SUPPORTING INFORMATION FOR:

Cyclo[18]carbon: smallest all-carbon electron acceptor

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Theoretical calculation methodology

General.

Geometry optimization was performed to explore minimum energy structures for ground state S_0 and first triplet excited state T_1 using density functional theory (DFT) in conjuntion with series of GGA, meta-GGA and hybride functionals (see Table S2). Ahlrichs' Def2-TZVP triple-ξ quality basis set[1,2] was used in all cases. The empirical Grimme D3 dispersion correction[3] with zero-damping was employed. Normal mode vibrational frequencies were also calculated in each case to confirm the presence of the local minimum, at the same level of theory. Electronic structures calculations and vertical excitation energies were calculated using TDA formalism[4] with the range-separated functional from Handy and coworkers' CAM-B3LYP[5] using Gaussian 16 (rev. A03)[6] and Ahlrichs' Def2-SVP basis set.[2,7] To visualize molecular structures and frontier molecular orbitals, we used the program Chemcraft 1.8.[8] CAM-B3LYP functional was used to study the vdW complexes of C_{18} with Fx fragments because it describes correctly the geometrical and electronic structure of C_{18} complex in the ground state and allows one to get reliable data for electronically excited states.[9] Also, CAM-B3LYP predicts accurately the internal reorganization energy for C_{18} that is in good agreement with the values obtained at the post-HF level (Table 1).

Amount of the exact (HF) exchange in DFT functionals

In order to explore role of HF exchange in the functional, user defined hybrid models implemented in Gaussian 16 were used. For selected B3LYP functional contribution of HF exchange were manually tuned from 0.05 to 1.00, while Slater and non-local exchange as well as local and non-local corerlation parts were mantain unchanged. In Gaussian any hybrid functional model is defined by the general form:

$P2E_X^{HF} + P1(P4E_X^{Slater} + P3\Delta E_x^{non\text{-}local}) + P6E_C^{local} + P5\Delta E_C^{non\text{-}local}$ (S1)

In this case, the route must contain the following internal overlay options keywords:

IOp(3/76=P1P2), IOp(3/77=P3P4) and **IOp(3/78=P5P6).**

For example, the formula for the B3LYP energy is:

$E_{B3LYP} = P2E_x^{HF} + P1(P4E_X^{LDA}+P3E_X^{B88}) +P6E_C^{VWN} + P5(E_C^{LYP}-E_C^{VWN})$ (S2)

In this work P1 parameter was set to 1.0, P2 varies from 0.05 to 1.00, while P4=(1 – P2). All other parameters (P3,P5, and P6) have been always set to 0.72, 0.81 and 1 correspondingly.

Analysis of excited states.

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out using a tool suggested recently by Plasser et al.[10,11] A key quantity is the parameter Ω:

$$\Omega(A,B)=\frac{1}{2}\sum_{\alpha\in A,\beta\in B}\left[\left(SP^{0i}\right)_{\alpha\beta}\left(P^{0i}S\right)_{\alpha\beta}+P^{0i}_{\alpha\beta}\left(SP^{0i}S\right)_{\alpha\beta}\right] \quad \text{(S3)}$$

$$X(F_i)=\sum_{A\in F_i}\Omega(A,A) \quad \text{(S4)}$$

$$\Delta q(\mathrm{CT}^{\mathrm{F_i}\to\mathrm{F_j}}) = \sum_{\mathrm{A}\in\mathrm{F_i},\mathrm{B}\in\mathrm{F_j}} \Omega(\mathrm{A},\mathrm{B}) + \Omega(\mathrm{B},\mathrm{A}) \quad \text{(S5)}$$

$$\Delta q(\mathrm{CS}^{\mathrm{F_i}\to\mathrm{F_j}}) = \sum_{\mathrm{A}\in\mathrm{F_i},\mathrm{B}\in\mathrm{F_j}} \Omega(\mathrm{A},\mathrm{B}) - \Omega(\mathrm{B},\mathrm{A}) \quad \text{(S6)}$$

where A and B are atoms, F_i and F_j are fragments, α and β are atomic orbitals, $\mathbf{P}^{0i}$ is the transition density matrix for the $\psi_0 \rightarrow \psi_i$ excitation, and S is the overlap matrix. $X(F_i)$ is the extent of exciton localization on the fragment F_i. $\Delta q(CT^{F_i\to F_j})$ is the total amount of the electron density transferred between fragments F_i and F_j in the $\psi_0 \rightarrow \psi_i$ excitation. $\Delta q(CS^{F_i\to F_j})$) is a measure of the charge separation between fragments F_i and F_j. Note that in the situation when charge transfer $(F_i \to F_j)$ is equal to the back transfer $(F_j \to F_i)$ there is no charge separation between the fragments and $CS^{F_i\to F_j}$ is equal to zero.

Electron transfer rates.

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

$$k_{ET} = \frac{2\pi}{\hbar^2} V^2 \, (FCWD) \quad \text{(S7)}$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:[12]

$$(FCWD) = (4\pi\lambda kT)^{-1/2} \cdot exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT \right] \quad \text{(S8)}$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD)[13,14] method was employed to calculate the electronic couplings in this work.

The reorganization energy for gas-phase calculation represents just by the internal term. The internal reorganization energy λ_i for $F_X \rightarrow C_{18}$ ET corresponds to the energy of structural change when denoted fragments going from neutral-state geometries to charged-state geometries – cation and anion radicals, respectively.

Interaction energies were calculated directly from electronic energies of particular CNOs and the electronic energies of individual fragments from which this object consists. For C_{18}+F_X complex interaction energy can be expressed as follows:

