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Supporting information for:

Photoinduced electron transfer in mechanically interlocked suit[3]ane systems

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Abstract:

Suitanes, a new class of two components mechanically interlocked systems, have recently been developed. In this work, we report a detailed study of photoinduced electron transfer processes in the suit[3]anes that consist of a 3-fold symmetric pyridinium-based (**$HC^{6+}\cdot 6PF_6^-$**) cage and substituted benzotrithiophenes, and other polycyclic aromatic guests. Analysis of electronic properties of the complexes shows that the electron transfer is favorable for complexes of **$HC^{6+}\cdot 6PF_6^-$** with strong donors, such as thiatruxene, benzotrithiophenes, and benzotrifuran. The photoinduced electron transfer for these complexes occurs on picosecond time scale. On the contrary, electron transfer does not occur in complexes of **$HC^{6+}\cdot 6PF_6^-$** with electron deficient benzotristhiazole and benzotrisoxazole. Our results open perspectives for the future design of mechanically interlocked systems for application in photovoltaic devices.

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Computational Methodology

Quantum-chemical calculations

Geometry optimizations were performed employing the DFT BLYP[1, 2] exchange–correlation functional with Ahlrichs' Def2-SVP basis set,[3, 4] and using the resolution of identity approximation (RI, alternatively termed density fitting)[5, 6] implemented in the ORCA 4.1.2 program.[7,8] Canonical energy decomposition analysis (EDA) was calculated using the Amsterdam Density Functional (ADF) program.[9] Electronic structures calculations and vertical excitation energies were calculated using TDA formalism[10] with the range-separated functional from Handy and coworkers' CAM-B3LYP[11] and Ahlrichs' Def2-SVP basis set,[3, 4] using Gaussian 16 (rev. A03)[12] The empirical dispersion D3 correction with Becke–Johnson damping,[13,14] was employed. The population analysis performed within Mulliken,[15,16] Lowdin,[17] Hirshfeld,[18] CM5,[19] schemes were carried out using code implemented in Gaussian 16. To visualize molecular structures, and frontier molecular orbitals, Chemcraft 1.8. program[20] was used.

Analysis of excited states

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes is carried out in terms of the transition density.[21-23] The analysis is convenient to perform in the Löwdin orthogonalized basis. The matrix ${}^{\lambda}\mathbf{C}$ of orthogonalized MO coefficients is 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^{*} constructed as a superposition of singly excited configurations (where an occupied MO ψ_i is replaced a virtual MO ψ_a) is computed,

$$T_{\alpha\beta}^{0i} = \sum_{ia} A_{i\to a}\, {}^{\lambda}C_{\alpha i}\, {}^{\lambda}C_{\beta a} \qquad (1)$$

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

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

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

The weights of local excitations on D and A are Ω(D,D) and Ω(A,A). The weight of electron transfer configurations D→A and A→D is 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

$$\Delta q(CS) = \sum \Omega(D,A) - \Omega(A,D) \qquad (3)$$

$$\Delta q(CT) = \sum \Omega(D,A) + \Omega(A,D) \qquad (4)$$

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[24,25] in the monopole approximation:

$$E_S^{eq}(Q,\varepsilon) = -\frac{1}{2} f(\varepsilon) Q^{+} D Q \qquad (5)$$

where the *f*(ε) 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.

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.[24,25] The GEPOL93 scheme[26] 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:

$$q_X^i = q_X^0 + \Delta_X^i, \quad \Delta_X^i = \sum_{Y \neq X} \sum_{\alpha \in X,\, \beta \in Y} (T_{\alpha\beta}^{0i} T_{\alpha\beta}^{0i} - T_{\beta\alpha}^{0i} T_{\beta\alpha}^{0i}), \qquad (6)$$

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 Y which is caused by the excitation $\psi_0 \rightarrow \psi_i$.

The non-equilibrium solvation energy for excited state ψ_i can be estimated as:[27]

$$E_S^{neq}(Q^0, \Delta, \varepsilon, n^2) = f(\varepsilon) \Delta^{+} D Q^0 - \frac{1}{2} f(n^2) \Delta^{+} D \Delta, \qquad (7)$$

In Eq. (7), 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. (6). By definition, the external (solvent) reorganization energy is the difference of the non-equilibrium (Eq. 7) and equilibrium (Eq. 5) solvation energies of the excited state.

Electron transfer rates

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

$$k_{ET} = \frac{2\pi}{\hbar} V^2 \left(FCWD\right) \qquad (8)$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:[28]

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (9)$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. ΔG^0 values were computed at vertical Franck-Condon geometry because the effect of internal geometry reorganization on the Gibbs energy is rather small for studied systems (see Table S9). The fragment charge difference (FCD)[29,30] 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 electron transfer (ET)[31,32] 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,

$$k = \sum_{n=0}^{\infty} k_{0\to n}, \text{ where } k_{0\to n} = \frac{2\pi}{\mathrm{h}} V_{0\to n}^2 \frac{1}{\sqrt{4\pi\lambda_s kT}} \exp\left[-\frac{(\Delta G + n\mathrm{h}\omega_i + \lambda_s)^2}{4\lambda_s kT}\right] \quad (10)$$

with

$$V_{0\to n}^2 = V^2 \frac{S^n}{n!} \exp(-S) \quad (11)$$

An effective value of the Huang-Rhys factor *S* is estimated from the internal reorganization energy λ_i,

$S = \lambda_i / \mathrm{h}\omega_i$

As seen, an additional parameter (as compared to the Marcus equation) enters the semi-classical expression - the frequency ω_i of a vibrational mode that effectively describes the nuclear intramolecular relaxation following the ET. Typically, in organic systems (including fullerene and nanotube derivatives) the main contribution to the internal reorganization energy is due to stretching of C=C bonds (the corresponding frequencies are found to be in the range 1400-1800 cm^{-1}). Thus, the effective frequency was set to 1600 cm^{-1}. We have demonstrated that varying the parameter ω_i within a reasonable range does not change significantly the computed ET rate (Table S8).

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 particular CT states were computed as a difference between equilibrium and non-equilibrium solvation energies. The internal reorganization energy λ_i corresponds to

the energy of structural changes when the molecule goes from the initial-state geometry to the final-state geometry.

Interaction energies

The interaction energies were calculated directly from the electronic energy of the complex and the electronic energies of the subsystems. For **$HC^{6+}\cdot 6PF_6^-\supset XXX$**, the interaction energy can be expressed as follows:

$$E_{\text{int}} = E_{HC^{6+}\cdot 6PF_6^-\supset XXX} - (E_{HC^{6+}\cdot 6PF_6^-} + E_{XXX}) \quad (12)$$

Quantum Theory of Atoms in Molecules (QTAIM)

Topological analysys of the electron distributions was conducted using the "Quantum Theory of Atoms in Molecules" (QTAIM) approach proposed by Bader.[33,34] The AIMALL suite of programs[35] was applied to evaluate the bond critical point properties and the associated bond descriptors – the electron density [$\rho(r)$] in bond critical points (BCPs), its Laplacian [$\nabla^2\rho(r)$], potential energy density [$V(r)$], kinetic energy density [$G(r)$], and total electron energy density [$H(r)$].

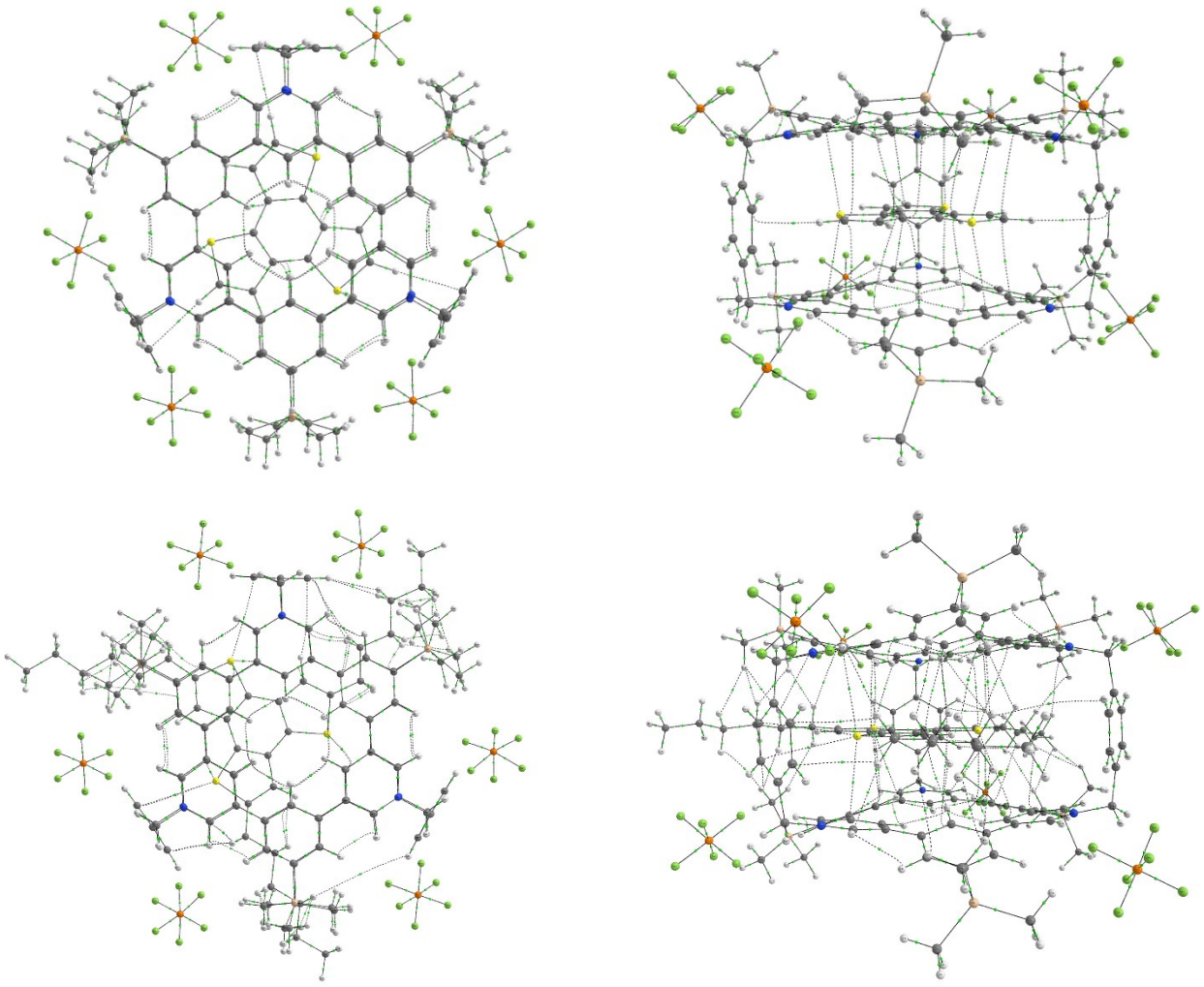
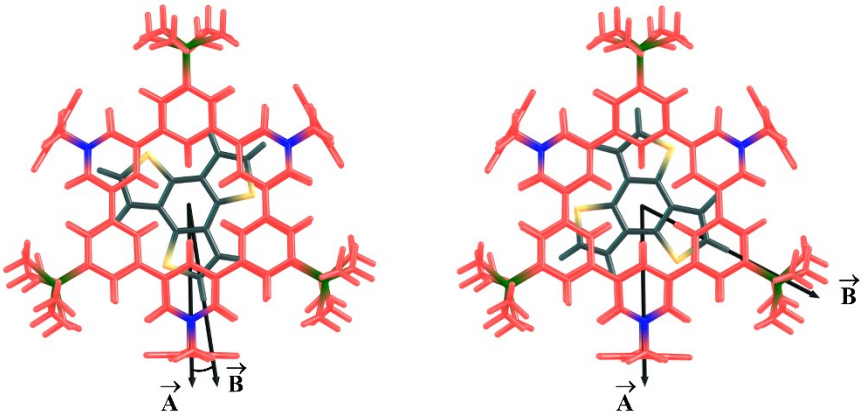


Figure S1. QTAIM molecular graph for **HC^{6+}·$6PF_6^-$⊃BTT** (top) and **HC^{6+}·$6PF_6^-$⊃BTT-$3C_6$** (bottom) complexes. Lines connecting the nuclei are the bond paths. Small green dots correspond to BCPs.



