

## Supporting information for:

### Host-guest complexes of perylene bisimide-based metallacage and fullerenes for efficient photoinduced charge separation

O. A. Stasyuk<sup>a</sup>, M. Solà<sup>\*a</sup> and A. J. Stasyuk<sup>\*a,b</sup>

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

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

#### Abstract

The discovery of coordination-driven self-assembly has greatly expanded the field of organic macrocyclic compounds. This approach enables the construction of precise supramolecular complexes, known as metallacages, assembled from organic ligands coordinated with metal centers. Metallacages come in various sizes and shapes, making them capable of hosting guest molecules of different sizes. In this work, we report the ground and excited state properties of non-covalent complexes between various fullerenes ( $C_{60}$ ,  $C_{70}$ ,  $Sc_3N@C_{80}$ ,  $Sc_3CH@C_{80}$ , and  $Sc_4O_3@C_{80}$ ) and  $Pt_6PBI_3$  metallacage, composed of perylene bisimide units and organoplatinum nodes. These complexes exhibit thermodynamically favorable photoinduced charge transfer from endohedral metallofullerenes to metallacage that occurs within picoseconds. Among the systems considered, the  $Pt_6PBI_3 \supset Sc_3N@C_{80}$  complex stands out as the most promising candidate for use in photovoltaics due to its ability to fast charge separation and slow charge recombination.

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## Computational Methodology

### Quantum-chemical calculations

Geometry optimization of the complexes was performed employing the DFT BLYP<sup>1,2</sup> exchange–correlation functional with Ahlrichs' def2-SVP basis set.<sup>3,4</sup> The empirical dispersion D3 correction was computed with the Becke–Johnson damping function.<sup>5,6</sup> Vertical excitation energies were calculated using TDA formalism<sup>7</sup> with the range-separated CAM-B3LYP<sup>8</sup> functional and def2-SVP basis set,<sup>3,4</sup> as implemented in the Gaussian16 (rev. A03) program.<sup>9</sup> The same program was used for population analysis and calculation of Mulliken,<sup>10,11</sup> Lowdin,<sup>12</sup> Hirshfeld,<sup>13</sup> and CM5,<sup>14</sup> charges. Interaction energy was computed using the BLYP functional coupled with TZVP basis<sup>15</sup> for the BLYP-D3(BJ)/def2-SVP optimized geometries. Its decomposition analysis (EDA)<sup>16,17</sup> was performed using the Amsterdam Density Functional (ADF) program.<sup>18</sup> Molecular structures and frontier molecular orbitals were visualized by Chemcraft 1.8. program.<sup>19</sup>

### Energy decomposition analysis

The interaction energy between Pt<sub>6</sub>PBI<sub>3</sub> metallacage 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  $\Delta E_{disp}$  was added to account for the dispersion correction:<sup>20-22</sup>

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

The term  $\Delta V_{elstat}$  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,  $\Delta E_{Pauli}$ , comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interactions,  $\Delta E_{oi}$ , 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  $\Delta E_{disp}$  accounts for the dispersion corrections.<sup>23,24</sup>

### 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.<sup>25-27</sup> The analysis was done in the Löwdin orthogonalized basis, which is more convenient. The matrix  ${}^{\lambda}\mathbf{C}$  of orthogonalized MO coefficients is obtained from the coefficients  $\mathbf{C}$  in the original basis  ${}^{\lambda}\mathbf{C} = \mathbf{S}^{1/2} \mathbf{C}$ , where  $\mathbf{S}$  is the atomic orbital overlap matrix. The transition density matrix  $T^{0i}$  for an excited state  $\Phi_i^*$  constructed as a superposition of singly excited configurations (where an occupied MO  $\psi_j$  is replaced a virtual MO  $\psi_a$ ) is computed as,

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

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

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

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

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

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

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

### Solvent Effects

The equilibrium solvation energy  $E_s^{\text{eq}}$  of a molecule (in the ground or excited state) in the medium with the dielectric constant  $\epsilon$  was estimated using a COSMO-like polarizable continuum model<sup>28-31</sup> in the monopole approximation:

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

where the  $f(\epsilon)$  is the dielectric scaling factor,  $f(\epsilon) = \frac{\epsilon - 1}{\epsilon}$ ,  $\mathbf{Q}$  – the vector of  $n$  atomic charges in the molecular system,  $\mathbf{D}$  is the  $n \times n$  symmetric matrix determined by the shape of the boundary surface between solute and solvent.  $\mathbf{D} = \mathbf{B}^+ \mathbf{A}^{-1} \mathbf{B}$ , where the  $m \times m$  matrix  $\mathbf{A}$  describes electrostatic interaction between  $m$  surface charges and the  $m \times n$   $\mathbf{B}$  matrix describes the interaction of the surface charges with  $n$  atomic charges of the solute.<sup>28,32</sup> The GEPOL93 scheme<sup>33</sup> was used to construct the molecular boundary surface.

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

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

where  $q_X^0$  is the atomic charge on A in the ground state and  $\Delta_X^i$  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  $\Phi_i^*$  can be estimated as:<sup>34</sup>

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

In Eq. (8),  $n^2$  (the refraction index squared) is the optical dielectric constant of the medium and the vector  $\Delta$  describes the change of atomic charges in the molecule by excitation in terms of atomic charges, see

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

### Electron transfer rates

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

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

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:<sup>35</sup>

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

where  $\lambda$  is the reorganization energy and  $\Delta G^0$  is the standard Gibbs energy change of the process. The fragment charge difference (FCD)<sup>36,37</sup> 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<sup>38,39</sup> 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  $\omega_i$ ,  $\hbar\omega_i \gg kT$ , is described quantum mechanically. Because ET occurs normally from the lowest vibrational level of the initial state, the rate  $k$  can be expressed as a sum over all channels connecting the initial state with the vibrational quantum number  $n = 0$  to manifold vibrational levels of the final state,

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

with

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

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

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

As seen, an additional parameter (as compared to the Marcus equation) enters the semi-classical expression - the frequency  $\omega_i$  of a vibrational mode that effectively describes the nuclear intramolecular relaxation following the ET. Typically, in organic systems (including fullerene and nanotube derivatives) the main contribution to the internal reorganization energy is due to stretching of C=C bonds (the corresponding frequencies are found to be in the range of 1400-1800  $\text{cm}^{-1}$ ). Thus, the effective frequency was set to 1600  $\text{cm}^{-1}$ . We have demonstrated that varying the parameter  $\omega_i$  within a reasonable range does not change significantly the computed ET rate (Table S4).

## Reorganization energy

The reorganization energy is usually divided into two parts,  $\lambda = \lambda_i + \lambda_s$ , including the internal and solvent terms. The solvent reorganization energy corresponds to the energy required to move solvent molecules from the position they occupy in the initial state to the location they have in the CT state, but without charge transfer having occurred. The  $\lambda_s$  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  $\lambda_i$  corresponds to the energy of structural changes when donor/acceptor fragments going from initial-state geometries to final-state geometries.

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

$$\lambda_i^1(C_{60}^* \rightarrow C_{60}^+) = \frac{1}{2} \left[ \left( (C_{60}^*)_+ - (C_{60}^*)_* \right) + \left( (C_{60}^+)_* - (C_{60}^+)_+ \right) \right] \quad (13)$$

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

## Complexation, interaction and deformation energies

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

$$E_{int} = E_{Cage \supset C_{xxx}} - (E_{Cage} + E_{C_{xxx}}) \quad (14)$$

Deformation energy for each of studied complexes has been determined using following equation:

$$E_{Strain} = (E_{Cage}^{Complex geom.} - E_{Cage}^{Eq. geom.}) + (E_{C_{xxx}}^{Complex geom.} - E_{C_{xxx}}^{Eq. geom.}) \quad (15)$$

At the same time, complexation energy comprises both interaction ( $\Delta E_{int.}$ ) and deformation ( $E_{def.}$ ) energies. Thus  $\Delta E_{Complex.}$  can be represented as following:

$$E_{Complex} = E_{int} + E_{def} \quad (16)$$

## Charge delocalization index

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

$$IPR = \Delta q^F \left( \sum_i^n \frac{1}{(\Delta q_i^F)^2} \right) \quad (17)$$

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

## Quantum Theory of Atoms in Molecules (QTAIM)

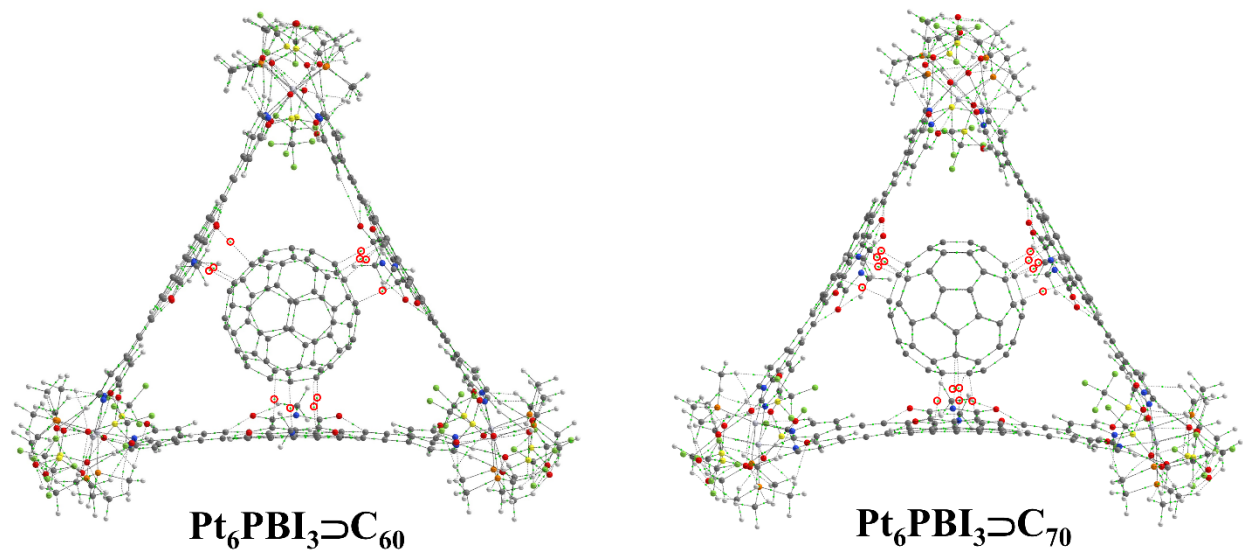
Topological analysis of the electron density distributions was conducted using the “Quantum Theory of Atoms in Molecules” (QTAIM) approach proposed by Bader.<sup>40,41</sup> Electron density properties measured at the bond critical point (BCP) give information about the character of different chemical bonds.<sup>42-44</sup> The AIMALL suite of programs<sup>45</sup> 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

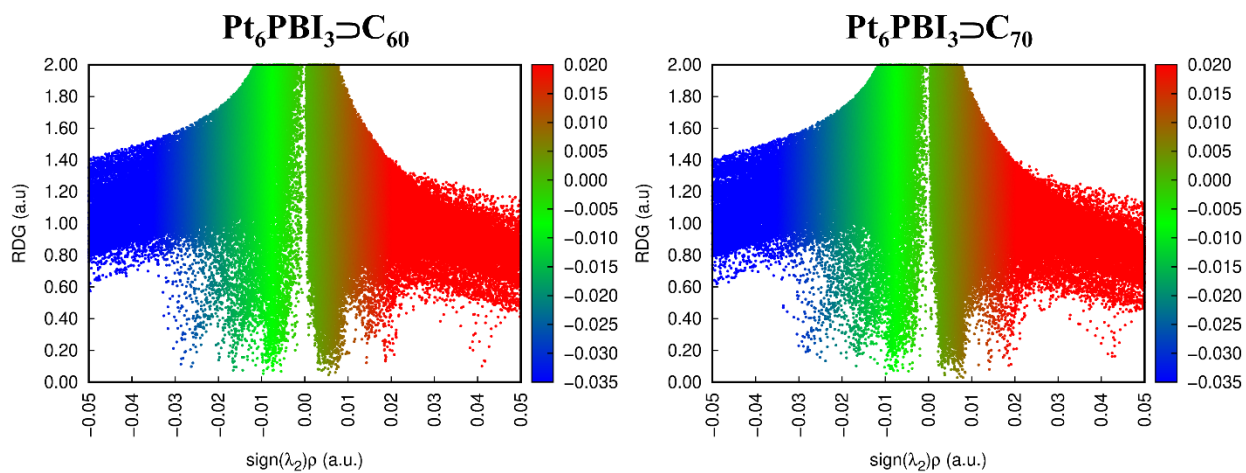
The NCI method<sup>46-48</sup> relies on two scalar fields to map local bonding properties: the electron density ( $\rho$ ) and the reduced-density gradient (RDG,  $s$ ) defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \quad (18)$$

The combination of  $s$  and  $\rho$  allows a rough partition of real space into bonding regions: high- $s$  low- $\rho$  corresponds to non-interacting density tails, low- $s$  high- $\rho$  to covalent bonds, and low- $s$  low- $\rho$  to non-covalent interactions. The NCI analysis was carried out at the BLYP-D3(BJ)/def2-SVP level using Multiwfn program.<sup>49</sup>

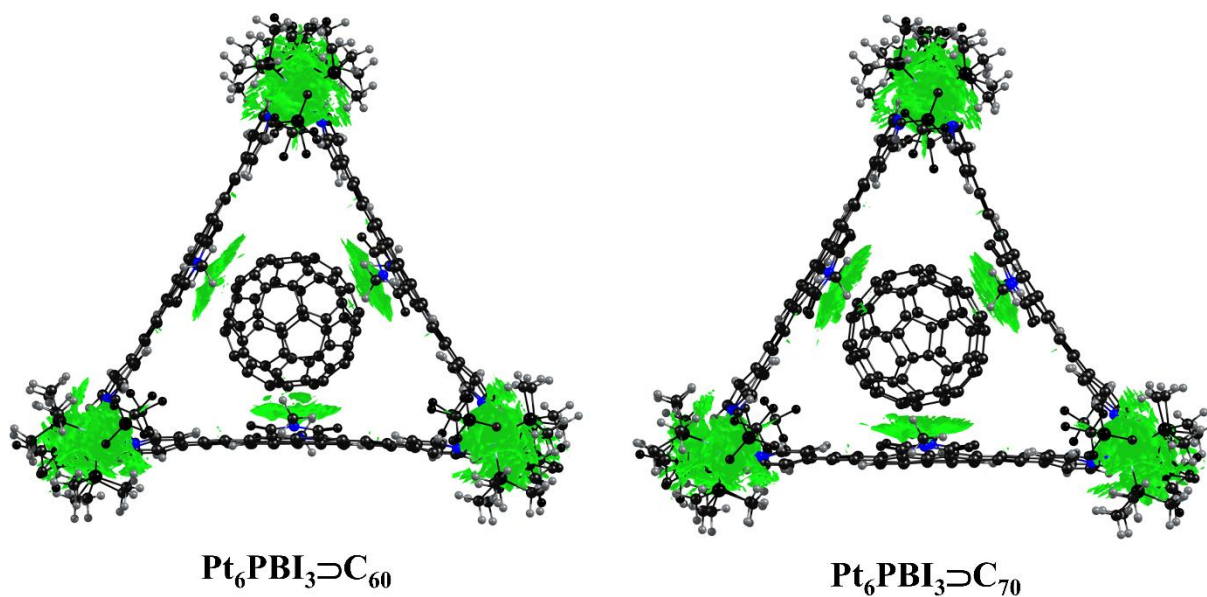


**Figure S1.** QTAIM molecular graph for **Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>60</sub>** and **Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>70</sub>** complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs. BCPs of interest corresponding to C...C contacts are marked by red circles.