$$E_{int} = E_{C18+Fx} - \left(E_{C18} + E_{F_X}\right) \quad \text{(S9)}$$

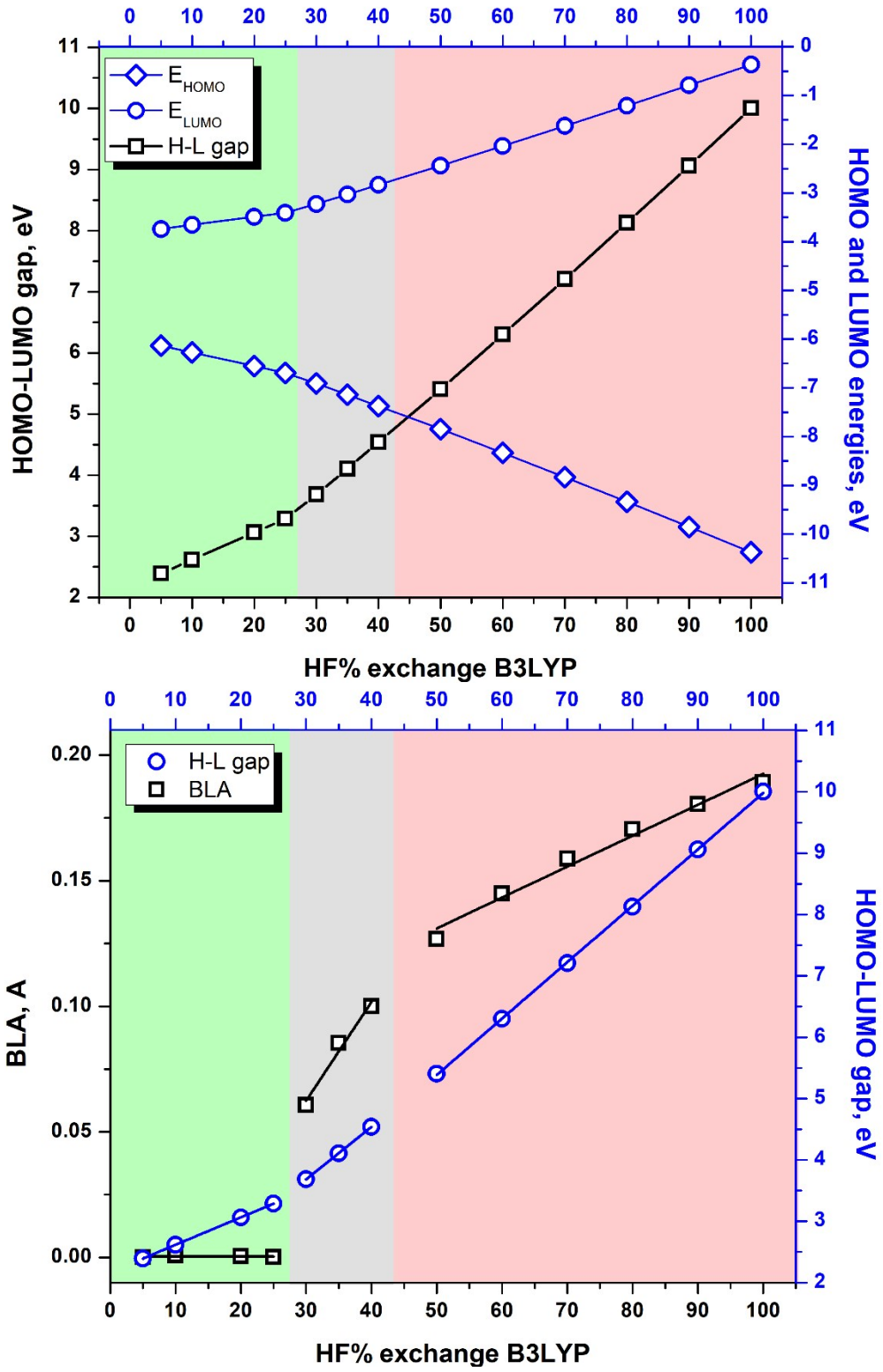
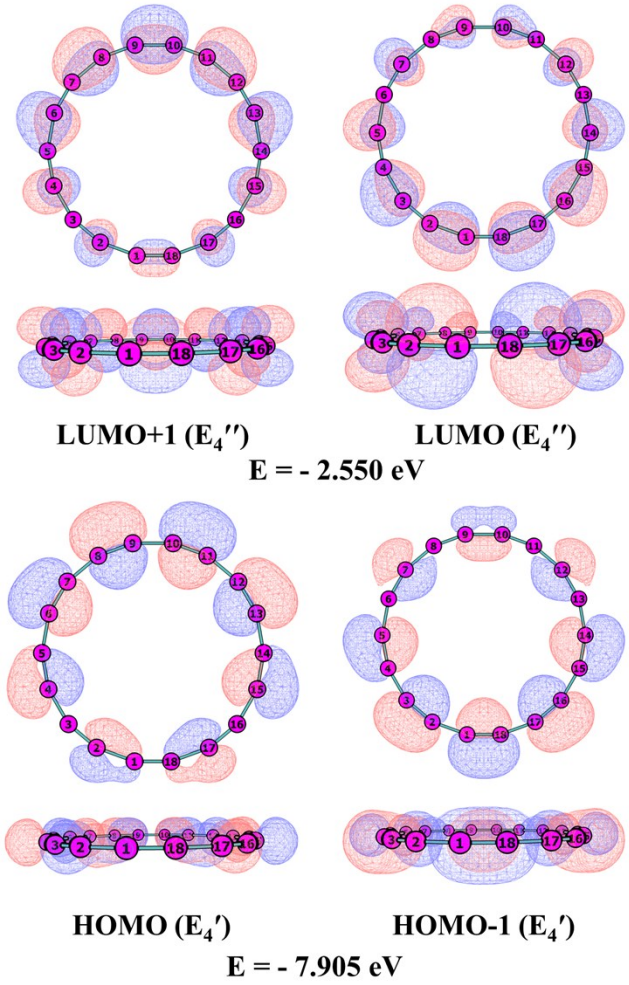


Figure S1. Dependence of HOMO (H) and LUMO (L) energies and H-L gap in cyclo[18]carbon (top) on the amount of exact exchange in B3LYP functional as well as comparison of BLA and H-L gap (bottom) on the amount of exact exchange in B3LYP functional.



Polyynic structure (M06-2X)				
Bond	**Bond type**	**Bond length**	**Character occupied MO**	**Character virtual MO**
C_1C_2	Long	1.345	Antibonding	Nonbonding
C_2C_3	Short	1.223	Bonding	Antibonding
C_3C_4	Long	1.345	Nonbonding	Bonding
C_4C_5	Short	1.223	Nonbonding	Antibonding
C_5C_6	Long	1.345	Bonding	Bonding
C_6C_7	Short	1.223	Antibonding	Antibonding
C_7C_8	Long	1.345	Bonding	Bonding
C_8C_9	Short	1.223	Nonbonding	Antibonding
C_9C_{10}	Long	1.345	Nonbonding	Bonding
$C_{10}C_{11}$	Short	1.223	Bonding	Antibonding
$C_{11}C_{12}$	Long	1.345	Antibonding	Bonding
$C_{12}C_{13}$	Short	1.223	Bonding	Antibonding
$C_{13}C_{14}$	Long	1.345	Antibonding	Nonbonding
$C_{14}C_{15}$	Short	1.223	Bonding	Nonbonding
$C_{15}C_{16}$	Long	1.345	Antibonding	Antibonding
$C_{16}C_{17}$	Short	1.223	Bonding	Bonding
$C_{17}C_{18}$	Long	1.345	Antibonding	Antibonding
$C_{18}C_1$	Short	1.223	Bonding	Nonbonding
		Long	Bonding – 2	Bonding – 2
			Nonbonding – 2	Nonbonding – 2
			Antibonding – 5	Antibonding – 5
		Short	Bonding – 6	Bonding – 1
			Nonbonding – 2	Nonbonding – 2
			Antibonding – 1	Antibonding – 6

