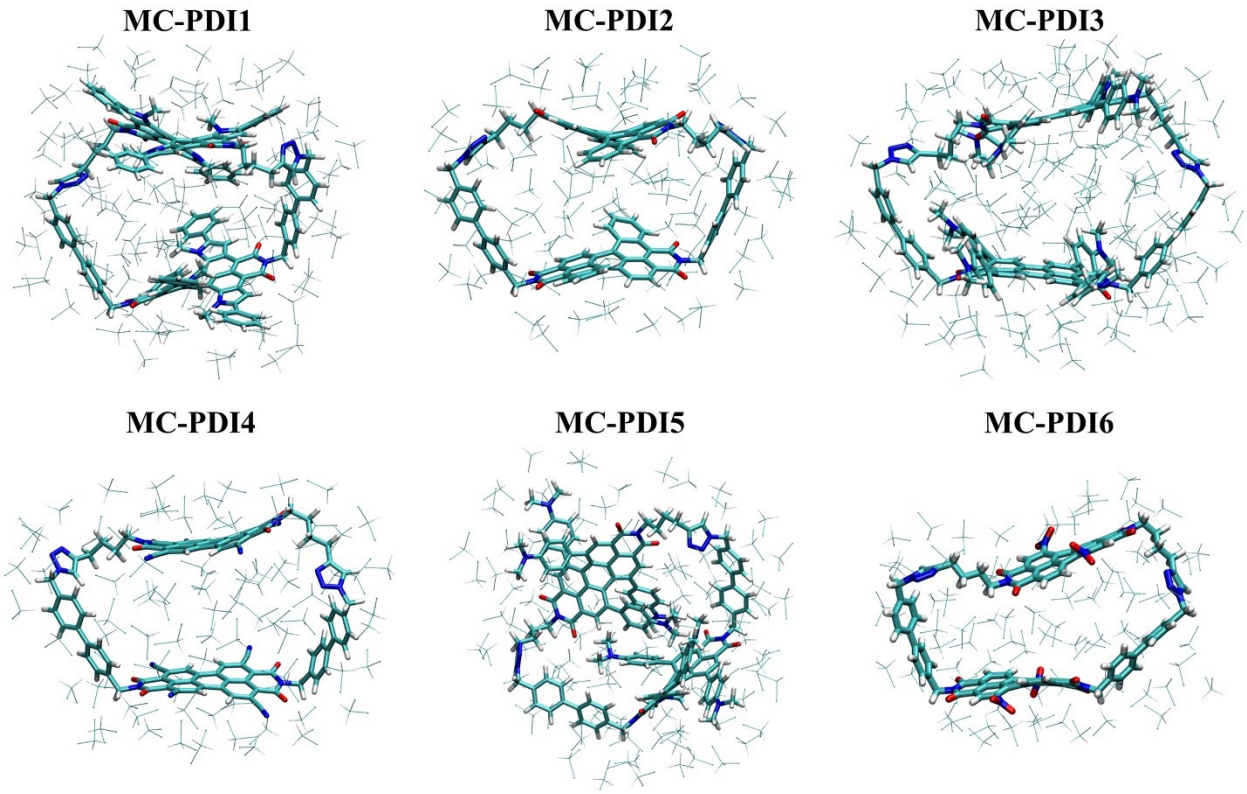

Figure S2. Structures of **MC-PDI1**, **MC-PDI2**, **MC-PDI3**, **MC-PDI4**, **MC-PDI5**, and **MC-PDI6** macrocycles optimized in DCM within QM1/QM2 (BLYP-D3(BJ)/def2-SVP//GFN2-xTB) approach.

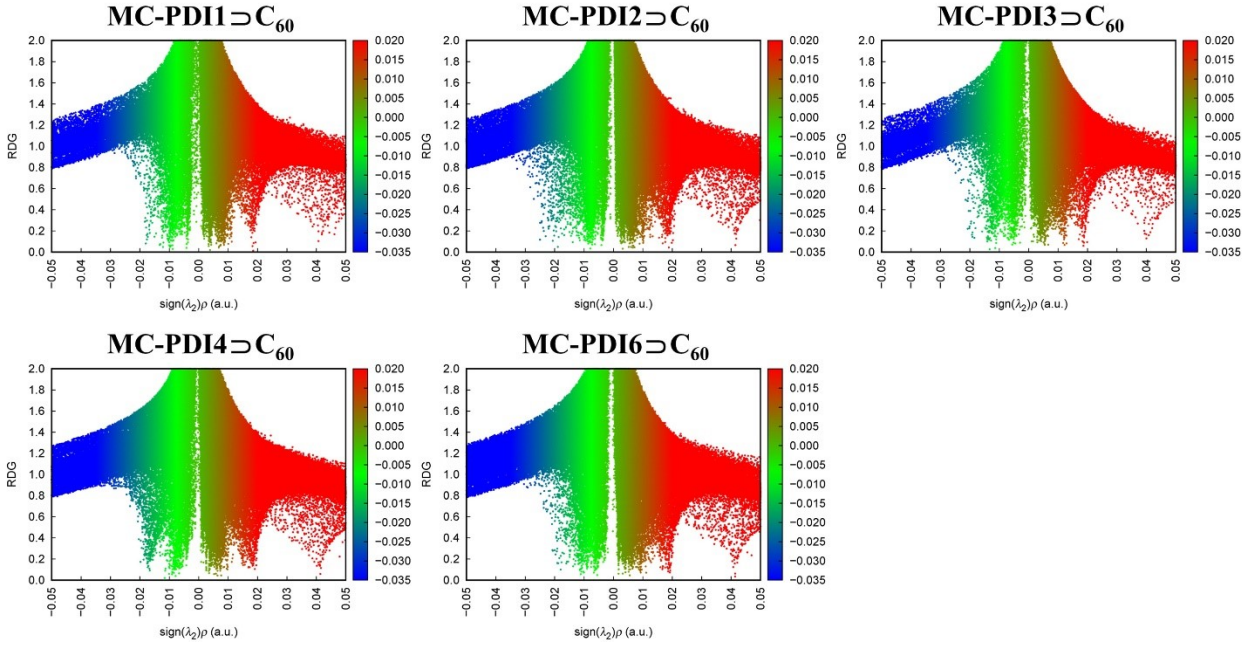

Figure S3. Plot of RDG *vs.* sign(λ2)×ρ for **MC-PDI1⊃C$_{60}$**, **MC-PDI2⊃C$_{60}$**, **MC-PDI3⊃C$_{60}$**, **MC-PDI4⊃C$_{60}$**, and **MC-PDI6⊃C$_{60}$** complexes.

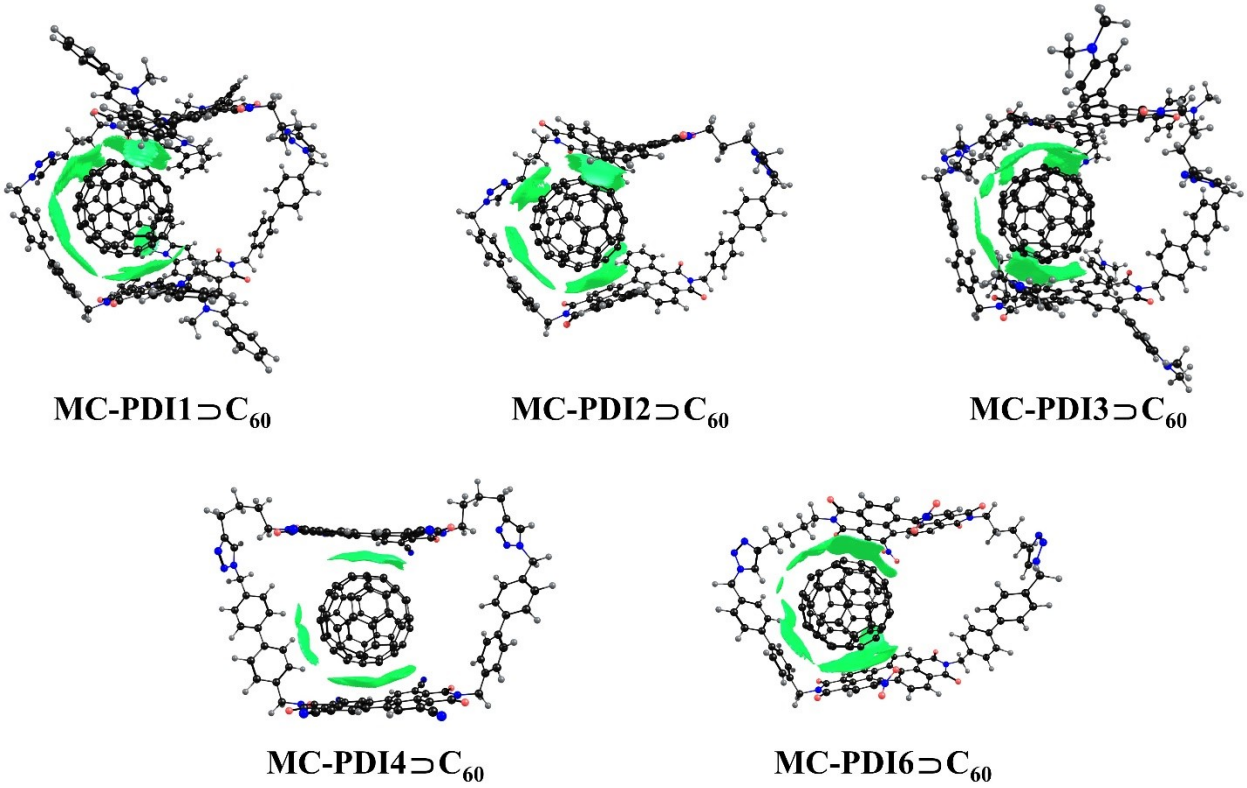

Figure S4. NCI isosurfaces of van der Waals interactions for **MC-PDI1⊃C_{60}**, **MC-PDI2⊃C_{60}**, **MC-PDI3⊃C_{60}**, **MC-PDI4⊃C_{60}**, and **MC-PDI6⊃C_{60}** complexes.

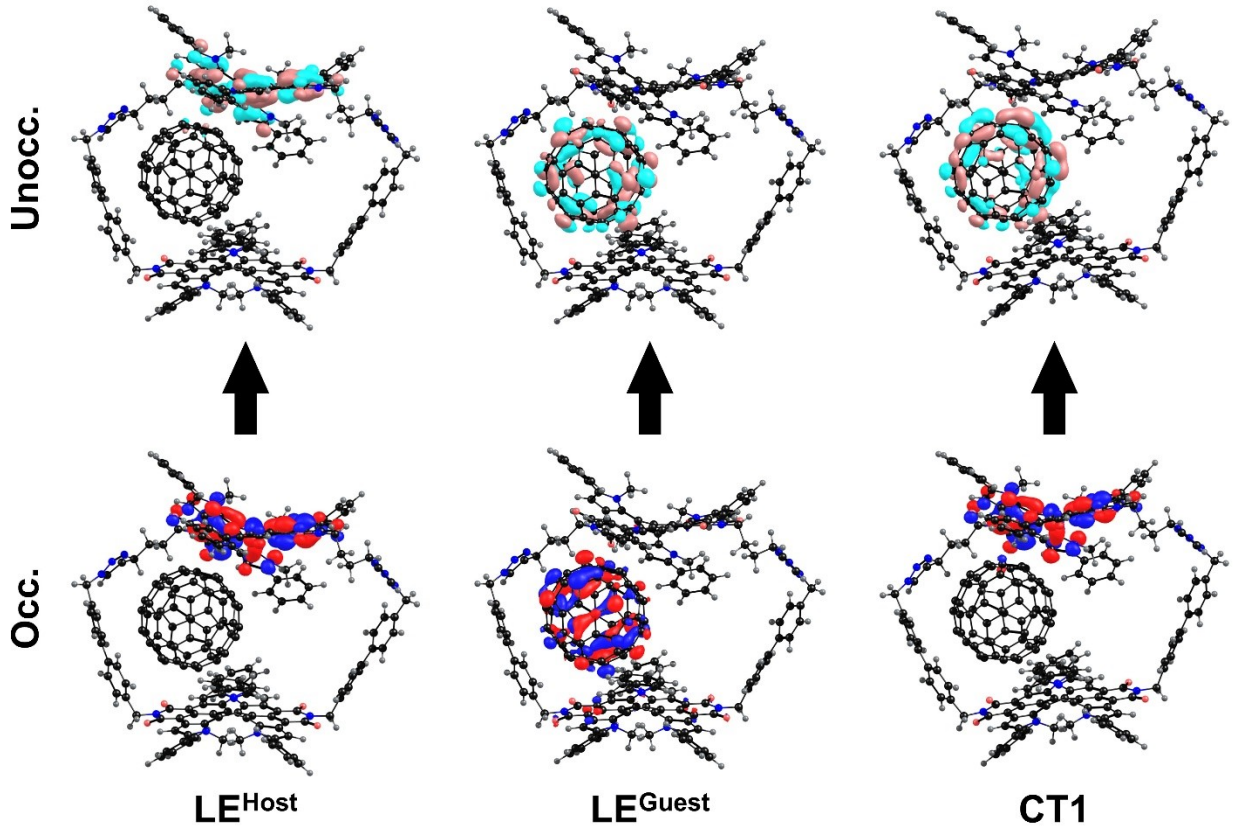

Figure S5. Natural transition orbitals representing lowest-lying singlet LE and CT excited states for **MC-PDI1⊃C_{60}** complex.

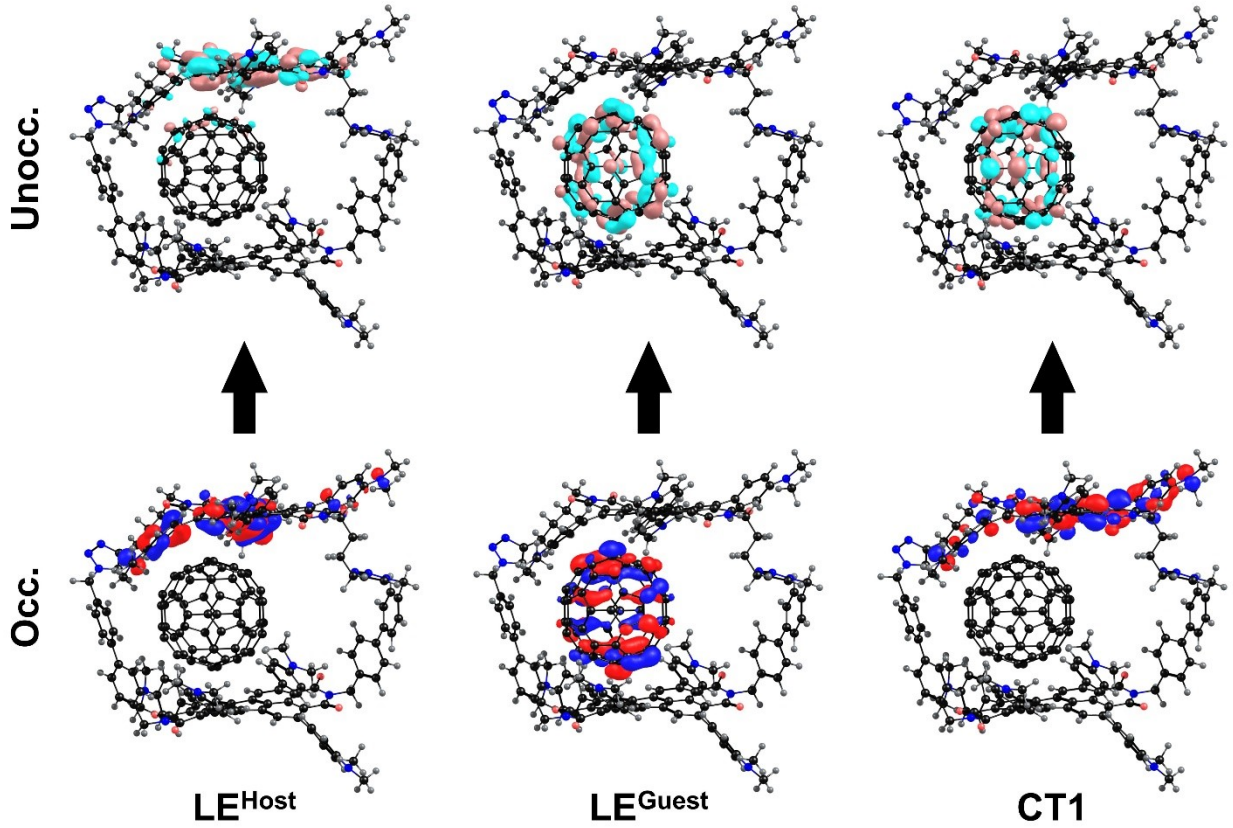

Figure S6. Natural transition orbitals representing lowest-lying singlet LE and CT excited states for **MC-PDI3⊃C_{60}** complex.