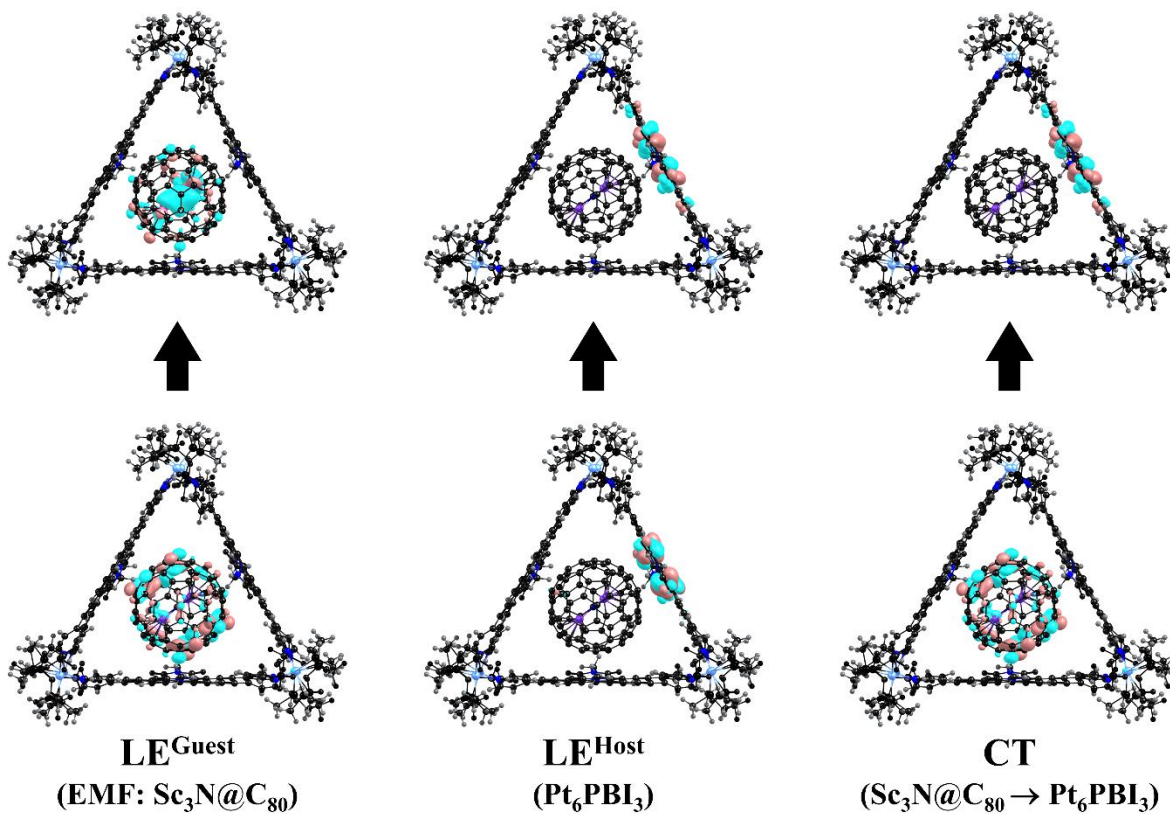


**Figure S2.** Plot of RDG vs.  $\text{sign}(\lambda_2)\rho$  for **Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>60</sub>** and **Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>70</sub>** complexes.

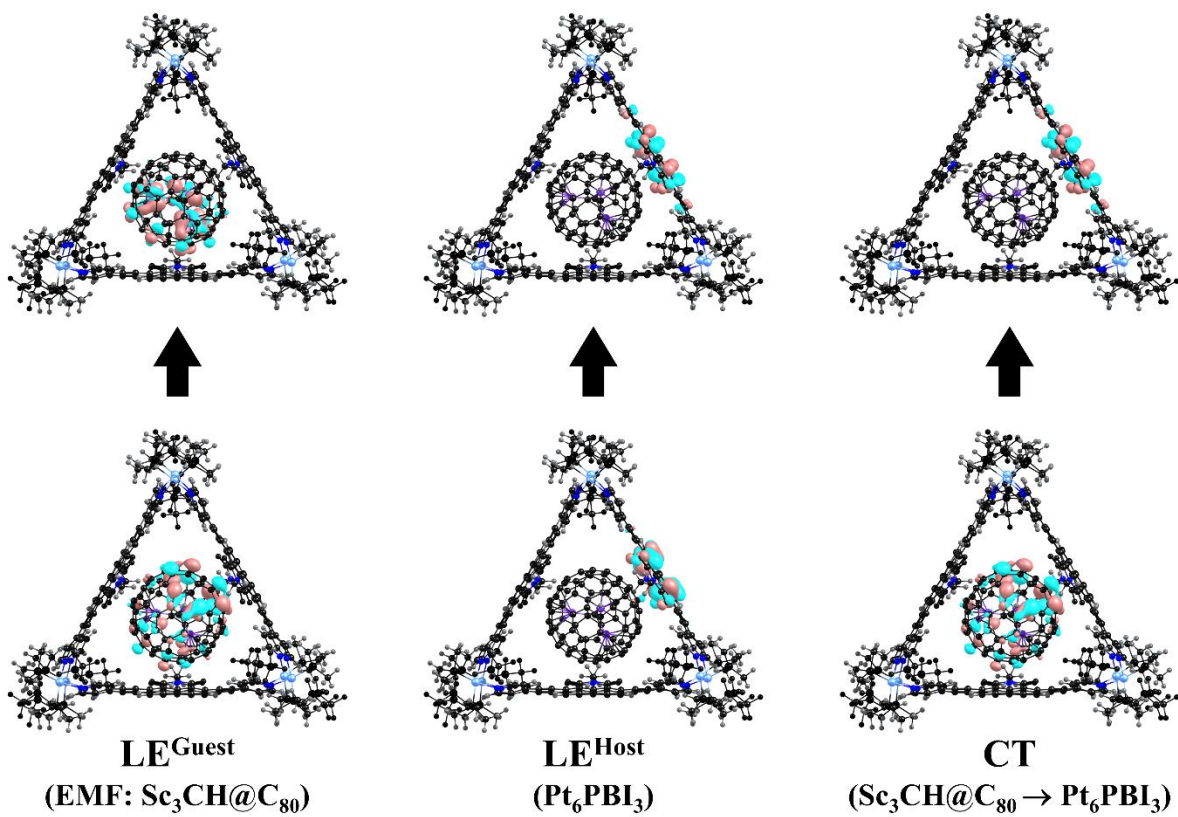




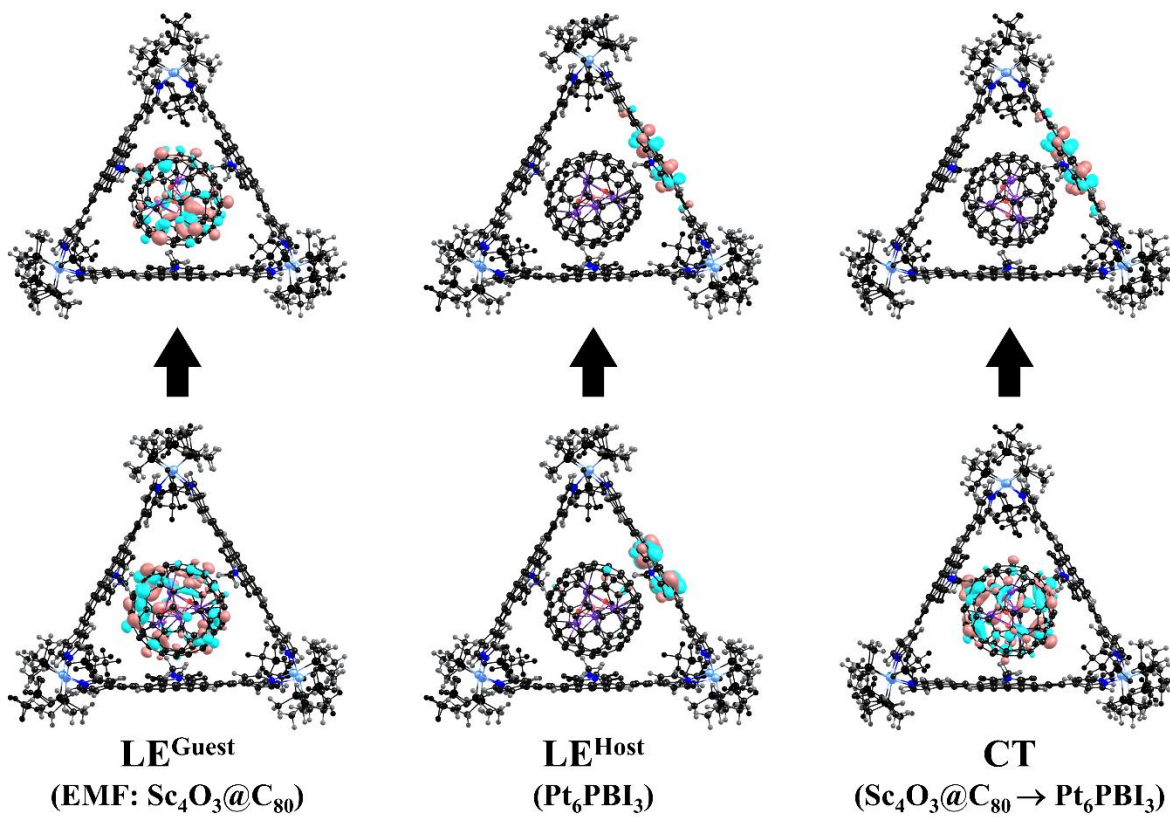
**Figure S3.** NCI isosurfaces for  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$  and  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$  complexes. Isosurfaces were generated for  $\text{RDG} = 0.65 \text{ a.u.}$



**Figure S4.** Frontier molecular orbitals representing  $\text{LE}^{\text{Guest}}$ ,  $\text{LE}^{\text{Host}}$ , and CT states in  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N}@C_{80}$  complex.



**Figure S5.** Frontier molecular orbitals representing LE<sup>Guest</sup>, LE<sup>Host</sup>, and CT states in Pt<sub>6</sub>PBI<sub>3</sub>⊃Sc<sub>3</sub>CH@C<sub>80</sub> complex.



**Figure S6.** Frontier molecular orbitals representing  $\text{LE}^{\text{Guest}}$ ,  $\text{LE}^{\text{Host}}$ , and CT states in  $\text{Pt}_6\text{PBI}_3@C_{80}$  complexes.

**Table S1.** Charge separation (in electrons) between the fragments in electronic ground state for  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$  and  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$  complexes.  $Q_{\text{Host}}$  - charge on  $\text{Pt}_6\text{PBI}_3$  host, and  $Q_{\text{C}_{60}}/Q_{\text{C}_{70}}$  - charge on fullerene moiety. Total charge of the complexes  $Q_{\text{Tot}} = 0$ .

Charge Scheme	$\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$		$\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$	
	$Q_{\text{Host}}$	$Q_{\text{C}_{60}}$	$Q_{\text{Host}}$	$Q_{\text{C}_{70}}$
Mulliken	-0.013	0.013	-0.024	0.024
Lowdin	0.018	-0.018	0.011	-0.011
Hirshfeld	-0.073	0.072	-0.100	0.100
CM5	-0.073	0.072	-0.096	0.096

**Table S2.** Parameters (electron density [ $\rho(r)$ ], its Laplacian [ $\nabla^2\rho(r)$ ], potential energy density [ $V(r)$ ], kinetic energy density [ $G(r)$ ], and total electron energy density [ $H(r)$ ] for selected bond critical points related to non-covalent interactions in  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$  and  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$  complexes computed in the gas phase.