Figure S2. Graphical representation of HOMO and LUMO and analysis of the wave function distribution for lowest energy polyynic C_{18} carbon cluster structure in singlet ground state obtained at M06-2X-D3(zero-damping)/Def2-TZVP level of theory.

Analysis of the C_{18} structure in first triplet state revealed that regardless of the applied functional the geometry of the T_1 corresponds to the polyynic structure. Important to note that polyynic structure in triplet excited state has smaller bond length alternation in comparison with ground state, i.e. the C≡C triple bonds become longer and the C–C single bonds become shorter. For example for M06-2X functional BLA for singlet ground state and first triplet electronic state were estimated 0.122Å and 0.052Å respectively. This observation is in good agreement with the analysis of a vibrational structure in electronic transitions of structurally similar polyynic chains,[15,16] and time-resolved resonance Raman measurements of first triplet state of diphenyl butadiyne.[17] The nature of such changes in BLA index is most likely similar to that in the simplest diacetylene molecule.[18] Qualitatively it can be explained as follow: during the electronic excitation the electron is removed from a bonding π-orbital and is placed into an antibonding π*-orbital. In the C_{18} cluster, the lowest π*-orbital is characterized by an additional bonding character of the wave function on C–C single bonds, and exhibits also a less number of wave function nodes on the C≡C triple bonds. All of this together leads to the partial equalization of the bonds

and decrease in BLA values. An increase of BLA in the triplet state of the cumulenic structures denotes the antiaromaticity of one of the π components according to Baird's rule.[19]

At the first look, these orbitals of C_{18} are not perfectly symmetric which does not agree with chemical intuitions. Note that HOMOs and LUMOs belong to two-dimensional irreducible representations E_4' and E_4''. The D_{9h} group has 12 irreducible representations – 4 one-dimensional and 8 two-dimensional. The character of the E_4' for the operations C_9 is $-2\cos(2\pi/18) \approx -1.879$. It means that by the rotation along the main axis by $2\pi/18$ each HOMO changes the sign and gets a small contribution of the paired MO. Obviously, if the HOMOs would be symmetric and change only the sign by the C_9 rotation the character will be exactly -2. The reflection σ_h is the only operation which has character of 2 (E_4') and -2 (E_4''). It means that each HOMOs and LUMOs are symmetric with respect to this operation (HOMOs remain unchanged, whereas LUMOs change the sign).

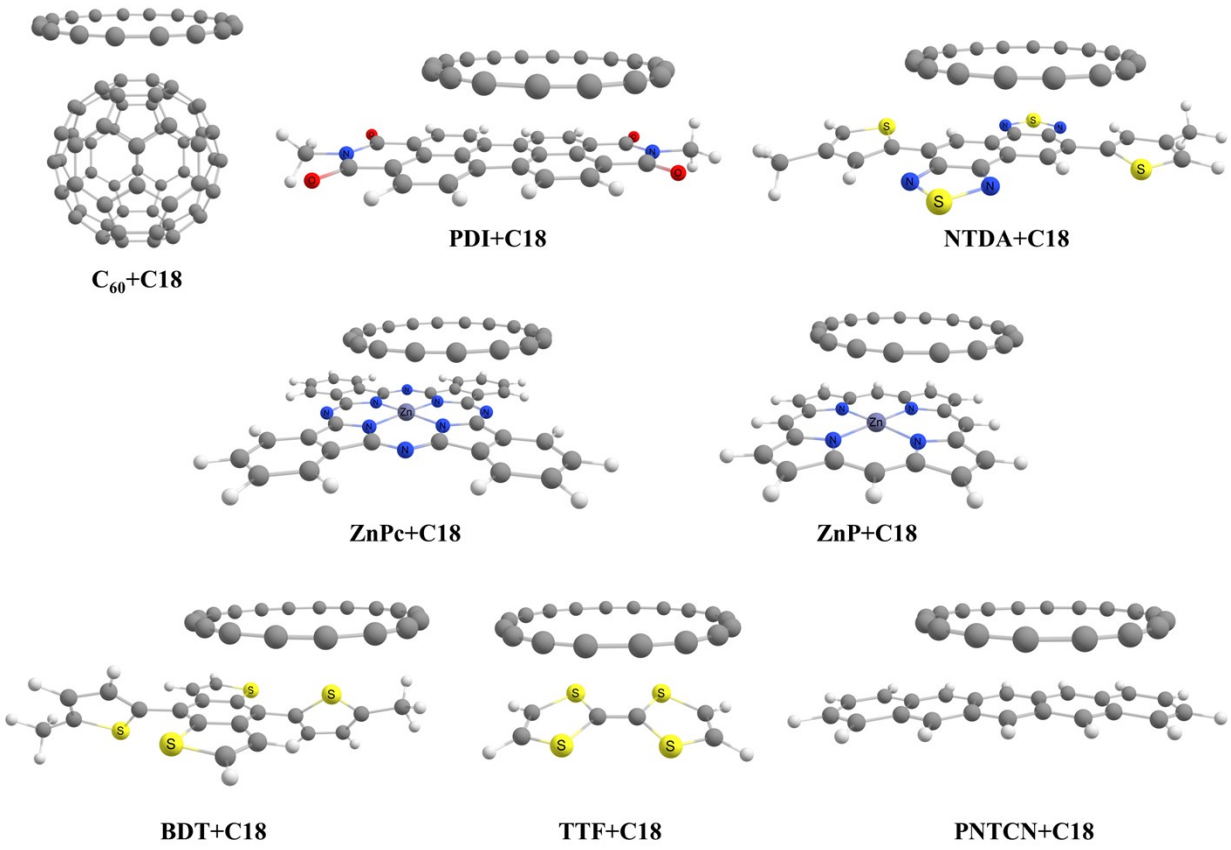


Figure S3. Structure of the C_{18} complexes optimized at the CAM-B3LYP-D3(zero-damping)/Def2-SVP level.