Conformer 1
$\phi = (\vec{A}, \vec{B}) = 7.8°$

Conformer 2
$\phi = (\vec{A}, \vec{B}) = 61.8°$

Figure S2. Structures of **HC^{6+}·$6PF_6^-$⊃BTT** conformers.

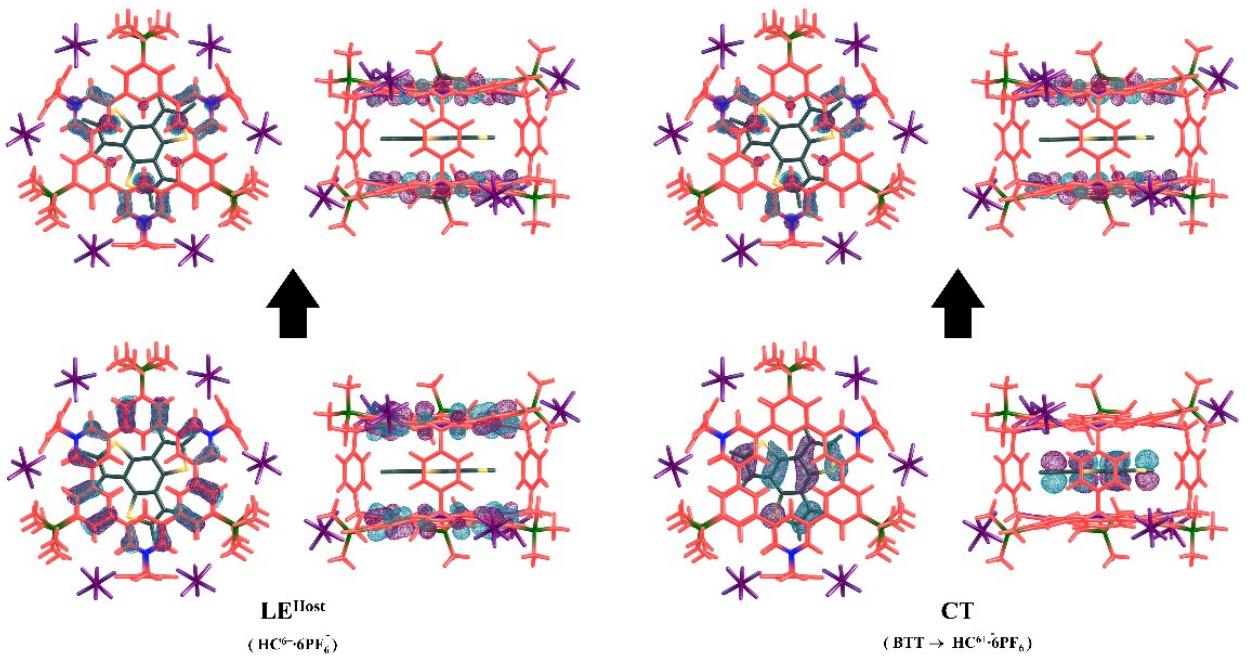


Figure S3. Frontier molecular orbitals representing lowest-lying singlet LE and CT excited states for **$HC^{6+}\cdot 6PF_6^-$⊃BTT c**omplex.

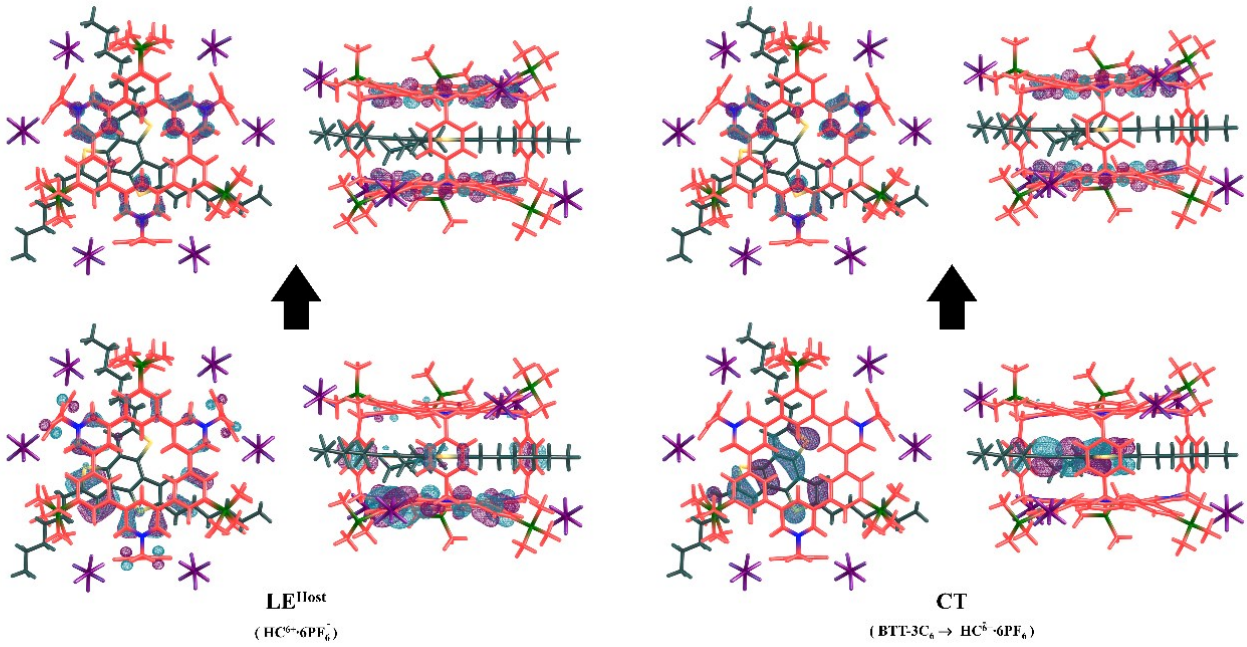


Figure S4. Frontier molecular orbitals representing lowest-lying singlet LE and CT excited states for **$HC^{6+}\cdot 6PF_6^-$⊃BTT-3C_6** complex.

Table S1. Charge separation between the fragments in electronic ground state for **$HC^{6+}\cdot 6PF_6^-$⊃BTT** and **$HC^{6+}\cdot 6PF_6^-$⊃BTT-$3C_6$** complexes. Q_{Tot} - total charge of the complex, Q_{Cage} - charge on [10]CPP, and Q_{BTT} - charge on fullerene moiety.

Charge	**$HC^{6+}\cdot 6PF_6^-$⊃BTT**			**$HC^{6+}\cdot 6PF_6^-$⊃BTT-$3C_6$**		
	Q_{Tot}	Q_{Cage}	Q_{BTT}	Q_{Tot}	Q_{Cage}	Q_{BTT-3C_6}
Mull.	0.000	-0.046	0.046	0.000	0.068	-0.068
Lowd.	0.000	-0.077	0.077	0.000	-0.017	0.017
Hirsh.	0.000	-0.068	0.068	0.000	0.035	-0.035
CM5	0.000	-0.071	0.071	0.000	0.013	-0.013

Table S2. HOMO and LUMO energies as well as HOMO-LUMO (HL) gap for isolated **BTT, BTT-$3C_6$,** and **$HC^{6+}\cdot 6PF_6^-$** in equilibrium geometry, complex geometry and in the field of point charges as well as for these units in complex.

Unit	Energy		
	HOMO	LUMO	HL gap
	BTT		
BTT in **$HC^{6+}\cdot 6PF_6^-$⊃BTT**	-8.941	-1.833	7.108
Isolated **BTT** in eq. geom.	-7.118	0.096	7.214
Isolated **BTT** in complex geom.	-7.115	0.078	7.193
Isolated **BTT** in complex geom.+ point charges	-8.747	-1.545	7.202
	BTT-$3C_6$		
BTT-$3C_6$ in **$HC^{6+}\cdot 6PF_6^-$⊃ BTT-$3C_6$**	-9.036	-2.004	7.032
Isolated **BTT-$3C_6$** in eq. geom.	-6.720	0.378	7.098
Isolated **BTT-$3C_6$** in complex geom.	-6.705	0.361	7.066
Isolated **BTT-$3C_6$**, in complex geom.+ point charges	-9.027	-2.043	6.984
	$HC^{6+}\cdot 6PF_6^-$		
$HC^{6+}\cdot 6PF_6^-$ in **$HC^{6+}\cdot 6PF_6^-$⊃BTT**	-9.240	-2.994	6.246
$HC^{6+}\cdot 6PF_6^-$ in **$HC^{6+}\cdot 6PF_6^-$⊃ BTT-$3C_6$**	-9.143	-3.659	5.484
Isolated **$HC^{6+}\cdot 6PF_6^-$** in eq. geom.	-9.296	-2.892	6.404
Isolated **$HC^{6+}\cdot 6PF_6^-$** in **$HC^{6+}\cdot 6PF_6^-$⊃BTT** complex geom.	-9.284	-3.062	6.222
Isolated **$HC^{6+}\cdot 6PF_6^-$** in **$HC^{6+}\cdot 6PF_6^-$⊃ BTT-$3C_6$** complex geom.	-9.146	-3.839	5.307

Table S3. EDA Results for **$HC^{6+}\cdot 6PF_6^-\supset$BTT** and **$HC^{6+}\cdot 6PF_6^-\supset$BTT-$3C_6$** investigated complexes.[a]

Complex	Energy terms				
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}
$HC^{6+}\cdot 6PF_6^-\supset$BTT	65.00	-32.94(25%)	-14.13(11%)	-83.19(64%)	-65.26
$HC^{6+}\cdot 6PF_6^-\supset$BTT-$3C_6$	122.06	-56.25(25%)	-32.48(15%)	-133.25(60%)	-99.93

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

Table S4. Selected bond critical points parameters (electron density [$\rho(r)$], its Laplacian [$\nabla^2\rho(r)$], potential energy density [$V(r)$], kinetic energy density [$G(r)$], and total electron energy density [$H(r)$] related to the non-covalent interactions of the fragments for studied **$HC^{6+}\cdot 6PF_6^-\supset$BTT** and **$HC^{6+}\cdot 6PF_6^-\supset$BTT-$3C_6$** complexes in the gas phase.