Bond critical points between fragments	Interaction	$\rho(r)$ , au	$\nabla^2\rho(r)$ , au	$V(r)$ , au	$G(r)$ , au	$H(r)$ , au
		<b><math>\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}</math></b>				
$\text{Pt}_6\text{PBI}_3 \cdots \text{C}_{60}$	C...C	5.81E-03	1.55E-02	-2.47E-03	3.17E-03	6.95E-04
		1.15E-02	3.61E-02	-5.61E-03	7.32E-03	1.71E-03
		7.26E-03	2.00E-02	-2.99E-03	3.99E-03	1.00E-03
		9.11E-03	2.70E-02	-3.92E-03	5.33E-03	1.41E-03
		9.48E-03	2.83E-02	-4.23E-03	5.65E-03	1.42E-03
		7.51E-03	2.33E-02	-3.39E-03	4.60E-03	1.21E-03
		7.24E-03	2.13E-02	-3.17E-03	4.25E-03	1.08E-03
		8.35E-03	2.32E-02	-3.54E-03	4.68E-03	1.13E-03
		8.49E-03	2.55E-02	-3.71E-03	5.05E-03	1.33E-03
		6.49E-03	1.68E-02	-2.64E-03	3.42E-03	7.84E-04
		<b><math>\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}</math></b>				
$\text{Pt}_6\text{PBI}_3 \cdots \text{C}_{60}$	C...C	5.75E-03	1.57E-02	-2.40E-03	3.16E-03	7.59E-04
		7.19E-03	2.14E-02	-3.16E-03	4.25E-03	1.09E-03
		8.77E-03	2.61E-02	-3.91E-03	5.22E-03	1.31E-03
		9.86E-03	3.12E-02	-4.57E-03	6.18E-03	1.61E-03
		9.37E-03	2.71E-02	-4.10E-03	5.43E-03	1.34E-03
		8.61E-03	2.66E-02	-3.95E-03	5.30E-03	1.35E-03
		3.93E-03	1.02E-02	-1.69E-03	2.12E-03	4.32E-04
		3.05E-03	8.97E-03	-1.46E-03	1.85E-03	3.91E-04
		9.53E-03	2.87E-02	-4.23E-03	5.70E-03	1.48E-03
		8.43E-03	2.61E-02	-3.86E-03	5.19E-03	1.33E-03
		8.91E-03	2.69E-02	-4.08E-03	5.40E-03	1.33E-03

		6.01E-03	1.67E-02	-2.52E-03	3.34E-03	8.22E-04
		1.02E-02	3.26E-02	-4.66E-03	6.40E-03	1.74E-03
		8.82E-03	2.52E-02	-3.76E-03	5.03E-03	1.27E-03
		5.53E-03	1.43E-02	-2.32E-03	2.95E-03	6.25E-04

**Table S3.** Excitation energies ( $E_x$ , eV) and dipole moments in the ground state ( $\mu_0$  in D), change in dipole moments between the ground state and the excited state of interest ( $\Delta\mu = \mu_i - \mu_0$ , D), as well as solvation energies ( $E_{solv}$ , eV) in acetonitrile calculated for  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$  and  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$  complexes.

	Supramolecular host-guest system	
	$\text{Pt}_6\text{PBI}_3\supset\text{C}_{60}$	$\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$
	Ground state (GS)	
$E_x$	0.000	0.000
$\mu_0$	0.87	2.11
$E_{solv}$	-5.291	-5.280
	$\text{LE}^{\text{Guest}} (\text{C}_{60}/\text{C}_{70})$	
$E_x$	2.499	2.284
$\Delta\mu$	0.41	0.06
$E_{solv}$	-5.292	-5.285
	$\text{LE}^{\text{Host}} ([\text{Pt}_6\text{PBI}_3])$	
$E_x$	2.692	2.678
$\Delta\mu$	0.26	1.11
$E_{solv}$	-5.326	-5.313
	Most absorptive ( $\text{Pt}_6\text{PBI}_3$ )	
$E_x$	2.741	2.739
$\mu_0$	0.42	2.06
$E_{solv}$	-5.342	-5.330
	CT ( $\text{C}_{60}/\text{C}_{70} \rightarrow \text{Pt}_6\text{PBI}_3$ )	
$E_x$	2.678	2.295
$\Delta\mu$	11.84	14.47
$E_{solv}$	-5.595	-5.617

**Table S4.** Computed semi-classical rates ( $k_x$  in  $\text{s}^{-1}$ ) and characteristic times ( $\tau$  in ns) for the CS process in  $\text{Pt}_6\text{PBI}_3\supset\text{C}_{70}$  complex in acetonitrile using different effective Huang-Rhys ( $S_{eff}$ ) factors.

$\hbar\omega_{eff}$	$\Delta G^0$ , eV	$ V $ , eV	$\lambda_s$	$\lambda_i$	$S_{eff}$	$k_x$ , $\text{s}^{-1}$	$\tau$ , ns
	$\text{LE}^{\text{Guest}} \rightarrow \text{CT}$						
1400	0.021	$2.42 \cdot 10^{-3}$	0.461	0.222	1.279	$3.05 \cdot 10^8$	3.28
1600					1.119	$3.54 \cdot 10^8$	2.82
1800					0.995	$3.99 \cdot 10^8$	2.51

**Table S5.** EDA results (in kcal/mol) for  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N@C}_{80}$ ,  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{CH@C}_{80}$ , and  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_4\text{O}_3\text{@C}_{80}$  complexes.

$\text{Pt}_6\text{PBI}_3\supset\text{C}_{xx}$	Energy terms				$\Delta E_{\text{int}}$	$\Delta E_{\text{def}}$	$\Delta E_{\text{complex}}$
	$\Delta E_{\text{Pauli}}$	$\Delta E_{\text{elstat}}$	$\Delta E_{\text{oi}}$	$\Delta E_{\text{disp}}$			
$\text{Sc}_3\text{N@C}_{80}$	115.98	-48.25 (25%)	-24.50 (12%)	-123.62 (63%)	-80.39	14.58	-65.81
$\text{Sc}_3\text{CH@C}_{80}$	115.99	-46.07 (24%)	-25.22 (13%)	-123.67 (63%)	-78.98	15.05	-63.93
$\text{Sc}_4\text{O}_3\text{@C}_{80}$	114.30	-47.47 (24%)	-24.19 (12%)	-123.70 (63%)	-81.06	13.24	-67.82

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

**Table S6.** Excitation energies ( $E_x$ , eV) and dipole moments in the ground state ( $\mu_0$ , D), change in dipole moments between the GS and excited state of interest ( $\Delta\mu = \mu_i - \mu_0$ , D), as well as solvation energies ( $E_{\text{solv}}$ , eV) in acetonitrile calculated for  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N@C}_{80}$ ,  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{CH@C}_{80}$ , and  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_4\text{O}_3\text{@C}_{80}$  complexes.

	Supramolecular system $\text{Pt}_6\text{PBI}_3\supset\text{C}_{xxx}$		
	$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N@C}_{80}$	$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{CH@C}_{80}$	$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_4\text{O}_3\text{@C}_{80}$
	Ground state (GS)		
$E_x$	0.000	0.000	0.000
$\mu_0$	2.77	1.46	1.16
$E_{\text{solv}}$	-4.834	-5.182	-5.313
	$\text{LE}^{\text{Guest}}(\text{C}_{xxx})$		
$E_x$	2.111	2.117	2.229
$\Delta\mu$	2.80	2.60	3.02
$E_{\text{solv}}$	-4.839	-5.220	-5.319
	$\text{LE}^{\text{Host}}([\text{Pt}_6\text{PBI}_3])$		
$E_x$	2.803	2.703	2.719
$\Delta\mu$	1.40	1.03	3.46
$E_{\text{solv}}$	-4.843	-5.226	-5.350
	CT ( $\text{C}_{xxx} \rightarrow \text{Pt}_6\text{PBI}_3$ )		
$E_x$	1.920	1.577	1.807
$\Delta\mu$	10.14	21.06	21.00
$E_{\text{solv}}$	-5.174	-5.757	-5.853

**Table S7.** Charge delocalization over the fragment index (IPR) in the CT state for  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N@C}_{80}$ ,  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{CH@C}_{80}$ , and  $\text{Pt}_6\text{PBI}_3\supset\text{Sc}_4\text{O}_3\text{@C}_{80}$  complexes.

	$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{N@C}_{80}$		$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_3\text{CH@C}_{80}$		$\text{Pt}_6\text{PBI}_3\supset\text{Sc}_4\text{O}_3\text{@C}_{80}$	
	$\text{Sc}_3\text{N@C}_{80}$	$\text{Pt}_6\text{PBI}_3$	$\text{Sc}_3\text{CH@C}_{80}$	$\text{Pt}_6\text{PBI}_3$	$\text{Sc}_4\text{O}_3\text{@C}_{80}$	$\text{Pt}_6\text{PBI}_3$
IPR	30.36	51.92	20.00	27.47	24.82	28.38

## Cartesian coordinates

### Pt<sub>6</sub>PBI<sub>3</sub> metallacage

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

Atom	X	Y	Z
7	10.1791790	3.3858180	5.7966760
6	10.2492890	3.7461950	4.4863670
6	9.0105440	3.5281890	6.4817260
6	9.1381740	4.2590830	3.8108550
1	11.2180920	3.5837510	3.9836370
6	7.8632170	4.0374090	5.8674930
1	9.0127140	3.2324730	7.5453900
6	7.9044640	4.4087370	4.4957100
1	9.2303470	4.5325770	2.7522710
1	6.9331460	4.1463140	6.4394370
6	6.7304710	4.8961290	3.8562810
6	5.6388190	5.2976500	3.4554610
6	4.4283400	5.7360920	2.8492520
6	4.4034050	5.8027340	1.4263600
6	3.2640860	6.0905600	3.5816080
6	3.2698060	6.1965940	0.7080880
1	5.3234050	5.5164790	0.9068310
6	3.2729920	6.0070570	5.0694430
6	2.0917790	6.5188040	2.8806150
6	2.0879130	6.5706290	1.4359020
8	4.2455950	5.6277830	5.7235950
7	2.0894610	6.3865980	5.7348850
6	0.9224960	6.8906530	3.6186730
6	0.9011320	6.9930990	0.7434780
6	0.9000990	6.8238850	5.1088360
6	2.1194060	6.3004050	7.2070910
6	-0.2354520	7.3261760	2.9205390
6	-0.2155840	7.3689490	1.4963660
8	-0.0904080	7.1236300	5.7764750
1	2.3125110	5.2564520	7.5181220
1	2.9416930	6.9267550	7.5998390
1	1.1459340	6.6459740	7.5862930
6	-1.4459160	7.7212920	3.5560870
1	-1.1332880	7.7071030	1.0048040
6	-2.5506610	8.0769110	3.9645270
6	3.2562960	6.2243510	-0.7706900
6	0.8834190	7.0081350	-0.7354260
6	-3.7808260	8.4279530	4.5870600
6	4.3798310	5.8686880	-1.5232820
6	2.0580030	6.6121080	-1.4634910
6	-0.2553530	7.3862630	-1.4537960
6	-4.8282760	9.0705780	3.8762520
6	-3.9962770	8.1351020	5.9618930
6	4.3791830	5.8494220	-2.9481090
1	5.3135310	5.5788930	-1.0309740
6	2.0334570	6.6023620	-2.9089210
1	-1.1667880	7.6980670	-0.9338800

### Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>60</sub>

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

Atom	X	Y	Z
7	10.0932210	3.4149440	5.8745120
6	10.1856060	3.7446590	4.5576070
6	8.8874980	3.4558030	6.5072920
6	9.0582240	4.1112020	3.8176530
1	11.1906550	3.6811970	4.1056830
6	7.7206790	3.8125970	5.8267050
1	8.8828790	3.2038900	7.5820080
6	7.7859290	4.1399520	4.4444070
1	9.1684730	4.3638800	2.7556520
1	6.7568940	3.8338730	6.3509920
6	6.5968070	4.4844510	3.7443520
6	5.4853160	4.7688270	3.3014480
6	4.2636650	5.1584770	2.6886970
6	4.2719350	5.3646640	1.2811940
6	3.0533690	5.3407690	3.4098260
6	3.1282150	5.7455690	0.5715580
1	5.2165160	5.1756230	0.7618530
6	2.9810020	4.9629900	4.8483430
6	1.9008230	5.8502400	2.7331910
6	1.9324660	6.0527460	1.3050130
8	3.9142520	4.4478080	5.4659450
7	1.7527930	5.1901300	5.5019940
6	0.7106750	6.1310060	3.4746110
6	0.7541570	6.5184160	0.6296920
6	0.6136170	5.7965480	4.9234440
6	1.6843240	4.7681080	6.9133000
6	-0.4058070	6.7030930	2.8086280
6	-0.3612130	6.8707570	1.3957360
8	-0.4013920	5.9966800	5.5910820
1	1.8795240	3.6816070	6.9846180
1	2.4620040	5.2909930	7.5004590
1	0.6799190	5.0127050	7.2902120
6	-1.5873720	7.1338640	3.4716750
1	-1.2613450	7.2730260	0.9206470
6	-2.6309230	7.6018850	3.9244110
6	3.1041050	5.7830030	-0.9042860
6	0.7350360	6.5729640	-0.8459940
6	-3.7839340	8.0945440	4.5951760
6	4.2141650	5.4074660	-1.6654920
6	1.8968940	6.1618120	-1.5842590
6	-0.4041970	6.9683690	-1.5523640
6	-4.7914260	8.8303160	3.9174470
6	-3.9564880	7.8605270	5.9870010
6	4.1899960	5.3597870	-3.0891870
1	5.1530890	5.1210860	-1.1815590
6	1.8449430	6.1114660	-3.0266960
1	-1.3028040	7.3017120	-1.0236650