Table S1. List of the exchange-correlation (XC) density functionals considered in this work. Types: GGA and meta-GGA – generalized gradient approximation; GH – global hybrid; RSH – range separated hybrid.

XC Functional	HF exchange %	year	type	References
BLYP	0	1988	GGA	20-22
M06L	0	2006	meta-GGA	23
M11L	0	2011	meta-GGA	23
TPSSh	10	2002	GH-meta-GGA	25
B3LYP	20	1993	GH-GGA	26-28
PBE0	25	1999	GH-GGA	29,30
M06	27	2008	GH-meta-GGA	31
HISSbPBE[a]	0 – 60 – 0[b]	2008	RSH-GGA	32
M06-2X	54	2008	GH-meta-GGA	31
CAMB3LYP	19 – 65	2004	RSH-GGA	5
wB97XD[a]	22 – 100	2008	RSH-GGA	33
M11[a]	42 – 100	2011	RSH-meta-GGA	34
M06-HF	100	2006	GH-meta-GGA	35

[a] Empirical dispersion efficiently included in the functional; [b] Percentage of HF exchange in the short, middle (only for HISSbPBE) and long range.

Table S2. Analysis of the 80 lowest singlet excitation energies (E_X, eV), major orbital contributions (HOMO(H)–LUMO(L)) and their weights, oscillator strength (f), charge separation (CS, *e*) quantities and the extent of exciton localization (X) of LE states of the studied F_X+C_{18} vdW complexes.

	F_X + C_{18} vdW complex							
	C_{60}+C_{18}	PDI+C_{18}	NTDA+C_{18}	ZnPc+C_{18}	ZnP+C_{18}	TTF+C_{18}	BDT+C_{18}	PNTCN+C_{18}
	LE1 (excitation on C_{18})							
E_x	2.571	2.583	2.588	2.593	2.581	2.591	2.569	2.604
X	0.99	0.98	0.98	0.97	0.90	0.99	0.90	0.98
Transition (weight)	H-6-L+3 (0.45)	H-2-L+1 (0.44)	H-1-L+1 (0.21)	H-1-L+2 (0.35)	H-3-L (0.38)	H-3-L (0.46)	H-2-L+3 (0.25)	H-3-L+1 (0.43)
f	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	LE2 (excitation on F_X)							
E_x	2.636	2.941	3.859	3.655	3.898	3.324	3.950	2.639
X	0.99	0.88	0.81	0.97	0.91	0.97	0.93	0.90
Transition (weight)	H-1-L (0.31)	H-L (0.86)	H-L+5 (0.44)	H-9-L (0.82)	H-6-L+5 (0.65)	H-L+4 (0.92)	H-L+4 (0.87)	H-L+4 (0.94)
f	< 0.001	0.576	0.007	< 0.001	0.001	< 0.001	0.332	0.062

	Most absorptive transition							
E_x	n/a*	2.941	2.849	4.398	4.055	6.027	3.950	4.681
X		0.88	0.75	0.85	0.84	0.91	0.93	0.63
Transition (weight)		H-L (0.86)	H-L (0.70)	H-5-L+1 (0.50)	H-L+4 (0.36)	H-4-L+6 (0.20)	H-L+4 (0.87)	H-6-L+4 (0.34)
f		0.576	0.366	0.579	0.571	0.759	0.332	1.146
Localization		PDI	NTDA	ZnPc	ZnP	C18	BDT	PNTCN
	CT1 ($F_X \rightarrow C_{18}$)							
E_x	3.613	3.167	3.003	2.185	2.607	1.991	2.629	2.135
Transition (weight)	H-L+3 (0.24)	H-L+1 (0.77)	H-L+1 (0.74)	H-L+2 (0.83)	H-L+3 (0.53)	H-L+1 (0.87)	H-L+3 (0.53)	H-L (0.59)
f	< 0.001	0.003	0.004	0.016	< 0.001	0.011	0.002	0.020
CS	0.81	0.80	0.81	0.97	0.86	0.97	0.96	0.92
	CT2 ($C_{18} \rightarrow F_X$)							
E_x	3.888	3.588	3.990	3.727	4.344	6.442	5.387	4.253
Transition (weight)	H-5-L+1 (0.42)	H-2-L (0.88)	H-3-L+4 (0.56)	H-1-L+1 (0.80)	H-4-L+1 (0.85)	H-1-L+4 (0.53)	H-2-L+4 (0.52)	H-2-L+4 (0.81)
f	< 0.001	0.002	0.006	0.013	0.004	< 0.001	0.003	0.013
CS	0.99	0.96	0.91	0.92	0.95	0.96	0.87	0.96

* No transition with f > 0.05 found within studied excited states.

Table S3. Internal reorganization energy for electron transfer in the complexes [Fx···C_{18}].

Complex	Internal reorganization energy		
	F_X, eV	C_{18}, eV	Total, eV
C_{60}+C_{18}	0.115	0.394	0.509
PDI+C_{18}	0.156	0.399	0.555
NTDA+C_{18}	0.180	0.401	0.581
ZnPc+C_{18}	0.093	0.393	0.486
ZnP+C_{18}	0.107	0.385	0.492
TTF+C_{18}	0.539	0.393	0.932
BDT+C_{18}	0.265	0.392	0.657
PNTCN+C_{18}	0.091	0.397	0.488

Cartesian coordinates.

1. Cartesian coordinated for C_{18} molecule in singlet ground state and 1st triplet electronic states optimized within different exchange-correlation (XC) functionals. Gas-phase. XC-D3(zero-damping)/Def2-TZVP

XC = BLYP. Singlet

Atom	X	Y	Z
6	3.518957000	1.151130000	0.000002000
6	3.699389000	-0.121752000	-0.000001000
6	3.435456000	-1.379972000	0.000001000
6	2.755463000	-2.471009000	-0.000001000
6	1.744684000	-3.265428000	0.000001000
6	0.522454000	-3.664091000	-0.000001000
6	-0.762477000	-3.622756000	0.000001000
6	-1.955061000	-3.142643000	-0.000001000
6	-2.912955000	-2.285200000	0.000001000
6	-3.517891000	-1.150812000	-0.000001000
6	-3.700299000	0.121783000	0.000001000
6	-3.434473000	1.379600000	-0.000001000
6	-2.756297000	2.471775000	0.000001000
6	-1.744191000	3.264501000	-0.000001000
6	-0.522613000	3.665154000	0.000001000
6	0.762254000	3.621792000	-0.000002000
6	1.955559000	3.143467000	0.000001000
6	2.912041000	2.284462000	-0.000001000