Bond critical points	Interaction	$\rho(r)$, au	$\nabla^2\rho(r)$, au	$V(r)$, au	$G(r)$, au	$H(r)$, au
	$HC^{6+}\cdot 6PF_6^-\supset$BTT					
BTT ⋯ $HC^{6+}\cdot 6PF_6^-$	π⋯π	7.06E-03	1.83E-02	-3.33E-03	3.95E-03	6.26E-04
		7.01E-03	1.83E-02	-3.30E-03	3.94E-03	6.39E-04
		6.92E-03	1.80E-02	-3.24E-03	3.87E-03	6.30E-04
		6.88E-03	1.78E-02	-3.23E-03	3.84E-03	6.13E-04
		6.87E-03	1.79E-02	-3.22E-03	3.85E-03	6.32E-04
		6.86E-03	1.78E-02	-3.23E-03	3.84E-03	6.15E-04
		5.46E-03	1.28E-02	-2.22E-03	2.71E-03	4.92E-04
		5.44E-03	1.26E-02	-2.21E-03	2.68E-03	4.76E-04
		5.35E-03	1.24E-02	-2.17E-03	2.64E-03	4.68E-04
		5.22E-03	1.21E-02	-2.13E-03	2.58E-03	4.48E-04
		5.21E-03	1.22E-02	-2.13E-03	2.59E-03	4.58E-04
		5.12E-03	1.18E-02	-2.09E-03	2.52E-03	4.32E-04
	CH⋯π	5.91E-03	1.63E-02	-2.85E-03	3.47E-03	6.15E-04
		5.54E-03	1.52E-02	-2.63E-03	3.21E-03	5.86E-04
		5.38E-03	1.49E-02	-2.56E-03	3.14E-03	5.78E-04
		3.91E-03	1.23E-02	-1.71E-03	2.40E-03	6.82E-04
		3.86E-03	1.21E-02	-1.70E-03	2.37E-03	6.65E-04
		3.83E-03	1.20E-02	-1.69E-03	2.34E-03	6.52E-04
		3.81E-03	1.20E-02	-1.67E-03	2.33E-03	6.61E-04
		3.77E-03	1.18E-02	-1.65E-03	2.31E-03	6.54E-04
		3.65E-03	1.14E-02	-1.61E-03	2.23E-03	6.26E-04
	$HC^{6+}\cdot 6PF_6^-\supset$BTT-$3C_6$					
BTT-$3C_6$ ⋯ $HC^{6+}\cdot 6PF_6^-$	π⋯π	6.92E-03	1.88E-02	-3.28E-03	3.99E-03	7.11E-04
		6.80E-03	1.91E-02	-3.31E-03	4.04E-03	7.33E-04
		6.70E-03	1.73E-02	-3.16E-03	3.74E-03	5.77E-04

		6.60E-03	1.68E-02	-3.08E-03	3.64E-03	5.62E-04
		6.57E-03	1.99E-02	-2.81E-03	3.90E-03	1.09E-03
		6.31E-03	1.95E-02	-2.63E-03	3.75E-03	1.12E-03
		5.91E-03	1.60E-02	-2.74E-03	3.37E-03	6.23E-04
		5.84E-03	1.62E-02	-2.78E-03	3.41E-03	6.34E-04
		4.63E-03	1.11E-02	-1.82E-03	2.30E-03	4.76E-04
		4.31E-03	1.12E-02	-2.08E-03	2.44E-03	3.59E-04
		4.26E-03	1.12E-02	-2.06E-03	2.43E-03	3.65E-04
		3.04E-03	7.86E-03	-1.24E-03	1.60E-03	3.63E-04
		3.01E-03	7.86E-03	-1.25E-03	1.61E-03	3.61E-04
		2.90E-03	7.27E-03	-1.20E-03	1.51E-03	3.07E-04
	CH···π	6.34E-03	1.97E-02	-3.22E-03	4.07E-03	8.49E-04
		6.17E-03	1.92E-02	-3.10E-03	3.95E-03	8.45E-04
		5.88E-03	1.90E-02	-2.89E-03	3.82E-03	9.28E-04
		5.74E-03	1.89E-02	-2.57E-03	3.65E-03	1.08E-03
		5.47E-03	1.79E-02	-2.70E-03	3.59E-03	8.91E-04
		5.39E-03	1.74E-02	-2.53E-03	3.44E-03	9.11E-04
		5.21E-03	1.75E-02	-2.30E-03	3.34E-03	1.04E-03
		5.18E-03	1.68E-02	-2.33E-03	3.27E-03	9.31E-04
		4.76E-03	1.50E-02	-1.91E-03	2.83E-03	9.23E-04
		4.61E-03	1.39E-02	-1.81E-03	2.64E-03	8.28E-04
		4.50E-03	1.37E-02	-1.75E-03	2.59E-03	8.37E-04
		4.40E-03	1.40E-02	-1.73E-03	2.61E-03	8.79E-04
		3.99E-03	1.15E-02	-1.63E-03	2.25E-03	6.28E-04
		3.89E-03	1.17E-02	-1.72E-03	2.33E-03	6.03E-04
		3.72E-03	1.12E-02	-1.64E-03	2.22E-03	5.84E-04
		3.20E-03	1.11E-02	-1.20E-03	1.99E-03	7.91E-04
		3.07E-03	9.70E-03	-1.23E-03	1.83E-03	6.00E-04
		3.01E-03	9.52E-03	-1.31E-03	1.85E-03	5.37E-04
		2.92E-03	9.00E-03	-1.19E-03	1.72E-03	5.29E-04
		2.58E-03	8.22E-03	-9.14E-04	1.49E-03	5.71E-04
		2.43E-03	9.39E-03	-9.77E-04	1.66E-03	6.86E-04
		2.32E-03	7.62E-03	-8.05E-04	1.36E-03	5.50E-04
		2.25E-03	6.67E-03	-8.61E-04	1.26E-03	4.03E-04
		1.47E-03	4.54E-03	-5.17E-04	8.26E-04	3.09E-04

Table S5. Excitation energies (E_x, eV) and dipole moments in ground state (μ_0, D), change in dipole moments between ground state and state of interest ($\Delta\mu = \mu_i - \mu_0$, D) and solvation energies (E_{solv}, eV) in ACN calculated for **HC^{6+}·$6PF_6^-$⊃BTT** and **HC^{6+}·$6PF_6^-$⊃BTT-$3C_6$** complexes.

	Supramolecular host-guest systems			
	HC^{6+}⊃BTT	**HC^{6+}⊃BTT-$3C_6$**	**HC^{6+}·$6PF_6^-$⊃BTT**	**HC^{6+}·$6PF_6^-$⊃BTT-$3C_6$**
	Ground state (GS)			
E_x	0.000	0.000	0.000	0.000
μ_0	0.06	8.73	0.20	1.13
E_{solv}	-29.991	-29.219	-3.402	-6.325
	LE^{Host} (**HC^{6+}·$6PF_6^-$**)			
E_x	4.288	4.219	4.143	4.187
$\Delta\mu$	0.86	2.45	0.20	2.15
E_{solv}	-29.739	-29.010	-3.276	-6.184
	Most absorptive transition			
E_x	4.808	5.093	4.817	5.119
$\Delta\mu$	2.44	2.78	1.93	4.63
E_{solv}	-29.961	-28.907	-3.332	-6.170
	CT (**BTT** → **HC^{6+}·$6PF_6^-$**)			
E_x	4.052	3.583	3.764	3.557
$\Delta\mu$	4.10	5.27	2.52	4.20
E_{solv}	-30.175	-29.182	-3.596	-6.264

Table S6. Excitation energies (E_x, eV), main singly excited configuration (HOMO(H)–LUMO(L)) and its weight (W), oscillator strength (f), extent of charge transfer (CT, e) or localization of exciton (X) computed for neutral **HC^{6+}·$6PF_6^-$⊃TruxS**, **HC^{6+}·$6PF_6^-$⊃BTF**, **HC^{6+}·$6PF_6^-$⊃BTTZ** and **HC^{6+}·$6PF_6^-$⊃BTOZ** complexes in the gas-phase (VAC).

	Supramolecular host-guest systems **HC^{6+}·$6PF_6^-$⊃XXX**			
	HC^{6+}·$6PF_6^-$⊃TruxS	**HC^{6+}·$6PF_6^-$⊃BTF**	**HC^{6+}·$6PF_6^-$⊃BTTZ**	**HC^{6+}·$6PF_6^-$⊃BTOZ**
	LE^{Host} (**HC^{6+}·$6PF_6^-$**)			
E_x	3.963	4.012	4.008	3.990
Transition (W)	H-4 – L+1 (0.23)	H-2 – L (0.22)	H – L (0.32)	H – L (0.25)
f	0.003	0.002	0.003	0.002
X	0.889	0.988	0.985	0.990
	CT (**XXX** → **HC^{6+}/HC^{6+}·$6PF_6^-$**)			
E_x	3.808	4.315	4.733	n/a*
Transition (W)	H – L (0.88)	H-1 – L+1 (0.46)	H-7 – L(0.63)	
f	<0.001	0.005	0.002	
CT	0.930	0.908	0.770	

* CT states for **HC^{6+}·$6PF_6^-$⊃BTOZ** complex are not found within considered number of excited states.

Table S7. Excitation energies (E_x, eV) and dipole moments in ground state (μ_0, D), change in dipole moments between ground state and state of interest ($\Delta\mu = \mu_i - \mu_0$, D) and solvation energies (E_{solv}, eV) in ACN calculated for **$HC^{6+}\cdot 6PF_6^-$⊃TruxS**, **$HC^{6+}\cdot 6PF_6^-$⊃BTF**, **$HC^{6+}\cdot 6PF_6^-$⊃BTTZ** and **$HC^{6+}\cdot 6PF_6^-$⊃BTOZ** complexes.

	Supramolecular host-guest systems			
	$HC^{6+}\cdot 6PF_6^-$⊃TruxS	**$HC^{6+}\cdot 6PF_6^-$⊃BTF**	**$HC^{6+}\cdot 6PF_6^-$⊃BTTZ**	**$HC^{6+}\cdot 6PF_6^-$⊃BTOZ**
	Ground state (GS)			
E_x	0.000	0.000	0.000	0.000
μ_0	1.00	0.19	0.13	0.44
E_{solv}	-2.900	-3.355	-3.328	-3.381
	LE^{Host} (**$HC^{6+}\cdot 6PF_6^-$**)			
E_x	4.074	4.143	4.123	4.209
$\Delta\mu$	0.53	0.57	0.07	0.78
E_{solv}	-2.788	-3.224	-3.214	-3.162
	CT (**BTT** $\rightarrow$ **$HC^{6+}\cdot 6PF_6^-$**)			
E_x	3.881	4.039	4.605	n/a
$\Delta\mu$	3.81	5.47	1.77	
E_{solv}	-2.818	-3.631	-3.456	

Table S8. Computed semi-classical rates (k_X in s^{-1}) and characteristic times (τ in ps) for the CT process in **$HC^{6+}\cdot 6PF_6^-$⊃BTT** complex in ACN solution using different effective Huang-Rhys (S_{eff}) factors.