6	-0.3053050	7.3792780	-2.8776630	6	-0.4708490	6.9507460	-2.9752360
6	-6.0266760	9.3685530	4.5290090	6	-5.9225260	9.2588460	4.6155500
1	-4.7061920	9.3376580	2.8190830	1	-4.6946990	9.0585630	2.8486100
6	-5.2235330	8.4520880	6.5508630	6	-5.1151460	8.3141190	6.6230920
1	-3.2040180	7.6580500	6.5524250	1	-3.1903190	7.3138490	6.5510370
6	3.1963400	6.2104220	-3.6468680	6	2.9904690	5.6890520	-3.7742420
6	5.5898230	5.4515710	-3.5822780	6	5.4038720	4.9946610	-3.7356320
6	0.8442490	6.9801140	-3.6106850	6	0.6509700	6.4938190	-3.7171160
6	-1.5314340	7.7717910	-3.4836400	6	-1.6775890	7.4095200	-3.5716550
7	-6.2180380	9.0488570	5.8371400	7	-6.0843980	8.9815490	5.9376320
1	-6.8529720	9.9047890	4.0368850	1	-6.7267850	9.8486780	4.1460180
1	-5.4448500	8.2524320	7.6138160	1	-5.3070040	8.1563910	7.6986640
6	3.1838780	6.1716760	-5.1379510	6	2.9452100	5.5945180	-5.2619520
6	6.6935080	5.0846060	-3.9837640	6	6.5284670	4.7057410	-4.1422900
6	0.7989680	6.9534510	-5.1000190	6	0.5751390	6.4196150	-5.2033500
6	-2.6407900	8.1205190	-3.8853590	6	-2.7532620	7.8575990	-3.9658380
8	4.1592260	5.8251010	-5.8052360	8	3.9010270	5.2081430	-5.9354610
7	1.9764550	6.5544320	-5.7651260	7	1.7293290	5.9697830	-5.8771750
6	7.9021560	4.6444950	-4.5921430	6	7.7743550	4.3706500	-4.7413420
8	-0.1994510	7.2543970	-5.7560720	8	-0.4295350	6.7208250	-5.8496110
6	-3.8610510	8.4713970	-4.5279220	6	-3.9360950	8.3281750	-4.6005720
6	1.9116670	6.5344970	-7.2385980	6	1.6314700	5.8933140	-7.3469190
6	9.1186530	4.5490530	-3.8664510	6	8.9840400	4.3682680	-3.9979400
6	7.9223530	4.2793280	-5.9661550	6	7.8446240	4.0272270	-6.1190710
6	-4.9685600	9.0032120	-3.8171790	6	-5.0020780	8.9211460	-3.8749330
6	-4.0015690	8.2887050	-5.9312670	6	-4.0797680	8.2084800	-6.0102850
1	1.1236530	5.8322730	-7.5696600	1	0.8186070	5.1995080	-7.6323690
1	1.6461790	7.5404090	-7.6135000	1	1.3833390	6.8901320	-7.7564940
1	2.8966760	6.2217010	-7.6165000	1	2.5998270	5.5405100	-7.7325470
6	10.2735500	4.0898040	-4.5053190	6	10.1807530	4.0072220	-4.6218730
1	9.1623400	4.8312800	-2.8070270	1	8.9883880	4.6418020	-2.9353840
6	9.1110390	3.8227490	-6.5419470	6	9.0742790	3.6711710	-6.6797190
1	7.0081430	4.3550520	-6.5682580	1	6.9365750	4.0352410	-6.7350310
6	-6.1479500	9.3094190	-4.5009610	6	-6.1541770	9.3318690	-4.5499120
1	-4.9085020	9.1786760	-2.7357030	1	-4.9342640	9.0543580	-2.7879080
6	-5.2129280	8.6079330	-6.5514940	6	-5.2619270	8.6350680	-6.6215270
1	-3.1632130	7.8942300	-6.5192420	1	-3.2701890	7.7714730	-6.6084340
7	10.2595160	3.7278190	-5.8170970	7	10.2141390	3.6532900	-5.9355620
1	9.1928820	3.5487000	-7.6070020	1	9.1920280	3.4057450	-7.7440620
7	-6.2633690	9.1047390	-5.8408460	7	-6.2806500	9.1736740	-5.8952490
1	-7.0243710	9.7586820	-4.0042280	1	-7.0058980	9.8128590	-4.0390330
1	-5.3772040	8.4832840	-7.6361010	1	-5.4330790	8.5568700	-7.7093450
78	-8.2210380	9.1824000	-6.7535720	78	-8.2555170	9.2716230	-6.7719530
78	-8.2166880	9.0925060	6.6411520	78	-8.0787250	9.0540450	6.7639600
7	10.7863370	0.6444080	5.8122950	7	10.7061590	0.7139740	5.9332010
6	9.7924590	0.0391390	6.5200570	6	9.6551980	0.1756110	6.6117330
6	10.9360950	0.3855710	4.4857750	6	10.8755450	0.4508700	4.6093160
6	8.8953390	-0.8411110	5.9086770	6	8.7095890	-0.6275790	5.9684530
1	9.7529100	0.2784320	7.5968420	1	9.6050660	0.4119180	7.6888910
6	10.0692830	-0.4764010	3.8099800	6	9.9633810	-0.3363560	3.9031900
1	11.7869350	0.8676600	3.9877860	1	11.7804100	0.8740220	4.1454640
6	9.0106650	-1.1050780	4.5159180	6	8.8393990	-0.8834490	4.5756570
1	8.1023590	-1.3217790	6.4952950	1	7.8663230	-1.0516380	6.5280440



1	10.2154740	-0.6596570	2.7382020	1	10.1224770	-0.5235800	2.8338730
6	8.0829970	-1.9692200	3.8702520	6	7.8682840	-1.6743370	3.9020130
6	7.2207180	-2.7335490	3.4392150	6	6.9724500	-2.3909500	3.4583470
6	6.2713880	-3.5692640	2.7869380	6	6.0339960	-3.2366390	2.8067560
6	6.2711920	-3.5562410	1.3621740	6	6.1055910	-3.3098600	1.3865710
6	5.3399460	-4.3928050	3.4731040	6	5.0531290	-3.9999990	3.4923900
6	5.3853900	-4.3237760	0.5993350	6	5.2558950	-4.1211110	0.6302220
1	7.0033350	-2.9018250	0.8786070	1	6.8499340	-2.6722010	0.9002390
6	5.3175690	-4.3974170	4.9627450	6	4.8836420	-3.8329380	4.9620950
6	4.4310720	-5.2076530	2.7252490	6	4.2123710	-4.8916630	2.7562550
6	4.4509630	-5.1784650	1.2798530	6	4.3154520	-4.9623300	1.3167190
8	6.0669550	-3.7081040	5.6561500	8	5.5503290	-3.0488330	5.6391870
7	4.3755860	-5.2442270	5.5818420	7	3.8850110	-4.6134480	5.5786330
6	3.5011390	-6.0484300	3.4171990	6	3.2420360	-5.6822120	3.4494020
6	3.5355560	-6.0033800	0.5396640	6	3.4254720	-5.8184340	0.5826560
6	3.4514790	-6.0749910	4.9085370	6	3.0580370	-5.5540950	4.9236670
6	4.3693410	-5.2348030	7.0568000	6	3.7143270	-4.4152200	7.0299300
6	2.6095530	-6.8656770	2.6708900	6	2.4170270	-6.5748430	2.7145540
6	2.6530530	-6.8256630	1.2472010	6	2.5234420	-6.6132590	1.2945260
8	2.6561060	-6.7722980	5.5395290	8	2.2256210	-6.2067770	5.5544860
1	5.3685220	-5.5198820	7.4353050	1	4.6596980	-4.6490030	7.5541830
1	4.1479000	-4.2151840	7.4242960	1	3.4678170	-3.3564200	7.2334510
1	3.6025650	-5.9469980	7.3967910	1	2.9051530	-5.0790500	7.3695170
6	1.6473690	-7.7314770	3.2618430	6	1.4677830	-7.4469930	3.3134110
1	1.9451630	-7.4722060	0.7188150	1	1.8390310	-7.2883850	0.7715660
6	0.7690770	-8.4992640	3.6527920	6	0.6432240	-8.2670260	3.7145570
6	5.3829680	-4.2688790	-0.8788040	6	5.2552730	-4.0784620	-0.8455880
6	3.5396930	-5.9555960	-0.9388640	6	3.4300070	-5.7810160	-0.8942290
6	-0.2154350	-9.3054500	4.2898040	6	-0.2752390	-9.1355590	4.3665520
6	6.2605310	-3.4412200	-1.5860430	6	6.1101660	-3.2310630	-1.5553750
6	4.4524250	-5.0770810	-1.6184370	6	4.3174920	-4.8822490	-1.5780360
6	2.6669500	-6.7371040	-1.7028050	6	2.5491790	-6.5587900	-1.6514590
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6	-6.8234090	7.3878830	11.7479930	6	-6.5958840	7.3131800	11.8299830
9	-5.6988750	6.6400300	11.7450580	9	-5.4760330	6.5596530	11.7822810
9	-7.7898090	6.7132670	12.4059280	9	-7.5487490	6.6296860	12.4983820
9	-6.5739010	8.5403120	12.4094760	9	-6.3227190	8.4499310	12.5085540
16	-9.5093520	11.0466440	3.6597090	16	-9.4312820	10.9734480	3.7686670
8	-10.6535370	11.6267280	4.4411700	8	-10.5391210	11.6111030	4.5568180
8	-9.6466460	9.5928340	3.2948360	8	-9.6300750	9.5186370	3.4369700
8	-8.1403750	11.4426970	4.1677600	8	-8.0397920	11.3296810	4.2469690
6	-9.5847860	11.9153980	1.9693720	6	-9.4999200	11.8086880	2.0604270
9	-10.7195240	11.5831750	1.3206220	9	-10.6483790	11.4932210	1.4280760
9	-8.5247490	11.5349510	1.2210730	9	-8.4574010	11.3830730	1.3113280
9	-9.5464790	13.2551290	2.1226060	9	-9.4237730	13.1495770	2.1843880
16	-7.1275890	8.1861520	-10.2358180	16	-7.2179960	8.3603310	-10.2774140
8	-7.9495630	7.1607100	-9.4869710	8	-8.0145380	7.3076450	-9.5386790
8	-5.9977740	8.7935570	-9.4397640	8	-6.0856480	8.9680250	-9.4847650
8	-7.9296250	9.1523150	-11.0524900	8	-8.0453530	9.3311020	-11.0626070
6	-6.2078930	7.1175040	-11.5114800	6	-6.3002550	7.3317740	-11.5867480
9	-5.4728150	6.1760630	-10.8711020	9	-5.5369390	6.3937800	-10.9748800
9	-5.3785790	7.8746660	-12.2590110	9	-5.4980180	8.1176390	-12.3341290
9	-7.0828350	6.4954660	-12.3288140	9	-7.1766020	6.7071920	-12.4005300
16	-4.6602190	-13.7640160	-3.8293010	16	-4.6687120	-13.6494930	-3.8041160
8	-5.7316130	-12.7897600	-4.2679970	8	-5.6758790	-12.6090330	-4.2454500
8	-3.3236410	-13.1363470	-3.5369200	8	-3.2849970	-13.1148010	-3.5471300
8	-4.6127950	-15.0357650	-4.6284940	8	-4.7270780	-14.9358700	-4.5777030
6	-5.2675200	-14.2916380	-2.1056570	6	-5.2817530	-14.0984020	-2.0597860
9	-5.3691720	-13.1996960	-1.3168170	9	-5.3008830	-12.9849380	-1.2942870
9	-4.3980330	-15.1593070	-1.5484590	9	-4.4606030	-15.0072480	-1.4953330
9	-6.4777760	-14.8806390	-2.1911190	9	-6.5284260	-14.6095500	-2.1140370
16	-4.6548840	-13.8148280	3.4424310	16	-4.7028690	-13.6578210	3.4941020
8	-3.2161100	-13.6763130	3.8905210	8	-3.2638260	-13.5628700	3.9541000
8	-5.3470620	-12.5119110	3.1431150	8	-5.3565350	-12.3348830	3.1957800
8	-5.4601210	-14.8033750	4.2375890	8	-5.5412980	-14.6261570	4.2792540



6	-4.4712330	-14.6048200	1.7218400
9	-3.7008580	-13.8099290	0.9471910
9	-5.6797590	-14.7498910	1.1407510
9	-3.8857020	-15.8160610	1.8186940

6	-4.5283090	-14.4436370	1.7702370
9	-3.7236440	-13.6704630	1.0084880
9	-5.7350800	-14.5432020	1.1759400
9	-3.9856140	-15.6746370	1.8648970
6	1.0562820	1.3525560	3.8679870
6	2.2228770	1.6875160	3.0443030
6	0.8088860	0.0105360	4.2242320
6	3.1011380	0.6726840	2.6120380
6	3.6216530	0.6882950	1.2393390
6	1.8298290	2.7538520	2.1206720
6	2.3287210	2.7669850	0.8033970
6	3.2450340	1.7185410	0.3516190
6	-1.6256340	0.3154430	3.7877650
6	-1.3703380	1.7115370	3.4172560
6	-0.5586210	-0.5188400	4.1842410
6	-0.0547910	2.2180300	3.4553140
6	0.4240210	3.0824360	2.3736320
6	-2.2558230	2.0547600	2.2992900
6	-1.7945970	2.8922530	1.2606310
6	-0.4268770	3.4129650	1.2999010
6	-1.4987030	-2.4067390	2.8549420
6	-2.6009490	-1.5359830	2.4385420
6	-0.4945180	-1.9050110	3.7098580
6	-2.6660190	-0.2042130	2.8970860
6	-3.0549050	0.8695000	1.9778310
6	-2.9118870	-1.8420470	1.0401280
6	-3.2785410	-0.8100650	0.1577410
6	-3.3567680	0.5706860	0.6331280
6	1.2566660	-3.0419320	2.3549090
6	0.2131420	-3.5675500	1.4673260
6	0.9127510	-2.2308260	3.4562150
6	-1.1382830	-3.2548210	1.7120310
6	-2.0190600	-2.9082420	0.5900160
6	0.7309440	-3.5435430	0.0939430
6	-0.1173320	-3.2213790	-0.9854240
6	-1.5240050	-2.8957640	-0.7321530
6	2.8411600	-0.7213570	2.9832190
6	3.1971700	-1.5631540	1.8389940
6	1.7190530	-1.0474700	3.7754210
6	2.4109400	-2.6880680	1.5286360
6	2.0868130	-2.9973740	0.1361430
6	3.6826700	-0.6952040	0.7612900
6	3.3725290	-0.9945340	-0.5827470
6	2.5595800	-2.1727720	-0.9003750
6	-0.7437200	-1.4832280	-2.4731960
6	0.3651370	-2.3490400	-2.0621230
6	1.6794610	-1.8366990	-2.0219900
6	-0.4960490	-0.1405170	-2.8288010
6	-2.5288090	0.5973640	-1.5909100
6	-2.7789920	-0.7983720	-1.2166520
6	-1.9114640	-1.8212560	-1.6529970
6	-1.4052090	0.9193480	-2.3800350
6	-0.9501020	2.9159340	-0.9605550

6	-2.1181180	2.5824870	-0.1379190
6	-2.8898990	1.4437400	-0.4466260
6	-0.6007160	2.1028690	-2.0601990
6	1.8107640	2.2723110	-1.4578870
6	1.4438650	3.1077350	-0.3131760
6	0.0942550	3.4256620	-0.0702600
6	0.8056880	1.7755540	-2.3138840
6	1.9385640	-0.4422990	-2.3929010
6	2.9856110	0.0771690	-1.5048200
6	2.9233150	1.4090040	-1.0461200
6	0.8704980	0.3893230	-2.7887370