XC = BLYP. Triplet

Atom	X	Y	Z
6	0.337123000	-3.671211000	0.000000000
6	-0.920810000	-3.566838000	0.000000000
6	-2.130715000	-3.051845000	0.000000000
6	-3.007733000	-2.134123000	0.000000000
6	-3.633244000	-0.991651000	0.000000000
6	-3.681271000	0.293963000	0.000000000
6	-3.423811000	1.551241000	0.000000000
6	-2.627041000	2.584850000	0.000000000
6	-1.611449000	3.343145000	0.000000000
6	-0.337123000	3.671212000	0.000000000
6	0.920810000	3.566838000	0.000000000
6	2.130715000	3.051845000	0.000000000
6	3.007733000	2.134123000	0.000000000
6	3.633244000	0.991651000	0.000000000
6	3.681271000	-0.293963000	0.000000000
6	3.423811000	-1.551241000	0.000000000
6	2.627041000	-2.584850000	0.000000000
6	1.611449000	-3.343145000	0.000000000

XC = M06L. Singlet

Atom	X	Y	Z
6	-3.472101000	-1.196815000	0.000002000
6	-3.672037000	0.062800000	-0.000002000
6	-3.429167000	1.314783000	0.000000000
6	-2.772535000	2.408114000	-0.000002000
6	-1.781760000	3.211135000	0.000001000
6	-0.575877000	3.626781000	0.000000000
6	0.699353000	3.605324000	0.000001000
6	1.890258000	3.148443000	-0.000001000
6	2.853471000	2.312331000	0.000001000
6	3.472069000	1.196932000	-0.000001000
6	3.672048000	-0.062725000	0.000001000
6	3.428877000	-1.314737000	-0.000001000
6	2.772763000	-2.408452000	0.000002000
6	1.781548000	-3.211033000	0.000000000
6	0.575859000	-3.627124000	0.000001000
6	-0.699363000	-3.605232000	-0.000003000
6	-1.890318000	-3.148544000	0.000000000
6	-2.853089000	-2.311982000	0.000000000

XC = M06L. Triplet

Atom	X	Y	Z
6	-1.795442000	3.177208000	-0.002096000
6	-0.619062000	3.606594000	-0.000988000
6	0.689426000	3.594731000	-0.000710000
6	1.857012000	3.141843000	-0.000596000
6	2.884983000	2.342445000	0.000677000
6	3.461010000	1.215797000	0.000159000
6	3.751600000	-0.036107000	0.001098000
6	3.436804000	-1.282309000	0.000204000
6	2.837550000	-2.396467000	0.001883000
6	1.795215000	-3.176709000	-0.001860000
6	0.619108000	-3.607145000	-0.000236000
6	-0.689299000	-3.593893000	-0.000751000
6	-1.857381000	-3.142557000	-0.000263000
6	-2.885165000	-2.342702000	0.000838000
6	-3.460828000	-1.216000000	0.000326000
6	-3.751120000	0.036064000	0.001042000
6	-3.436282000	1.282206000	0.000070000
6	-2.838129000	2.397000000	0.001203000

XC = M11L. Singlet

Atom	X	Y	Z
6	-2.432566000	-2.712380000	-0.000012000

XC = M11L. Triplet

Atom	X	Y	Z
6	-0.456115000	-3.431582000	0.000155000

6	-3.214030000	-1.717078000	-0.000040000
6	-3.607724000	-0.514528000	-0.000050000
6	-3.566067000	0.750142000	-0.000068000
6	-3.094224000	1.924280000	-0.000070000
6	-2.249262000	2.866175000	-0.000062000
6	-1.133053000	3.462172000	-0.000018000
6	0.119671000	3.640948000	0.000026000
6	1.357925000	3.380476000	0.000034000
6	2.432520000	2.712348000	0.000021000
6	3.213951000	1.717025000	0.000004000
6	3.607755000	0.514509000	0.000002000
6	3.566145000	-0.750158000	0.000016000
6	3.094227000	-1.924275000	0.000028000
6	2.249234000	-2.866125000	0.000047000
6	1.133084000	-3.462248000	0.000059000
6	-0.119666000	-3.640862000	0.000052000
6	-1.357921000	-3.380421000	0.000029000

6	-1.661570000	-3.058706000	-0.000477000
6	-2.788047000	-2.460544000	-0.000381000
6	-3.408455000	-1.354847000	-0.000280000
6	-3.923178000	-0.186145000	-0.000416000
6	-3.539831000	1.031211000	-0.000502000
6	-3.051371000	2.202921000	-0.000277000
6	-1.977497000	2.892053000	0.000477000
6	-0.816182000	3.387116000	0.000458000
6	0.456115000	3.431586000	0.000003000
6	1.661572000	3.058711000	-0.000459000
6	2.788044000	2.460542000	-0.000194000
6	3.408457000	1.354847000	0.000043000
6	3.923174000	0.186144000	0.000024000
6	3.539835000	-1.031213000	0.000002000
6	3.051370000	-2.202920000	0.000194000
6	1.977497000	-2.892055000	0.000876000
6	0.816182000	-3.387118000	0.000753000

XC = TPSSh. Singlet

Atom	X	Y	Z
6	2.964893000	-2.183282000	0.000038000
6	3.533338000	-1.037269000	0.000014000
6	3.674716000	0.233191000	0.000065000
6	3.373392000	1.476448000	0.000039000
6	2.665125000	2.540588000	0.000078000
6	1.635037000	3.299153000	0.000031000
6	0.408440000	3.659032000	0.000050000
6	-0.868259000	3.578121000	-0.000004000
6	-2.039309000	3.065607000	0.000015000
6	-2.965387000	2.183037000	-0.000038000
6	-3.532901000	1.037644000	-0.000018000
6	-3.675038000	-0.233703000	-0.000067000
6	-3.373376000	-1.475893000	-0.000036000
6	-2.665002000	-2.541135000	-0.000073000
6	-1.635328000	-3.298642000	-0.000029000
6	-0.407971000	-3.659371000	-0.000053000
6	0.867724000	-3.577933000	0.000005000
6	2.039904000	-3.065593000	-0.000015000