$h\omega_{eff}$	ΔG^0, eV	|Vij|, eV	λ_s	λ_i	S_{eff} [a]	k_X, s^{-1}	τ, ps
	$LE^{Host} \rightarrow$ CT						
1200	-0.379	$1.16\cdot10^{-3}$	0.166	0.171	1.149	$2.757\cdot10^{10}$	36
1400					0.985	$2.603\cdot10^{10}$	38
1600					0.862	$2.503\cdot10^{10}$	40
1800					0.766	$2.383\cdot10^{10}$	42

[a] An effective value of the Huang-Rhys factor $S_{eff} = \lambda_i / h\omega_{eff}$, *where* $h\omega_{eff}$ *is set to* $1600\ cm^{-1}$.

Table S9. Electron transfer parameters computed for **$HC^{6+}\cdot 6PF_6^-$⊃BTT** in relaxed and Frank-Condon geometries: excitation energy of the lowest LE (E_X, eV), exciton localization (X) on **$HC^{6+}\cdot 6PF_6$** fragment, extent of charge transfer (CT, e), Gibbs energy (ΔG^0, eV), electronic coupling ($|V_{ij}|$, eV), internal and solvent reorganization energies (λ_i and λ_s, eV) and electron transfer rate (k_{ET}, s^{-1}).

$HC^{6+}\cdot 6PF_6^-$⊃XXX	E_X[a]	CT[b]	ΔG^0 [c]	$\|V_{ij}\|$	Reorg. Energy		k_{ET}
					λ_i	λ_s	
BTT FC_geometry	E=4.14 X=0.97	E=3.76 CT=0.95	-0.38	$1.16\cdot10^{-3}$	0.171	0.166	$2.50\cdot10^{10}$
BTT relaxed_geometry	E=4.20 X=0.97	E=3.67 CT=0.98	-0.53	$1.16\cdot10^{-3}$	0.193	0.248	$1.96\cdot10^{10}$

[a] The lowest LE states localized on **$HC^{6+}\cdot 6PF_6^-$** cage; [b] electron transfer from **XXX** to **$HC^{6+}\cdot 6PF_6^-$**; [c] Gibbs energy of electron transfer LE $\rightarrow$ CT

Cartesian coordinates

$HC^{6+}\cdot 6PF_6^-\supset$BTT

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

Atom	X	Y	Z
16	-2.473930000	1.948334000	0.001597000
16	-0.395481000	-3.140635000	0.012534000
16	2.972814000	1.204347000	0.007470000
6	0.119733000	1.448502000	0.006902000
6	-1.146090000	0.783451000	0.007410000
6	-1.258508000	-0.644476000	0.009626000
6	-0.049771000	-1.408376000	0.012215000
6	1.243192000	-0.791703000	0.011941000
6	1.300268000	0.637217000	0.009558000
6	-0.024415000	2.887407000	0.003350000
1	0.822239000	3.584371000	0.004925000
6	-1.339985000	3.295212000	0.000324000
6	-2.432930000	-1.488393000	0.009859000
1	-3.459510000	-1.102678000	0.011047000
6	-2.128777000	-2.831686000	0.011702000
6	2.561395000	-1.386304000	0.013801000
1	2.741725000	-2.468026000	0.018939000
6	3.572333000	-0.450854000	0.011614000
1	4.654581000	-0.624195000	0.014621000
1	-2.820812000	-3.681829000	0.014382000
1	-1.730963000	4.319313000	-0.001010000
14	3.784286000	-6.612515000	-4.347007000
7	5.638175000	-0.044004000	-3.176249000
6	4.974543000	-1.228733000	-3.251450000
1	5.587106000	-2.129136000	-3.147306000
6	3.582330000	-1.266186000	-3.429995000
6	2.923596000	-0.021671000	-3.553466000
1	1.852500000	-0.015538000	-3.775841000
6	2.847589000	-2.552970000	-3.527802000
6	1.452334000	-2.585507000	-3.334235000
1	0.937516000	-1.681624000	-2.990725000
6	3.509905000	-3.765005000	-3.842222000
1	4.595948000	-3.756073000	-4.000778000
6	2.817340000	-4.984942000	-3.992075000
6	7.125396000	-0.060015000	-2.899066000
1	7.517532000	-0.988835000	-3.347451000
6	7.330185000	-0.019962000	-1.400876000
6	7.394277000	-1.218409000	-0.659375000
1	7.435781000	-2.186827000	-1.180234000
6	5.634034000	-6.193761000	-4.181958000
1	5.971574000	-5.462075000	-4.945255000
1	6.235277000	-7.114666000	-4.327451000
1	5.884528000	-5.794366000	-3.177263000
14	3.857056000	-6.581324000	4.362376000
7	5.645817000	0.059237000	3.191333000
6	5.009490000	-1.138374000	3.228029000

$HC^{6+}\cdot 6PF_6^-\supset$BTT-$3C_6$

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

Atom	X	Y	Z
16	6.942831000	9.544043000	7.599718000
16	7.875256000	14.963052000	7.647403000
16	12.094104000	11.441825000	7.562429000
6	9.367250000	10.596097000	7.572542000
6	7.990773000	10.975247000	7.598105000
6	7.578818000	12.338498000	7.620380000
6	8.595321000	13.343108000	7.619345000
6	9.980513000	13.017512000	7.603075000
6	10.340070000	11.634855000	7.575420000
6	9.537042000	9.159106000	7.553636000
1	10.518909000	8.672914000	7.530175000
6	8.356120000	8.449818000	7.564996000
6	8.139189000	6.961055000	7.538838000
1	7.452449000	6.711894000	6.701919000
1	7.611615000	6.647531000	8.465739000
6	9.435381000	6.145183000	7.385703000
1	10.093871000	6.324095000	8.262740000
1	9.996550000	6.518181000	6.504002000
6	9.175434000	4.638717000	7.225899000
1	8.658622000	4.257144000	8.130992000
1	8.471347000	4.482671000	6.381125000
6	10.450375000	3.814148000	6.977898000
1	11.185765000	4.009087000	7.791930000
1	10.936427000	4.171571000	6.039292000
6	10.205179000	2.296168000	6.873360000
1	9.433754000	2.108858000	6.095808000
1	9.762029000	1.939063000	7.827207000
6	11.476920000	1.496236000	6.549344000
1	11.268013000	0.411030000	6.492117000
1	11.909179000	1.802710000	5.574067000
1	12.256502000	1.643426000	7.324917000
6	6.249754000	12.905490000	7.648087000
1	5.336321000	12.300711000	7.655334000
6	6.224420000	14.283071000	7.666792000
6	5.032075000	15.198845000	7.699737000
1	5.076296000	15.885716000	6.827340000
1	5.110425000	15.867372000	8.584033000
6	3.671004000	14.479657000	7.718132000
1	3.623958000	13.811553000	8.604685000
1	3.591339000	13.828551000	6.821400000
6	2.485378000	15.460596000	7.749251000
1	2.543294000	16.136207000	6.867517000
1	2.573988000	16.116117000	8.643440000
6	1.112775000	14.765641000	7.764641000
1	1.028468000	14.110282000	6.867762000
1	1.060798000	14.083908000	8.643943000

1	5.631470000	-2.028165000	3.083389000	6	-0.078412000	15.742319000	7.801554000
6	3.617078000	-1.197927000	3.436504000	1	0.010360000	16.387373000	8.700186000
6	2.931273000	0.026114000	3.567104000	1	-0.012460000	16.427376000	6.930581000
1	1.859942000	0.014736000	3.788042000	6	-1.442062000	15.033534000	7.803408000
6	2.916903000	-2.505787000	3.545506000	1	-2.276094000	15.760332000	7.833785000
6	1.518371000	-2.557397000	3.353562000	1	-1.576892000	14.411309000	6.893835000
1	0.989134000	-1.661906000	3.010020000	1	-1.550834000	14.366445000	8.684165000
6	3.608428000	-3.700181000	3.875267000	6	11.136513000	13.880167000	7.626504000
1	4.690044000	-3.675769000	4.051356000	1	11.070812000	14.972845000	7.661561000
6	2.924134000	-4.933474000	4.010312000	6	12.341056000	13.212255000	7.621346000
6	7.132544000	0.082059000	2.912344000	6	13.736518000	13.770290000	7.688593000
1	7.574785000	-0.788188000	3.421406000	1	14.238112000	13.369934000	8.596844000
6	7.334380000	0.048411000	1.413373000	1	14.329708000	13.391751000	6.828090000
6	7.403851000	-1.192732000	0.744209000	6	13.790955000	15.309471000	7.710180000
1	7.452885000	-2.125503000	1.319582000	1	13.323113000	15.697775000	6.780031000
6	4.538551000	-6.545553000	6.124523000	1	13.171375000	15.683242000	8.554028000
1	3.721449000	-6.405690000	6.861515000	6	15.220694000	15.864300000	7.844059000
1	5.044826000	-7.506271000	6.353277000	1	15.871191000	15.405586000	7.070164000
1	5.280352000	-5.735255000	6.244386000	1	15.643451000	15.548395000	8.821068000
7	-2.869170000	-4.864230000	-3.177866000	6	15.290854000	17.397501000	7.727002000
6	-1.513848000	-4.907957000	-3.221361000	1	14.922217000	17.704635000	6.722041000
1	-1.049484000	-5.890069000	-3.083175000	1	14.587018000	17.857787000	8.457853000
6	-0.770356000	-3.729076000	-3.428954000	6	16.703524000	17.969768000	7.952760000
6	-1.491461000	-2.525070000	-3.554506000	1	17.403562000	17.498500000	7.229296000
1	-0.949338000	-1.600977000	-3.775514000	1	17.058598000	17.662330000	8.960867000
6	0.712685000	-3.771638000	-3.536136000	6	16.767728000	19.500096000	7.821828000
6	1.406083000	-4.964180000	-3.867395000	1	17.794736000	19.875473000	7.993029000
1	0.847899000	-5.889407000	-4.051259000	1	16.456283000	19.832549000	6.810095000
6	-3.628365000	-6.143351000	-2.900724000	1	16.103697000	19.997409000	8.559038000
1	-3.095460000	-6.957953000	-3.414985000	14	1.414277000	14.961526000	12.981308000
6	-3.693210000	-6.342139000	-1.402636000	14	14.372513000	14.912150000	
6	-2.623727000	-6.980263000	-0.737722000	12.169210000			
1	-1.821249000	-7.455726000	-1.315542000	14	7.808387000	3.598401000	12.144439000
6	3.426701000	-7.176865000	-6.114746000	7	7.790675000	16.858813000	10.858068000
1	3.701559000	-6.389215000	-6.845763000	7	12.655559000	8.345177000	10.673620000
1	4.022023000	-8.083715000	-6.349013000	7	2.841750000	8.406070000	10.959075000
1	2.358405000	-7.431666000	-6.237988000	6	2.940089000	14.041640000	12.209277000
14	3.831068000	6.596560000	-4.319884000	6	2.917820000	12.651952000	11.953854000
6	4.998200000	1.151199000	-3.223823000	1	2.024887000	12.082480000	12.248326000
1	5.617298000	2.044109000	-3.088536000	6	4.030612000	11.967330000	11.399973000
6	3.605441000	1.205356000	-3.430856000	6	5.191435000	12.707575000	11.082263000
6	2.901163000	2.511283000	-3.538157000	1	6.034478000	12.211016000	10.587788000
6	1.503288000	2.558586000	-3.342355000	6	5.272378000	14.089616000	11.366081000
1	0.976170000	1.659346000	-3.005597000	6	4.137551000	14.735874000	11.917362000
6	3.589014000	3.709498000	-3.860862000	1	4.200467000	15.800669000	12.184778000
1	4.670159000	3.689118000	-4.039896000	6	0.322624000	13.661410000	13.803139000
6	2.902529000	4.943054000	-3.981829000	1	-0.099490000	12.939708000	13.073443000
1	7.562840000	0.810743000	-3.411588000	1	-0.539159000	14.158628000	14.293676000
6	7.334511000	1.223013000	-0.731328000	1	0.865142000	13.097535000	14.588785000
1	7.332292000	2.158596000	-1.304583000	6	0.535843000	15.789368000	11.523309000
6	4.503939000	6.584562000	-6.085692000	1	1.207337000	16.489680000	10.986449000
1	3.686283000	6.439500000	-6.821024000	1	-0.337450000	16.371983000	11.881449000
1	4.996364000	7.553881000	-6.308399000	1	0.164498000	15.038078000	10.798622000