**Pt<sub>6</sub>PBI<sub>3</sub>⊃C<sub>70</sub>**

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

Atom	X	Y	Z
7	10.0862130	3.4346680	5.8034580
6	10.1472020	3.7591240	4.4835640
6	8.9098390	3.5441440	6.4814060
6	9.0181830	4.2036390	3.7902460
1	11.1267340	3.6284310	3.9921610
6	7.7428220	3.9793290	5.8482290
1	8.9273010	3.2874480	7.5548580
6	7.7765960	4.3167280	4.4674410
1	9.1027020	4.4540840	2.7253510
1	6.8038140	4.0578370	6.4105500
6	6.5899440	4.7497040	3.8142860
6	5.4876930	5.1099980	3.4045680
6	4.2789540	5.5518580	2.8022670
6	4.2916430	5.7556650	1.3938070
6	3.0714840	5.7514220	3.5224340
6	3.1487340	6.1250860	0.6795220
1	5.2326330	5.5453960	0.8763140
6	2.9986880	5.3812720	4.9624240
6	1.9168070	6.2453850	2.8386980
6	1.9482910	6.4284730	1.4076430
8	3.9356640	4.8779320	5.5846750
7	1.7669750	5.5983950	5.6107450
6	0.7167160	6.5034340	3.5712220
6	0.7556030	6.8386880	0.7209390
6	0.6191350	6.1775640	5.0221320
6	1.6969820	5.1767830	7.0218530
6	-0.4111720	7.0391860	2.8934180
6	-0.3674290	7.1838960	1.4777190
8	-0.4034340	6.3606280	5.6832980
1	1.8930930	4.0902380	7.0935330
1	2.4737160	5.7001560	7.6095060
1	0.6916020	5.4196530	7.3972020
6	-1.6085480	7.4395140	3.5461400
1	-1.2797510	7.5452660	0.9927800

**Pt<sub>6</sub>PBI<sub>3</sub>⊃Sc<sub>3</sub>N@C<sub>80</sub>**

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

Atom	X	Y	Z
7	9.9323717	-3.186148	5.753901
6	9.7705720	-3.122174	4.429838
6	9.3967821	-2.234133	6.517103
6	9.0935885	-2.088296	3.818812
1	10.1988400	-3.912349	3.830957
6	8.7000146	-1.164344	5.992161
1	9.4907690	-2.369590	7.584145
6	8.5478676	-1.070535	4.605702
1	8.9873103	-2.070311	2.746124
1	8.2708388	-0.410797	6.632973
6	7.8547216	-0.001939	4.011830
6	7.2384044	0.931409	3.553167
6	6.5896097	1.964048	2.854385
6	6.7235661	1.980383	1.459535
6	5.8251814	2.938795	3.494339
6	6.1054906	2.936150	0.675382
1	7.3066680	1.188968	1.018738
6	5.6609075	2.888034	4.953156
6	5.2061405	3.944575	2.723760
6	5.3335035	3.946962	1.307547
8	6.1794032	2.038356	5.650452
7	4.8718754	3.878487	5.510053
6	4.4421688	4.935985	3.371546
6	4.6484272	4.931548	0.548810
6	4.2693467	4.919716	4.829388
6	4.6622838	3.859501	6.947587
6	3.8329329	5.934479	2.610675
6	3.9415647	5.916023	1.214750
8	3.6385273	5.759314	5.442183
1	5.1587115	2.980520	7.350066
1	5.0747368	4.765331	7.391775
1	3.5936530	3.824771	7.157191
6	3.0755260	6.958898	3.205164
1	3.4276151	6.696154	0.678200

6	-2.6730090	7.8690150	3.9880470	6	2.4017288	7.883801	3.595529
6	3.1107850	6.0848100	-0.7955510	6	6.1547392	2.877573	-0.779176
6	0.7176630	6.7971100	-0.7544400	6	4.6362924	4.826900	-0.904230
6	-3.8537160	8.3124770	4.6441830	6	1.6346490	8.882270	4.220966
6	4.2185230	5.6831370	-1.5462380	6	6.9138431	1.936688	-1.451095
6	1.8768660	6.3554740	-1.4782630	6	5.3561425	3.776315	-1.533578
6	-0.4423690	7.1071770	-1.4698780	6	3.8978802	5.691849	-1.689851
6	-4.8900120	8.9887810	3.9486060	6	0.7387566	9.685890	3.511510
6	-4.0279710	8.0848180	6.0369670	6	1.7305876	9.071847	5.603763
6	4.1529310	5.4571830	-2.9505630	6	6.8195577	1.764045	-2.837822
1	5.1808250	5.4875720	-1.0634220	1	7.5873397	1.282030	-0.923001
6	1.7891080	6.1444210	-2.9038640	6	5.2430153	3.595812	-2.937914
1	-1.3357810	7.4747830	-0.9553410	1	3.3589136	6.518558	-1.258080
6	-0.5379870	6.9486360	-2.8817920	6	3.7861708	5.522510	-3.076152
6	-6.0488690	9.3651990	4.6305690	6	-0.0243625	10.606483	4.200842
1	-4.7943100	9.2101110	2.8782380	1	0.6296176	9.585788	2.443543
6	-5.2146420	8.4855570	6.6566720	6	0.9396302	10.029753	6.203848
1	-3.2407290	7.5833370	6.6138300	1	2.4047311	8.459487	6.181244
6	2.9209910	5.6541060	-3.6289810	6	5.9405603	2.553976	-3.581664
6	5.3543130	5.0422690	-3.5886730	6	7.6120340	0.772020	-3.442079
6	0.5692250	6.4193230	-3.5971880	6	4.4291840	4.456342	-3.702596
6	-1.7539790	7.3529030	-3.4977300	6	3.0166642	6.468011	-3.776624
7	-6.2097780	9.0946200	5.9541310	7	0.0732676	10.776143	5.518914
1	-6.8773820	9.9056850	4.1446890	1	-0.7366431	11.227852	3.676546
1	-5.4109350	8.3307460	7.7317160	1	0.9568197	10.177506	7.274448
6	2.8228640	5.3378340	-5.0825190	6	5.7500254	2.287924	-5.014055
6	6.4687780	4.7283750	-4.0042430	6	8.3645353	-0.081307	-3.852070
6	0.4481130	6.1517120	-5.0573680	6	4.2599403	4.249134	-5.145150
6	-2.8258540	7.7866840	-3.9172300	6	2.3599032	7.376816	-4.228308
8	3.7575160	4.8610050	-5.7274320	8	6.2709051	1.352737	-5.590440
7	1.5791950	5.6049660	-5.6985140	7	4.9210194	3.164188	-5.691689
6	7.6865220	4.3531590	-4.6360090	6	9.1028789	-1.097896	-4.483843
8	-0.5766370	6.3659750	-5.7067390	8	3.5775957	4.966424	-5.850170
6	-4.0023420	8.2398010	-4.5754570	6	1.6001949	8.426558	-4.773112
6	1.4281360	5.3099040	-7.1354850	6	4.7140246	2.949612	-7.113823
6	8.9229900	4.3420020	-3.9389160	6	10.2602073	-1.647994	-3.927671
6	7.6966220	3.9792290	-6.0076140	6	8.6515014	-1.618372	-5.701137
6	-5.0738640	8.8538230	-3.8759590	6	0.9524043	9.333825	-3.929023
6	-4.1319860	8.0848540	-5.9830230	6	1.4577417	8.603343	-6.152390
1	0.5806040	4.6156590	-7.2857440	1	3.6671150	2.710531	-7.300791
1	1.2034030	6.2411900	-7.6887180	1	4.9655160	3.859818	-7.657072
1	2.3699050	4.8647050	-7.4902040	1	5.3505063	2.127226	-7.429552
6	10.0885200	3.9484220	-4.6013130	6	10.8858172	-2.689486	-4.583413
1	8.9730710	4.6347790	-2.8826520	1	10.6561485	-1.276325	-2.995665
6	8.8982020	3.5957490	-6.6090860	6	9.3329341	-2.670787	-6.275097
1	6.7641650	3.9883980	-6.5859920	1	7.7724457	-1.202883	-6.166732
6	-6.2184930	9.2486720	-4.5726120	6	0.2145292	10.357200	-4.484279
1	-5.0172120	9.0133690	-2.7918560	1	1.0242693	9.240621	-2.857404

6	-5.3055360	8.5012760	-6.6171170	6	0.7062097	9.665114	-6.616591
1	-3.3191780	7.6275230	-6.5612300	1	1.9287561	7.914601	-6.835507
7	10.0662160	3.5743570	-5.9096580	7	10.4266604	-3.204344	-5.722597
1	8.9699360	3.3140850	-7.6731670	1	8.9908868	-3.092890	-7.208799
7	-6.3314120	9.0581110	-5.9150110	7	0.1024974	10.528346	-5.800821
1	-7.0774600	9.7371640	-4.0813450	1	-0.2975764	11.064157	-3.848049
1	-5.4654100	8.3966340	-7.7043130	1	0.5401917	9.814869	-7.674528
78	-8.3033950	9.1005510	-6.8069880	78	-1.1932683	12.076675	-6.357343
78	-8.2139500	9.0688200	6.7551880	78	-1.3959707	12.014498	6.345530
7	10.6864610	0.7138730	5.9013830	7	9.1706225	-5.787288	5.525413
6	9.6532430	0.1875370	6.6157930	6	8.0120963	-5.511355	6.129006
6	10.8433710	0.3967690	4.5880670	6	9.1478902	-6.293015	4.292930
6	8.7167960	-0.6629110	6.0217240	6	6.7919633	-5.703712	5.514198
1	9.6166320	0.4637240	7.6835460	1	8.0626400	-5.120084	7.135684
6	9.9426960	-0.4448290	3.9314900	6	7.9756307	-6.512304	3.596547
1	11.7322880	0.8143670	4.0923550	1	10.1075424	-6.482352	3.832817
6	8.8400820	-0.9866890	4.6425400	6	6.7588100	-6.195739	4.205030
1	7.8872570	-1.0744730	6.6104620	1	5.8687559	-5.464075	6.017086
1	10.0953560	-0.6793970	2.8706430	1	8.0058083	-6.909405	2.594028
6	7.8844420	-1.8319250	4.0145850	6	5.5238149	-6.323837	3.544661
6	7.0020720	-2.5759080	3.5893250	6	4.3915792	-6.350635	3.120929
6	6.0719380	-3.4368920	2.9459550	6	3.1336758	-6.442371	2.499708
6	6.2017260	-3.5886790	1.5366250	6	3.0885798	-6.615276	1.112191
6	5.0159790	-4.1040750	3.6204910	6	1.9459621	-6.336133	3.228145
6	5.3104530	-4.3541100	0.7799050	6	1.8888868	-6.682257	0.424425
1	7.0008340	-3.0184240	1.0531860	1	4.0321949	-6.657332	0.593778
6	4.7502040	-3.8077930	5.0542460	6	1.9925345	-5.990580	4.654959
6	4.1724580	-5.0025160	2.8950790	6	0.7163510	-6.540761	2.570112
6	4.3110800	-5.1259960	1.4644860	6	0.6780793	-6.735397	1.162877
8	5.3796240	-2.9706520	5.7033340	8	3.0283401	-5.767206	5.251314
7	3.6911520	-4.5120840	5.6606820	7	0.7719609	-5.908333	5.299584
6	3.1573440	-5.7341040	3.5861290	6	-0.4789605	-6.517407	3.316159
6	3.4008460	-5.9634260	0.7352810	6	-0.5734328	-6.915591	0.516769
6	2.9009560	-5.5051640	5.0362860	6	-0.4638272	-6.188681	4.746350
6	3.4105910	-4.1712050	7.0673120	6	0.7615606	-5.521189	6.699858
6	2.3526680	-6.6580680	2.8665050	6	-1.6895614	-6.787982	2.675050
6	2.4866430	-6.7411150	1.4514250	6	-1.7183067	-6.994297	1.291298
8	2.0299190	-6.1056420	5.6662240	8	-1.4629425	-6.139493	5.437004
1	4.3093000	-4.3530650	7.6855560	1	1.7897623	-5.372282	7.018354
1	3.1591790	-3.0965890	7.1439550	1	0.1900371	-4.600609	6.817123
1	2.5709780	-4.7966240	7.4060550	1	0.2879757	-6.303418	7.292410
6	1.3954660	-7.5157700	3.4740320	6	-2.9046826	-6.843735	3.379267
1	1.8052530	-7.4231490	0.9331730	1	-2.6832008	-7.171703	0.846148
6	0.5779710	-8.3441120	3.8724690	6	-4.0012273	-6.941432	3.878391
6	5.2893840	-4.2875380	-0.6944410	6	1.8316613	-6.660152	-1.029762
6	3.3968080	-5.9168540	-0.7402970	6	-0.6231888	-6.963904	-0.938460
6	-0.3435950	-9.2403010	4.4803630	6	-5.2190759	-7.034040	4.573973
6	6.1457350	-3.4397970	-1.4018280	6	2.9634793	-6.455443	-1.795333