XC = TPSSh. Triplet

Atom	X	Y	Z
6	-2.066727000	3.068848000	0.000024000
6	-2.954910000	2.174337000	0.000070000
6	-3.607653000	1.052768000	0.000123000
6	-3.673325000	-0.225654000	0.000147000
6	-3.445714000	-1.481521000	0.000164000
6	-2.661542000	-2.519386000	0.000150000
6	-1.667543000	-3.290704000	0.000124000
6	-0.400792000	-3.635246000	0.000080000
6	0.848826000	-3.555681000	0.000025000
6	2.066727000	-3.068848000	-0.000031000
6	2.954910000	-2.174337000	-0.000085000
6	3.607653000	-1.052768000	-0.000121000
6	3.673325000	0.225654000	-0.000146000
6	3.445714000	1.481521000	-0.000155000
6	2.661542000	2.519386000	-0.000144000
6	1.667543000	3.290704000	-0.000119000
6	0.400792000	3.635246000	-0.000077000
6	-0.848826000	3.555681000	-0.000031000

XC = B3LYP. Singlet

Atom	X	Y	Z
6	-3.121856000	1.941117000	0.000009000
6	-3.597576000	0.756426000	0.000052000
6	-3.639337000	-0.519751000	0.000050000
6	-3.242191000	-1.733056000	0.000053000
6	-2.453801000	-2.737444000	0.000040000
6	-1.369712000	-3.411675000	0.000059000
6	-0.120137000	-3.674220000	0.000036000
6	1.143689000	-3.493753000	0.000021000
6	2.269779000	-2.891858000	-0.000015000
6	3.121944000	-1.941248000	-0.000018000
6	3.597671000	-0.756334000	-0.000039000

XC = B3LYP. Triplet

Atom	X	Y	Z
6	-0.508351000	3.535550000	0.000128000
6	-1.778643000	3.193078000	0.000315000
6	-2.741466000	2.390209000	0.000510000
6	-3.569468000	1.383249000	0.000664000
6	-3.704904000	0.113753000	0.000582000
6	-3.658171000	-1.164515000	0.000479000
6	-2.894143000	-2.218771000	0.000148000
6	-1.986716000	-3.085860000	-0.000158000
6	-0.736990000	-3.495398000	-0.000390000
6	0.508351000	-3.535550000	-0.000512000
6	1.778643000	-3.193078000	-0.000535000

6	3.639504000	0.519642000	-0.000036000
6	3.241981000	1.733031000	-0.000061000
6	2.453931000	2.737430000	-0.000058000
6	1.369517000	3.411517000	-0.000056000
6	0.120218000	3.674392000	-0.000018000
6	-1.143770000	3.493628000	-0.000018000
6	-2.269856000	2.892157000	-0.000001000
6	2.741466000	-2.390209000	-0.000418000
6	3.569468000	-1.383249000	-0.000283000
6	3.704906000	-0.113753000	-0.000200000
6	3.658172000	1.164515000	-0.000099000
6	2.894142000	2.218770000	-0.000114000
6	1.986715000	3.085859000	-0.000101000
6	0.736990000	3.495398000	-0.000014000

XC = PBE0. Singlet

Atom	X	Y	Z
6	3.163395000	-1.868642000	0.000008000
6	3.611786000	-0.674102000	0.000054000
6	3.624590000	0.601997000	0.000050000
6	3.200223000	1.805298000	0.000050000
6	2.389661000	2.790981000	0.000037000
6	1.291141000	3.440040000	0.000060000
6	0.036599000	3.673946000	0.000038000
6	-1.222091000	3.464903000	0.000022000
6	-2.333632000	2.837964000	-0.000016000
6	-3.163507000	1.868771000	-0.000018000
6	-3.611978000	0.674019000	-0.000038000
6	-3.624797000	-0.601869000	-0.000034000
6	-3.199981000	-1.805237000	-0.000063000
6	-2.389776000	-2.790933000	-0.000061000
6	-1.290918000	-3.439843000	-0.000057000
6	-0.036669000	-3.674141000	-0.000015000
6	1.222197000	-3.464812000	-0.000016000
6	2.333757000	-2.838340000	-0.000002000

XC = PBE0. Triplet

Atom	X	Y	Z
6	0.512184000	-3.531812000	0.000312000
6	1.781853000	-3.188604000	0.000426000
6	2.743453000	-2.385627000	0.000467000
6	3.570150000	-1.378438000	0.000484000
6	3.703736000	-0.109428000	0.000396000
6	3.655622000	1.168106000	0.000299000
6	2.890269000	2.220582000	0.000128000
6	1.982124000	3.085694000	-0.000033000
6	0.732152000	3.493099000	-0.000203000
6	-0.512184000	3.531812000	-0.000327000
6	-1.781853000	3.188604000	-0.000423000
6	-2.743453000	2.385627000	-0.000460000
6	-3.570150000	1.378438000	-0.000462000
6	-3.703736000	0.109428000	-0.000386000
6	-3.655622000	-1.168106000	-0.000280000
6	-2.890268000	-2.220582000	-0.000134000
6	-1.982124000	-3.085694000	0.000024000
6	-0.732152000	-3.493099000	0.000173000

XC = M06. Singlet

Atom	X	Y	Z
6	-1.151147000	3.489607000	0.000022000
6	-2.295768000	2.868272000	0.000033000
6	-3.124884000	1.933163000	0.000047000
6	-3.602574000	0.721547000	0.000059000
6	-3.636762000	-0.527739000	0.000057000
6	-3.223591000	-1.762853000	0.000044000
6	-2.446560000	-2.741679000	0.000031000
6	-1.336167000	-3.422291000	0.000017000
6	-0.111777000	-3.672773000	0.000001000
6	1.176342000	-3.480512000	-0.000020000
6	2.275318000	-2.885432000	-0.000039000
6	3.138547000	-1.910214000	-0.000051000
6	3.597888000	-0.747932000	-0.000054000
6	3.632000000	0.554008000	-0.000051000
6	3.236624000	1.739565000	-0.000047000
6	2.426154000	2.759041000	-0.000039000
6	1.361283000	3.413208000	-0.000017000
6	0.085073000	3.673012000	0.000007000