1	5.255967000	5.785050000	-6.214525000	6	2.082255000	16.230746000	14.206136000
14	3.774441000	6.629012000	4.311149000	1	2.707432000	17.005890000	13.716827000
6	4.978693000	1.241261000	3.277052000	1	2.677427000	15.756391000	15.012075000
1	5.588442000	2.144268000	3.181471000	1	1.234968000	16.760820000	14.687798000
6	3.586036000	1.273433000	3.452311000	6	6.557398000	14.811511000	11.161332000
6	2.846523000	2.558039000	3.543859000	6	7.796764000	14.135009000	11.193352000
6	1.452216000	2.585456000	3.344046000	1	7.801164000	13.061313000	11.402560000
1	0.939684000	1.676815000	3.010103000	6	9.032570000	14.800999000	11.029904000
6	3.504847000	3.774825000	3.846604000	6	8.979091000	16.198284000	10.858654000
1	4.590317000	3.770664000	4.008774000	1	9.872341000	16.814221000	10.714713000
6	2.810000000	4.995755000	3.976189000	6	6.602553000	16.209389000	10.989607000
1	7.520844000	1.011325000	3.363311000	1	5.704313000	16.834246000	10.960305000
6	7.329092000	1.248184000	0.671196000	6	7.782612000	18.342731000	10.547270000
1	7.319901000	2.217958000	1.190969000	1	8.696158000	18.773361000	10.991932000
6	5.624364000	6.213533000	4.139164000	1	6.907350000	18.777410000	11.059957000
1	5.968957000	5.492134000	4.909070000	6	7.726038000	18.526186000	9.043353000
1	6.223651000	7.137914000	4.270078000	6	8.916084000	18.587802000	8.288068000
1	5.869539000	5.803130000	3.137640000	1	9.891064000	18.648857000	8.792620000
14	-7.632563000	0.023992000	-4.343321000	6	8.863829000	18.584167000	6.885605000
6	-3.563063000	-3.697183000	-3.258254000	1	9.798570000	18.643220000	6.309760000
1	-4.649506000	-3.777781000	-3.158798000	6	10.326447000	14.071107000	11.088563000
6	-2.898976000	-2.472770000	-3.435818000	6	10.354142000	12.679593000	10.851286000
6	-3.645628000	-1.192896000	-3.536836000	1	9.446516000	12.177859000	10.500357000
6	-2.975690000	0.032125000	-3.347198000	6	11.540931000	11.934978000	11.017689000
1	-1.934112000	0.026482000	-3.008042000	6	12.728018000	12.626812000	11.367479000
6	-5.027082000	-1.160670000	-3.848275000	1	13.656831000	12.062173000	11.528568000
1	-5.563229000	-2.105706000	-4.003531000	6	12.755843000	14.024185000	11.573684000
6	-5.737684000	0.048885000	-3.998055000	6	11.535629000	14.724295000	11.436392000
1	-4.629345000	-6.016011000	-3.347215000	1	11.526828000	15.801681000	11.654317000
6	-4.754216000	-5.786695000	-0.656918000	6	14.367534000	14.838308000	14.053899000
1	-5.610972000	-5.329175000	-1.174190000	1	13.491191000	15.364676000	14.482674000
6	-8.192864000	-1.787458000	-4.173744000	1	15.280235000	15.327464000	14.452659000
1	-7.731340000	-2.446361000	-4.938458000	1	14.358219000	13.793420000	14.424085000
1	-9.291650000	-1.848173000	-4.314099000	6	14.306213000	16.695881000	11.548697000
1	-7.967408000	-2.202994000	-3.169666000	1	14.210770000	16.767583000	10.448261000
7	-2.790870000	4.914584000	-3.190944000	1	15.242188000	17.218932000	11.833032000
6	-1.432995000	4.932435000	-3.265797000	1	13.474690000	17.262861000	12.015787000
1	-0.960443000	5.913839000	-3.164604000	6	15.830701000	13.944578000	11.448130000
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9	0.925528455	2.934664608	12.478229075
9	1.164296084	4.287672078	10.735633192
9	3.304081192	4.444468555	10.995190102
9	3.031982111	3.048868736	12.761940763
15	13.186792245	3.581065698	3.583460498
9	13.333464916	4.913373710	2.620610504
9	13.306569127	2.303613604	4.501613160
9	14.504850097	2.894592816	2.756673218
9	14.271333000	4.253449539	4.495425004
9	12.132169667	4.417794137	4.235411874
9	12.398852905	3.016148009	2.472626338
15	17.021482633	10.000908917	11.853046396
9	15.854611800	10.865603024	11.177497463
9	18.158500626	9.117157477	12.528539999
9	15.903419041	9.112055441	12.591927237
9	16.965251451	9.005221025	10.596687689
9	18.122768150	10.886608810	11.114124268
9	17.021271628	10.996697299	13.103203945
15	-1.563617741	10.024855636	3.361732200
9	-0.393403638	10.886936557	4.034832411
9	-2.704053017	9.143602156	2.688739510
9	-0.449008446	9.129588248	2.625380368
9	-1.511235630	9.032523250	4.620907946
9	-2.661461299	10.916904625	4.098134351
9	-1.559557660	11.017087529	2.108755612

$HC^{6+}\cdot 6PF_6^-$⊃TruxS

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

Atom	X	Y	Z
16	2.894163000	1.417526000	-0.035038000
16	-0.130521000	-3.189959000	-0.020068000
16	-2.606308000	1.730642000	-0.038003000
6	0.227225000	1.417963000	-0.037209000
6	1.353760000	0.532245000	-0.032527000
6	1.207725000	-0.882828000	-0.025971000

$HC^{6+}\cdot 6PF_6^-$⊃BTF

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

Atom	X	Y	Z
6	0.122675000	1.448749000	0.009120000
6	-1.133816000	0.775745000	0.009107000
6	-1.260124000	-0.640096000	0.012234000
6	-0.049003000	-1.391743000	0.014784000
6	1.240397000	-0.793111000	0.015071000
6	1.285859000	0.631616000	0.011658000

6	-0.123414000	-1.414518000	-0.027980000	6	-0.189378000	2.865111000	0.007002000
6	-1.276091000	-0.580940000	-0.032949000	1	0.519539000	3.696799000	0.011352000
6	-1.071133000	0.837121000	-0.037036000	6	-1.561323000	2.956316000	0.004375000
6	0.624617000	2.824222000	-0.040302000	6	-2.330859000	-1.618545000	0.014704000
6	2.047080000	2.976442000	-0.042347000	1	-3.405603000	-1.420562000	0.019088000
6	2.224932000	-1.932688000	-0.013496000	6	-1.723729000	-2.852264000	0.016715000
6	1.641666000	-3.239475000	-0.009318000	6	2.623099000	-1.231023000	0.018578000
6	-2.693880000	-0.937651000	-0.027213000	1	2.988841000	-2.260820000	0.027271000
6	-3.534990000	0.220033000	-0.028295000	6	3.388253000	-0.088482000	0.015536000
6	3.637828000	-1.836450000	-0.001698000	1	4.467408000	0.090008000	0.016467000
6	4.415601000	-3.005042000	0.020446000	1	-2.108757000	-3.876074000	0.018543000
1	4.136484000	-0.859409000	-0.005899000	1	-2.255384000	3.801699000	0.002272000
1	5.508285000	-2.920299000	0.034332000	8	-2.153645000	1.699492000	0.005728000
6	2.415323000	-4.410379000	0.007460000	8	2.595639000	1.052725000	0.011468000
6	3.812836000	-4.282249000	0.026708000	8	-0.339301000	-2.736707000	0.016939000
1	1.948099000	-5.403402000	0.005541000	14	3.751655000	-6.613047000	-4.372623000
1	4.435813000	-5.186140000	0.048678000	7	5.641882000	-0.064964000	-3.142310000
6	2.668872000	4.235171000	-0.050667000	6	4.973623000	-1.246823000	-3.221727000
6	1.854583000	5.378653000	-0.050806000	1	5.585475000	-2.149902000	-3.138148000
1	3.762210000	4.331091000	-0.059479000	6	3.578740000	-1.278687000	-3.381382000
1	2.320580000	6.372877000	-0.055955000	6	2.922758000	-0.030489000	-3.484432000
6	-0.169729000	3.996290000	-0.041512000	1	1.849991000	-0.019239000	-3.698834000
6	0.447351000	5.256718000	-0.044651000	6	2.838599000	-2.562235000	-3.484174000
1	-1.264644000	3.932984000	-0.039256000	6	1.445822000	-2.593217000	-3.272875000
1	-0.176331000	6.158427000	-0.043506000	1	0.937964000	-1.690838000	-2.915246000
6	-4.936097000	0.133564000	-0.017054000	6	3.493066000	-3.772330000	-3.822370000
6	-5.522356000	-1.141659000	0.000594000	1	4.576862000	-3.764704000	-3.995866000
1	-5.563466000	1.033964000	-0.022303000	6	2.794978000	-4.988290000	-3.978589000
1	-6.616568000	-1.231132000	0.016874000	6	7.134234000	-0.087900000	-2.889065000
6	-3.315613000	-2.209545000	-0.016470000	1	7.512454000	-1.023542000	-3.335156000
6	-4.716181000	-2.301243000	-0.000375000	6	7.360308000	-0.035248000	-1.394554000
1	-2.716474000	-3.128079000	-0.017467000	6	7.407260000	-1.227254000	-0.641315000
1	-5.186766000	-3.291140000	0.012176000	1	7.430812000	-2.201352000	-1.152671000
14	3.690626000	-6.720327000	-3.996966000	6	5.604483000	-6.206739000	-4.210267000
7	5.672482000	-0.087000000	-3.218448000	1	5.941839000	-5.463496000	-4.962405000
6	4.991084000	-1.263691000	-3.220118000	1	6.199607000	-7.128247000	-4.375828000
1	5.594071000	-2.167000000	-3.088556000	1	5.862826000	-5.826747000	-3.200079000
6	3.589946000	-1.288105000	-3.379608000	14	3.876227000	-6.557394000	4.368274000
6	2.948331000	-0.036186000	-3.506031000	7	5.649986000	0.084374000	3.166592000
1	1.870406000	-0.017049000	-3.685663000	6	5.019556000	-1.116229000	3.213321000
6	2.835095000	-2.569933000	-3.443750000	1	5.649060000	-2.004423000	3.093495000
6	1.428398000	-2.569216000	-3.326654000	6	3.624213000	-1.180711000	3.400721000
1	0.913962000	-1.635816000	-3.078832000	6	2.930800000	0.041870000	3.507756000
6	3.490842000	-3.807853000	-3.659151000	1	1.857952000	0.027318000	3.721376000
1	4.582310000	-3.834861000	-3.774674000	6	2.928342000	-2.490939000	3.511574000
6	2.783415000	-5.024098000	-3.774335000	6	1.532985000	-2.550941000	3.299687000
6	7.162422000	-0.104700000	-2.934969000	1	1.003737000	-1.658533000	2.948268000
1	7.577624000	-1.010756000	-3.408159000	6	3.620641000	-3.680042000	3.859185000
6	7.368344000	-0.085793000	-1.431952000	1	4.698763000	-3.649061000	4.054235000
6	7.606413000	-1.280566000	-0.723458000	6	2.941108000	-4.916560000	3.988588000
1	7.795627000	-2.217539000	-1.266874000	6	7.142591000	0.110822000	2.912838000
6	5.493621000	-6.362334000	-4.419620000	1	7.578611000	-0.752785000	3.438434000
1	5.591340000	-5.783026000	-5.360198000	6	7.366764000	0.061314000	1.417785000