6	4.2921940	-5.0230440	-1.4205080	6	0.5740666	-6.776275	-1.679644
6	2.4939680	-6.6679330	-1.4983600	6	-1.8136144	-7.114377	-1.624880
6	-1.0454010	-10.2205270	3.7303270	6	-6.4144320	-7.340398	3.918372
6	-0.5907890	-9.1735990	5.8791100	6	-5.2688352	-6.815567	5.954522
6	6.0253590	-3.2237510	-2.8039070	6	2.9089541	-6.366326	-3.192542
1	6.9249130	-2.8722830	-0.8839560	1	3.9330069	-6.343662	-1.339109
6	4.1618820	-4.8325890	-2.8456110	6	0.5105021	-6.675760	-3.096389
1	1.8205860	-7.3843900	-1.0175250	1	-2.7413622	-7.281813	-1.103263
6	2.3829280	-6.5340330	-2.9116430	6	-1.8810256	-7.033904	-3.021831
6	-1.9753020	-11.0447380	4.3678090	6	-7.5821008	-7.417003	4.649735
1	-0.8730230	-10.3297630	2.6522550	1	-6.4299519	-7.511758	2.853746
6	-1.5357350	-10.0283620	6.4529440	6	-6.4818909	-6.920309	6.604619
1	-0.0540420	-8.4434650	6.4977940	1	-4.3662777	-6.566356	6.489433
6	5.0047020	-3.8978850	-3.5263730	6	1.6836193	-6.465095	-3.849703
6	6.9603950	-2.3345040	-3.4011910	6	4.1247617	-6.186266	-3.875059
6	3.1862240	-5.5738460	-3.5828700	6	-0.7260700	-6.783111	-3.764522
6	1.4633550	-7.3920570	-3.5744110	6	-3.1342716	-7.194645	-3.639143
7	-2.2272180	-10.9282800	5.6998410	7	-7.6148296	-7.220779	5.968146
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6	3.0010900	-5.3442750	-5.0426210	6	-0.8165196	-6.631340	-5.223450
6	0.6755470	-8.2163860	-4.0356700	6	-4.2559626	-7.371604	-4.055286
8	5.4847440	-2.7752620	-5.5868160	8	2.6146053	-6.189907	-6.008329
7	3.8205010	-4.3640750	-5.6401370	7	0.3786405	-6.433209	-5.890994
6	8.8076870	-0.7551720	-4.4474530	6	6.5263618	-5.907765	-4.869177
8	2.1726720	-5.9460110	-5.7275820	8	-1.8687093	-6.672133	-5.831018
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6	3.5963020	-4.1237590	-7.0777870	6	0.3409882	-6.296722	-7.337235
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9	14.0199480	1.3289540	1.2612590	9	13.5016596	-4.168941	1.638368
9	16.0065900	1.4025880	2.1912090	9	14.5684326	-5.725364	2.689868
9	15.1153370	3.2309010	1.3673640	9	15.0979073	-3.657020	2.995673
16	-7.3306330	7.8801010	10.1049840	16	-1.9100202	10.897802	9.161977
8	-8.6244480	8.6154660	10.3121250	8	-2.2212080	12.311159	9.168283
8	-6.2043360	8.6921650	9.5088510	8	-0.6327360	10.556092	8.568753
8	-7.4817580	6.4973200	9.5250010	8	-3.0020290	10.026885	8.822475
6	-6.7212400	7.5617550	11.8770650	6	-1.5878259	10.566426	10.990038
9	-5.5625010	6.8680650	11.8600410	9	-1.2610870	9.291875	11.218985
9	-7.6379740	6.8552840	12.5713300	9	-2.6478057	10.859338	11.746924
9	-6.5112650	8.7376280	12.5102010	9	-0.5681723	11.324257	11.415798
16	-9.6081000	10.8522340	3.6974560	16	-1.1417286	13.849354	3.741620
8	-10.7802130	11.4212320	4.4438750	8	-1.6241212	15.164231	4.062963
8	-9.6871480	9.3791660	3.3967790	8	-2.1304768	12.789244	3.774663
8	-8.2601540	11.3237710	4.1995310	8	0.1295230	13.491944	4.339689
6	-9.6967490	11.6425150	1.9692200	6	-0.7236020	13.922597	1.907672
9	-10.8155940	11.2477410	1.3283730	9	-1.7991907	14.219349	1.178400
9	-8.6199890	11.2597940	1.2456490	9	-0.2852030	12.716720	1.511749
9	-9.6982880	12.9878460	2.0626200	9	0.2301638	14.811001	1.642348
16	-7.2241100	8.1218820	-10.2800950	16	-1.9137410	11.402742	-9.561675
8	-8.0253840	7.0910510	-9.5156340	8	-1.1530322	10.576308	-8.642412
8	-6.1078270	8.7654210	-9.4929100	8	-1.3705330	11.517264	-10.879766
8	-8.0460820	9.0579220	-11.1114310	8	-2.4230521	12.626974	-8.976612
6	-6.2798450	7.0505590	-11.5350610	6	-3.4945905	10.402682	-9.797396
9	-5.5272300	6.1364740	-10.8748850	9	-3.2522764	9.146672	-10.178070
9	-5.4640970	7.8106430	-12.2942140	9	-4.3021757	10.962608	-10.698149
9	-7.1391680	6.3952400	-12.3426720	9	-4.1826065	10.335318	-8.641948
16	-4.8477980	-13.6011930	-4.0130420	16	-11.7634568	-6.669159	-4.416352
8	-5.7804040	-12.4805590	-4.4221480	8	-11.5721343	-5.273308	-4.118777

8	-3.4233940	-13.1767690	-3.7697320	8	-10.6012695	-7.510347	-4.213707
8	-5.0150590	-14.8657130	-4.8050960	8	-12.5226503	-6.951288	-5.613620
6	-5.4637210	-14.0298210	-2.2640550	6	-12.9185154	-7.269347	-3.053637
9	-5.4284980	-12.9193590	-1.4940850	9	-12.3863384	-7.069552	-1.844504
9	-4.6761670	-14.9742290	-1.7101720	9	-13.1498842	-8.580775	-3.183491
9	-6.7312790	-14.4877330	-2.3072590	9	-14.0991783	-6.646221	-3.087173
16	-4.7661150	-13.6943590	3.3065820	16	-10.6792337	-8.946095	4.993846
8	-3.3221230	-13.6493870	3.7572070	8	-9.3980272	-9.535691	5.308735
8	-5.3916290	-12.3471220	3.0611020	8	-10.6131306	-7.724331	4.226189
8	-5.6218700	-14.6706700	4.0638020	8	-11.6767271	-8.987262	6.029376
6	-4.6327390	-14.4251500	1.5545640	6	-11.3614020	-10.179365	3.726189
9	-3.8323080	-13.6398010	0.8012120	9	-10.5699977	-10.264539	2.649807
9	-5.8525480	-14.4881570	0.9822640	9	-12.5833140	-9.839531	3.303422
9	-4.1067110	-15.6659720	1.5998040	9	-11.4468275	-11.406241	4.256914
6	-0.9664970	2.2371010	-2.4950790	21	1.4561056	-1.087815	-0.713576
6	-2.1150020	1.9685200	-1.6302570	21	-1.1405014	0.634297	-1.135850
6	-0.4195040	1.2040920	-3.2886140	21	-0.8459100	0.448225	2.030769
6	-2.6788670	0.6822200	-1.5951770	7	-0.0799162	-0.068314	0.195678
6	-3.0796590	0.1110830	-0.3144660	6	0.2064325	-0.174111	4.318018
6	-3.0133690	0.8622710	0.9034070	6	0.0461979	1.230689	4.133046
6	-2.9131490	0.1024410	2.1122870	6	1.1721921	1.913930	3.596730
6	1.8838160	1.9376360	-2.6920700	6	2.2900316	-0.963763	-3.034870
6	1.3098640	2.9932030	-1.8588570	6	-0.8868311	-1.085582	4.109180
6	1.0341870	1.0519420	-3.3893930	6	-2.8847755	-1.475924	2.818750
6	-0.0840350	3.1454030	-1.7644280	6	-2.1738396	-0.622435	3.709196
6	-0.6943810	3.4441870	-0.4707970	6	-2.3718630	0.797998	3.618124
6	0.1001600	3.6706250	0.7002180	6	-1.3879443	2.768032	2.850269
6	-0.5284770	3.4340130	1.9660770	6	-0.2610068	3.423518	2.268360
6	-2.4299540	2.2192740	0.8679720	6	1.0248837	3.016660	2.690920
6	-1.9491620	2.7206350	-0.3880510	6	-0.3823991	3.908777	0.942315
6	-1.7841870	2.7128150	2.0507380	6	-2.5535019	2.524495	2.060605
6	2.4815900	-0.8682630	-2.7434310	6	-3.3917533	2.149351	-0.190530
6	3.3537070	0.0533660	-2.0126960	6	-2.6452337	2.952485	0.707540
6	1.3396570	-0.3816960	-3.4157460	6	-1.5652633	3.683857	0.172067
6	3.0609200	1.4267130	-1.9874150	6	-3.7109404	-0.946854	1.774602
6	3.2167980	2.1733680	-0.7415560	6	-3.7907684	0.445545	1.575959
6	3.7576510	1.5688280	0.4419180	6	-3.1391531	1.300297	2.511204
6	3.3830740	2.1623240	1.6933750	6	-3.9354801	0.904091	0.241092
6	1.5621230	3.4956260	0.5991580	6	3.8915774	-0.189755	1.347350
6	2.1306740	3.1292920	-0.6610870	6	3.6968550	1.198402	1.158293
6	2.2937270	3.1122510	1.7660760	6	2.1356717	3.011908	1.795274
6	0.0019480	-2.3084890	-2.5776230	6	2.9772715	1.911485	2.144160
6	1.1831980	-2.8034650	-1.8725040	6	3.3082581	-0.865908	2.461112
6	0.0744880	-1.1159390	-3.3315190	6	1.4155304	-0.854518	3.973684
6	2.3940990	-2.0941530	-1.9515110	6	2.5177368	-0.169307	3.406650
6	3.2075700	-1.9250080	-0.7531820	6	2.3820068	1.232153	3.250182
6	2.8455200	-2.5339670	0.4889860	6	1.1271515	-3.702822	1.686507
6	3.3660520	-1.9271740	1.6738790	6	1.8311165	-2.849549	2.568542

6	4.0654360	0.1235850	0.4154770	6	2.9684980	-2.188815	2.042808
6	3.8100480	-0.6073710	-0.7926940	6	1.0791517	-2.182278	3.562904
6	3.9741360	-0.6141690	1.6427970	6	-2.1848258	-3.191210	-1.300122
6	-2.1285870	-0.3887780	-2.4270750	6	-3.7606994	-1.391238	-0.666514
6	-2.1889840	-1.6192830	-1.6370710	6	-3.0298655	-2.096013	-1.651376
6	-1.0130220	-0.1358260	-3.2543670	6	-3.9391383	0.001519	-0.867060
6	-1.1501040	-2.5621130	-1.7127110	6	-1.0684519	-3.186452	-2.193100
6	-0.6832100	-3.2243880	-0.4964740	6	1.3613205	-2.964403	-2.339892
6	-1.3167670	-3.0051790	0.7726760	6	0.2164895	-3.598169	-1.769715
6	-0.5170880	-3.2335920	1.9423970	6	0.3256420	-4.075961	-0.444710
6	1.5838060	-3.2943590	0.5728740	6	-0.2672956	0.002116	-3.823513
6	0.7570900	-3.3707870	-0.5952040	6	-0.1068228	-1.386324	-3.588629
6	0.9226190	-3.3779980	1.8421730	6	-1.2272828	-2.089670	-3.095779
6	-2.4028660	-2.0064350	0.8510930	6	1.1862257	-1.852496	-3.220763
6	-2.7780310	-1.3050630	-0.3401980	6	-3.3969728	0.690211	-2.000339
6	-2.6120920	-1.3150490	2.0869990	6	-2.5929716	-0.012217	-2.955205
6	0.4445240	-2.3333360	3.9187440	6	-2.4414541	-1.412229	-2.764118
6	-0.8139850	-2.5811710	3.2159600	6	-1.4882133	0.687356	-3.533591
6	-1.8518990	-1.6375350	3.2884590	6	-3.0557579	2.033194	-1.577409
6	0.6201550	-1.1453640	4.6634650	6	-1.1868326	3.543196	-1.202170
6	2.9242710	-0.8893810	3.7549720	6	-1.9050305	2.705120	-2.100132
6	2.7237480	-2.1044490	2.9695350	6	-1.1476899	2.029466	-3.109827
6	1.5176210	-2.8191220	3.0536440	6	2.5970602	-2.790187	-1.622229
6	1.8857660	-0.4106520	4.5820870	6	2.6354505	-3.168658	-0.235469
6	2.3275220	1.9128300	3.8064020	6	1.5174257	-3.852136	0.315424
6	3.3990590	1.4090720	2.9450240	6	3.3555536	-2.338814	0.672453
6	3.6915420	0.0366470	2.9201380	6	-0.2877523	-3.854043	1.769065
6	1.5802180	1.0229990	4.6077900	6	-1.0475895	-3.139585	2.723969
6	-0.5236970	2.2127610	4.0005160	6	-0.3407335	-2.321740	3.638633
6	0.2515900	3.1239060	3.1616630	6	-2.3415523	-2.711901	2.343803
6	1.6434760	2.9669090	3.0619750	6	-0.7848258	-4.086347	0.448588
6	0.1259210	1.1749010	4.7055620	6	-3.6835618	-1.855629	0.669485
6	-1.6841480	-0.4122780	4.0710690	6	-2.0531547	-3.608751	0.045657
6	-2.3421130	0.6645900	3.3299520	6	-2.8378954	-2.947126	1.022577
6	-1.7797430	1.9513110	3.2982070	6	3.1805945	-1.535262	-2.060084
6	-0.4665950	-0.1651160	4.7416300	6	3.6560263	0.749343	-1.288360
				6	3.8039334	-0.653624	-1.112892
				6	3.9282430	-1.094536	0.238377
				6	0.8171383	0.901443	-3.594797
				6	2.8273257	1.297492	-2.319882
				6	2.0888846	0.441687	-3.167216
				6	-1.2689206	1.718344	3.826800
				6	0.2349899	3.682718	-1.274757
				6	2.2829551	2.532881	-1.849925
				6	0.9899285	2.962154	-2.230394
				6	0.2786118	2.147919	-3.147800
				6	0.7292817	3.912413	0.046679
				6	3.6056137	1.652060	-0.178035

6	1.9914799	3.422233	0.450097
6	2.7671077	2.750582	-0.526059

**Pt<sub>6</sub>PBI<sub>3</sub>⊃Sc<sub>3</sub>CH@C<sub>80</sub>**

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

Atom	X	Y	Z
21	1.7439920	0.2313130	-0.1390030
21	-0.8019210	0.3337340	2.3903440
21	-1.0414520	-1.9740930	-0.3332800
6	-0.2636580	-0.1499470	0.4011840
1	-0.8263930	0.6099380	-0.2083970
6	2.1454670	2.9275600	1.8092220
6	1.8716480	3.2947760	0.4482680
6	2.5907340	2.5656760	-0.5864110
6	0.1467510	-4.3061940	-0.1391040
6	1.1061580	2.9587130	2.8129850
6	-1.3138200	2.6676720	3.1685160
6	-0.2319560	3.3545360	2.4690640
6	-0.4810430	3.8181190	1.1347500
6	-0.0473280	3.5142570	-1.1637380
6	0.6237670	2.7376010	-2.1659010
6	1.9616530	2.2851480	-1.8547060
6	-0.1547580	1.9004400	-3.0312360
6	-1.4737780	3.3716460	-0.9570530
6	-3.3522920	1.7824070	-1.1155260
6	-2.2441940	2.4452920	-1.7491210
6	-1.5819750	1.7554650	-2.8256480
6	-2.5408760	2.3759730	2.4653440
6	-2.7733740	2.7964850	1.1016320
6	-1.7402700	3.5496680	0.4592070
6	-3.6011150	1.9508080	0.3002370
6	3.8412970	-1.2857040	0.1672380
6	3.6245140	-0.8638610	-1.2000270
6	2.5136560	1.0520330	-2.3723090
6	3.5544780	0.5799880	-1.4537870
6	3.8983300	-0.3327080	1.2756660
6	3.0249210	1.8035920	2.0995550
6	3.7207110	1.0794170	1.0611470
6	3.5883580	1.5362130	-0.3214350
6	1.6249260	-0.9594240	4.1736330
6	2.6794730	-0.2709440	3.4782680
6	3.4083110	-0.9976170	2.4717350
6	2.5289560	1.1434590	3.2948000
6	-2.8386910	-1.6313200	3.3838580
6	-3.8909920	0.2798220	2.1548820
6	-3.7952350	-1.1310370	2.4005610
6	-4.1484570	0.7133670	0.8181860
6	-2.3157630	-2.8934740	2.8862610
6	-0.2864140	-4.0536860	2.1561960
6	-0.9713210	-3.3046310	3.1709240
6	-0.1772110	-2.4631870	4.0260000
6	-2.5482180	-3.5865460	-0.8492670
6	-2.2543620	-3.9000950	0.5551020
6	-2.9427330	-3.1719720	1.6000960
6	-0.9067360	-4.3010390	0.8666790