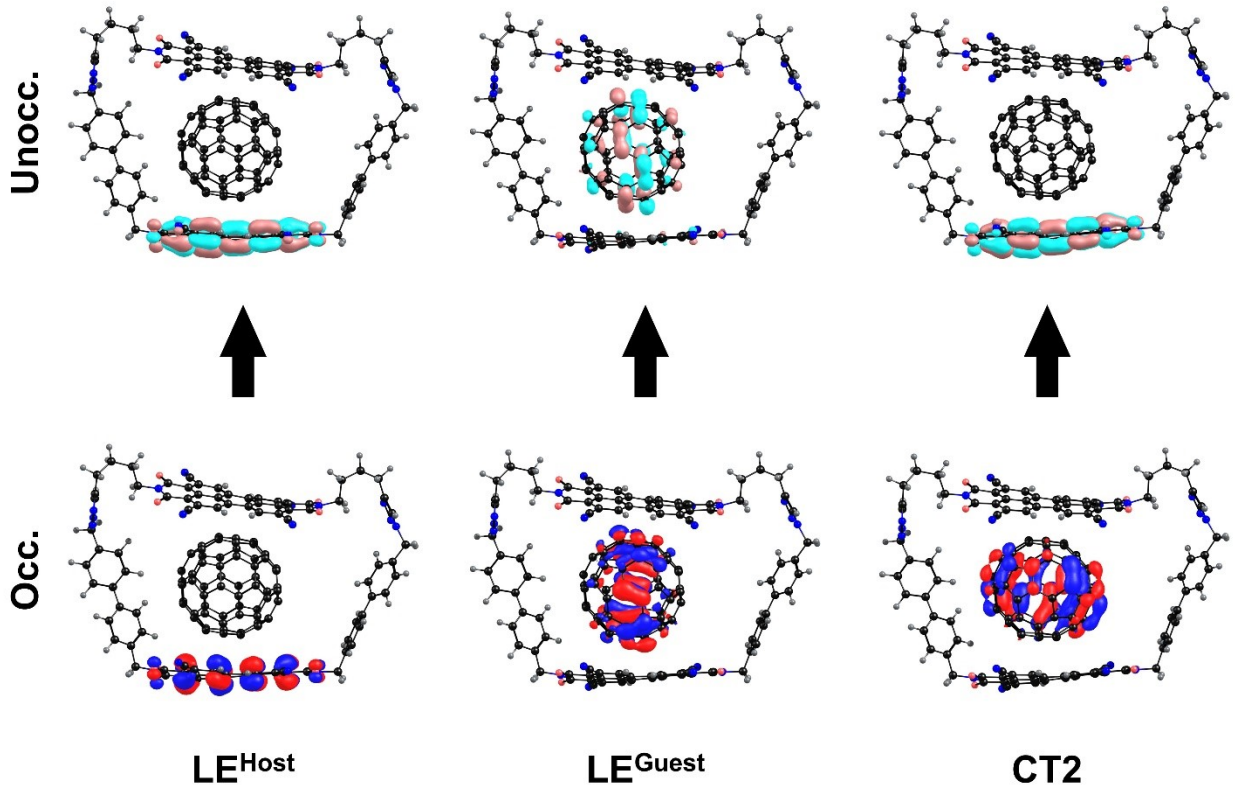

Figure S7. Natural transition orbitals representing lowest-lying singlet LE and CT excited states for **MC-PDI4⊃C_{60}** complex.

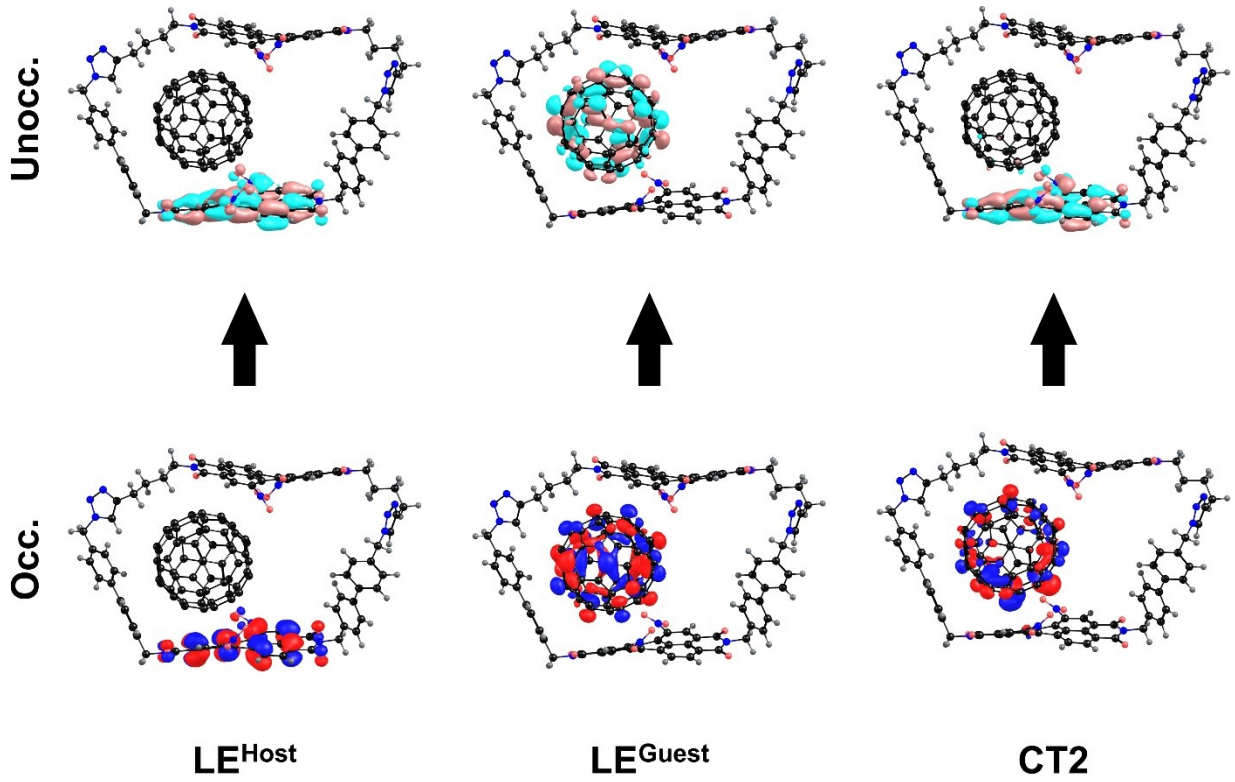

Figure S8. Natural transition orbitals representing lowest-lying singlet LE and CT excited states for **MC-PDI6⊃C_{60}** complex.

Table S1. HOMO and LUMO energies, as well as HOMO-LUMO (HL) gap for individual PDIs considered in this work.

PDI	HOMO	LUMO	HL Gap	PDI	HOMO	LUMO	HL Gap
Bay-substituted PDIs							
1	-7.615	-3.141	4.473	**24**	-6.424	-2.362	4.063
2	-7.598	-3.099	4.499	**25**	-7.013	-2.632	4.381
3	-7.532	-3.014	4.517	**26**	-7.026	-2.805	4.221
4	-6.717	-2.446	4.271	**27**	-7.462	-2.983	4.479
5	-7.438	-3.229	4.209	**28**	-6.813	-2.776	4.038
6	-6.036	-2.226	3.810	**29**	-6.926	-2.882	4.044
7	-6.561	-2.540	4.022	**30**	-7.775	-3.236	4.539
8	-6.863	-2.715	4.148	**31**	-7.884	-3.470	4.414
9	-6.907	-2.785	4.123	**32**	-6.572	-2.593	3.979
10	-6.751	-2.840	3.911	**33**	-6.586	-2.445	4.141
11	-7.457	-2.984	4.473	**34**	-7.966	-3.526	4.440
12	-6.894	-2.768	4.125	**35**	-6.900	-2.579	4.321
13	-6.980	-2.868	4.113	**36**	-7.344	-3.014	4.331
14	-7.778	-3.230	4.547	**37**	-6.365	-2.455	3.910
15	-7.873	-3.459	4.414	**38**	-6.815	-2.635	4.180
16	-6.761	-2.650	4.111	**39**	-7.029	-2.728	4.301
17	-6.722	-2.422	4.300	**40**	-6.262	-2.283	3.979
18	-7.948	-3.524	4.424	**41**	-6.961	-2.634	4.327
19	-6.938	-2.580	4.358	**42**	-6.989	-2.812	4.177
20	-7.354	-3.009	4.345	**43**	-7.377	-2.913	4.464
21	-6.430	-2.456	3.974	**44**	-7.583	-3.167	4.417
22	-6.841	-2.620	4.221	**45**	-6.929	-2.632	4.296
23	-7.043	-2.723	4.320	**46**	-7.627	-3.189	4.437
Ortho-substituted PDIs							
1	-7.786	-3.164	4.622	**10**	-7.607	-3.131	4.477
2	-7.160	-2.745	4.415	**11**	-7.691	-3.225	4.466
3	-7.218	-2.822	4.396	**12**	-6.340	-2.242	4.097
4	-7.803	-3.156	4.647	**13**	-6.985	-2.554	4.431
5	-8.454	-3.974	4.480	**14**	-7.182	-2.717	4.465
6	-7.888	-3.223	4.665	**15**	-7.211	-2.614	4.597
7	-7.714	-3.128	4.586	**16**	-7.175	-2.771	4.403
8	-6.779	-2.318	4.461	**17**	-6.955	-2.430	4.525
9	-7.194	-2.566	4.628				
π-extended PDIs							
1	-6.776	-3.186	3.589	**19**	-7.776	-3.085	4.691
2	-7.038	-2.947	4.091	**20**	-7.607	-2.862	4.745
3	-6.940	-2.974	3.966	**21**	-7.520	-2.837	4.683
4	-6.750	-2.784	3.966	**22**	-7.344	-2.934	4.409
5	-7.058	-2.938	4.119	**23**	-7.279	-2.878	4.401

6	-6.958	-2.957	4.001	**24**	-7.080	-2.235	4.845
7	-6.750	-2.760	3.990	**25**	-7.470	-2.636	4.833
8	-6.044	-2.515	3.529	**26**	-7.462	-2.800	4.662
9	-6.661	-2.878	3.783	**27**	-7.435	-2.819	4.616
10	-6.700	-2.833	3.867	**28**	-7.395	-2.817	4.578
11	-6.452	-2.679	3.773	**29**	-7.312	-2.893	4.418
12	-7.579	-2.415	5.164	**30**	-7.281	-2.863	4.418
13	-7.653	-2.475	5.179	**31**	-7.200	-2.628	4.572
14	-7.462	-2.478	4.985	**32**	-7.304	-3.094	4.210
15	-7.214	-2.528	4.686	**33**	-7.075	-2.756	4.319
16	-6.834	-2.608	4.226	**34**	-6.760	-2.607	4.153
17	-7.284	-2.475	4.809	**35**	-7.181	-2.676	4.505
18	-7.344	-2.892	4.452				

Table S2. Charge separation (in electrons) between the fragments in electronic ground state for **MC-PDI1⊃C$_{60}$**, **MC-PDI2⊃C$_{60}$**, **MC-PDI3⊃C$_{60}$**, **MC-PDI4⊃C$_{60}$**, and **MC-PDI6⊃C$_{60}$** complexes. Q_{Host} is charge on host (**MC-PDI1**, **MC-PDI2**, **MC-PDI3**, **MC-PDI4**, and **MC-PDI16**), and Q_{C60} is charge on C_{60} fullerene. Total charge of the complexes $Q_{Tot} = 0$.

Complex	Charge Scheme					
	Mulliken		Löwdin		CM5	
	Q_{Host}	Q_{C60}	Q_{Host}	Q_{C60}	Q_{Host}	Q_{C60}
MC-PDI1⊃C$_{60}$	0.055	-0.055	0.021	-0.021	-0.127	0.127
MC-PDI2⊃C$_{60}$	0.025	-0.025	0.018	-0.018	-0.086	0.086
MC-PDI3⊃C$_{60}$	0.024	-0.024	0.001	-0.001	-0.143	0.143
MC-PDI4⊃C$_{60}$	-0.044	0.044	-0.030	0.030	-0.129	0.129
MC-PDI6⊃C$_{60}$	0.023	-0.023	0.018	-0.018	-0.108	0.108

Table S3. Parameters (electron density [ρ(r)], its Laplacian [∇2ρ(r)], potential energy density [V(r)], kinetic energy density [G(r)], and total electron energy density [H(r)]) for selected bond critical points related to non-covalent interactions in **MC-PDI1⊃C$_{60}$**, **MC-PDI2⊃C$_{60}$**, **MC-PDI3⊃C$_{60}$**, **MC-PDI4⊃C$_{60}$**, and **MC-PDI6⊃C$_{60}$** complexes computed in the gas phase.

Bond critical points between fragments	Interaction	*ρ(r)*, a.u.	$\nabla^2\rho(r)$, a.u.	*V(r)*, a.u.	*G(r)*, a.u.	*H(r)*, a.u.
		MC-PDI1⊃C$_{60}$				
PDI1 ⋯ C$_{60}$	π···π	3.70E-03	8.68E-03	-1.48E-03	1.82E-03	3.46E-04
		1.08E-02	3.06E-02	-4.77E-03	6.21E-03	1.44E-03
		9.00E-03	2.78E-02	-3.97E-03	5.46E-03	1.49E-03
		6.14E-03	1.73E-02	-2.64E-03	3.48E-03	8.48E-04
	CH···π	6.43E-03	2.20E-02	-2.84E-03	4.18E-03	1.34E-03
		1.04E-02	3.47E-02	-5.61E-03	7.14E-03	1.53E-03
		3.08E-03	9.53E-03	-1.17E-03	1.78E-03	6.04E-04
		6.61E-03	2.25E-02	-2.84E-03	4.24E-03	1.39E-03
		6.42E-03	2.34E-02	-2.83E-03	4.34E-03	1.51E-03