1	6.040347000	-7.315951000	-4.567427000	6	7.419342000	-1.187530000	0.761340000
1	6.016396000	-5.814548000	-3.608038000	1	7.455582000	-2.114691000	1.346891000
14	3.743469000	-6.707569000	4.184867000	6	4.522379000	-6.507579000	6.143529000
7	5.658598000	-0.106311000	3.174786000	1	3.690565000	-6.364616000	6.863285000
6	4.986570000	-1.288205000	3.191892000	1	5.026188000	-7.465470000	6.388965000
1	5.596172000	-2.188767000	3.072146000	1	5.259635000	-5.694518000	6.272586000
6	3.585428000	-1.320878000	3.351494000	7	-2.888935000	-4.857821000	-3.142670000
6	2.933746000	-0.072602000	3.459392000	6	-1.532950000	-4.905995000	-3.171573000
1	1.855746000	-0.060756000	3.639450000	1	-1.073935000	-5.892240000	-3.042717000
6	2.839388000	-2.606052000	3.435458000	6	-0.782706000	-3.727928000	-3.363972000
6	1.433933000	-2.618570000	3.295584000	6	-1.499455000	-2.520491000	-3.486693000
1	0.916771000	-1.696526000	3.012081000	1	-0.953087000	-1.597168000	-3.700900000
6	3.498864000	-3.833244000	3.690917000	6	0.700145000	-3.774954000	-3.478490000
1	4.589922000	-3.847171000	3.818260000	6	1.385633000	-4.965319000	-3.833941000
6	2.799248000	-5.053528000	3.824996000	1	0.821534000	-5.885363000	-4.025384000
6	7.149769000	-0.113975000	2.896510000	6	-3.655601000	-6.138657000	-2.889215000
1	7.569043000	-1.018566000	3.368824000	1	-3.127008000	-6.945522000	-3.419883000
6	7.362170000	-0.089996000	1.394432000	6	-3.719856000	-6.362835000	-1.394906000
6	7.603660000	-1.282434000	0.683171000	6	-2.653765000	-7.019291000	-0.742120000
1	7.791798000	-2.220716000	1.224782000	1	-1.859940000	-7.498928000	-1.328429000
6	4.091087000	-6.779950000	6.034848000	6	3.381242000	-7.136626000	-6.150322000
1	3.154403000	-6.779204000	6.627580000	1	3.657395000	-6.334716000	-6.865182000
1	4.643004000	-7.710619000	6.280595000	1	3.969465000	-8.041832000	-6.407709000
1	4.711799000	-5.924610000	6.369866000	1	2.310671000	-7.381725000	-6.273333000
7	-2.940056000	-4.821649000	-3.233154000	14	3.846893000	6.567286000	-4.350951000
6	-1.583197000	-4.877558000	-3.315445000	6	5.005403000	1.133271000	-3.170129000
1	-1.144487000	-5.878487000	-3.284816000	1	5.630510000	2.023428000	-3.041218000
6	-0.812912000	-3.703380000	-3.423574000	6	3.609969000	1.194087000	-3.361916000
6	-1.529823000	-2.486638000	-3.483430000	6	2.909830000	2.502185000	-3.476333000
1	-0.971807000	-1.561078000	-3.643911000	6	1.512782000	2.557072000	-3.276311000
6	0.674517000	-3.752816000	-3.485644000	1	0.983648000	1.665078000	-2.923615000
6	1.373430000	-4.965773000	-3.707164000	6	3.599652000	3.692014000	-3.825397000
1	0.813181000	-5.898209000	-3.864119000	1	4.679051000	3.663643000	-4.013542000
6	-3.702232000	-6.106730000	-2.968386000	6	2.915928000	4.924805000	-3.968334000
1	-3.158026000	-6.916754000	-3.484672000	1	7.568078000	0.775206000	-3.417296000
6	-3.783278000	-6.321105000	-1.468342000	6	7.392940000	1.214414000	-0.738175000
6	-2.665551000	-6.826922000	-0.767810000	1	7.405573000	2.144155000	-1.320776000
1	-1.796790000	-7.217949000	-1.315928000	6	4.486253000	6.519229000	-6.128674000
6	2.797527000	-7.690697000	-5.342616000	1	3.653389000	6.366329000	-6.845133000
1	2.825227000	-7.161407000	-6.316179000	1	4.980364000	7.481004000	-6.378579000
1	3.289979000	-8.674570000	-5.485064000	1	5.230381000	5.712349000	-6.257337000
1	1.737121000	-7.894565000	-5.087947000	14	3.741872000	6.634964000	4.327599000
14	3.997588000	6.586858000	-4.168992000	6	4.975312000	1.264085000	3.224212000
6	5.044209000	1.115095000	-3.323685000	1	5.582106000	2.168928000	3.125478000
1	5.690882000	1.996442000	-3.294782000	6	3.580128000	1.291883000	3.386777000
6	3.643640000	1.193337000	-3.450227000	6	2.835122000	2.573607000	3.483774000
6	2.943407000	2.504441000	-3.535835000	6	1.439887000	2.596670000	3.289921000
6	1.544201000	2.570201000	-3.355429000	1	0.930767000	1.689572000	2.946698000
1	0.997517000	1.666070000	-3.069805000	6	3.487837000	3.789327000	3.803591000
6	3.641729000	3.708606000	-3.802642000	1	4.573838000	3.788673000	3.962235000
1	4.726265000	3.682949000	-3.979263000	6	2.786290000	5.003456000	3.958923000
6	2.986965000	4.957297000	-3.893949000	1	7.518873000	1.046493000	3.360703000
1	7.596761000	0.778732000	-3.434679000	6	7.387689000	1.253873000	0.664369000

6	7.219313000	1.123918000	-0.717514000	1	7.394330000	2.228590000	1.174935000
1	7.112022000	2.076715000	-1.254850000	6	5.593969000	6.233478000	4.147062000
6	5.331963000	6.238885000	-5.453320000	1	5.942445000	5.497481000	4.901258000
1	4.896646000	5.934283000	-6.426172000	1	6.187842000	7.158241000	4.298328000
1	5.929213000	7.157002000	-5.629854000	1	5.841770000	5.846163000	3.137037000
1	6.042378000	5.451478000	-5.127213000	14	-7.613534000	0.052717000	-4.381335000
14	3.905196000	6.572406000	4.112984000	6	-3.578235000	-3.687996000	-3.222951000
6	5.020587000	1.092141000	3.262723000	1	-4.666235000	-3.766213000	-3.138956000
1	5.660202000	1.978206000	3.224288000	6	-2.908397000	-2.464192000	-3.384237000
6	3.619411000	1.161508000	3.386474000	6	-3.649438000	-1.181234000	-3.489063000
6	2.909311000	2.468377000	3.457030000	6	-2.979587000	0.040655000	-3.279282000
6	1.509061000	2.520385000	3.287755000	1	-1.944111000	0.029579000	-2.921673000
1	0.967335000	1.607595000	3.021189000	6	-5.024425000	-1.143119000	-3.828131000
6	3.601772000	3.682569000	3.696643000	1	-5.559807000	-2.085674000	-4.000616000
1	4.689683000	3.670252000	3.847153000	6	-5.728076000	0.069359000	-3.986630000
6	2.938282000	4.925895000	3.781355000	1	-4.655842000	-5.996730000	-3.332885000
1	7.576418000	0.770917000	3.400224000	6	-4.771874000	-5.805020000	-0.638273000
6	7.216176000	1.122004000	0.683193000	1	-5.627691000	-5.335993000	-1.146764000
1	7.106447000	2.073169000	1.222860000	6	-8.187549000	-1.755103000	-4.218016000
6	5.678293000	6.290496000	3.517370000	1	-7.712048000	-2.419275000	-4.969485000
1	6.210432000	5.538151000	4.135556000	1	-9.283077000	-1.810131000	-4.383989000
1	6.256467000	7.233138000	3.603056000	1	-7.987932000	-2.168004000	-3.207431000
1	5.718394000	5.971955000	2.454990000	7	-2.775113000	4.927504000	-3.153762000
14	-7.693592000	0.215313000	-3.972822000	6	-1.417211000	4.940027000	-3.230974000
6	-3.618806000	-3.643651000	-3.243310000	1	-0.941686000	5.921702000	-3.147108000
1	-4.704931000	-3.715738000	-3.134685000	6	-0.691291000	3.748114000	-3.388266000
6	-2.936953000	-2.416676000	-3.383252000	6	-1.443856000	2.555711000	-3.491699000
6	-3.668227000	-1.120946000	-3.450944000	1	-0.916903000	1.620565000	-3.703142000
6	-2.962989000	0.097146000	-3.340588000	6	0.790687000	3.748661000	-3.486587000
1	-1.896172000	0.078289000	-3.098225000	6	1.513194000	4.921363000	-3.817721000
6	-5.069230000	-1.067872000	-3.659293000	1	0.965911000	5.857169000	-3.989438000
1	-5.641320000	-1.998604000	-3.767660000	6	-3.501689000	6.231587000	-2.900578000
6	-5.768432000	0.153337000	-3.773001000	1	-2.880450000	7.026948000	-3.346638000
1	-4.696146000	-6.002547000	-3.435700000	6	-3.659886000	6.400059000	-1.405964000
6	-4.927245000	-5.923758000	-0.746913000	6	-2.648743000	7.032067000	-0.651922000
1	-5.831568000	-5.596911000	-1.280188000	1	-1.816359000	7.539514000	-1.162422000
6	-8.284631000	-1.511589000	-4.448304000	6	2.570237000	7.969083000	-4.179451000
1	-7.836782000	-1.853575000	-5.403410000	1	1.758259000	7.896288000	-4.932657000
1	-9.384815000	-1.505877000	-4.588699000	1	3.072094000	8.945771000	-4.337530000
1	-8.065301000	-2.264475000	-3.662742000	1	2.111421000	7.995953000	-3.169317000
7	-2.724348000	5.004861000	-3.231736000	14	-7.614341000	-0.079889000	4.351636000
6	-1.365083000	5.003451000	-3.257635000	7	-2.747268000	-4.940352000	3.164300000
1	-0.881529000	5.978488000	-3.146093000	6	-3.471804000	-3.793793000	3.208789000
6	-0.646048000	3.800102000	-3.414163000	1	-4.555766000	-3.894324000	3.088136000
6	-1.410940000	2.617044000	-3.516002000	6	-2.830306000	-2.553180000	3.397580000
1	-0.889561000	1.672870000	-3.692514000	6	-1.425241000	-2.564248000	3.509497000
6	0.840211000	3.785443000	-3.498624000	1	-0.902038000	-1.627893000	3.724801000
6	1.581439000	4.965337000	-3.759328000	6	-3.616957000	-1.294998000	3.505217000
1	1.056520000	5.919891000	-3.897793000	6	-2.970473000	-0.056980000	3.293125000
6	-3.452808000	6.305080000	-2.945805000	1	-1.931733000	-0.045714000	2.945386000
1	-2.866369000	7.118777000	-3.405301000	6	-4.993671000	-1.299392000	3.849575000
6	-3.588681000	6.461394000	-1.442772000	1	-5.506534000	-2.248083000	4.044892000
6	-2.647385000	7.215866000	-0.712943000	6	-5.724935000	-0.092432000	3.975690000