XC = M06. Triplet

Atom	X	Y	Z
6	-1.831800000	-3.191234000	0.000020000
6	-0.653301000	-3.602009000	0.000036000
6	0.658395000	-3.601335000	0.000048000
6	1.836093000	-3.188718000	0.000050000
6	2.827486000	-2.342130000	0.000053000
6	3.487728000	-1.266564000	0.000044000
6	3.682187000	0.002674000	0.000036000
6	3.486026000	1.271220000	0.000017000
6	2.823998000	2.346108000	0.000005000
6	1.831799000	3.191233000	-0.000021000
6	0.653301000	3.602010000	-0.000033000
6	-0.658395000	3.601337000	-0.000051000
6	-1.836091000	3.188713000	-0.000055000
6	-2.827486000	2.342130000	-0.000057000
6	-3.487730000	1.266565000	-0.000048000
6	-3.682185000	-0.002674000	-0.000033000
6	-3.486029000	-1.271220000	-0.000016000
6	-2.823995000	-2.346105000	0.000004000

XC = HISSbPBE. Singlet

Atom	X	Y	Z

XC = HISSbPBE. Triplet

Atom	X	Y	Z

6	1.925302000	-3.116163000	0.000028000
6	2.899868000	-2.240528000	0.000027000
6	3.477945000	-1.149581000	0.000056000
6	3.661636000	0.147635000	0.000048000
6	3.403246000	1.354935000	0.000064000
6	2.710074000	2.466707000	0.000039000
6	1.736071000	3.225429000	0.000041000
6	0.490443000	3.631530000	0.000007000
6	-0.743380000	3.586726000	0.000006000
6	-1.958636000	3.097148000	-0.000028000
6	-2.875024000	2.269761000	-0.000028000
6	-3.491336000	1.113605000	-0.000057000
6	-3.661448000	-0.109259000	-0.000047000
6	-3.390351000	-1.391066000	-0.000062000
6	-2.734531000	-2.437124000	-0.000040000
6	-1.702935000	-3.244795000	-0.000042000
6	-0.528178000	-3.624633000	-0.000008000
6	0.781235000	-3.580326000	-0.000005000
6	-0.319364000	3.622267000	0.000052000
6	-1.526587000	3.336882000	0.000056000
6	-2.582054000	2.574192000	0.000117000
6	-3.347622000	1.581515000	0.000060000
6	-3.645447000	0.334237000	0.000063000
6	-3.587021000	-0.940805000	-0.000018000
6	-3.013641000	-2.061396000	0.000016000
6	-2.121447000	-3.004412000	-0.000018000
6	-0.982636000	-3.501023000	0.000024000
6	0.318167000	-3.643060000	-0.000019000
6	1.516704000	-3.320455000	0.000001000
6	2.596620000	-2.592925000	-0.000036000
6	3.330009000	-1.574173000	-0.000032000
6	3.669805000	-0.336908000	-0.000060000
6	3.568161000	0.936394000	-0.000061000
6	3.032018000	2.077117000	-0.000075000
6	2.109025000	2.990013000	-0.000042000
6	0.985311000	3.522542000	-0.000029000

XC = M06-2X. Singlet

Atom	X	Y	Z
6	1.725548000	-3.269351000	0.000042000
6	2.780878000	-2.436021000	0.000017000
6	3.423712000	-1.395556000	0.000071000
6	3.696323000	-0.078849000	0.000036000
6	3.519769000	1.131465000	0.000074000
6	2.882104000	2.315395000	0.000028000
6	1.968830000	3.129142000	0.000053000
6	0.719319000	3.626282000	-0.000005000
6	-0.503279000	3.662611000	0.000017000
6	-1.779905000	3.240235000	-0.000041000
6	-2.739866000	2.482260000	-0.000016000
6	-3.446492000	1.338034000	-0.000068000
6	-3.694576000	0.140294000	-0.000034000
6	-3.500301000	-1.190310000	-0.000074000
6	-2.920347000	-2.267214000	-0.000027000
6	-1.916200000	-3.161429000	-0.000055000
6	-0.779813000	-3.613603000	0.000002000
6	0.564296000	-3.653385000	-0.000020000

XC = M06-2X. Triplet

Atom	X	Y	Z
6	3.360096000	-1.508059000	0.000048000
6	3.710007000	-0.267965000	0.000015000
6	3.554442000	0.981149000	0.000064000
6	3.000512000	2.173700000	0.000035000
6	2.095213000	3.019981000	0.000063000
6	0.883304000	3.571349000	0.000037000
6	-0.345265000	3.659852000	0.000047000
6	-1.626891000	3.293461000	0.000014000
6	-2.643222000	2.588778000	0.000009000
6	-3.370734000	1.488157000	-0.000027000
6	-3.709410000	0.280878000	-0.000033000
6	-3.545642000	-1.003001000	-0.000064000
6	-3.008317000	-2.163215000	-0.000051000
6	-2.076973000	-3.025332000	-0.000070000
6	-0.895724000	-3.563619000	-0.000032000
6	0.358598000	-3.652171000	-0.000046000
6	1.609094000	-3.295807000	0.000006000
6	2.650910000	-2.578135000	-0.000015000

XC = CAMB3LYP. Singlet

Atom	X	Y	Z
6	-1.572820000	-3.334546000	0.000038000
6	-0.275710000	-3.676626000	0.000021000
6	0.938596000	-3.565475000	0.000067000
6	2.152115000	-2.993720000	0.000037000
6	3.010836000	-2.127991000	0.000070000
6	3.572950000	-0.909978000	0.000030000
6	3.674291000	0.305184000	0.000051000
6	3.321938000	1.599547000	-0.000001000
6	2.618506000	2.595574000	0.000015000
6	1.516577000	3.360612000	-0.000038000

XC = CAMB3LYP. Triplet

Atom	X	Y	Z
6	-2.868416000	-2.387070000	-0.000464000
6	-3.446844000	-1.244477000	-0.000351000
6	-3.754163000	-0.020711000	-0.000105000
6	-3.451153000	1.253909000	-0.000163000
6	-2.867033000	2.345155000	0.000234000
6	-1.820025000	3.164899000	0.000096000
6	-0.671690000	3.593395000	0.000261000
6	0.664826000	3.594586000	0.000088000
6	1.813977000	3.168350000	0.000041000
6	2.862488000	2.350447000	0.000018000

6	0.337484000	3.671456000	-0.000019000
6	-0.998408000	3.549253000	-0.000066000
6	-2.101417000	3.029389000	-0.000038000
6	-3.046245000	2.077112000	-0.000072000
6	-3.557063000	0.969885000	-0.000030000
6	-3.668741000	-0.366926000	-0.000051000
6	-3.348304000	-1.543450000	0.000001000
6	-2.574582000	-2.639301000	-0.000017000
6	3.448751000	1.260429000	-0.000102000
6	3.754099000	-0.013728000	0.000047000
6	3.449217000	-1.237997000	0.000059000
6	2.873035000	-2.381845000	0.000358000
6	1.827439000	-3.136618000	0.000268000
6	0.654151000	-3.583843000	0.000203000
6	-0.647266000	-3.584882000	-0.000118000
6	-1.821393000	-3.140001000	-0.000370000