Linker ⋯ C_{60}	π···π	9.96E-03	3.00E-02	-4.31E-03	5.90E-03	1.59E-03
		9.60E-03	2.96E-02	-4.07E-03	5.74E-03	1.67E-03
		7.67E-03	2.24E-02	-3.68E-03	4.65E-03	9.64E-04
	CH···π	5.88E-03	1.81E-02	-2.56E-03	3.55E-03	9.88E-04
		3.80E-03	1.13E-02	-1.56E-03	2.19E-03	6.26E-04
		7.66E-03	2.51E-02	-3.65E-03	4.97E-03	1.32E-03
		MC-PDI2⊃C_{60}				
PDI2 ⋯ C_{60}	π···π	8.67E-03	2.51E-02	-3.80E-03	5.04E-03	1.24E-03
		7.89E-03	2.26E-02	-3.35E-03	4.50E-03	1.15E-03
		9.66E-03	3.02E-02	-4.52E-03	6.04E-03	1.52E-03
		9.30E-03	2.79E-02	-4.19E-03	5.58E-03	1.39E-03
		8.59E-03	2.62E-02	-3.81E-03	5.18E-03	1.37E-03
		8.90E-03	2.66E-02	-3.95E-03	5.29E-03	1.35E-03
		7.31E-03	2.04E-02	-3.06E-03	4.08E-03	1.02E-03
		9.13E-03	2.98E-02	-3.92E-03	5.68E-03	1.76E-03
	CH···π	7.34E-03	2.24E-02	-3.48E-03	4.54E-03	1.07E-03
Linker ⋯ C_{60}	π···π	7.54E-03	2.18E-02	-3.54E-03	4.50E-03	9.60E-04
		3.67E-03	8.42E-03	-1.42E-03	1.76E-03	3.44E-04
		4.11E-03	9.12E-03	-1.56E-03	1.92E-03	3.60E-04
		1.02E-02	3.21E-02	-4.56E-03	6.29E-03	1.73E-03
	CH···π	4.15E-03	1.26E-02	-1.70E-03	2.43E-03	7.29E-04
		7.15E-03	2.13E-02	-3.34E-03	4.33E-03	9.86E-04
		MC-PDI3⊃C_{60}				
PDI3 ⋯ C_{60}	π···π	6.00E-03	1.48E-02	-2.40E-03	3.05E-03	6.52E-04
		6.69E-03	1.76E-02	-2.68E-03	3.53E-03	8.57E-04
		8.30E-03	2.45E-02	-3.61E-03	4.87E-03	1.26E-03
		5.70E-03	1.52E-02	-2.40E-03	3.10E-03	6.95E-04
		1.20E-02	3.67E-02	-5.78E-03	7.47E-03	1.70E-03
	CH···π	1.24E-02	4.16E-02	-6.63E-03	8.52E-03	1.88E-03
		2.30E-03	6.44E-03	-8.00E-04	1.21E-03	4.05E-04
		8.50E-03	2.79E-02	-4.11E-03	5.54E-03	1.44E-03
		7.10E-03	2.46E-02	-3.71E-03	4.93E-03	1.22E-03
		5.27E-03	1.74E-02	-2.56E-03	3.46E-03	8.92E-04
Linker ⋯ C_{60}	π···π	4.60E-03	1.13E-02	-1.75E-03	2.29E-03	5.42E-04
		4.26E-03	1.16E-02	-1.86E-03	2.39E-03	5.25E-04
		5.81E-03	1.63E-02	-2.28E-03	3.18E-03	9.01E-04
	CH···π	4.90E-03	1.48E-02	-2.06E-03	2.88E-03	8.14E-04
		5.81E-03	1.75E-02	-2.54E-03	3.46E-03	9.20E-04
		1.01E-02	2.88E-02	-5.35E-03	6.28E-03	9.29E-04
		MC-PDI4⊃C_{60}				
PDI4 ⋯ C_{60}	π···π	7.85E-03	2.31E-02	-3.34E-03	4.55E-03	1.21E-03
		9.08E-03	2.64E-02	-3.92E-03	5.25E-03	1.34E-03
		8.56E-03	2.57E-02	-3.72E-03	5.07E-03	1.35E-03
		1.16E-02	3.71E-02	-5.87E-03	7.57E-03	1.71E-03
		1.01E-02	3.10E-02	-4.74E-03	6.25E-03	1.51E-03
		4.35E-03	1.04E-02	-1.75E-03	2.18E-03	4.29E-04

		4.05E-03	1.01E-02	-1.71E-03	2.12E-03	4.06E-04
Linker ⋯ C_{60}	π···π	4.05E-03	1.01E-02	-1.71E-03	2.12E-03	4.06E-04
	CH···π	4.47E-03	1.26E-02	-1.86E-03	2.50E-03	6.49E-04
		MC-PDI6⊃C_{60}				
PDI6 ⋯ C_{60}	π···π	6.49E-03	2.02E-02	-3.24E-03	4.14E-03	9.02E-04
		7.75E-03	2.33E-02	-3.55E-03	4.69E-03	1.14E-03
		1.01E-02	3.05E-02	-4.45E-03	6.04E-03	1.59E-03
		6.00E-03	1.91E-02	-3.14E-03	3.95E-03	8.16E-04
		9.27E-03	2.82E-02	-4.27E-03	5.66E-03	1.39E-03
		1.10E-02	3.46E-02	-5.30E-03	6.98E-03	1.68E-03
		6.61E-03	2.10E-02	-3.47E-03	4.36E-03	8.95E-04
		1.08E-02	3.75E-02	-6.61E-03	7.99E-03	1.38E-03
Linker ⋯ C_{60}	π···π	6.78E-03	1.89E-02	-2.82E-03	3.77E-03	9.49E-04
	CH···π	5.91E-03	1.90E-02	-2.43E-03	3.59E-03	1.16E-03
		3.52E-03	1.07E-02	-1.40E-03	2.04E-03	6.36E-04
		5.52E-03	1.60E-02	-2.31E-03	3.15E-03	8.43E-04
		4.30E-03	1.32E-02	-1.75E-03	2.52E-03	7.73E-04
		6.23E-03	1.99E-02	-3.05E-03	4.02E-03	9.66E-04

Table S4. Excitation energies (E_x, eV) and dipole moments in the ground state (μ_0, D), change in dipole moments between the GS and state of interest ($\Delta\mu = \mu_i - \mu_0$, D), as well as solvation energies (E_{solv}, eV) in DCM calculated for **MC-PDI1⊃C_{60}**, **MC-PDI2⊃C_{60}**, **MC-PDI3⊃C_{60}**, **MC-PDI4⊃C_{60}**, and **MC-PDI6⊃C_{60}** complexes.

	Host-guest system				
	MC-PDI1⊃C_{60}	**MC-PDI3⊃C_{60}**	**MC-PDI2⊃C_{60}**	**MC-PDI4⊃C_{60}**	**MC-PDI6⊃C_{60}**
	Ground state (GS)				
E_x	0.000	0.000	0.000	0.000	0.000
μ_0	6.38	8.13	6.86	2.38	11.44
E_{solv}	-1.906	-2.387	-1.395	-2.591	-1.656
	LE^{Host} (**MC-PDIs**)				
E_x	1.761	2.315	1.850	2.500	2.349
$\Delta\mu$	1.61	3.66	1.31	3.26	1.00
E_{solv}	-1.914	-2.449	-1.389	-2.645	-1.675
	LE^{Guest} (**C_{60}**)				
E_x	2.524	2.426	2.416	2.427	2.533
$\Delta\mu$	0.66	1.89	1.68	1.48	0.58
E_{solv}	-1.909	-2.403	-1.400	-2.617	-1.638
	CT1 (**MC-PDI → C_{60}**)				
E_x	1.679	2.096	2.112	n/f[a]	
$\Delta\mu$	28.09	19.62	25.39		
E_{solv}	-2.432	-2.918	-1.991		
	CT2 (**C_{60} → MC-PDI**)				

E_x	n/f[a]	2.088	1.932	2.136
$\Delta\mu$		26.96	25.01	22.29
E_{solv}		-2.047	-3.439	-1.855

[a] states of interest are not found within the studied range of energies.

Cartesian coordinates

MC-PDI1

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	-1.24755014	-7.47882519	2.83667220
6	-3.10129301	-5.26525107	3.13027022
6	-0.24181698	-8.52640035	2.68541332
6	-1.87473522	-6.90780399	1.68428799
6	-2.84810662	-5.84587953	1.83936218
8	0.35544437	-9.05886042	3.64748070
7	0.04983291	-8.94995891	1.37324661
6	-1.52678416	-7.36484114	0.37611014
6	-3.56800336	-5.32822998	0.70218228
6	-0.58171831	-8.46724333	0.20688198
8	-0.30215495	-8.98157319	-0.89401329
6	-3.81591329	-3.98944901	3.16521743
6	-4.78816163	-4.56334205	0.96978016
6	-4.82041848	-3.76180644	2.16300451
6	-5.82977702	-2.74166144	2.35240825
6	-5.73027318	-1.83902315	3.45959420
6	-6.91036762	-2.63022360	1.42239241
6	-6.69574246	-0.74672999	3.61057885
6	-7.96842860	-1.63209269	1.63532370
8	-6.58283206	0.15971677	4.46058427
7	-7.77734961	-0.72425699	2.70578567
8	-8.99447498	-1.54768022	0.93756198
6	-5.92485500	-4.50940326	0.13735889
6	-6.96760334	-3.52470679	0.32218305
7	-6.25571259	-5.29803025	-0.96938773
6	-7.87937655	-3.69017130	-0.77247383
6	-7.42829108	-4.76015230	-1.55064391
1	-8.73238836	-3.04834810	-0.98944949
6	-3.03530159	-5.63139231	-0.57023085
6	-2.06121225	-6.68589426	-0.75381666
7	-3.29993511	-5.05868510	-1.82097000
6	-1.81930903	-6.77389261	-2.15816284
6	-2.56478040	-5.77305178	-2.78911402
1	-1.16808745	-7.48738168	-2.65897841
6	-2.59683472	-5.95582589	4.25393777
6	-1.63322266	-7.02337008	4.12731083
7	-2.84044527	-5.74582888	5.61720818
6	-1.24649325	-7.37933587	5.46020357
6	-1.98437397	-6.58642755	6.35079179
1	-0.45496155	-8.07532703	5.73207070
6	-3.63815557	-2.97541351	4.12694765
6	-4.61309565	-1.93299500	4.33072814
7	-2.58990011	-2.78719061	5.03146466
6	-4.16265849	-1.18230582	5.46331415
6	-2.93210668	-1.70457677	5.87524779
1	-4.71144326	-0.37734245	5.94535171
6	-2.16171135	-1.31229405	7.06272529
6	-1.17306560	-2.14522917	7.65393329

MC-PDI2

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	-1.60112361	6.26445982	-0.07419456
6	-0.42711087	6.01829269	0.65493622
6	-1.88525037	5.55992998	-1.24410456
6	0.52331731	5.08304655	0.20326206
1	-0.23976452	6.60167771	1.56063675
6	-3.10149604	5.91578197	-1.99664207
6	-0.97709377	4.57173517	-1.73717110
6	0.28603154	4.40727880	-1.05396829
8	-3.83033476	6.86492409	-1.66885304
7	-3.38204377	5.14354077	-3.12492827
6	-1.29587025	3.80635090	-2.89121336
6	1.30156133	3.61243917	-1.65156583
6	-2.58117979	4.07507260	-3.59520375
6	-0.37467751	2.79132264	-3.33930164
6	0.93624380	2.69068404	-2.69954966
8	-2.98721805	3.44263078	-4.58144260
6	1.77116813	4.81401526	0.91954349
6	2.67423085	3.83903215	-1.18850240
6	1.95506949	5.01746687	2.33414967
6	2.87562485	4.37721310	0.13912690
6	3.80235422	3.63661399	-2.00877094
6	3.30153196	5.04939127	2.90282188
6	4.21363079	4.53824577	0.66388137
6	5.09760186	3.94058962	-1.54888043
6	4.43425430	4.89095117	2.02450461
6	5.31261832	4.37479848	-0.23875700
6	5.84170807	5.01884386	2.50175775
6	6.68528742	4.74427394	0.16802911
8	6.16562346	5.14031701	3.69495397
7	6.86956682	5.01820583	1.53450087
8	7.62147159	4.80882940	-0.63160529
1	5.96592746	3.83220234	-2.21084182
1	-2.32968478	7.01190876	0.26175701
6	3.41985413	5.23692071	4.32154872
6	2.30111322	5.34145092	5.13631823
1	4.42177132	5.26928365	4.74905689
1	2.42194180	5.45490717	6.22223436
6	0.83292530	5.08933529	3.22184600
6	0.99425098	5.24233296	4.58952457
1	-0.17310675	4.94038536	2.81952319
1	0.11340161	5.23214210	5.24683154
6	1.80485219	1.61848131	-3.08603395
6	1.46203370	0.72370425	-4.08834496
1	2.73845384	1.48396543	-2.53427524
1	2.13335587	-0.10399237	-4.35166247
6	-0.67544677	1.86014674	-4.39231480
6	0.21934726	0.86473223	-4.76067939
1	-1.64025220	1.94529128	-4.89576034

6	-2.48349085	-0.09843978	7.72952677	1	-0.05482141	0.16067732	-5.55777307
6	-0.55438927	-1.78693861	8.86475334	1	3.68205978	3.29139685	-3.04078635
1	-0.90466167	-3.09946041	7.19499744	6	1.57501411	-6.98125733	2.30409113
6	-1.88615358	0.24192444	8.95051465	6	0.38817212	-6.41667963	2.79175969
1	-3.21422720	0.58795301	7.28986096	6	1.82975093	-7.05264534	0.93332120
6	-0.91252754	-0.59904011	9.52870957	6	-0.57792302	-5.88363873	1.91442401
1	0.19729113	-2.45855087	9.30087809	1	0.20872876	-6.42604861	3.87038370
1	-2.19129994	1.17274723	9.44906550	6	3.10106075	-7.66106704	0.49400802
1	-0.44686151	-0.34157192	10.48987065	6	0.86703618	-6.57591370	-0.01337374
6	-1.80419459	-6.50598683	7.80623063	6	-0.36977849	-6.01636891	0.48909007
6	-1.13907388	-7.56400284	8.48775615	8	3.95957424	-8.07333777	1.28759333
6	-2.13461911	-5.33999385	8.54886154	7	3.30502366	-7.73207195	-0.88751032
6	-0.77662687	-7.43257963	9.83718193	6	1.10352470	-6.69582265	-1.41148451
1	-0.88910364	-8.48927779	7.95277684	6	-1.39080788	-5.63112942	-0.42461513
6	-1.77859426	-5.21763412	9.90319186	6	2.39054142	-7.29039932	-1.87278474
1	-2.62694364	-4.49453025	8.06193840	6	0.13398539	-6.17222002	-2.33952387
6	-1.08989339	-6.25809819	10.55411382	6	-1.06577742	-5.52330530	-1.82491096
1	-0.22532317	-8.24514528	10.33183877	8	2.72616510	-7.40803775	-3.06015926
1	-2.02205997	-4.28421558	10.42982187	6	-1.82058786	-5.27890220	2.40015795
1	-0.78228425	-6.17153886	11.60493441	6	-2.75132594	-5.48299787	0.10185314
6	-2.61986889	-5.51468361	-4.23349998	6	-1.98156159	-4.74313233	3.72925898
6	-1.53667675	-5.94286772	-5.05401502	6	-2.94047440	-5.28419609	1.52334399
6	-3.74151848	-4.92171743	-4.86797034	6	-3.89618592	-5.60186333	-0.71031310
6	-1.56899952	-5.75869583	-6.44382962	6	-3.31843395	-4.56412696	4.28220864
1	-0.65189627	-6.40649125	-4.59532524	6	-4.27289851	-5.12096545	2.06874477
6	-3.77829684	-4.76159427	-6.26350717	6	-5.18915234	-5.51639249	-0.17168304
1	-4.60924769	-4.60574317	-4.28191667	6	-4.46614340	-4.83121091	3.44836518
6	-2.68871928	-5.16445405	-7.05876587	6	-5.39279773	-5.28546971	1.18963497
1	-0.70650593	-6.07840803	-7.04372061	6	-5.85695163	-4.73514537	3.97455041
1	-4.67669470	-4.32375599	-6.72188008	6	-6.77657439	-5.21919661	1.69839550
1	-2.70296417	-5.01106410	-8.14671226	8	-6.14615732	-4.46655447	5.14993885
6	-7.94685808	-5.20646310	-2.85040108	7	-6.91894554	-4.94653676	3.06178212
6	-9.28795316	-4.91713778	-3.21974936	8	-7.77461960	-5.38997117	0.98353406
6	-7.10421118	-5.82070065	-3.81444216	1	-6.05551760	-5.61416550	-0.83384525
6	-9.76132338	-5.22110048	-4.50543255	1	2.33561522	-7.36359865	2.99476381
1	-9.96382963	-4.44397149	-2.49638963	6	-3.41841591	-4.10371994	5.64108107
6	-7.57542084	-6.11602480	-5.10314593	6	-2.29431768	-3.76613887	6.38235626
1	-6.06075142	-6.04202056	-3.57373955	1	-4.41642342	-4.00420906	6.06869437
6	-8.90748171	-5.82382085	-5.45528091	1	-2.41042563	-3.40368484	7.41351140
1	-10.79914126	-4.97753457	-4.77238563	6	-0.85437132	-4.32049510	4.50672299
1	-6.88565736	-6.55672800	-5.83646400	6	-0.99794681	-3.84375477	5.80273703
1	-9.27605807	-6.05444661	-6.46381273	1	0.13865668	-4.33139599	4.04661760
6	-3.78299371	-3.67773176	-1.99759275	1	-0.11829695	-3.50025096	6.36529136
1	-3.14698644	-3.16084716	-2.73816576	6	-1.88467047	-4.77977809	-2.73701859
1	-4.83423544	-3.63125471	-2.33195699	6	-1.67249374	-4.82503855	-4.10628812
1	-3.70031187	-3.14091609	-1.03781535	1	-2.67668790	-4.13509371	-2.34063660
6	-5.86488816	-6.71656808	-1.09025579	1	-2.31509679	-4.23656486	-4.77547701
1	-5.05641887	-6.87833047	-1.82310118	6	0.26916545	-6.25709822	-3.76557263
1	-5.52951907	-7.08270418	-0.10405708	6	-0.62701853	-5.63785585	-4.62381156
1	-6.74360074	-7.30912538	-1.39891769	1	1.11287660	-6.82206898	-4.16206896
6	-1.21346150	-3.20823675	4.72238676	1	-0.50150621	-5.75499684	-5.71048385
1	-1.16301883	-3.48728667	3.65746804	1	-3.79829066	-5.78545455	-1.78334693
1	-0.53091856	-2.35637712	4.88127190	6	-4.60478298	5.47090264	-3.89283737
1	-0.87929478	-4.07168303	5.32243944	1	-4.39912246	5.25347838	-4.95378107
6	-4.11024974	-5.21222712	6.13585317	1	-4.77077066	6.55454890	-3.77798666
1	-4.50749984	-5.90071603	6.90219080	6	-8.30795719	-4.79967928	3.57196385