**Pt<sub>6</sub>PBI<sub>3</sub>⊃Sc<sub>4</sub>O<sub>3</sub>@C<sub>80</sub>**

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

Atom	X	Y	Z
21	-1.3723410	-1.3356340	-0.5539350
21	-0.6722550	1.4101860	0.4407070
21	0.3089760	-0.7380590	2.3481100
21	1.8231440	0.1235550	-0.5512570
8	-0.1159040	0.1312790	-1.0416920
8	-1.2681320	-0.3968340	1.1958400
8	1.0501640	0.6790710	1.1809700
6	0.1997470	-4.1827950	-0.0313730
6	0.2817440	-3.7784450	-1.4018870
6	-0.9475170	-3.3419960	-2.0323070
6	-2.6141030	2.7121820	1.7710970
6	1.2977690	-3.9897820	0.8844630
6	3.1950190	-2.5322920	1.4056570
6	2.5076290	-3.3549680	0.4513050
6	2.6194080	-3.0095150	-0.9401800
6	1.5496520	-2.1699380	-2.8636710
6	0.3341080	-1.6485720	-3.4312350
6	-0.9148990	-2.2720040	-3.0106240
6	0.3026250	-0.2584690	-3.7835300
6	2.6806090	-1.2985090	-2.5635170
6	3.3945870	0.9875090	-1.9285370
6	2.6501780	0.1161770	-2.8603050
6	1.4391910	0.6174090	-3.4851070
6	3.9291240	-1.3481880	0.9985750
6	4.0201310	-0.9664890	-0.4001560
6	3.3367590	-1.8161200	-1.3566880
6	4.0841640	0.4552700	-0.7177760
6	-3.8832930	-1.7219680	0.4490230
6	-3.7712120	-1.3364480	-0.9508630
6	-2.1551460	-1.5334700	-2.9041970
6	-2.9988130	-2.1788970	-1.8725040
6	-3.1288720	-2.8546250	0.9733350
6	-1.0446770	-4.1054380	0.7155970
6	-2.2585130	-3.6172020	0.1110160
6	-2.2327390	-3.3165500	-1.3293250
6	-0.8945840	-2.2146780	3.9518880
6	-1.5580210	-3.0384100	2.9425280
6	-2.7965480	-2.5754580	2.3723010
6	-0.7089890	-3.8361680	2.1052760
6	2.1666440	1.2573580	3.7601370
6	3.7556760	1.0292860	1.7943550
6	2.9472530	1.8418070	2.6661220
6	3.8570570	1.4014500	0.3813800
6	0.9261430	2.0264930	3.8886900
6	-1.5520990	1.8843120	3.6962980
6	-0.3195900	1.3900840	4.2553090
6	-0.2875950	-0.0303810	4.5792210
6	-0.1930690	3.9369550	0.8722920
6	-0.2629810	3.5124150	2.2568590

6	-4.2345090	-0.2335800	-0.2847100	6	0.9566800	3.0871500	2.8976780
6	-4.0365020	-1.6308950	-0.0544800	6	-1.5097580	2.9335340	2.6959890
6	-3.8612480	-2.0758220	1.3057030	6	3.0677010	2.4917140	-0.1252220
6	-3.3598360	-2.3936220	-1.1018960	6	2.2288780	3.2901010	0.7357690
6	-3.7335830	0.4320160	-1.4789570	6	2.1954270	2.9699840	2.1368210
6	-1.9531450	0.3990200	-3.1826130	6	1.0412220	3.8161130	0.1197510
6	-2.9968080	-0.2848480	-2.4757670	6	2.7543060	2.2320570	-1.5218930
6	-2.8270070	-1.7071250	-2.2613350	6	0.8931120	1.9308290	-3.1385880
6	1.1372860	-3.9034250	1.9425530	6	1.5253060	2.7270660	-2.1225190
6	1.9210740	-3.0024120	2.7425320	6	0.6966030	3.5390990	-1.2692890
6	1.2478200	-2.3082020	3.8102560	6	-2.6912250	1.0161340	3.3947290
6	3.0320080	-2.3453460	2.1042510	6	-2.6416770	-0.4014190	3.6338730
6	0.4235510	-0.2564250	4.6017790	6	-1.4198310	-0.8997100	4.2500570
6	0.2515400	1.1668080	4.4157300	6	-3.3403590	-1.2738330	2.7132770
6	1.3344500	1.8500140	3.7390890	6	0.5700720	-2.1787350	4.1194300
6	-1.1174490	1.6540600	4.2087920	6	1.3966300	-2.8973870	3.1567120
6	-0.6975040	-1.1932600	4.5079310	6	0.7436600	-3.7615510	2.2064280
6	-3.0990010	1.1587060	3.0059410	6	2.6378580	-2.2925500	2.7268180
6	-2.0392570	-0.7487120	4.2107210	6	0.9508920	-0.8095300	4.5292230
6	-2.2527970	0.6988380	4.1052580	6	3.8306300	-0.3715930	2.0814160
6	1.4102440	-4.0790380	0.5330820	6	2.1726550	-0.1656950	4.0061150
6	2.2602270	-2.9858980	-1.4891580	6	3.0320880	-0.9574010	3.1497850
6	2.4717170	-3.3718750	-0.1226810	6	-3.3400030	1.5280850	2.2028040
6	3.3068250	-2.5325060	0.6921330	6	-3.8810850	1.0458400	-0.1512210
6	-1.4678310	-3.5986950	-1.8723170	6	-3.9541120	0.6548020	1.2339260
6	1.0027730	-3.2513440	-2.1712310	6	-4.0102930	-0.7474670	1.5287440
6	-0.0896580	-3.9256800	-1.5045370	6	-1.3066070	3.7408180	-0.0511060
6	0.5718950	3.7929630	0.1249870	6	-3.1817980	2.2404660	-0.5750630
6	-0.7538100	-0.2991360	-3.6171670	6	-2.5238260	3.0904290	0.3828860
6	0.7716650	-2.1682760	-3.1216650	6	1.5222790	-3.2208470	-1.8656000
6	-0.5660520	-1.6960840	-3.3677650	6	-0.5580190	1.8614670	-3.2375720
6	-1.6559690	-2.4208160	-2.7191900	6	-2.6502050	2.0226730	-1.9188870
6	0.3636240	0.6347330	-3.5275000	6	-1.3921100	2.6024630	-2.3273940
6	2.8054710	-1.7410450	-2.0111800	6	-0.7473310	3.4797400	-1.3737320
6	1.6746730	0.1737340	-3.1826980	6	-0.9284680	0.5092180	-3.6433210
6	1.8786030	-1.2412000	-3.0256230	6	-3.7820070	0.0798570	-1.2291690
7	9.8274100	-3.3283430	6.2759980	6	-2.1502210	-0.0988560	-3.1675080
6	10.2274160	-3.0803600	4.9994150	6	-3.0213580	0.6868850	-2.3284040
6	8.8467400	-2.5735960	6.8451860	7	10.1301630	-3.3357150	5.4923050
6	9.6410760	-2.0664900	4.2372820	6	10.3456700	-3.2259690	4.1534320
1	11.0505610	-3.7001260	4.6034550	6	9.3238070	-2.4430010	6.1317790
6	8.2246590	-1.5383100	6.1419020	6	9.7571620	-2.2040520	3.4027420
1	8.5653620	-2.8365030	7.8797060	1	11.0239920	-3.9654650	3.6928510
6	8.6110370	-1.2694340	4.8001860	6	8.7049100	-1.3976940	5.4416560
1	9.9876330	-1.8951670	3.2104740	1	9.1837090	-2.5942530	7.2164360
1	7.4376750	-0.9390700	6.6169050	6	8.9146280	-1.2587790	4.0419570
6	7.9701180	-0.2248290	4.0774440	1	9.9580390	-2.1432150	2.3258050
6	7.3310560	0.7192490	3.6157060	1	8.0567700	-0.6878810	5.9710630
6	6.6656810	1.7976280	2.9709330	6	8.2808770	-0.1895660	3.3493480
6	6.8728210	1.9447600	1.5691010	6	7.6477780	0.7901010	2.9587830
6	5.8004670	2.7008730	3.6452170	6	6.9555370	1.8982670	2.4001130
6	6.2348380	2.9334990	0.8141350	6	7.0617230	2.0903280	0.9940920
1	7.5157900	1.2011760	1.0878380	6	6.1306260	2.7699070	3.1617100
6	5.4555500	2.4654660	5.0768800	6	6.3555090	3.0891050	0.3174360
6	5.2212000	3.7906210	2.9213820	1	7.6740160	1.3676580	0.4458680
6	5.4216740	3.9011740	1.4958810	6	5.8772420	2.4777370	4.6021060



8	5.8693750	1.4970970	5.7157830	6	5.4907740	3.8738410	2.5148050
7	4.5874750	3.4069720	5.6741430	6	5.5969870	4.0366640	1.0848120
6	4.3956460	4.7370540	3.6047010	8	6.3610480	1.5061180	5.1853070
6	4.7382060	4.9308700	0.7659890	7	5.0066000	3.3621710	5.2762740
6	4.0629620	4.5544770	5.0435410	6	4.6849370	4.7740000	3.2794200
6	4.1837240	3.2003750	7.0770770	6	4.8693510	5.0922240	0.4372090
6	3.8473390	5.8339400	2.8882760	6	4.4190130	4.5169550	4.7202460
6	4.0249010	5.8994170	1.4780390	6	4.6669860	3.0797400	6.6829580
8	3.3421730	5.3246360	5.6797890	6	4.0813460	5.8891020	2.6412550
1	4.6691280	2.2808980	7.4372210	6	4.1885530	6.0215780	1.2286610
1	4.4871730	4.0711810	7.6871710	8	3.6970930	5.2306990	5.4177600
1	3.0824230	3.1127150	7.1370400	1	5.2000630	2.1652000	6.9828050
6	3.0971580	6.8776240	3.4945440	1	4.9621470	3.9341970	7.3195040
1	3.5355530	6.7290480	0.9586110	1	3.5728590	2.9468940	6.7787270
6	2.4682120	7.8558460	3.8950040	6	3.3259420	6.8796240	3.3258910
6	6.2678790	2.9236640	-0.6635510	1	3.6608330	6.8653090	0.7733170
6	4.7145910	4.8779490	-0.7086800	6	2.6759250	7.8152510	3.7895390
6	1.7545230	8.9142120	4.5214730	6	6.2648230	3.1108840	-1.1564490
6	6.9903450	1.9637460	-1.3780760	6	4.7673980	5.1055750	-1.0354270
6	5.4364370	3.8413370	-1.3916370	6	1.9424180	8.8238020	4.4727340
6	3.9214110	5.7518660	-1.4564600	6	6.8896620	2.1399490	-1.9432480
6	1.3093760	10.0541690	3.8023470	6	5.4209780	4.0791090	-1.7988420
6	1.4725190	8.8556090	5.9139790	6	3.9681860	6.0352940	-1.7060010
6	6.8531040	1.7926570	-2.7851760	6	1.4565000	9.9804350	3.8085290
1	7.6635060	1.2716570	-0.8620190	6	1.6790570	8.6983480	5.8644020
6	5.2661390	3.6754080	-2.8155900	6	6.6760090	2.0331490	-3.3474820
1	3.3676470	6.5605270	-0.9699400	1	7.5472330	1.3923080	-1.4895890
6	3.7541800	5.6211770	-2.8641730	6	5.1874540	3.9900150	-3.2211440
6	0.5957590	11.0546390	4.4661330	1	3.4629270	6.8365740	-1.1580820
1	1.5184730	10.1578060	2.7302980	6	3.7407200	5.9806050	-3.1111240
6	0.7512530	9.8907940	6.5144530	6	0.7264160	10.9329060	4.5227810
1	1.8145230	7.9981710	6.5072410	1	1.6485870	10.1344260	2.7393130
6	5.9510950	2.6247820	-3.5047210	6	0.9391070	9.6878420	6.5174770
6	7.6192550	0.7641240	-3.3975820	1	2.0511000	7.8263620	6.4170030
6	4.3970310	4.5513990	-3.5408200	6	5.7979260	2.9467900	-3.9865330
6	2.9498390	6.6012440	-3.5084600	6	7.3633080	0.9782460	-4.0103310
7	0.3131140	10.9598500	5.7933110	6	4.3280800	4.9329930	-3.8689870
1	0.2557940	11.9733470	3.9642080	6	2.9233570	6.9998340	-3.6715800
1	0.5109820	9.9043340	7.5915310	7	0.4658190	10.7756770	5.8486500
6	5.7160630	2.3837730	-4.9592440	1	0.3568280	11.8643850	4.0649120
6	8.3223270	-0.1334800	-3.8590480	1	0.7142070	9.6498250	7.5972960
6	4.1510280	4.3468460	-4.9940810	6	5.5112130	2.7920200	-5.4410650
6	2.2918980	7.5499700	-3.9334430	6	8.0438100	0.0326190	-4.4057360
8	6.2532880	1.4680440	-5.5840330	6	4.0355860	4.8192800	-5.3253610
7	4.8162000	3.2630480	-5.6034030	6	2.2371420	7.9545950	-4.0331180
6	9.0051820	-1.1168190	-4.6282850	8	5.9920150	1.8854080	-6.1216790
8	3.3985490	5.0565890	-5.6629190	7	4.6395370	3.7464170	-6.0130860
6	1.5803100	8.5958640	-4.5840830	6	8.7943210	-1.0497610	-4.9415270
6	4.5367400	3.0591590	-7.0375280	8	3.2973970	5.5957220	-5.9334790
6	9.9937120	-1.9763300	-4.0853270	6	1.4657280	8.9880440	-4.6329300
6	8.6869620	-1.2593530	-6.0073570	6	4.3183840	3.6348290	-7.4482050
6	1.1010240	9.7334640	-3.8827780	6	9.7463600	-1.7472120	-4.1520150
6	1.3487950	8.5367380	-5.9853550	6	8.6149590	-1.4760270	-6.2852760
1	3.4523320	2.9006370	-7.1861220	6	0.9495860	10.0805410	-3.8882100
1	4.8272920	3.9614240	-7.6073250	6	1.1951420	8.9504240	-6.0281480
1	5.1110610	2.1831860	-7.3740790	1	3.2257850	3.5224200	-7.5783360