1	-1.899412000	7.825560000	-1.240064000	6	-3.470193000	-6.246886000	2.911369000
6	2.792348000	7.934540000	-4.705777000	1	-4.434526000	-6.193866000	3.439912000
1	2.270405000	7.671500000	-5.648162000	6	-3.629890000	-6.416484000	1.416973000
1	3.344951000	8.877992000	-4.892251000	6	-4.738959000	-5.835845000	0.764207000
1	2.032266000	8.157205000	-3.928194000	1	-5.557322000	-5.401875000	1.352232000
14	-7.685461000	0.066189000	4.108728000	6	-7.899801000	-0.650618000	6.130520000
7	-2.914968000	-4.895932000	3.150356000	1	-7.349805000	-0.005874000	6.846188000
6	-3.601846000	-3.722551000	3.171172000	1	-8.980217000	-0.590907000	6.377082000
1	-4.686032000	-3.799442000	3.046623000	1	-7.578958000	-1.699639000	6.264337000
6	-2.930280000	-2.493455000	3.338256000	7	-2.901367000	4.844981000	3.151624000
6	-1.524148000	-2.555109000	3.455656000	6	-1.546178000	4.899814000	3.195492000
1	-0.974946000	-1.628873000	3.643245000	1	-1.092018000	5.888982000	3.073445000
6	-3.670901000	-1.204255000	3.417143000	6	-0.791902000	3.724318000	3.384871000
6	-2.978012000	0.019560000	3.285162000	6	-1.503661000	2.512836000	3.497204000
1	-1.916598000	0.006091000	3.018601000	1	-0.954409000	1.591585000	3.712593000
6	-5.066594000	-1.161982000	3.655453000	6	0.690951000	3.776989000	3.493692000
1	-5.625733000	-2.099902000	3.775743000	6	1.375488000	4.973285000	3.831669000
6	-5.775552000	0.053968000	3.779179000	1	0.810608000	5.893208000	4.020998000
6	-3.669491000	-6.180458000	2.861610000	6	-3.672545000	6.123928000	2.900310000
1	-4.658503000	-6.096727000	3.343455000	1	-3.144019000	6.932602000	3.428274000
6	-3.767713000	-6.357118000	1.358070000	6	-3.743253000	6.347495000	1.406122000
6	-4.919647000	-5.942285000	0.659444000	6	-2.687627000	7.017909000	0.750672000
1	-5.818702000	-5.630800000	1.210666000	1	-1.901037000	7.509324000	1.336851000
6	-7.954209000	-0.181060000	5.956512000	6	3.391055000	7.173329000	6.104861000
1	-7.493942000	0.633797000	6.550493000	1	3.679939000	6.379123000	6.823303000
1	-9.040385000	-0.189300000	6.183068000	1	3.978635000	8.083269000	6.346558000
1	-7.532208000	-1.144286000	6.307547000	1	2.321133000	7.414937000	6.239715000
7	-2.777908000	4.927376000	3.155726000	6	-3.494266000	3.776960000	-3.182893000
6	-1.418425000	4.934985000	3.174705000	1	-4.578145000	3.872170000	-3.056071000
1	-0.942951000	5.913320000	3.058278000	6	-2.848164000	2.538257000	-3.372381000
6	-0.689855000	3.737553000	3.331962000	6	-3.629884000	1.277193000	-3.486746000
6	-1.446747000	2.550356000	3.442496000	6	-5.003281000	1.278394000	-3.843201000
1	-0.919527000	1.610175000	3.622598000	1	-5.517631000	2.226859000	-4.035919000
6	0.796736000	3.733744000	3.412621000	1	-4.466123000	6.175851000	-3.428626000
6	1.531456000	4.921317000	3.649950000	6	-4.759475000	5.804651000	-0.750368000
1	1.000042000	5.875935000	3.763526000	1	-5.573065000	5.356686000	-1.334664000
6	-3.511958000	6.227423000	2.883943000	6	-7.881812000	0.634022000	-6.159418000
1	-2.943874000	7.034647000	3.377018000	1	-7.323897000	-0.005534000	-6.873597000
6	-3.615947000	6.422163000	1.383329000	1	-8.959616000	0.575182000	-6.417333000
6	-2.661316000	7.196734000	0.692852000	1	-7.560526000	1.684199000	-6.282820000
1	-1.924244000	7.792422000	1.250532000	6	-3.585284000	3.670797000	3.214467000
6	3.818281000	6.930600000	5.960205000	1	-4.672602000	3.743421000	3.118471000
1	4.289795000	6.123709000	6.556282000	6	-2.911086000	2.449390000	3.379970000
1	4.355426000	7.874231000	6.188683000	6	-3.647713000	1.163463000	3.485223000
1	2.771957000	7.049009000	6.306991000	6	-5.025303000	1.121769000	3.812084000
6	-3.452282000	3.858192000	-3.313689000	1	-5.567161000	2.063140000	3.969599000
1	-4.538035000	3.978130000	-3.266190000	1	-4.670579000	5.979294000	3.348214000
6	-2.822522000	2.604701000	-3.439419000	6	-4.789267000	5.774988000	0.652138000
6	-3.610643000	1.342076000	-3.498955000	1	-5.637063000	5.293376000	1.162173000
6	-5.011524000	1.344733000	-3.713903000	6	-8.193092000	1.724640000	4.170923000
1	-5.538011000	2.296420000	-3.872171000	1	-7.727367000	2.395165000	4.922883000
1	-4.429223000	6.247584000	-3.457702000	1	-9.290387000	1.776750000	4.325784000
6	-4.600465000	5.761049000	-0.749333000	1	-7.984923000	2.131843000	3.159780000

1	-5.390379000	5.234040000	-1.303046000	6	-1.388419000	-4.946081000	3.226768000
6	-8.108733000	1.519180000	-5.267971000	1	-0.908022000	-5.924219000	3.130513000
1	-7.670930000	1.270280000	-6.255456000	6	-0.667182000	-3.751777000	3.392117000
1	-9.208720000	1.580851000	-5.398318000	6	0.814767000	-3.746981000	3.496029000
1	-7.761552000	2.532494000	-4.978733000	6	1.539684000	-4.918259000	3.825886000
6	-3.498424000	3.776372000	3.241928000	1	0.995233000	-5.857586000	3.986744000
1	-4.585525000	3.888634000	3.198352000	1	-2.846045000	-7.040114000	3.357284000
6	-2.858606000	2.527867000	3.370811000	6	-2.611761000	-7.033964000	0.660321000
6	-3.634485000	1.258826000	3.447255000	1	-1.770528000	-7.529252000	1.168141000
6	-5.032309000	1.250904000	3.686640000	6	2.602100000	-7.961990000	4.202824000
1	-5.566923000	2.199626000	3.829998000	1	1.791225000	-7.888343000	4.957120000
1	-4.498996000	6.148552000	3.371728000	1	3.106096000	-8.937253000	4.362913000
6	-4.613547000	5.740514000	0.652005000	1	2.141863000	-7.992715000	3.193468000
1	-5.412215000	5.196745000	1.176361000	6	5.229265000	-6.776574000	3.068004000
6	-8.330388000	1.738232000	3.503589000	1	5.816725000	-7.692829000	3.283358000
1	-7.942905000	2.580193000	4.113747000	1	4.784583000	-6.886969000	2.057401000
1	-9.435513000	1.767654000	3.593231000	1	5.930298000	-5.923402000	3.060613000
1	-8.078804000	1.923714000	2.438684000	6	-8.478501000	-1.152686000	3.058707000
6	-1.558457000	-4.944182000	3.244906000	1	-8.342021000	-0.726339000	2.043402000
1	-1.110949000	-5.941114000	3.199644000	1	-8.096979000	-2.188975000	3.066903000
6	-0.798292000	-3.766241000	3.382464000	1	-9.567532000	-1.193201000	3.267081000
6	0.687823000	-3.804405000	3.467407000	6	-8.494763000	1.114111000	-3.090638000
6	1.391442000	-5.008900000	3.724369000	1	-9.582237000	1.149255000	-3.307994000
1	0.835329000	-5.943618000	3.878099000	1	-8.364177000	0.683993000	-2.076171000
1	-3.112334000	-6.998472000	3.350515000	1	-8.119157000	2.152600000	-3.090875000
6	-2.657310000	-6.844119000	0.633153000	6	3.273012000	-7.906333000	-3.081340000
1	-1.782205000	-7.247014000	1.162457000	1	2.185888000	-8.100625000	-3.082214000
6	2.618693000	-8.114156000	3.607670000	1	3.786788000	-8.865619000	-3.297841000
1	1.696993000	-8.188131000	4.221154000	1	3.579429000	-7.577425000	-2.066885000
1	3.146627000	-9.083627000	3.715472000	6	5.206020000	6.789064000	-3.057734000
1	2.330087000	-8.010583000	2.541069000	1	4.767873000	6.885771000	-2.042910000
6	5.342251000	-6.636040000	3.171128000	1	5.915684000	5.942995000	-3.062897000
1	5.904127000	-7.584548000	3.293602000	1	5.782386000	7.713277000	-3.269158000
1	5.147011000	-6.501516000	2.087414000	6	3.244417000	7.915217000	3.030318000
1	6.016293000	-5.822953000	3.511525000	1	3.755125000	8.878841000	3.234417000
6	-8.406845000	-1.361139000	3.092790000	1	3.543978000	7.579649000	2.015961000
1	-8.170289000	-1.266178000	2.013043000	1	2.156423000	8.104218000	3.039079000
1	-8.047904000	-2.349473000	3.447215000	15	-0.748085000	-8.555880000	-4.220747000
1	-9.511435000	-1.371290000	3.192905000	9	-1.489583000	-7.180513000	-4.851328000
6	-8.333222000	0.712086000	-2.254215000	9	0.006045000	-9.823573000	-3.529020000
1	-9.435701000	0.832381000	-2.272548000	9	0.654987000	-8.083325000	-4.970200000
1	-8.093270000	-0.063871000	-1.498902000	9	-2.156127000	-8.893505000	-3.406083000
1	-7.897931000	1.675938000	-1.917952000	9	-1.214046000	-9.423414000	-5.509927000
6	3.537611000	-7.570988000	-2.305438000	9	-0.278152000	-7.592474000	-2.874907000
1	2.478061000	-7.675975000	-1.992748000	15	-7.047657000	4.921121000	-4.231163000
1	3.976082000	-8.589006000	-2.345487000	9	-5.485672000	4.878061000	-4.861754000
1	4.080269000	-7.002324000	-1.523128000	9	-8.522616000	4.899536000	-3.539537000
6	4.750768000	6.971379000	-2.468362000	9	-7.337451000	3.469380000	-4.980949000
1	3.961121000	7.170117000	-1.715110000	9	-6.638003000	6.309872000	-3.416353000
1	5.381812000	6.135130000	-2.102365000	9	-7.567248000	5.757693000	-5.520315000
1	5.393410000	7.873574000	-2.526302000	9	-6.447260000	4.033113000	-2.885573000
6	3.036055000	7.910851000	3.092405000	15	-0.760510000	8.563466000	4.204453000
1	3.581508000	8.871429000	3.192394000	9	-1.218142000	9.445653000	5.486459000