1	-4.00227932	-4.20132828	6.56114944	1	-8.25845764	-4.96988079	4.65936569
1	-4.83568307	-5.15850252	5.30961046	1	-8.92180601	-5.58425534	3.09966575
6	6.43354438	3.65007214	1.14455117	7	-8.46294103	5.52615218	-1.58657602
6	4.36536968	4.25542785	-0.79242416	7	-9.23347848	5.56758573	-0.50586642
6	7.46227712	3.18132188	2.07491823	1	-8.92693591	3.72414313	1.66682804
6	5.07512823	3.76815970	1.56798129	6	-8.97170440	4.61974246	-2.48085285
6	4.05094439	4.13130306	0.60827270	1	-8.29109260	1.51525385	2.57222696
8	8.63873293	2.96422217	1.72207364	6	-9.65410785	2.90308850	1.64618585
7	7.07472406	2.94828832	3.40823404	7	-10.24938772	4.69570629	-0.69961680
6	4.73559831	3.54034418	2.93993043	6	-9.29867292	1.65120656	2.15962832
6	2.69914688	4.38515755	1.03298874	1	-11.16668829	5.28579669	1.06305131
6	5.77308315	3.17177803	3.91846652	1	-11.11253835	-1.85660298	1.18645518
8	5.54935539	3.01566681	5.13380061	6	-11.22542135	4.42771453	0.36780899
6	3.24651486	4.27895200	-1.73476227	6	-10.12432222	4.07149371	-1.90569261
6	1.82373278	5.11182373	0.10738773	1	-10.32687811	-4.13984660	1.83698322
6	2.02288776	4.90096237	-1.30225444	6	-10.33873586	-1.96469110	1.95727988
6	1.02690245	5.32118294	-2.27087520	6	-10.91709095	3.10633447	1.05042213
6	1.20525539	5.01340035	-3.65585359	6	-9.88919628	-3.24916711	2.31021470
6	-0.12630484	6.05369471	-1.84475817	6	-10.19536990	0.55480830	2.10149894
6	0.25358297	5.51478948	-4.65397371	6	-9.76671279	-0.80257724	2.53395227
6	-1.16874027	6.44994496	-2.81553623	1	-12.23638481	4.42222356	-0.07907001
8	0.42944236	5.39081381	-5.88082269	6	-8.85343068	-3.41993086	3.25068274
7	-0.90924934	6.15154861	-4.17816755	6	-11.83668981	2.04070637	1.03562021
8	-2.21288456	7.03937640	-2.49331453	6	-11.48405287	0.78758834	1.56178118
6	0.79455635	6.01212472	0.46762955	6	-8.73758961	-0.98704344	3.49361478
6	-0.21607024	6.44646287	-0.47817829	6	-8.29099697	-2.26846059	3.84490762
7	0.54112816	6.64149925	1.69148797	1	-12.83205622	2.18885221	0.59107000
6	-1.12411772	7.28771484	0.25408886	1	-8.28431361	-0.11515198	3.98273357
6	-0.63187879	7.41236269	1.55931870	1	-12.22583838	-0.02169667	1.54642782
1	-2.02370754	7.76050638	-0.14445713	1	-7.48945636	-2.38378118	4.58426556
6	2.36314432	3.97576862	2.34208506	6	-5.83798927	4.69157858	-3.41246983
6	3.36921695	3.62618416	3.32352906	6	-8.36993226	4.31868876	-3.82934918
7	1.10876114	3.89241357	2.95588401	6	-7.09851494	5.10874690	-4.18859108
6	2.67682916	3.43564641	4.56234420	1	-9.14129931	4.50313314	-4.60574220
6	1.30650610	3.59434818	4.32148582	1	-8.16711795	3.22800354	-3.87787213
1	3.14420888	3.22040780	5.52321202	1	-5.98130789	4.87624745	-2.33402768
6	5.73357285	4.32872687	-1.13675213	1	-5.65764689	3.60340134	-3.53241809
6	6.77696824	3.99975674	-0.18809902	1	-7.29410363	6.19145002	-4.04531310
7	6.34425077	4.66679290	-2.35206824	1	-6.91687706	4.97486941	-5.27449410
6	8.01776041	4.10174397	-0.89435592	1	-10.82762083	3.30902992	-2.24926124
6	7.73630205	4.49306456	-2.20476419	6	8.24835915	5.31741929	1.98900143
1	9.00909605	3.89632438	-0.49372875	1	8.75463594	5.79612813	1.13404889
6	3.27299538	3.78949129	-3.05831267	1	8.16660456	6.04621071	2.81151524
6	2.29717805	4.19431982	-4.04507606	6	4.60307397	-8.28374676	-1.35784404
7	4.16049639	2.89678369	-3.66084830	1	4.41251053	-8.86669924	-2.27212789
6	2.68584619	3.57356235	-5.27755804	1	4.94771017	-8.95456235	-0.55488870
6	3.80660291	2.77318693	-5.02224466	7	9.45412265	2.66280903	-2.01212957
1	2.19432737	3.71949013	-6.23921318	7	9.62199493	1.65775658	-2.85316615
6	4.55021070	1.94571803	-5.98588079	1	9.08979867	-1.50561737	-4.75504730
6	3.89007055	1.46897679	-7.15289270	1	7.54125037	-3.40962535	-4.32754870
6	5.93180799	1.64061360	-5.83223323	6	10.23908427	2.47324694	-0.90012419
6	4.57946441	0.72010718	-8.11989690	6	9.10569654	-2.01430000	-3.77911916
1	2.82390306	1.67826331	-7.30518766	6	8.25332471	-3.10956821	-3.54832220
6	6.61795252	0.89742037	-6.80644028	1	7.30735485	-5.62869316	-4.16364463
1	6.48546198	2.00652425	-4.96186728	7	10.52396351	0.80846376	-2.30322964
6	5.94876897	0.43305725	-7.95449580	1	5.74847078	-7.50786046	-3.75331976

1	4.03135684	0.35493753	-9.00018038
1	7.68864296	0.69332354	-6.67646024
1	6.49226848	-0.13565489	-8.72157152
6	8.68881254	4.56788857	-3.31970717
6	10.06450704	4.79895796	-3.05403686
6	8.30310496	4.27520932	-4.65518533
6	11.01905004	4.70708721	-4.07817456
1	10.37714126	5.05978120	-2.03371958
6	9.26168985	4.19121937	-5.68218463
1	7.25200796	4.07248722	-4.88768810
6	10.62448393	4.40475557	-5.39724918
1	12.08252601	4.86498482	-3.84748140
1	8.94440477	3.95068278	-6.70827882
1	11.37458389	4.32580248	-6.19622102
6	0.22548029	3.54628362	5.31214104
6	0.46146476	2.89777177	6.55330310
6	-1.02315482	4.19698182	5.12964639
6	-0.51328516	2.88201687	7.55622467
1	1.42516785	2.40522443	6.73014184
6	-2.00176246	4.17845106	6.13989589
1	-1.22825939	4.74767220	4.20675260
6	-1.75965101	3.50939559	7.35581884
1	-0.29918338	2.36946243	8.50043133
1	-2.95025588	4.71367275	5.98618007
1	-2.52699943	3.48867879	8.14348593
6	-1.18583997	8.21591426	2.66112589
6	-1.94545777	9.38175873	2.36593384
6	-1.01471329	7.85382917	4.02612064
6	-2.49314795	10.15991308	3.40002187
1	-2.08203342	9.68676902	1.32082291
6	-1.56313090	8.63623786	5.05437214
1	-0.46981210	6.94409287	4.29418784
6	-2.30107322	9.79582343	4.74898164
1	-3.06794676	11.06424094	3.16107535
1	-1.42827159	8.32630436	6.09889299
1	-2.73348163	10.41074264	5.55161779
6	-0.12691282	3.60223079	2.21050712
1	-0.67743391	2.78968258	2.71715185
1	-0.78313475	4.48586449	2.12161919
1	0.14578007	3.25973546	1.19849629
6	1.57877861	6.91049545	2.70065748
1	2.56687928	6.69126792	2.26995731
1	1.55454908	7.97931081	2.96636364
1	1.44170838	6.31310648	3.61686385
6	4.93411095	1.90580397	-2.89935161
1	4.45151408	1.75307480	-1.91837627
1	4.93006819	0.94877881	-3.44373765
1	5.97960931	2.21649293	-2.73795946
6	5.74744561	5.58665151	-3.33661287
1	5.37874076	5.07555453	-4.24169329
1	4.89810555	6.11043625	-2.86992662
1	6.49648077	6.34351007	-3.62971448
6	8.10803745	2.42801110	4.33256073
1	7.88788150	2.83247935	5.33101270
6	1.11709736	-9.96508684	1.19220940
1	0.82290500	-10.60575084	0.34599233
1	10.98298673	-0.15741295	-4.09466249
6	6.95587126	-5.81366924	-3.13950962
6	6.07875660	-6.88800414	-2.90840425
6	10.93395658	-0.40897831	-3.01982615
6	10.92866278	1.26731878	-1.08019226
6	9.99706066	-1.57718667	-2.77833662
6	8.26764789	-3.80703542	-2.31366470
6	7.38162718	-4.97777758	-2.07836700
6	5.61634395	-7.18062028	-1.61068658
1	11.95822243	-0.65079648	-2.68135772
1	11.64545447	0.72441735	-0.46013630
6	10.00500053	-2.25153680	-1.53674024
6	6.93480611	-5.29378034	-0.76988828
6	9.15780015	-3.34865327	-1.30865458
6	6.08184407	-6.38323737	-0.53852837
1	10.69641194	-1.93110666	-0.74238890
1	7.23950833	-4.65637221	0.07176187
1	5.75415928	-6.62651792	0.48241569
1	9.21686321	-3.86857922	-0.34383281
6	9.27380287	2.99837069	1.39128521
6	10.24111126	3.43062974	0.25852163
6	9.03292863	4.07646804	2.46545496
1	8.30102049	2.70525607	0.94921255
1	9.67722616	2.08982138	1.88779350
1	10.00805754	4.43766589	2.85782326
1	8.49762833	3.61767738	3.32014642
1	9.93813207	4.42081655	-0.12652463
1	11.26563637	3.52345649	0.67363748

7	8.13388362	-1.80992911	0.78761853
7	8.45757132	-2.67914486	-0.15924988
1	7.70711516	-5.19346314	-2.13443387
1	5.65344848	-6.51453116	-1.79919490
6	8.86292150	-2.07161000	1.92524757
6	7.58168244	-5.76044474	-1.20344082
6	6.41160088	-6.50789740	-1.00459897
1	4.70307734	-8.66238874	-1.59835559
7	9.40649107	-3.49460463	0.34710278
1	2.55053065	-9.84272480	-1.17134435
1	9.94291096	-4.49873605	-1.41666738
6	4.25874425	-8.63545569	-0.59224786
6	3.04735120	-9.30705831	-0.35178766
6	9.74470888	-4.74473386	-0.35819381
6	9.69309109	-3.15950586	1.64200519
6	8.57655390	-5.70224127	-0.20847797
6	6.19699543	-7.21092406	0.20633279
6	4.92778978	-7.94578482	0.45074001
6	2.46392656	-9.30514057	0.93271165
1	10.67439158	-5.13811402	0.09104008
1	10.42708832	-3.71027474	2.23268784
6	8.38554056	-6.42098126	0.99033756
6	4.34093391	-7.95432903	1.74038177
6	7.21400418	-7.16684360	1.19509591
6	3.13019357	-8.61768999	1.97408575
1	9.16157250	-6.38076352	1.76843562
1	4.82986707	-7.41567600	2.56416287
1	2.67300323	-8.58720450	2.96937522
1	7.07964109	-7.73222161	2.12647846
6	8.46359159	0.19179541	3.05595520
6	8.64888920	-1.32934947	3.21756896
6	8.15127947	0.88815641	4.39098255
1	9.36794745	0.64228794	2.60357808
1	7.63607506	0.37333161	2.34317436
1	8.91835712	0.61278469	5.14441862
1	7.18553817	0.50819897	4.78698624
1	9.48636545	-1.55408554	3.90837252
1	7.74882291	-1.75373744	3.71543277
1	9.07911290	2.83123236	4.00035642
1	1.13894104	-10.55589542	2.12206522
6	-1.88887946	6.58888032	-5.19791523
1	-1.31056424	7.06142169	-6.01168948
6	-8.77989559	0.35778425	2.87168202
1	-8.79103815	0.62070821	3.94202665
7	-4.71453833	8.26221639	-5.82265091
7	-5.19789483	8.89681603	-4.76042218
1	-9.21335638	7.20614242	-2.60810881
6	-5.33591468	7.04380238	-5.94859608
1	-9.66002747	5.21789390	-1.19780676
6	-8.39720419	6.76664143	-2.01687432
7	-6.13207703	8.09728802	-4.19928087
6	-8.64583535	5.63725197	-1.22119729
1	-6.20458359	9.27692920	-2.49050696
1	-6.53585745	4.42316080	2.02670059
6	-6.84646108	8.52165539	-2.97937873
6	-6.25780950	6.93560549	-4.90495322

1	-7.02106169	2.40826949	3.41431677
6	-7.23833402	3.66811604	1.64945349
6	-7.11220422	7.34507400	-2.06504087
6	-7.51943132	2.54093382	2.44451548
6	-7.61677988	5.05797777	-0.43687960
6	-7.88589393	3.86075093	0.40335786
1	-7.79848203	9.00217435	-3.27616311
6	-8.46008073	1.57352308	2.01896486
6	-6.07418504	6.77357254	-1.29290960
6	-6.32907730	5.65414166	-0.48392006
6	-8.81379286	2.87679245	-0.02216832
6	-9.09012322	1.75303727	0.77040817
1	-5.05948999	7.19598033	-1.34070557
1	-9.31488792	2.97954779	-0.99469783
1	-5.51275032	5.21557889	0.10562804
1	-9.80327548	0.99905585	0.42031841
6	-2.73258340	5.42950854	-5.77805026
6	-4.96521856	6.03862920	-7.00050635
6	-3.43944574	5.80269864	-7.11284216
1	-5.36610902	6.34866806	-7.98947654
1	-5.47639309	5.08678184	-6.75840902
1	-3.47660261	5.10055060	-5.02433488
1	-2.07235936	4.55862365	-5.94182187
1	-2.96534763	6.70515721	-7.55317290
1	-3.29513203	4.99507137	-7.85659980
1	-6.98122090	6.16032696	-4.64995996
1	-2.52989672	7.33942098	-4.71406767
1	-9.75713011	-0.05427781	2.57696616