6	10.6001160	-2.9357840	-4.9018320	1	4.6280690	4.5573950	-7.9737050
1	10.2839310	-1.9056460	-3.0295590	1	4.8527090	2.7592260	-7.8467730
6	9.3335480	-2.2370520	-6.7670690	6	10.4497610	-2.8224320	-4.6993730
1	7.9328680	-0.6067040	-6.4649990	1	9.9318620	-1.4559750	-3.1105890
6	0.4250740	10.7407010	-4.5760350	6	9.3519490	-2.5599100	-6.7716680
1	1.2619090	9.8339040	-2.8020720	1	7.8981550	-0.9619700	-6.9378480
6	0.6600290	9.5766990	-6.6157920	6	0.1883910	11.0590650	-4.5324460
1	1.7100970	7.6786040	-6.5660850	1	1.1409460	10.1651060	-2.8111010
7	10.2673130	-3.0614280	-6.2152390	6	0.4231470	9.9602950	-6.6086030
1	9.1236860	-2.3742930	-7.8421470	1	1.5856590	8.1276350	-6.6402930
7	0.2095530	10.6551790	-5.9165310	7	10.2464140	-3.2199070	-5.9850360
1	0.0643210	11.6612000	-4.0865390	1	9.2506340	-2.9158000	-7.8119220
1	0.4580810	9.5828640	-7.7012020	7	-0.0729370	10.9885950	-5.8656470
78	-1.1998960	12.0028300	-6.8509200	1	-0.2154710	11.9411100	-4.0067600
78	-1.2363410	12.2157240	6.6128570	1	0.1813340	9.9774380	-7.6858130
7	8.8295850	-5.9266850	6.0941370	78	-1.6406250	12.2211920	-6.6996550
6	7.5592730	-5.7943100	6.5666220	78	-1.0796960	11.9789550	6.7507690
6	9.0464680	-6.2824820	4.7988960	7	8.9379440	-5.8502950	5.7709050
6	6.4519620	-5.9983610	5.7414250	6	7.7720170	-5.5653100	6.4135010
1	7.4654940	-5.5556800	7.6372020	6	8.9188830	-6.3473990	4.5042990
6	7.9833740	-6.5014930	3.9171010	6	6.5346610	-5.7479900	5.7910970
1	10.1019280	-6.3997860	4.4972990	1	7.8690780	-5.2186410	7.4543370
6	6.6503360	-6.3509740	4.3775300	6	7.7163380	-6.5514970	3.8223360
1	5.4329800	-5.8885230	6.1332240	1	9.9001100	-6.5928660	4.0616910
1	8.1910120	-6.7873360	2.8783010	6	6.4859690	-6.2387530	4.4575200
6	5.5078120	-6.5411120	3.5501920	1	5.6045860	-5.5120960	6.3234910
6	4.3851830	-6.6560970	3.0605850	1	7.7342240	-6.9509290	2.8005690
6	3.1212910	-6.8164430	2.4322460	6	5.2327190	-6.4060070	3.8058050
6	3.1019630	-6.9819920	1.0202320	6	4.0849940	-6.5055020	3.3745860
6	1.8899840	-6.7697060	3.1440450	6	2.8255850	-6.6700160	2.7354190
6	1.9109390	-7.0884670	0.2951360	6	2.8395990	-6.8993710	1.3317890
1	4.0690610	-6.9527060	0.5087870	6	1.5778640	-6.5714460	3.4082290
6	1.8812160	-6.3710130	4.5801640	6	1.6666850	-7.0033360	0.5782660
6	0.6669520	-7.0282250	2.4481020	1	3.8204490	-6.9170880	0.8469230
6	0.6724830	-7.1984490	1.0146280	6	1.5409880	-6.1138380	4.8241930
8	2.9017560	-6.0818670	5.2067010	6	0.3681640	-6.8380030	2.6914300
7	0.6131450	-6.2903410	5.1976640	6	0.4070020	-7.0563320	1.2656240
6	-0.5717950	-7.0327480	3.1631500	8	2.5489120	-5.7703410	5.4440690
6	-0.5705010	-7.3739160	0.3160010	7	0.2644790	-6.0473840	5.4256650
6	-0.6153600	-6.6252080	4.5949510	6	-0.8853230	-6.8168130	3.3787470
6	0.5374960	-5.8105520	6.5904130	6	-0.8208210	-7.2280340	0.5401220
6	-1.7778860	-7.3388930	2.4728930	6	-0.9538220	-6.3972900	4.8067040
6	-1.7461980	-7.5138990	1.0616390	6	0.1669620	-5.5574530	6.8132910
8	-1.6550980	-6.5252840	5.2492450	6	-2.0770020	-7.1363870	2.6683210
1	1.5633170	-5.6236500	6.9410140	6	-2.0157780	-7.3352530	1.2608640
1	-0.0641910	-4.8825990	6.6288070	8	-2.0029490	-6.3040390	5.4464180
1	0.0367560	-6.5674770	7.2212370	1	1.1876590	-5.3625920	7.1750940
6	-3.0361400	-7.4166130	3.1277430	1	-0.4399570	-4.6324470	6.8407940
1	-2.7060200	-7.6915380	0.5664930	1	-0.3385560	-6.3131680	7.4417840
6	-4.1386630	-7.4901300	3.6683940	6	-3.3443010	-7.2282830	3.3035520
6	1.8855630	-6.9669400	-1.1758970	1	-2.9652700	-7.5185720	0.7478270
6	-0.5942060	-7.2685670	-1.1574750	6	-4.4497870	-7.3369050	3.8318800
6	-5.2457130	-7.4707900	4.5636960	6	1.6838880	-6.9225600	-0.8952410
6	3.0483780	-6.7147820	-1.9090410	6	-0.8018600	-7.1701920	-0.9361960
6	0.6258770	-6.9952440	-1.8661040	6	-5.5773000	-7.3672440	4.7004740
6	-1.7923420	-7.3071480	-1.8767330	6	2.8693620	-6.6940570	-1.5986170

6	-6.5660310	-7.8279950	4.1917190	6	0.4432450	-6.9490720	-1.6192750
6	-5.0165990	-7.0685000	5.9095130	6	-1.9801150	-7.2085290	-1.6879250
6	3.0301070	-6.4320300	-3.3043160	6	-6.8763910	-7.7537150	4.2854040
1	4.0264070	-6.6989000	-1.4184120	6	-5.3965100	-6.9891730	6.0604790
6	0.5791890	-6.6825540	-3.2754920	6	2.8947380	-6.4462260	-3.0003690
1	-2.7389900	-7.5322150	-1.3756070	1	3.8318990	-6.6660370	-1.0791560
6	-1.8621240	-7.0090720	-3.2674890	6	0.4420400	-6.6806490	-3.0385120
6	-7.5916260	-7.7553820	5.1395110	1	-2.9453230	-7.3925240	-1.2055060
1	-6.7944770	-8.1581820	3.1706670	6	-2.0033090	-6.9687380	-3.0917260
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1	-4.0035740	-6.7944630	6.2296530	1	-7.0681120	-8.0671230	3.2516140
6	1.7844610	-6.3763790	-3.9835230	6	-6.4936190	-6.9868310	6.9242400
6	4.2855270	-6.2189210	-3.9370350	1	-4.4012370	-6.6931490	6.4149850
6	-0.6745480	-6.6556340	-3.9653300	6	1.6713510	-6.4077010	-3.7183740
6	-3.1406840	-7.0686470	-3.8853790	6	4.1713060	-6.2436100	-3.5932490
7	-7.3520010	-7.3482630	6.4143230	6	-0.7898520	-6.6601760	-3.7666120
1	-8.6245700	-8.0436210	4.9071680	6	-3.2614550	-7.0424620	-3.7486980
1	-5.9664310	-6.7259760	7.8598930	7	-7.7371330	-7.3414270	6.4942870
6	1.7443320	-5.9819290	-5.4184420	1	-8.9477650	-8.0314860	4.9335000
6	5.4299400	-6.0999480	-4.3724090	1	-6.4098820	-6.7096890	7.9889170
6	-0.7525380	-6.2391570	-5.3964700	6	1.6802410	-6.0607190	-5.1656210
6	-4.2753120	-7.1690870	-4.3499960	6	5.3370510	-6.1310620	-3.9699730
8	2.7465140	-5.6926140	-6.0737990	6	-0.8182690	-6.2952410	-5.2138660
7	0.4732180	-5.9264120	-6.0260390	6	-4.3769610	-7.1561000	-4.2548430
6	6.6710650	-5.9359280	-5.0479210	8	2.7064020	-5.8041160	-5.7971320
8	-1.8151760	-6.1514370	-6.0137090	7	0.4298770	-6.0155020	-5.8150220
6	-5.4728760	-7.1907830	-5.1187400	6	6.6262630	-6.0074270	-4.5580160
6	0.4517180	-5.5026780	-7.4387830	8	-1.8593320	-6.2215370	-5.8683810
6	7.9175540	-6.1754010	-4.4121620	6	-5.5370960	-7.1926860	-5.0786020
6	6.6889210	-5.5327680	-6.4113880	6	0.4573420	-5.6409970	-7.2414110
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1	1.0561210	-6.2005180	-8.0477740	1	-0.5791590	-5.6322760	-7.6103290
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1	7.9584340	-6.5061400	-3.3667820	1	1.0694300	-6.3678150	-7.8073970
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1	-4.1083440	14.8794450	8.8780180	1	-2.3783550	13.7336150	9.7832870
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1	-0.6929520	15.9911610	7.7541940	1	-3.9269540	14.4889370	9.2231460
1	0.9334110	16.1107540	7.0089540	6	0.0759730	15.3339300	7.2105180
1	-0.4975380	15.6778290	5.9835100	1	-0.6111190	15.6986020	7.9939460
6	0.6767980	13.7789650	9.1589980	1	1.0224890	15.9041200	7.2840830
1	1.0133460	12.7661580	9.4442900	1	-0.3825310	15.4812440	6.2155350
1	1.4560280	14.5400280	9.3621290	6	0.9001290	13.4618940	9.2809430
1	-0.2361820	13.9856200	9.7416480	1	1.2597440	12.4418850	9.5072190
6	1.9492460	13.4866620	6.5838530	1	1.6749410	14.2247130	9.4937780
1	1.8414480	13.6049970	5.4918330	1	0.0044310	13.6242840	9.9034640
1	2.6694060	14.2292560	6.9787000	6	2.0722430	13.3247360	6.6380820
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6	1.0980180	13.2407640	-9.1828710	1	-2.9602100	13.2507100	-9.9404140
1	0.2861150	13.3713260	-9.9196270	1	-4.3479870	14.3646850	-9.5627860
1	1.9185110	13.9611140	-9.3711080	6	0.4352100	13.6762360	-9.0978170
1	1.4454340	12.1977290	-9.2983350	1	-0.4143360	13.7450900	-9.8001570
6	0.1102100	15.2636390	-7.2940920	1	1.1869760	14.4610430	-9.3133990
1	-0.2361400	15.4727550	-6.2627500	1	0.8598290	12.6650690	-9.2368670
1	1.0327370	15.8362580	-7.5135440	6	-0.6584970	15.5969870	-7.1600270
1	-0.6751030	15.5716250	-8.0066490	1	-0.9756490	15.7688650	-6.1120810
6	-3.5527840	14.5930190	-6.7890740	1	0.1984420	16.2508260	-7.4152100
1	-3.8690910	14.1938030	-5.8081800	1	-1.4990110	15.8339940	-7.8355770
1	-2.7529550	15.3223970	-6.5711120	6	-4.2036890	14.6044060	-6.4924100
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6	10.3948770	-8.2016760	-7.4828110	1	12.1235230	-7.2439930	-9.4529880
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9	0.0637570	16.2888030	2.0315680	9	-2.0219360	15.4968020	1.4914200
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8	0.2523030	10.2018690	-9.5077360	16	-1.4792000	10.7606480	-10.1903890
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6	-1.0093460	9.0354260	-11.5535530	8	-0.1609940	10.5738860	-9.4790570
9	-1.0387800	7.8520940	-10.8939530	8	-1.5942670	12.0090690	-11.0099640
9	0.0998400	9.0720110	-12.3205310	6	-1.4718130	9.3424890	-11.4564350
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16	-11.3175520	-8.5869000	5.4329010	9	-13.1386430	-10.5898590	-4.9696450
8	-10.0848090	-9.4227000	5.6966410	9	-14.2861320	-8.8378040	-4.3136900
8	-11.0401730	-7.3000680	4.7000520	16	-11.6197640	-8.6433600	5.3475780
8	-12.2780530	-8.4921850	6.5818090	8	-10.3983210	-9.4691170	5.6849670

6	-12.2521500	-9.6272790	4.1467940
9	-11.4903350	-9.8034610	3.0443130
9	-13.3986950	-9.0137870	3.7861900
9	-12.5525460	-10.8400070	4.6613740

8	-11.3077330	-7.3624900	4.6171180
8	-12.6422540	-8.5412120	6.4406680
6	-12.4728900	-9.7030220	4.0213080
9	-11.6393560	-9.8976070	2.9748770
9	-13.5921860	-9.0960330	3.5748250
9	-12.8082260	-10.9071650	4.5345560

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