1	3.001684000	7.656123000	2.013294000
1	2.000184000	8.096627000	3.444188000
15	-0.882557067	-8.576466217	-4.100690285
9	-1.613967356	-7.214552797	-4.770256202
9	-0.137019659	-9.829362301	-3.373143294
9	0.522583770	-8.137603066	-4.866840350
9	-2.291013203	-8.877233405	-3.273136364
9	-1.358398871	-9.478428032	-5.362184527
9	-0.400417181	-7.577809700	-2.784648462
15	-7.011998119	5.022373107	-4.133454800
9	-5.469295751	4.971830827	-4.808607451
9	-8.467017152	5.006529897	-3.400469550
9	-7.337174264	3.582565559	-4.891858387
9	-6.565004465	6.396270034	-3.313802095
9	-7.559730777	5.879618122	-5.397020935
9	-6.383235596	4.111271713	-2.815732025
15	-0.548944169	8.605432603	4.168083673
9	-0.978861233	9.525644568	5.432863491
9	-0.117684970	7.588348995	2.848361583
9	0.847271132	8.117228855	4.920193068
9	-1.954491602	8.956760835	3.354456278
9	-1.322390461	7.271903110	4.846839987
9	0.233506594	9.829489373	3.430461901
15	7.727622342	-3.815627408	4.197772686
9	8.747348204	-3.894570198	5.456921872
9	6.623386181	-3.688734034	2.884298913
9	6.617520058	-4.785741823	4.958548106
9	8.725217165	-2.769903835	3.376697545
9	6.955803035	-2.481481367	4.877666552
9	8.399923532	-5.102545175	3.458549869
15	-7.161415160	-4.764525202	4.244965064
9	-7.733009497	-5.592694600	5.517334418
9	-6.507508336	-3.886344768	2.917353058
9	-7.429132090	-3.308806248	4.995243453
9	-6.770427197	-6.159908973	3.431907473
9	-5.614231408	-4.766578893	4.910758133
9	-8.618987198	-4.700416046	3.519664011
15	7.839024684	3.529430753	-4.136305038
9	7.021760209	2.217849448	-4.807222365
9	8.554278547	4.798592855	-3.406499798
9	6.758954039	4.530679727	-4.900791523
9	8.800947069	2.456697745	-3.309972279
9	8.858193121	3.567396250	-5.397671649
9	6.732382672	3.448365599	-2.820138488
9	-0.298462000	7.584919000	2.865622000
9	0.644971000	8.094977000	4.951867000
9	-2.171271000	8.895465000	3.392545000
9	-1.502202000	7.196554000	4.852266000
9	-0.006559000	9.821950000	3.495626000
15	7.801739000	-3.631445000	4.212700000
9	8.802520000	-3.674401000	5.488681000
9	6.715243000	-3.543363000	2.880482000
9	6.701504000	-4.618794000	4.965656000
9	8.787278000	-2.571398000	3.396503000
9	6.988557000	-2.308683000	4.866759000
9	8.514613000	-4.910026000	3.497603000
15	-7.031213000	-4.944391000	4.231676000
9	-7.561049000	-5.780751000	5.516602000
9	-6.420699000	-4.055888000	2.889789000
9	-7.322138000	-3.492353000	4.980476000
9	-6.619106000	-6.332810000	3.417899000
9	-5.473309000	-4.905251000	4.871862000
9	-8.501664000	-4.918815000	3.530439000
15	7.777485000	3.638362000	-4.213677000
9	6.955507000	2.311402000	-4.848159000
9	8.499610000	4.922146000	-3.517511000
9	6.668446000	4.620878000	-4.960490000
9	8.772370000	2.584192000	-3.401780000
9	8.762246000	3.671179000	-5.502465000
9	6.707354000	3.560840000	-2.868394000

$HC^{6+}\cdot 6PF_6^-\supset$BTTZ

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

Atom	X	Y	Z
16	2.934304000	1.279906000	-0.005686000
16	-2.514942000	1.875293000	-0.006258000
16	-0.305929000	-3.140701000	0.004092000
6	1.273331000	-0.736414000	-0.003697000

$HC^{6+}\cdot 6PF_6^-\supset$BTOZ

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

Atom	X	Y	Z
8	2.404070000	1.426983000	-0.017152000
8	-2.383888000	1.342329000	-0.010216000
8	0.083183000	-2.761785000	-0.019828000
6	1.355962000	-0.568048000	-0.022655000

6	1.276602000	0.695200000	-0.006288000	6	1.158086000	0.843984000	-0.018468000
6	0.062156000	1.445566000	-0.008519000	6	-0.131951000	1.432103000	-0.016808000
6	-1.178994000	0.732500000	-0.006325000	6	-1.255845000	0.554737000	-0.015028000
6	-1.221879000	-0.694203000	-0.004176000	6	-1.120059000	-0.856481000	-0.018320000
6	0.016195000	-1.412604000	-0.001718000	6	0.201693000	-1.391210000	-0.020683000
6	3.472910000	-0.422029000	0.000950000	6	3.291450000	0.354690000	-0.021926000
6	-1.310389000	3.193028000	-0.006658000	6	-1.898716000	2.646925000	-0.010355000
6	-2.049106000	-2.756320000	0.004961000	6	-1.289027000	-2.993784000	-0.017872000
1	-2.782466000	-3.576768000	0.009731000	1	-1.599881000	-4.045520000	-0.018506000
1	-1.654418000	4.238244000	-0.004805000	1	-2.654551000	3.441641000	-0.008014000
1	4.550017000	-0.646562000	0.005583000	1	4.357709000	0.611348000	-0.024321000
7	-0.054880000	2.828111000	-0.010104000	7	-0.597754000	2.754128000	-0.014364000
7	-2.360931000	-1.486536000	-0.001334000	7	-2.032335000	-1.920656000	-0.017349000
7	2.528841000	-1.326760000	-0.001126000	7	2.733779000	-0.825613000	-0.025377000
14	3.639418000	-6.657644000	-4.539573000	14	3.639521000	-6.679032000	-4.477935000
7	5.634167000	-0.150809000	-3.192936000	7	5.641141000	-0.172585000	-3.159899000
6	4.948923000	-1.324041000	-3.264090000	6	4.953818000	-1.343924000	-3.232071000
1	5.541417000	-2.235936000	-3.142281000	1	5.545800000	-2.257094000	-3.117765000
6	3.558550000	-1.336264000	-3.464227000	6	3.561918000	-1.353423000	-3.425098000
6	2.924830000	-0.079816000	-3.601452000	6	2.930132000	-0.095457000	-3.553978000
1	1.857368000	-0.054178000	-3.841120000	1	1.862319000	-0.067768000	-3.792229000
6	2.799883000	-2.606586000	-3.580408000	6	2.800415000	-2.622581000	-3.541949000
6	1.406333000	-2.615043000	-3.375838000	6	1.406079000	-2.629126000	-3.341079000
1	0.912994000	-1.708692000	-3.006993000	1	0.911591000	-1.718570000	-2.984051000
6	3.434653000	-3.821933000	-3.935360000	6	3.434010000	-3.840707000	-3.889449000
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6	2.715139000	-5.022377000	-4.114715000	6	2.713713000	-5.041398000	-4.063635000
6	7.117675000	-0.188408000	-2.899210000	6	7.130871000	-0.211656000	-2.890507000
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6	7.310574000	-0.085307000	-1.402323000	6	7.350344000	-0.101150000	-1.398083000
6	7.358178000	-1.251082000	-0.609312000	6	7.412372000	-1.262117000	-0.600269000
1	7.388955000	-2.241766000	-1.087106000	1	7.442337000	-2.254890000	-1.073647000
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7	5.633196000	0.161752000	3.195208000	7	5.638085000	0.165748000	3.157480000
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6	2.924216000	0.081498000	3.603546000	6	2.922318000	0.090604000	3.514262000
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6	2.953432000	-2.449093000	3.593025000	6	2.947612000	-2.441159000	3.515979000
6	1.559760000	-2.531039000	3.382344000	6	1.553535000	-2.520492000	3.305781000
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6	2.998998000	-4.863847000	4.118654000	6	2.989249000	-4.859703000	4.026075000
6	7.116724000	0.205765000	2.903216000	6	7.129711000	0.206985000	2.900197000
1	7.582614000	-0.630419000	3.447691000	1	7.579126000	-0.628905000	3.458495000
6	7.310657000	0.106366000	1.406161000	6	7.354177000	0.103693000	1.408184000
6	7.370205000	-1.163571000	0.791762000	6	7.427160000	-1.167821000	0.799920000

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