MC-PDI3

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	-3.26670913	-2.71311818	4.44523039
6	-4.07939518	-2.19911951	3.40490654
6	-2.72482364	-1.80036873	5.39770396
6	-4.40388865	-0.84616458	3.27480051
1	-4.51144333	-2.92887499	2.71437725
6	-1.79840403	-2.26074033	6.45997597
6	-2.99414956	-0.39061761	5.27451593
6	-3.83117497	0.08971412	4.20180581
8	-1.32903239	-3.40709805	6.52661327
7	-1.45887148	-1.33048207	7.45910717
6	-2.42352866	0.55032116	6.20188094
6	-4.07547183	1.49788993	4.06406957
6	-1.79606441	0.03762070	7.44396355
6	-2.57997600	1.95069266	5.98973045
6	-3.43233506	2.38073182	4.94133914
8	-1.58150882	0.73118994	8.44569940
1	-3.55101248	3.46025243	4.80273521
6	-5.34089137	-0.37241569	2.24199911
6	-4.96943973	1.98528509	2.99885337
6	-5.93050954	-1.24403741	1.30990336
6	-5.63610738	1.03203995	2.15529440
6	-5.18934016	3.35406731	2.76732374

MC-PDI4

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	-2.22493778	-5.18163611	-1.13645582
6	-0.83819180	-5.01964221	-1.38762171
6	-2.69371615	-5.41050076	0.17149821
6	0.10417175	-5.07364607	-0.35211363
1	-0.51688063	-4.89864505	-2.42672526
6	-4.12268794	-5.76017452	0.40043585
6	-1.76342214	-5.38911478	1.24912455
6	-0.35627211	-5.23310702	0.99761631
8	-4.93478106	-5.82743369	-0.52290551
7	-4.48503407	-6.08959864	1.71533168
6	-2.24822449	-5.53248210	2.57940656
6	0.56592671	-5.27685655	2.09873111
6	-3.67676279	-5.84582174	2.83319986
6	-1.33631412	-5.45675718	3.65205382
6	0.05694499	-5.34821292	3.40198124
8	-4.13071479	-5.96741450	3.97337192
1	0.73435126	-5.35223690	4.26159477
6	1.54902002	-5.03179299	-0.61851610
6	2.01083333	-5.32940940	1.82223145
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6	6.89544320	-10.59916134	-4.98490473
1	6.70479958	-11.68578590	-5.01320787
1	7.19454509	-10.28231595	-6.00611913
1	7.76000197	-10.41971217	-4.30771441
6	4.56730737	-10.69576378	-4.02156873
1	4.74376413	-11.76372448	-4.23072746
1	4.42876397	-10.55968512	-2.92682887
1	3.60246056	-10.41196859	-4.48917589
6	9.86896518	-3.75404127	-1.32772414
1	10.68636080	-3.01599782	-1.31676075
6	-0.71224286	-1.83550773	8.64308266
1	-1.05473690	-2.87059730	8.80426524
7	9.05528736	-1.45351601	3.59558019
7	9.14906304	-0.88681520	4.78915365
1	7.74432679	-3.80818293	7.26147563
1	5.33437720	-3.87964644	7.74890182
6	9.28419342	-2.80241302	3.70862170
6	7.22947325	-2.87603834	7.53725083
6	5.85353727	-2.91372798	7.80074913
1	3.37210277	-3.46071052	6.93958821
7	9.45252315	-1.85845110	5.68063332
1	0.88641338	-3.49644552	7.17014277
1	10.01274800	-2.35887135	7.62835964
6	2.87677084	-2.73138202	7.59571773
6	1.47994308	-2.75374156	7.71391990
6	9.38697856	-1.59500505	7.13045616
6	9.54837048	-3.06902610	5.05591160
6	7.94122071	-1.65700375	7.59752093
6	5.13523136	-1.73106254	8.11755717
6	3.65428322	-1.75048236	8.26639616
6	0.80012938	-1.78971498	8.49193719
1	9.83535661	-0.60361689	7.32205237
1	9.75272479	-3.99589128	5.59637193
6	7.25217762	-0.49152465	7.98852108

6	2.96479738	-0.77447946	9.03127361
6	5.86891863	-0.52582639	8.23559359
6	1.56172063	-0.78893800	9.13379507
1	7.80308977	0.45581695	8.08369390
1	3.52776707	0.00424539	9.56379372
1	1.05868229	-0.01234466	9.72684678
1	5.34721185	0.40962651	8.47667663
6	9.49951673	-3.15497828	1.17229565
6	9.19732411	-3.76397186	2.55491847
6	9.57092894	-4.25020074	0.09818649
1	8.72020498	-2.41166198	0.91491204
1	10.46150416	-2.60353051	1.20286320
1	8.63286405	-4.83760426	0.09621906
1	10.36733714	-4.97250885	0.37420557
1	8.17993672	-4.21603926	2.53553985
1	9.87904565	-4.61745781	2.75133482
1	10.17213062	-4.60002940	-1.96776514
1	-1.01715130	-1.20595386	9.49086522
6	-0.95614971	2.12553830	-8.64073094
1	-1.39688461	1.24266092	-9.13102542
6	-10.19624841	2.72291507	-0.80524217
1	-10.53788270	3.58723438	-0.21472967
7	-5.43060940	1.51852295	-10.29220750
7	-6.36252413	2.27258086	-10.85943192
1	-9.54811323	2.55906414	-9.58431215
6	-4.97630160	2.13180065	-9.14947803
1	-10.47524445	2.23391970	-7.30233396
6	-9.32618578	3.29247296	-8.79577364
7	-6.50270428	3.38434669	-10.09968699
6	-9.85701905	3.11642341	-7.51277544
1	-7.17686974	5.33617573	-10.55509158
1	-10.25480877	5.76626781	-4.40830885
6	-7.60752445	4.34291311	-10.32712464
6	-5.65749251	3.34459802	-9.02761626
1	-10.49802286	5.19325295	-2.00104011
6	-10.16575940	4.71648223	-4.09573031
6	-8.45976703	4.37158871	-9.07125699
6	-10.30094433	4.39534977	-2.73047780
6	-9.54615838	4.02099414	-6.46704508
6	-9.89317740	3.70848569	-5.05552229
1	-8.16118012	3.96962362	-11.20763384
6	-10.15960023	3.06478618	-2.28296687
6	-8.22069497	5.32879302	-8.06538848
6	-8.76083457	5.16043382	-6.77967830
6	-9.82897474	2.36236345	-4.60557605
6	-9.94726805	2.04780532	-3.24351015
1	-7.54997045	6.17714512	-8.26754988
1	-9.63098696	1.56177790	-5.33304917
1	-8.49050729	5.88086646	-5.99489179
1	-9.83784332	1.01124641	-2.89863695
6	-2.04808314	3.09096463	-8.14679857
6	-4.05480361	1.45991557	-8.16861854
6	-3.17496495	2.42013796	-7.34275211
1	-3.43435804	0.70297624	-8.68574340
1	-4.70461848	0.89399382	-7.46857741
1	-2.47705074	3.59345774	-9.04108713

1	-1.58323976	3.88755191	-7.53362609
1	-2.73507094	1.85970851	-6.49413908
1	-3.81086605	3.20974065	-6.89209222
1	-5.63153416	4.13268277	-8.27352533
1	-0.30886725	2.63516296	-9.37007885
1	-10.86728577	1.86605783	-0.62784266

MC-PDI5

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	3.31172813	3.82422339	1.79463527
6	3.22171900	2.43499596	2.07293277
6	4.33284343	4.36796668	1.01036338
6	4.21411815	1.55982492	1.51560913
6	4.36166325	5.81736080	0.72849109
6	5.38445580	3.52995689	0.54973791
6	5.38072281	2.14052786	0.89497750
8	3.52697211	6.61486947	1.17617977
7	5.41291780	6.28550394	-0.09249227
6	6.43494302	4.05349379	-0.25411744
6	6.54864453	1.34865931	0.60518784
6	6.41614506	5.47225349	-0.66414487
6	7.43168390	3.19584874	-0.73715542
6	7.50502213	1.83698417	-0.34391794
8	7.24483218	5.95519705	-1.45237578
6	4.15138328	0.08699024	1.49007636
6	6.65907492	0.07662006	1.33121750
6	2.95682977	-0.69574327	1.35898703
6	5.41399524	-0.60045798	1.59654897
6	7.88895286	-0.52675022	1.75190403
6	3.02223878	-2.08884700	1.62812367
6	5.43410746	-1.98713291	1.95695040
6	7.86077197	-1.86521564	2.21470307
6	4.21744404	-2.72588364	1.99143780
6	6.67667502	-2.60742014	2.26884540
6	4.23881662	-4.16714305	2.33367616
6	6.70723146	-4.00810798	2.73412969
8	3.22810144	-4.88338464	2.29221904
7	5.48659943	-4.71124721	2.73147669
8	7.74631188	-4.56863622	3.11738281
1	8.15520227	3.60414483	-1.45222130
1	8.78501446	-2.35034600	2.55056206
1	2.11220994	-2.69555444	1.54479904
1	2.56354311	4.51166035	2.20737416
6	2.12949144	1.98786008	2.96511185
6	2.29867507	0.93625144	3.90183322
6	0.87344413	2.65080203	2.97613793
6	1.27880632	0.54804602	4.77547726
6	-0.15055453	2.29531882	3.85770737
6	0.00871838	1.21063267	4.77586107
1	3.25887424	0.40948651	3.96252262
1	0.67156468	3.45187832	2.25270592
1	1.47119821	-0.27545768	5.47035285
1	-1.09692231	2.84544148	3.80220606

MC-PDI6

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute macrocycle shown

Atom	X	Y	Z
6	-0.83738864	-3.51184449	2.11962148
6	-2.17664434	-3.88914836	1.93368624
6	0.12309925	-3.80025764	1.14885672
6	-2.61300050	-4.54873489	0.76891684
1	-2.87558801	-3.63460264	2.73028921
6	1.55064558	-3.45702199	1.39554422
6	-0.28599806	-4.40945278	-0.07150061
6	-1.66651470	-4.74016981	-0.29870522
8	1.91771122	-2.85097558	2.40731350
7	2.47724685	-3.87017633	0.41674605
6	0.68456316	-4.69546987	-1.07004616
6	-2.07929823	-5.27486243	-1.56856611
6	2.12745268	-4.44649168	-0.81658205
6	0.29985770	-5.31191961	-2.25904953
6	-1.05261862	-5.63065414	-2.47671091
8	2.99906021	-4.75550554	-1.63522718
6	-3.98024007	-5.05351309	0.59256563
6	-3.51584000	-5.37050662	-1.84679336
6	-4.92859194	-5.20686120	1.63053485
6	-4.43166551	-5.36241200	-0.73714924
6	-4.04180669	-5.44050934	-3.15174893
6	-6.28409117	-5.50059586	1.41013830
6	-5.81931152	-5.64895536	-0.97729468
1	-3.38991439	-5.30903633	-4.02281165
6	-5.41132490	-5.65853541	-3.38112031
6	-6.73665400	-5.72536814	0.11074706
6	-6.29320601	-5.82171336	-2.30803456
6	-8.16541890	-6.06820410	-0.11403306
6	-7.71967270	-6.13913956	-2.56827318
8	-8.96748824	-6.17065029	0.82396938
7	-8.56314492	-6.28607661	-1.44200060
8	-8.17047680	-6.27356494	-3.70805406
1	1.05226706	-5.59485600	-3.00280817
1	-5.79706889	-5.72519832	-4.40571387
1	-6.97011259	-5.57550885	2.26047381
1	-0.53592362	-3.01413322	3.04677970
7	-4.52474523	-5.15733595	3.05651511
8	-3.71279049	-6.00009315	3.44186795
8	-5.05169423	-4.29242925	3.77519664
7	-1.29770043	-6.51644401	-3.64487489
8	-2.04518975	-7.49056658	-3.47651551
8	-0.68142696	-6.27157705	-4.69108975
6	5.36067886	3.90110518	-2.81655757
6	3.99448435	4.08059892	-2.53404341

6	1.67996901	-0.09187966	0.91260924	6	6.33401167	4.23408351	-1.87288830
6	1.65923385	0.93014662	-0.07525603	6	3.55365698	4.57708130	-1.29280772
6	0.42995298	-0.47353425	1.46800796	1	3.28677294	3.80438663	-3.31724333
6	0.48642854	1.59491865	-0.43045485	6	7.77303395	4.12917412	-2.22656453
6	-0.75179380	0.19217290	1.14269170	6	5.93257516	4.66383500	-0.57704475
6	-0.75179733	1.28131325	0.21580274	6	4.53578964	4.77748384	-0.25416908
1	2.59424258	1.23119241	-0.56449824	8	8.15666442	3.74650968	-3.33635960
1	0.38991656	-1.26217272	2.23012083	7	8.70385757	4.48457861	-1.22896145
1	0.54079761	2.38554016	-1.18784366	6	6.92052829	4.98289584	0.39726241
1	-1.67223727	-0.11160101	1.64728636	6	4.13987655	5.10947298	1.08506977
6	9.18043743	0.19629304	1.75177992	6	8.37245771	4.88690547	0.07899623
6	10.38455111	-0.45093483	1.37579461	6	6.52992817	5.42524116	1.65921684
6	9.28054805	1.55344473	2.15239411	6	5.16402579	5.50348846	1.97637676
6	11.60876367	0.22649531	1.33456812	8	9.25206274	5.13880763	0.90623643
6	10.49398587	2.24629897	2.11759177	6	2.15667623	4.94033804	-1.00350545
6	11.69167184	1.61449140	1.65611096	6	2.71969762	5.01393137	1.43748018
1	10.34394524	-1.50334934	1.06218536	6	1.15050806	5.16872270	-1.96701894
1	8.38174920	2.08036517	2.50170387	6	1.75550322	5.08308489	0.37239206
1	12.50738657	-0.31328989	1.02453339	6	2.25318774	4.88212777	2.76104344
1	10.51897609	3.28818978	2.45128132	6	-0.18005001	5.50101182	-1.65004169
6	8.49695304	0.95719364	-1.00112169	6	0.38052306	5.32362106	0.71076528
6	9.76795370	1.43379305	-1.41234933	1	2.95849271	4.68975458	3.57589017
6	8.18355543	-0.38859206	-1.32781204	6	0.88647754	4.99374281	3.07455159
6	10.67021972	0.62741546	-2.11546299	6	-0.56638486	5.59954606	-0.31542625
6	9.07766082	-1.21375631	-2.01182481	6	-0.04064682	5.29922831	2.07149205
6	10.35495572	-0.72852998	-2.43331663	6	-1.91415226	6.12415593	0.03341651
1	10.07093334	2.45540269	-1.14560455	6	-1.45219085	5.60056702	2.42792281
1	7.20477146	-0.80065133	-1.04773930	8	-2.67781338	6.59103368	-0.81651612
1	8.77214035	-2.24015304	-2.23576244	7	-2.26078221	6.12024668	1.39521270
7	12.87569450	2.32349227	1.51008635	8	-1.89288903	5.46968585	3.57315907
7	-1.89748646	2.01685467	-0.03972601	1	7.27880167	5.75354161	2.38719536
7	-1.01085580	0.82580003	5.62765491	1	0.54553296	4.88639404	4.11165635
6	-3.08460756	1.79222504	0.78180024	1	-0.90150552	5.71402510	-2.44789517
1	-2.88873061	1.96659872	1.86314034	1	5.67098411	3.52655273	-3.79842783
1	-3.88406605	2.48259067	0.46854516	7	1.45511594	5.18273980	-3.42144834
1	-3.46031512	0.75711496	0.67351332	8	1.06148725	4.21881316	-4.09205550
6	-1.80098884	3.25328279	-0.82063098	8	2.04640765	6.17032229	-3.86503205
1	-2.76378498	3.78871862	-0.77950484	7	4.86436095	6.16031172	3.26967891
1	-1.02261889	3.93712362	-0.42296712	8	4.05035837	7.09070759	3.25993021
1	-1.55852053	3.06084393	-1.88689724	8	5.49655379	5.77132725	4.26201121
6	-0.77948591	-0.22911375	6.60832462	6	3.92859860	-3.74340871	0.69607390
1	-1.75128989	-0.57009281	7.00609738	1	4.03120350	-3.06164784	1.55360300
1	-0.29759897	-1.10360461	6.13758320	6	10.15132153	4.31492081	-1.54394296
1	-0.13771354	0.09887636	7.45845341	1	10.69655085	5.06537584	-0.95057551
6	-2.12561838	1.73872263	5.88244181	7	8.72049900	-5.81316368	2.93616257
1	-1.80486639	2.65275182	6.43233558	7	10.01995465	-5.57119453	2.88750144
1	-2.61576023	2.06371656	4.94789288	1	10.34051543	-4.34233648	-0.94456480
1	-2.88559519	1.21599370	6.48753510	6	8.26351144	-6.14267829	1.68467884
6	14.12361403	1.58956177	1.28658355	1	10.13160938	-2.00549074	-1.66297405
1	14.06497858	0.96654074	0.37130059	6	10.94016142	-3.57808903	-0.43517282
1	14.94430170	2.31471063	1.15129535	7	10.42130383	-5.76025713	1.60576797
1	14.38188876	0.92992797	2.14439429	6	10.82717956	-2.24691620	-0.84969751
6	12.98054914	3.66556229	2.08554823	1	12.43394040	-5.46226913	2.05316426
1	13.97247455	4.08227185	1.83977984	1	11.83281575	1.03506022	1.38177251
1	12.20916699	4.33962837	1.66213439	6	11.77013676	-5.35619658	1.17657710
1	12.86201371	3.65670561	3.19284840	6	9.35874683	-6.11683689	0.81973663

7	11.24735027	-1.54489278	-3.12012596	1	11.24578514	3.37406937	0.80031917
6	10.80539254	-2.87009648	-3.55234348	6	11.47385900	1.25922449	0.36740932
1	10.45450520	-3.47574276	-2.69348215	6	11.76962970	-3.92812694	0.65092163
1	9.96764394	-2.82896089	-4.28585525	6	11.13882970	2.58360739	0.04599564
1	11.65256727	-3.39358683	-4.02651725	6	11.54564284	-1.21094258	-0.20083958
6	12.34505218	-0.93787245	-3.87712665	6	11.29928243	0.20986026	-0.57207425
1	12.96622203	-0.27642321	-3.24387612	1	12.09594354	-6.06994794	0.39562829
1	13.00743239	-1.73348051	-4.26245834	6	10.61475050	2.90674668	-1.22310631
1	11.98134914	-0.33863722	-4.74412487	6	12.53190365	-2.91683753	1.26546246
1	11.64045169	1.04354897	-2.40523501	6	12.42808811	-1.58091571	0.84236197
6	-7.70503171	2.59216138	0.17743676	6	10.79966697	0.55223807	-1.85738143
6	-7.56037980	1.47196641	-0.67626034	6	10.45413007	1.87374958	-2.17199431
6	-7.09158291	2.66022554	1.43501154	1	13.19942626	-3.17020856	2.10109929
6	-6.74045396	0.37612708	-0.24848210	1	10.66114138	-0.22633000	-2.61850190
6	-7.22381433	3.87036577	2.27090663	1	13.03508423	-0.81744469	1.34764213
6	-6.36252192	1.53635552	1.91898766	1	10.00539366	2.10991803	-3.14567841
6	-6.27043101	0.35295866	1.11379436	6	4.58264368	-5.10307915	0.99761856
8	-7.89909873	4.85825570	1.94139871	6	6.80250134	-6.32098067	1.38899920
7	-6.53204001	3.87060707	3.50258715	6	6.07186963	-4.95586080	1.33496879
6	-5.67520789	1.58851520	3.16605980	1	6.32662027	-6.96092565	2.16112724
6	-5.64385668	-0.82032931	1.66189806	1	6.68089714	-6.82872888	0.41063415
6	-5.71787659	2.82058772	3.98006323	1	4.47430316	-5.75377219	0.10907506
6	-4.85529472	0.51769867	3.54995855	1	4.04591910	-5.59888916	1.83256078
6	-4.78200634	-0.67832388	2.79757898	1	6.57051104	-4.32187136	0.57103753
8	-5.06824964	2.96031130	5.02908908	1	6.19851684	-4.43122463	2.30484034
6	-6.28930109	-0.72766906	-1.10798641	1	9.45229759	-6.31139002	-0.25072908
6	-5.89824927	-2.08484232	0.96654136	1	4.40148958	-3.28140210	-0.18968932
6	-6.02309619	-0.62346573	-2.51401792	1	10.27221072	4.52688453	-2.61723749
6	-6.07226883	-1.99687418	-0.45997590	6	-9.96811767	-6.68725373	-1.69816385
6	-5.91047302	-3.36974621	1.60006227	1	-10.31225886	-7.18899777	-0.78309069
6	-5.88279616	-1.81633705	-3.26748471	6	-3.54691310	6.76263992	1.77702906
6	-5.95473705	-3.18472144	-1.25242156	1	-3.63408614	7.68558163	1.18208155
6	-5.88833336	-4.52270908	0.78393150	7	-11.23513332	-2.11271022	0.73711522
6	-5.89635197	-3.07939891	-2.67057586	7	-11.31310904	-0.93097648	1.33324403
6	-5.85351403	-4.45016901	-0.61378196	1	-10.40003908	1.99329138	-1.15378264
6	-5.71352038	-4.28603294	-3.49769461	1	-8.27403172	3.29231665	-0.97139542
6	-5.72645389	-5.68036319	-1.41739579	6	-11.77223919	-2.03280875	-0.52241866
8	-5.57317037	-4.24776490	-4.72940508	6	-10.06595045	2.37028476	-0.17502769
7	-5.67747280	-5.52508180	-2.81391393	6	-8.86924711	3.09395764	-0.07095979
8	-5.64420156	-6.81710448	-0.91828122	1	-7.42647346	5.45227449	-0.55050396
1	-4.21778454	0.63548398	4.43149996	7	-11.91886970	-0.08471799	0.47298196
1	-5.88246156	-5.50871311	1.25683259	1	-5.35996980	6.80563064	-0.29809304
1	-5.71181797	-1.76257771	-4.34938642	1	-12.79048292	1.76153553	0.08363883
1	-8.31029074	3.44251399	-0.15641389	6	-6.77781858	5.28268864	0.32132258
6	-8.28492117	1.45453547	-1.96652472	6	-5.61061677	6.05418001	0.46109656
6	-8.92339962	0.27331697	-2.42386324	6	-12.13738231	1.31935338	0.85831157
6	-8.38207702	2.60446869	-2.79384911	6	-12.21849857	-0.71764356	-0.69956032
6	-9.56315990	0.21461310	-3.66441401	6	-10.83218152	2.08521049	0.97604638
6	-9.02659080	2.56080219	-4.03150099	6	-8.39348855	3.53890727	1.18946829
6	-9.60422711	1.35356512	-4.52265574	6	-7.13412429	4.32110397	1.30207640
1	-8.92212470	-0.62365849	-1.79141125	6	-4.76896384	5.88897291	1.58038128
1	-7.88537519	3.53608177	-2.49063501	1	-12.68755602	1.32436358	1.81823326
1	-10.04898344	-0.72283932	-3.95153580	1	-12.70351426	-0.20496138	-1.53388786
1	-9.03660733	3.46450498	-4.64819275	6	-10.35963799	2.50913042	2.23389222
6	-5.74989952	0.65933913	-3.19012680	6	-6.26708722	4.14341080	2.40958307
6	-5.03719716	1.69712863	-2.52730474	6	-9.15579159	3.22378814	2.34141785

6	-6.06765113	0.87365775	-4.55735772
6	-4.65772126	2.86998363	-3.17618465
6	-5.68832745	2.03917185	-5.22841566
6	-4.96364350	3.07708796	-4.56040100
1	-4.75356350	1.56515437	-1.47646251
1	-6.66671831	0.12367726	-5.09262220
1	-4.08556607	3.61939427	-2.62176149
1	-5.98695619	2.17787399	-6.27182572
6	-5.96946877	-3.56674299	3.06853012
6	-5.27551953	-4.63315744	3.69420674
6	-6.77743726	-2.75516585	3.89904517
6	-5.40424103	-4.89786497	5.06025283
6	-6.91310255	-2.99944950	5.27158931
6	-6.23548018	-4.09316337	5.89130979
1	-4.59480914	-5.25351370	3.09542341
1	-7.34074269	-1.92493249	3.45906791
1	-4.85540406	-5.74065762	5.48969746
1	-7.57285869	-2.34043040	5.84670063
6	-3.71917559	-1.66527684	3.09659154
6	-3.24331675	-1.92171363	4.40838229
6	-3.05665695	-2.32083928	2.02941759
6	-2.16363449	-2.78098133	4.63529001
6	-1.98407343	-3.18614787	2.24506776
6	-1.49739484	-3.42611467	3.55632789
1	-3.75169248	-1.47180836	5.27104478
1	-3.35502804	-2.11879892	0.99473349
1	-1.48850031	-3.62350312	1.37383226
7	-6.39601214	-4.37985741	7.25310947
7	-4.56124173	4.21039881	-5.22556842
7	-10.16026257	1.28101230	-5.80690955
6	-3.86630696	5.28005485	-4.51422429
1	-4.39270524	5.53695460	-3.57546372
1	-2.81546099	5.01516503	-4.25703906
1	-3.86069496	6.18966981	-5.13898161
6	-4.60848791	4.24917453	-6.68523736
1	-4.10869485	5.16691960	-7.03954769
1	-4.08000662	3.37816297	-7.12757804
1	-5.65065877	4.24434542	-7.07089702
6	-10.70360151	-0.00512782	-6.25011711
1	-11.58772524	-0.32954164	-5.65395011
1	-10.99815838	0.07179511	-7.31247451
1	-9.93640986	-0.79719429	-6.15891560
6	-10.84656955	2.46804028	-6.34364572
1	-11.77926671	2.70571843	-5.78397412
1	-10.19634936	3.35970894	-6.30354881
1	-11.11535278	2.29023519	-7.40117409
6	-7.45838016	-3.67723108	7.97856335
1	-7.28157249	-2.58411696	7.98121461
1	-8.46741136	-3.85386769	7.53976167
1	-7.46978596	-4.01973105	9.02695857
6	-6.09000189	-5.74334015	7.70978510
1	-5.01508132	-5.98332976	7.58556162
1	-6.33735195	-5.82779019	8.78371645
1	-6.66456784	-6.51609534	7.14824390
7	-0.39292203	-4.28166535	3.78982956
6	0.68626456	-3.73174085	4.63385163
6	-5.10372918	4.91283435	2.54290242
1	-10.94557929	2.29100228	3.13853020
1	-6.50417866	3.38546424	3.16663643
1	-4.43416571	4.76306610	3.39880485
1	-8.81317940	3.55863673	3.33037247
6	-10.88526796	-4.35934468	-1.04554536
6	-11.81547298	-3.20720461	-1.46415016
6	-10.89109724	-5.51083172	-2.06124101
1	-9.85572179	-3.96075510	-0.93710061
1	-11.17995189	-4.73635290	-0.04827879
1	-10.60961958	-5.12868789	-3.06079304
1	-11.91818475	-5.92020134	-2.17107629
1	-11.54563514	-2.85742023	-2.48148618
1	-12.86034311	-3.57848901	-1.55319077
1	-9.94932961	-7.42762438	-2.51469896
1	-3.44109347	7.04092778	2.83786146

1	1.44924683	-4.51002966	4.81805347
1	1.19654375	-2.86802941	4.14918645
1	0.30047882	-3.39243042	5.61218503
6	0.10037172	-5.05093512	2.64025738
1	0.55909026	-4.41159179	1.85351050
1	0.88177723	-5.75042492	2.98311243
1	-0.73077895	-5.62401472	2.18697694
1	-1.84378591	-2.96924146	5.66777240
6	5.51851825	-6.09547246	3.26323566
1	4.46606349	-6.38297958	3.41410829
6	-5.49636360	-6.75570861	-3.61922681
1	-5.84146650	-6.51730882	-4.63707798
7	6.30820075	-7.84167852	-2.25398812
7	5.74026923	-8.30180218	-3.35892507
1	3.29291777	-7.45430233	-3.81362509
1	0.96389888	-6.63841057	-3.70941595
6	5.97194379	-8.64909265	-1.19456248
6	2.46876241	-8.17874874	-3.87070890
6	1.14424128	-7.71822540	-3.81348889
1	-2.07519983	-9.84571870	-2.61772342
7	5.03185520	-9.40365880	-3.02282376
1	-4.44321597	-9.05943615	-2.53798613
1	4.64148847	-9.88727907	-5.00352686
6	-2.35118343	-8.90247434	-3.10939305
6	-3.68163381	-8.45494461	-3.05132742
6	4.17989894	-10.06781318	-4.01292691
6	5.14063201	-9.65748618	-1.68629897
6	2.74660458	-9.56143645	-3.95843657
6	0.05089185	-8.62225006	-3.84703738
6	-1.35251212	-8.14066122	-3.76487204
6	-4.05585411	-7.23169469	-3.64850237
1	4.21896788	-11.15706556	-3.83058444
1	4.64401406	-10.50583734	-1.21102709
6	1.66851915	-10.46736005	-3.99598410
6	-1.73141560	-6.90491232	-4.34557627
6	0.34063303	-10.00652672	-3.95145688
6	-3.05909426	-6.45691033	-4.28496116
1	1.86295799	-11.54744668	-4.06848694
1	-0.99476590	-6.30934775	-4.90190274
1	-3.32667820	-5.50157789	-4.75446560
1	-0.47890222	-10.73516373	-4.01817946
6	5.67280465	-7.29541828	0.96303426
6	6.44977340	-8.39626771	0.20265699
6	6.23997561	-7.12119084	2.37649027
1	5.73827480	-6.33948697	0.40334182
1	4.59749059	-7.56094680	1.01193071
1	7.31580612	-6.87153728	2.31768870
1	6.18063778	-8.09336021	2.90998199
1	7.52655596	-8.12964438	0.17360271
1	6.38512402	-9.34300522	0.77339057
1	6.02419893	-6.05125185	4.24493849
1	-6.15440835	-7.53335402	-3.20556011
6	5.43049172	7.72765879	-0.40940650
1	6.46366707	7.98026708	-0.69212261
6	-6.63077828	5.09634250	4.33655789
1	-6.33459368	4.79029002	5.35314455

7	1.32492403	9.25827671	-2.40527127
7	0.25438486	9.63786465	-1.72326296
1	0.19081910	9.91735120	1.49386163
6	2.28810565	10.23395772	-2.34117964
1	-1.27520494	8.48722051	2.86426769
6	-0.89600002	9.96056128	1.34117323
7	0.52632741	10.85539460	-1.19715918
6	-1.73458922	9.14229055	2.11270834
1	0.01642404	12.41925171	0.06022043
1	-5.90449875	9.20164829	2.15155339
6	-0.51790810	11.64926744	-0.52912713
6	1.77834229	11.26536844	-1.54881943
1	-7.37162071	7.44765353	3.11601231
6	-5.44388792	8.32607524	2.62618735
6	-1.42469123	10.81054504	0.34697210
6	-6.27870382	7.34544482	3.18594257
6	-3.14384833	9.13870879	1.91701437
6	-4.03194671	8.18235833	2.63826734
1	-1.10789312	12.16819104	-1.31012525
6	-5.73372200	6.20550741	3.81714875
6	-2.82288142	10.85298574	0.17719794
6	-3.66523942	10.03956227	0.95483894
6	-3.49629896	7.04836763	3.30365228
6	-4.32827912	6.08648116	3.89446799
1	-3.25637742	11.49629099	-0.60421353
1	-2.41418907	6.87454741	3.32959029
1	-4.74333611	10.07632264	0.76137879
1	-3.88131352	5.21514506	4.39290536
6	4.46519147	8.11869369	-1.53855795
6	3.63937101	10.08911448	-2.98134647
6	4.71277710	9.56457999	-1.99770270
1	3.96179381	11.07057974	-3.38196848
1	3.55694573	9.39572138	-3.84391924
1	3.42276634	7.99924121	-1.18583236
1	4.59570539	7.42902772	-2.39736156
1	4.73352933	10.23815339	-1.11352131
1	5.70737958	9.63336542	-2.48809420
1	2.19882198	12.21005803	-1.20287645
1	5.17904264	8.27808986	0.51518939
1	-7.68409889	5.41967928	4.34802841

MC-PDI1⊃C60

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute complex shown

Atom	X	Y	Z
6	3.57229967	6.09369436	3.31840762
6	1.01948552	5.70035419	2.01178996
6	4.91955821	6.12748080	3.89031118
6	2.50433229	5.44985265	4.01357839
6	1.19975661	5.34542886	3.39400965
8	5.89590202	6.63198965	3.29831030
7	5.09974530	5.54223331	5.15743237
6	2.73249954	4.89184657	5.30945070
6	0.06365992	4.86037790	4.13578734
6	4.07215792	4.93546043	5.90865049

MC-PDI2⊃C60

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute complex shown

Atom	X	Y	Z
6	-7.16270468	3.96076847	0.80867252
6	-6.75585196	3.45463641	-0.43949900
6	-7.22242998	3.13751582	1.93690789
6	-6.44564373	2.09328595	-0.61012474
1	-6.74132409	4.12713212	-1.30259359
6	-7.69374742	3.69330622	3.22321525
6	-6.89400266	1.74752168	1.82614986
6	-6.60340755	1.20637818	0.51921142
8	-8.06737194	4.87334808	3.34866090
7	-7.75316993	2.81290583	4.30574169

8	4.33951374	4.44621226	7.02694320	6	-6.89142796	0.90845410	2.96813385
6	-0.18621067	5.20781801	1.34547940	6	-6.56596067	-0.20452969	0.34631713
6	-1.26781611	5.12685924	3.57067259	6	-7.39605231	1.44019971	4.26050345
6	-1.38701825	5.12160747	2.13302050	6	-6.45835888	-0.45746628	2.83467322
6	-2.68125422	5.05799223	1.48402175	6	-6.37074294	-1.04386151	1.50278089
6	-2.76778671	4.93807920	0.06185253	8	-7.56121424	0.74569250	5.27211497
6	-3.87342163	5.12286163	2.26783036	6	-6.03777973	1.51948845	-1.89468933
6	-4.07043235	4.84860441	-0.59721105	6	-6.74483901	-0.69934619	-1.01854657
6	-5.18827426	5.09492267	1.62260783	6	-5.33758518	2.24263068	-2.92163227
8	-4.21305203	4.66086446	-1.82246320	6	-6.37944622	0.15920500	-2.12228349
7	-5.21275489	4.97391656	0.22136233	6	-7.29058152	-1.96422693	-1.30461080
8	-6.26481720	5.19434977	2.25187539	6	-5.24357342	1.68812186	-4.26686287
6	-2.45523362	5.36963691	4.29834855	6	-6.37872994	-0.35828459	-3.47129243
6	-3.76096518	5.32641898	3.67027590	6	-7.39480241	-2.42665450	-2.62607622
7	-2.64109658	5.66742767	5.65368314	6	-5.86857832	0.42083158	-4.54449516
6	-4.72050293	5.53911930	4.70727388	6	-6.92002123	-1.66616574	-3.69944788
6	-4.02329969	5.75271444	5.90091306	6	-5.94696914	-0.13021118	-5.91778681
1	-5.80348684	5.50470994	4.59952550	6	-6.98996717	-2.23324121	-5.05984451
6	0.34547232	4.19701350	5.35034812	8	-5.63122841	0.49049070	-6.94514246
6	1.65877545	4.22855557	5.96537648	7	-6.40034673	-1.46765890	-6.07126064
7	-0.49083454	3.42141244	6.15978826	8	-7.52888760	-3.32505742	-5.31159546
6	1.54968581	3.50273155	7.19257994	1	-7.82347752	-3.41196279	-2.82751833
6	0.24647933	3.00686269	7.28696975	1	-7.43248079	5.01897076	0.89486891
1	2.32840101	3.36992555	7.94199559	6	-4.47647981	2.41532989	-5.23699343
6	2.02908435	6.48948422	1.41678476	6	-3.82464649	3.59413691	-4.91069004
6	3.30983209	6.69538743	2.05746359	1	-4.38253387	1.99736535	-6.24020512
7	2.03252811	7.19321141	0.20590932	1	-3.22540922	4.11508949	-5.66857128
6	4.08299910	7.51613041	1.17648139	6	-4.62285945	3.44818843	-2.62452406
6	3.29629232	7.80018154	0.05855241	6	-3.88239600	4.11155526	-3.58986179
1	5.10886453	7.85041965	1.32507360	1	-4.59867145	3.80509106	-1.59108786
6	-0.29558245	4.88436709	-0.02287902	1	-3.31698986	5.01707736	-3.33099847
6	-1.57181521	4.82305421	-0.69493135	6	-5.97951834	-2.41825481	1.39762560
7	0.70838396	4.63662611	-0.96312921	6	-5.65236415	-3.17427263	2.51516991
6	-1.28751181	4.63856316	-2.08221674	1	-5.84977377	-2.86633538	0.41020844
6	0.10067795	4.52198714	-2.23244969	1	-5.30638257	-4.20881431	2.38911843
1	-2.01914245	4.64126158	-2.88692083	6	-6.08800483	-1.26374586	3.95935240
6	0.83129269	4.41948623	-3.50314181	6	-5.69294534	-2.58582294	3.80737318
6	2.19926306	4.77154840	-3.64862837	1	-6.09602654	-0.80278947	4.94661312
6	0.11712274	4.04712716	-4.67561484	1	-5.38347319	-3.16711489	4.68768445
6	2.81696606	4.75297561	-4.91032931	1	-7.66672491	-2.58448012	-0.48746655
1	2.78388167	5.08132526	-2.77728831	6	6.56048454	0.26551227	-0.99646712
6	0.73582258	4.03566264	-5.93337491	6	6.07163187	1.47051366	-0.46378757
1	-0.94420824	3.78287829	-4.59910728	6	6.39922183	-0.94851534	-0.32312603
6	2.09360421	4.38954817	-6.05802249	6	5.39654502	1.49808449	0.77072500
1	3.87418693	5.02899049	-5.00331094	1	6.24657040	2.39941536	-1.01353155
1	0.15825353	3.75801733	-6.82699835	6	6.86298368	-2.19637464	-0.96651460
1	2.57423797	4.38855100	-7.04601970	6	5.78703009	-0.97303560	0.97060888
6	3.71510262	8.53075642	-1.14507276	6	5.32924890	0.27427558	1.53784422
6	4.72474117	9.52931742	-1.05047213	8	7.30041541	-2.24144238	-2.12536149
6	3.20573967	8.20513012	-2.43018796	7	6.79735788	-3.35190460	-0.17400894
6	5.19929736	10.18183080	-2.19950095	6	5.60695170	-2.19566114	1.67014143
1	5.14993973	9.78938860	-0.07038261	6	4.81430486	0.28774495	2.86101369
6	3.68572982	8.85983513	-3.57759020	6	6.20084330	-3.43467062	1.10895242
1	2.45543234	7.41517509	-2.54111063	6	4.79713314	-2.21365024	2.86324416
6	4.68087213	9.85369113	-3.46904869	6	4.37538939	-0.94931660	3.44848303
1	5.97751711	10.95166601	-2.10120864	8	6.19207285	-4.53193233	1.68880850

1	3.27967105	8.59337532	-4.56344527	6	4.79079561	2.70944839	1.33137832
1	5.03503836	10.37958932	-4.36785879	6	4.76483424	1.57673316	3.54607297
6	-0.31614516	2.20494758	8.38224867	6	4.34597647	3.83351394	0.54933462
6	0.54453615	1.37066527	9.14563868	6	4.67876929	2.77574034	2.74828370
6	-1.68167034	2.28907963	8.76563116	6	4.86825045	1.69013372	4.94586720
6	0.06336625	0.66233942	10.25879182	6	4.06303240	5.10896274	1.20312683
1	1.59848419	1.27527372	8.85551873	6	4.50730999	4.05458409	3.39396809
6	-2.16234945	1.57880050	9.87822240	6	4.84162130	2.94917195	5.56730732
1	-2.36740745	2.94882710	8.22233408	6	4.22880439	5.22141104	2.63170311
6	-1.29304176	0.76631390	10.63287360	6	4.63859971	4.11372421	4.81971103
1	0.75052139	0.02733412	10.83647439	6	4.05655708	6.51228914	3.35090063
1	-3.21243511	1.68957385	10.18399399	6	4.60614908	5.40965438	5.52261279
1	-1.66761276	0.24414454	11.52649248	8	3.65478574	7.56813401	2.84133147
6	-4.61433532	5.96344436	7.22808485	7	4.37552590	6.53681100	4.73217923
6	-5.92152143	6.51867759	7.32568361	8	4.75493826	5.51449194	6.75335600
6	-3.97688681	5.54035198	8.42201935	1	4.98682488	3.02377665	6.65166377
6	-6.56713300	6.62270862	8.56633230	1	7.06581541	0.27085909	-1.96865677
1	-6.43358353	6.86808381	6.41821353	6	3.63928284	6.20222491	0.37569125
6	-4.62432406	5.65247088	9.66264146	6	3.45946528	6.05897092	-0.99167753
1	-2.98039472	5.08882473	8.38892879	1	3.44339977	7.16340515	0.84765925
6	-5.92286815	6.19047662	9.74254190	1	3.13000244	6.92885386	-1.57670307
1	-7.58371695	7.03748238	8.60753493	6	4.09356040	3.71953317	-0.85554623
1	-4.10217318	5.29062944	10.55945786	6	3.66004329	4.79802338	-1.61177372
1	-6.43976158	6.27320902	10.70885713	1	4.19136872	2.74342062	-1.33438700
6	-1.67052532	2.70569796	5.65071893	1	3.45668612	4.66817406	-2.68306948
1	-2.62123363	3.14050186	6.00594580	6	3.43229669	-0.96172435	4.52490777
1	-1.65682144	2.73784390	4.55149151	6	2.96317762	-2.15236799	5.05880394
1	-1.60052102	1.65229310	5.96404507	1	3.02235337	-0.00867256	4.87751872
6	-1.61482716	6.28487855	6.50745184	1	2.22048257	-2.13593620	5.86737799
1	-1.17106459	5.57407983	7.22413874	6	4.30543796	-3.41885342	3.46329045
1	-0.80744092	6.67842827	5.86972822	6	3.42249191	-3.38915844	4.53313231
1	-2.06540275	7.12096084	7.06829480	1	4.60819992	-4.36991417	3.02779162
6	2.02228694	4.08624638	-0.59322565	1	3.04568872	-4.33379927	4.94987075
1	2.82036234	4.84937760	-0.59992701	1	5.03041522	0.79640258	5.56013457
1	1.95563554	3.65442548	0.42041600	6	-8.31798170	3.32509417	5.57294930
1	2.28525963	3.27449522	-1.29133931	1	-8.71017925	2.45225055	6.11316831
6	0.81446827	7.68718549	-0.45940859	1	-9.16980300	3.97902895	5.32069868
1	0.98474886	8.72337591	-0.79563187	6	4.29515449	7.85595008	5.41491020
1	0.52392017	7.07725084	-1.32996745	1	4.66920994	8.60932669	4.70307568
1	-0.01568480	7.68034990	0.26603042	1	4.97476672	7.79162299	6.28138092
6	6.78052948	-6.96732104	-0.22191016	7	-7.32459782	7.17954014	7.50167037
6	4.18551845	-7.21458765	1.01805294	7	-6.88764224	8.43167823	7.47836110
6	8.09120797	-6.66417587	-0.80710543	1	-4.26506316	10.01797126	6.06379430
6	5.59280685	-6.86973083	-1.01361313	6	-6.70490317	6.49314587	8.51887242
6	4.29634158	-7.09475474	-0.40901701	1	-1.97712525	9.52867987	5.23706649
8	9.15609569	-6.72136383	-0.16288485	6	-3.48535616	9.71437977	6.77633692
7	8.11468871	-6.29922679	-2.17111890	7	-6.00091041	8.56651489	8.48842633
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6	3.09798059	-7.19841552	-1.20369269	1	-5.74827020	10.58507206	8.07515664
6	6.98687337	-6.29049602	-3.01988401	1	0.63122411	7.28628846	8.30342371
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6	1.90467074	-7.76302830	-0.54669827	1	2.95729290	6.83429533	7.56538373
6	1.73561137	-7.47681506	0.85822899	6	1.02992209	7.81410542	7.42753299
6	0.48546250	-7.71946532	1.54808169	6	-3.79609972	9.59866139	8.14783828
6	0.31142493	-7.30379171	2.90752274	6	2.33800840	7.54523155	7.00827307

6	-0.56867254	-8.39531428	0.87117931	6	-1.16522250	9.03729760	7.20621897
6	-0.92371204	-7.63094708	3.63005348	6	0.21503628	8.74251121	6.73253709
6	-1.80866366	-8.75372930	1.57972189	1	-5.22064267	10.07401193	9.71670042
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8	-2.73469293	-9.39112295	1.05825941	6	-1.49437057	8.91861953	8.58039912
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6	-1.13322097	-9.65204766	-1.33388514	1	0.18203620	10.14710736	5.06136624
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7	3.47501649	-5.69225196	3.68678519	1	7.64520895	-5.22034878	0.13218186
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1	3.97365750	-8.02218200	4.53904979	6	2.31629868	-4.25356273	-1.85092476
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6	11.24838438	-0.88004579	4.56865484	6	-2.14398003	-1.57758376	1.50234880
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1	9.21249330	1.92117474	6.82109675	6	-0.96846274	-2.19431776	1.97613690
7	12.60355188	-2.65763444	2.16336938	6	0.27437341	-1.42182975	2.07085505
1	7.59680512	3.70808578	7.41254843	6	-2.12538696	-0.16496309	1.10294667
1	13.56694491	-2.22153221	3.95658336	6	-0.92800692	0.57780134	1.19261292
6	8.80042557	2.55352866	6.02209528	6	0.29370464	-0.06301354	1.68569564
6	7.88354567	3.56999413	6.36021638	6	3.06309758	-0.31765042	-0.79559278
6	13.17655151	-1.66168342	3.08614349	6	2.47897630	-0.39613886	0.54541845
6	12.58300410	-2.66856549	0.79394589	6	1.42118500	0.46005063	0.90924417
6	12.15986561	-0.61914989	3.52183728	6	2.56573927	0.61143709	-1.72754495
6	10.22860018	1.34309200	4.29456839	6	2.71424586	-1.09207050	-3.53983590
6	9.23162998	2.37749753	4.68305246	6	3.23584292	-2.05694407	-2.56606969

6	7.37507155	4.44836736	5.37825334
1	14.02788181	-1.18472282	2.56759715
1	13.13114440	-1.93826342	0.19258931
6	12.08959815	0.62234210	2.85965523
6	8.69576809	3.24743147	3.70241892
6	11.14318322	1.58731423	3.23865802
6	7.79636538	4.26282567	4.04258706
1	12.79393365	0.84518769	2.04428766
1	8.98094242	3.11887451	2.64992962
1	7.42198900	4.93726680	3.26805472
1	11.12753577	2.55323351	2.71760643
6	10.07577910	-3.84320730	-1.45166246
6	11.42668729	-4.33937537	-0.88405153
6	9.74663659	-4.48445010	-2.81371273
1	9.26291803	-4.03683369	-0.72353002
1	10.12270635	-2.74231247	-1.57722028
1	10.61158134	-4.35212465	-3.49810523
1	8.89478851	-3.95641697	-3.28239279
1	11.38785365	-5.44059052	-0.79116559
1	12.22726354	-4.09100194	-1.60697251
1	10.18764842	-6.55113766	-2.22165548
1	6.89821356	6.55802061	5.42981508
6	-3.06166234	-8.86056982	3.71861294
1	-2.69791117	-9.02671651	4.74709431
6	-6.53832023	5.01942049	-0.44957914
1	-6.37451822	5.47582283	-1.43831606
7	-6.49908261	-6.82081727	0.03243475
7	-7.27741285	-6.24570308	-0.87843153
1	-9.03033393	-3.05031830	-3.06076126
6	-6.94424357	-6.49008778	1.28817997
1	-8.64030667	-0.61198858	-3.03396548
6	-8.92372539	-2.53573738	-2.09493753
7	-8.23781614	-5.54842209	-0.21175240
6	-8.70343507	-1.14960492	-2.07926715
1	-9.28366021	-5.14533042	-1.96141351
1	-9.14884477	1.41280548	1.09976794
6	-9.26294190	-4.77067600	-0.92333168
6	-8.07399093	-5.68219201	1.13316532
1	-8.25592556	3.72294775	1.28078738
6	-8.50018476	1.80284199	0.30276636
6	-9.02595370	-3.26835974	-0.89391248
6	-8.00129659	3.10986713	0.40709449
6	-8.56657697	-0.44808428	-0.85634340
6	-8.18427100	0.98640445	-0.81159906
1	-10.23218460	-5.00951009	-0.44399019
6	-7.16840827	3.64561946	-0.59908589
6	-8.94454228	-2.56864084	0.32866231
6	-8.71122804	-1.18855008	0.34782686
6	-7.39615429	1.55151779	-1.84548639
6	-6.89657515	2.85717128	-1.73832815
1	-9.04262113	-3.09626069	1.28546326
1	-7.12282549	0.93643942	-2.71255616
1	-8.60012212	-0.69012573	1.31858167
1	-6.24620383	3.27127649	-2.51756238
6	-4.25654767	-7.89229731	3.74573716
6	-6.25807422	-6.86219157	2.57526163
6	3.41182545	-1.67506783	-1.22152834
6	2.38600202	0.21698609	-3.12806415
6	0.31549676	0.16124218	-4.50683578
6	0.65612533	-1.19934076	-4.93339301
6	1.83244788	-1.81479639	-4.45991069
6	1.16528609	0.85861787	-3.62294427
6	-0.80577098	1.71295216	-2.36036850
6	-1.68662817	0.99353721	-3.28265134
6	-1.13751269	0.23225999	-4.33431270
6	0.59212402	1.64546695	-2.52522881
6	0.89967187	1.42596444	-0.06220221
6	-0.55393146	1.49879421	0.11160348
6	-1.38964805	1.63682035	-1.01810764
6	1.45916051	1.49637193	-1.35469152

6	-5.03748900	-7.78182863	2.42742217
1	-7.00060862	-7.31589173	3.26670404
1	-5.94734747	-5.91787933	3.07181709
1	-3.90236784	-6.88825214	4.05692615
1	-4.94105491	-8.23469810	4.55279185
1	-4.37866345	-7.39834596	1.62618677
1	-5.36240637	-8.78986800	2.10336842
1	-8.75182181	-5.23410092	1.85903161
1	-3.35603081	-9.82904781	3.27715227
1	-7.18058765	5.67521362	0.15820578
6	-0.34786653	-1.81192254	3.62662527
6	0.28159142	-0.68103568	2.93548135
6	-0.15834311	-3.12595966	3.15159176
6	1.07665682	-0.90464155	1.79532286
6	0.96701003	-0.00876260	0.64032949
6	-0.65072102	0.44723925	2.96859540
6	-0.75343931	1.31419893	1.86191374
6	0.07336692	1.08189398	0.67204890
6	-2.56434990	-3.63987468	3.54763116
6	-2.75781036	-2.27642346	4.04523913
6	-1.29069739	-4.05654931	3.10988347
6	-1.67118216	-1.38040144	4.08296061
6	-1.85739880	0.01330782	3.67522810
6	-4.07369046	-1.81246999	3.60397565
6	-4.25502264	-0.46767854	3.21566082
6	-3.12489717	0.46549680	3.25409853
6	-2.31914494	-5.23376067	1.17054986
6	-3.64121076	-4.79748022	1.62804152
6	-1.16654490	-4.86458772	1.89485439
6	-3.76339105	-4.02121705	2.79698133
6	-4.69716921	-2.89103440	2.83131232
6	-4.45028982	-4.47717529	0.44804818
6	-5.35242405	-3.39538299	0.48102849
6	-5.47533527	-2.58397657	1.69597854
6	0.04789459	-4.38101321	-0.22203233
6	-1.15317114	-4.75912800	-0.97586449
6	0.04079320	-4.43040515	1.18479568
6	-2.31187918	-5.17672617	-0.29415170
6	-3.62873346	-4.71331918	-0.74039200
6	-1.26207791	-3.86610611	-2.13068765
6	-2.52825276	-3.42435617	-2.56519194
6	-3.73439366	-3.85441678	-1.85404087
6	1.26938265	-2.26985695	1.29706601
6	1.27787874	-2.21785919	-0.16692986
6	0.66738755	-3.35908578	1.96153605
6	0.67913742	-3.25456198	-0.91296162
6	-0.13048346	-2.93564616	-2.09234507
6	1.09086811	-0.82158245	-0.57281338
6	0.31243622	-0.51565027	-1.70755848
6	-0.30995527	-1.59278391	-2.48150273
6	-4.03628582	-1.59413190	-2.50746990
6	-2.71368765	-2.02704961	-2.96941035
6	-1.62573377	-1.13004541	-2.92602106
6	-4.21866629	-0.28232453	-2.02544129
6	-5.63853571	-1.13716254	-0.17280649
6	-5.45762642	-2.49918428	-0.67357576

6	-4.66902845	-2.72497503	-1.82167422
6	-5.03633177	-0.05061284	-0.83421450
6	-4.43186735	0.98697888	1.34663271
6	-5.06344957	-0.14936544	2.03725112
6	-5.65393203	-1.18861936	1.29086986
6	-4.41810094	1.03127944	-0.06186565
6	-2.06044226	1.82635206	-0.04642754
6	-2.07004080	1.77828512	1.41786553
6	-3.23394866	1.36662737	2.10267418
6	-3.21371420	1.46516330	-0.77314400
6	-1.81720940	0.23629398	-2.43034191
6	-0.61665001	0.61732003	-1.67582153
6	-0.73632356	1.39809815	-0.50771353
6	-3.08997474	0.65220823	-1.98792804

MC-PDI3⊃C60

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute complex shown

Atom	X	Y	Z
6	7.07484878	1.20964896	0.01609489
6	6.31165387	2.33105713	-0.39790656
6	7.20559662	0.10811182	-0.87897178
6	5.68493548	2.41283120	-1.64878345
1	6.24329366	3.17446116	0.29495648
6	7.79990312	-1.17775050	-0.44316854
6	6.65541700	0.19197230	-2.20504267
6	5.83171213	1.31602141	-2.56165684
8	8.01983295	-1.47525010	0.74077892
7	8.09022938	-2.11753288	-1.44871984
6	6.93174079	-0.81783135	-3.18758693
6	5.16457274	1.32510456	-3.83009474
6	7.65393565	-2.04387316	-2.78611343
6	6.43907674	-0.67175137	-4.51688628
6	5.48560200	0.34153276	-4.77160925
8	7.83511829	-3.02350854	-3.52215564
1	5.05398339	0.40285975	-5.77652540
6	4.94027728	3.60808543	-2.07860224
6	4.23021687	2.41164373	-4.14403977
6	4.86580238	4.76499467	-1.28991109
6	4.23388425	3.58880201	-3.32223702
6	3.29880978	2.31255657	-5.18076758
6	4.17007768	5.92654068	-1.69169105
1	5.37332564	4.79899830	-0.32197926
6	3.47661570	4.73536856	-3.74213822
1	3.16583147	1.34546449	-5.67944310
6	2.43945515	3.38208065	-5.54838801
6	3.49521484	5.92869237	-2.94027570
6	2.65530960	4.64686140	-4.91570516
6	2.74149969	7.11944140	-3.39366880
6	2.09345237	5.88615944	-5.47967462
8	2.66322347	8.17932049	-2.75418200
7	2.10289429	7.02581240	-4.64306948
8	1.62941009	5.97562936	-6.62456270
6	7.73708296	1.30664444	1.34407131
6	7.02890157	1.80863792	2.46395531

MC-PDI4⊃C60

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute complex shown

Atom	X	Y	Z
6	-5.20533314	-1.39543880	-3.52216881
6	-3.94496158	-1.85973121	-3.97283522
6	-5.85498736	-2.04049287	-2.44744815
6	-3.29274234	-2.93991775	-3.36072754
1	-3.48172989	-1.33389385	-4.81323731
6	-7.15838745	-1.53371338	-1.95377748
6	-5.22281549	-3.15210820	-1.81786881
6	-3.92437882	-3.59207960	-2.24891003
8	-7.66831947	-0.49456010	-2.38268216
7	-7.80278801	-2.28556316	-0.96168353
6	-5.89401063	-3.82232138	-0.75329830
6	-3.27154710	-4.65657383	-1.54083910
6	-7.27198196	-3.43364359	-0.36163908
6	-5.24036725	-4.87990657	-0.08470691
6	-3.93531844	-5.26888092	-0.46920364
8	-7.92582282	-4.06746737	0.47227095
1	-3.46062385	-6.07913752	0.09093094
6	-1.98473618	-3.42062982	-3.82610594
6	-1.92220639	-5.06354554	-1.94239933
6	-1.32697322	-2.84366321	-4.92266986
6	-1.33802946	-4.48967865	-3.12038016
6	-1.15357596	-5.94620334	-1.16967534
6	-0.09534895	-3.34788028	-5.40532106
1	-1.75818119	-1.98413785	-5.44385053
6	-0.06006919	-4.96581342	-3.57632589
1	-1.52200179	-6.30807819	-0.20522097
6	0.13126305	-6.36920577	-1.58657391
6	0.52815250	-4.43795752	-4.76136509
6	0.65074633	-5.94954375	-2.83180181
6	1.74689867	-5.05309100	-5.33963042
6	1.89452993	-6.55447748	-3.36621226
8	2.22297548	-4.68284982	-6.41958197
7	2.32280624	-6.11784044	-4.63483227
8	2.50639081	-7.44507947	-2.76952284
6	0.46164050	-2.67992368	-6.54878537
7	0.77466673	-2.00755727	-7.45876544

6	9.09371025	0.94607812	1.54921593	6	0.88955104	-7.17485776	-0.67355462
6	7.61252669	1.88762433	3.73594387	7	1.44618473	-7.75749735	0.17960881
6	9.70287729	1.04274446	2.80287477	6	-5.82946461	-5.59722860	1.01184075
6	8.97404460	1.50902137	3.94514051	7	-6.17665684	-6.24835101	1.92542393
1	5.97491627	2.09491338	2.34658575	6	-5.76017124	-0.26177623	-4.20946630
1	9.68530207	0.56998928	0.70400100	7	-6.07273796	0.66092395	-4.86550512
1	7.00112043	2.24564966	4.56975635	6	2.28730073	5.11401762	5.82425752
1	10.75226808	0.74026001	2.89694304	6	3.44906798	4.57149175	5.22324582
6	4.16884724	7.04564062	-0.69351794	6	1.37855669	5.87913079	5.05786629
6	5.06705478	8.13085337	-0.76982667	6	3.76104741	4.80835954	3.87548949
6	3.36541724	6.94339828	0.46217348	1	4.09674240	3.94270815	5.84193863
6	5.14466485	9.09551686	0.24599187	6	0.12011217	6.36456279	5.67026136
6	3.42352868	7.90383770	1.48392813	6	1.67036372	6.13544030	3.68581178
6	4.30192286	9.02281633	1.39562928	6	2.88261703	5.63344451	3.09391770
1	5.75006538	8.20266021	-1.62819784	8	-0.13141769	6.22799797	6.87197430
1	2.69003532	6.08576186	0.57236283	7	-0.81034511	6.96151777	4.80394804
1	5.89048455	9.89180593	0.14664104	6	0.73228673	6.86019376	2.89581014
1	2.77499718	7.77648268	2.35830787	6	3.15609388	5.90559027	1.71140345
6	1.30674589	3.07836787	-6.44980544	6	-0.53702961	7.34080587	3.47973462
6	1.37888394	2.06042804	-7.43755782	6	1.01171980	7.09706649	1.53025316
6	0.03571547	3.68913090	-6.27078046	6	2.21766884	6.63048293	0.96028781
6	0.27339606	1.69007797	-8.21453844	8	-1.35125242	8.02038355	2.84958422
6	-1.07928089	3.34287504	-7.02909011	1	2.38405311	6.81906796	-0.10432422
6	-0.99676264	2.33018266	-8.04148482	6	4.90780687	4.16567341	3.22264229
1	2.33093000	1.54619875	-7.62506528	6	4.36976560	5.36054157	1.09416153
1	-0.09876010	4.41591317	-5.46415531	6	5.66837325	3.18132591	3.87383427
1	0.40406164	0.89844917	-8.96266334	6	5.20411743	4.47273667	1.85222052
1	-2.03994120	3.81104437	-6.78941143	6	4.70573183	5.63731888	-0.24046743
6	6.95294157	-1.42608396	-5.68635532	6	6.74122580	2.52074325	3.22955388
6	6.09353655	-1.94489382	-6.68609108	1	5.42218738	2.87534095	4.89393217
6	8.34871400	-1.53062793	-5.91351922	6	6.33053615	3.84453251	1.21346881
6	6.59807419	-2.60383687	-7.81966563	1	4.09594925	6.31999420	-0.83927116
6	8.86624855	-2.14540017	-7.05365244	6	5.83677968	5.05318528	-0.85583440
6	8.00364738	-2.72587446	-8.03613735	6	7.11229567	2.87784327	1.91197965
1	5.00247459	-1.87592586	-6.55440418	6	6.65400260	4.15301310	-0.13761879
1	9.03783943	-1.10525586	-5.17264005	6	8.30858843	2.27085932	1.28349656
1	5.88758201	-3.02102509	-8.54025349	6	7.83270333	3.55083227	-0.79527038
1	9.95282249	-2.17147172	-7.19082449	8	9.02820140	1.46033468	1.88303051
7	-2.09060733	1.98321167	-8.80178162	7	8.61054847	2.67009969	-0.02535731
7	8.51333250	-3.37062859	-9.16503572	8	8.14631851	3.81395366	-1.96021035
7	9.57510168	1.61932342	5.19515076	6	7.37817564	1.46634251	3.96968853
7	4.32412611	10.00651721	2.40171617	7	7.75291349	0.60695297	4.67699110
6	10.84395009	0.92840940	5.43974301	6	6.08104586	5.41926490	-2.21987010
1	10.76948688	-0.17039332	5.28004010	7	6.11744378	5.83594371	-3.31770729
1	11.64825149	1.30421907	4.77567341	6	0.10044347	7.77483333	0.65017017
1	11.15734308	1.10706273	6.48254854	7	-0.53532503	8.28987350	-0.19180790
6	8.73344454	1.91280349	6.35603932	6	2.07930431	4.82140398	7.21515444
1	7.99368840	1.10702997	6.56244837	7	2.04305912	4.51788117	8.34874559
1	9.37513750	2.03303132	7.24671834	6	3.33242101	-6.95445045	-5.33934308
1	8.16534456	2.85143548	6.20606936	1	3.91860040	-7.47677536	-4.56890255
6	3.85088897	9.62633774	3.73961311	6	9.82311384	2.10375788	-0.67525923
1	4.44827831	8.79911176	4.19160019	1	10.52025056	1.85574616	0.14105947
1	3.92615956	10.49881536	4.41216908	7	6.20399416	-8.72782622	-5.50583176
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MC-PDI6⊃C60

QM1//QM2: BLYP-D3(BJ)/def2-SVP//GFN2-xTB

Only solute complex shown

Atom	X	Y	Z
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