XC = wB97XD. Singlet

Atom	X	Y	Z
6	-2.319693000	-2.873503000	0.000037000
6	-1.136922000	-3.513484000	0.000023000
6	0.070227000	-3.691969000	0.000065000
6	1.387700000	-3.422105000	0.000039000
6	2.427342000	-2.783153000	0.000068000
6	3.263444000	-1.729781000	0.000032000
6	3.648941000	-0.571986000	0.000050000
6	3.612044000	0.772380000	0.000002000
6	3.162689000	1.906920000	0.000013000
6	2.270167000	2.912911000	-0.000036000
6	1.196753000	3.493337000	-0.000021000
6	-0.133548000	3.690393000	-0.000063000
6	-1.328998000	3.445465000	-0.000040000
6	-2.474788000	2.741396000	-0.000071000
6	-3.232927000	1.785224000	-0.000034000
6	-3.658174000	0.509396000	-0.000049000
6	-3.624320000	-0.710384000	-0.000001000
6	-3.129938000	-1.961057000	-0.000013000

XC = wB97XD. Triplet

Atom	X	Y	Z
6	-0.978727000	3.525637000	-0.000030000
6	-2.145485000	3.063799000	-0.000316000
6	-3.032073000	2.085792000	-0.000324000
6	-3.652543000	0.974145000	-0.000317000
6	-3.679741000	-0.318960000	0.000131000
6	-3.419359000	-1.594108000	0.000531000
6	-2.619058000	-2.575757000	0.000394000
6	-1.569337000	-3.384749000	0.000240000
6	-0.343251000	-3.642851000	-0.000044000
6	0.987722000	-3.587173000	-0.000240000
6	2.111460000	-3.022682000	-0.000320000
6	3.083726000	-2.130121000	-0.000281000
6	3.596623000	-0.960578000	-0.000182000
6	3.748130000	0.326083000	-0.000019000
6	3.367295000	1.572325000	0.000131000
6	2.660877000	2.628168000	0.000223000
6	1.541875000	3.337898000	0.000266000
6	0.341865000	3.703132000	0.000157000

XC = M11. Singlet

Atom	X	Y	Z
6	2.319731000	2.887062000	0.000039000
6	1.123204000	3.528699000	0.000020000
6	-0.079070000	3.702065000	0.000066000
6	-1.408226000	3.424888000	0.000037000
6	-2.440906000	2.785361000	0.000069000
6	-3.281046000	1.718805000	0.000031000
6	-3.661024000	0.565052000	0.000051000
6	-3.618738000	-0.791940000	0.000001000
6	-3.167696000	-1.919790000	0.000016000
6	-2.262642000	-2.931882000	-0.000037000
6	-1.192124000	-3.505831000	-0.000020000
6	0.151693000	-3.699739000	-0.000066000
6	1.340855000	-3.451922000	-0.000040000
6	2.495085000	-2.737087000	-0.000073000
6	3.246762000	-1.782920000	-0.000031000
6	3.671298000	-0.493239000	-0.000050000
6	3.633448000	0.720838000	0.000002000
6	3.129397000	1.981580000	-0.000015000

XC = M11. Triplet

Atom	X	Y	Z
6	3.240183000	-1.763213000	0.000089000
6	3.680036000	-0.533643000	0.000364000
6	3.626724000	0.709408000	0.000274000
6	3.150647000	1.957146000	0.000086000
6	2.326554000	2.863030000	-0.000028000
6	1.138520000	3.511876000	-0.000116000
6	-0.065062000	3.687644000	-0.000125000
6	-1.394679000	3.413871000	-0.000085000
6	-2.438458000	2.784823000	-0.000023000
6	-3.267502000	1.722842000	0.000059000
6	-3.675243000	0.560318000	0.000095000
6	-3.614260000	-0.761482000	0.000103000
6	-3.167182000	-1.934696000	0.000045000
6	-2.286489000	-2.880429000	-0.000041000
6	-1.163365000	-3.492301000	-0.000143000
6	0.096603000	-3.670049000	-0.000224000
6	1.355907000	-3.412531000	-0.000205000
6	2.457069000	-2.762614000	-0.000126000

XC = M06-HF. Singlet

XC = M06-HF. Triplet

Atom	X	Y	Z
6	-2.582416000	-2.666275000	0.000006000
6	-1.438145000	-3.420793000	-0.000004000
6	-0.263739000	-3.701191000	0.000005000
6	1.097866000	-3.544645000	-0.000003000
6	2.178018000	-3.005225000	0.000004000
6	3.120794000	-2.010280000	-0.000004000
6	3.601794000	-0.902778000	0.000003000
6	3.683732000	0.465512000	-0.000005000
6	3.339224000	1.622691000	0.000004000
6	2.522350000	2.723408000	-0.000004000
6	1.514172000	3.387806000	0.000005000
6	0.181002000	3.706241000	-0.000003000
6	-1.018469000	3.568125000	0.000004000
6	-2.244508000	2.955635000	-0.000004000
6	-3.075359000	2.079546000	0.000004000
6	-3.620869000	0.822114000	-0.000007000
6	-3.693381000	-0.383161000	0.000004000
6	-3.302067000	-1.696732000	-0.000005000
6	2.771668000	-2.579353000	-0.000721000
6	3.391229000	-1.410539000	0.000128000
6	3.710822000	-0.222006000	0.000277000
6	3.506748000	1.116914000	0.001187000
6	2.974564000	2.207546000	0.000069000
6	1.969770000	3.135322000	0.000510000
6	0.859041000	3.611224000	-0.000383000
6	-0.510347000	3.676497000	-0.000385000
6	-1.661114000	3.307978000	-0.000453000
6	-2.749873000	2.480122000	-0.000594000
6	-3.383579000	1.445209000	-0.000210000
6	-3.714612000	0.131743000	-0.000204000
6	-3.510661000	-1.081830000	0.000300000
6	-3.005938000	-2.304879000	0.000332000
6	-1.989727000	-3.067595000	0.000421000
6	-0.815278000	-3.572340000	0.000058000
6	0.470252000	-3.632549000	-0.000096000
6	1.687035000	-3.241464000	-0.000237000

2. Cartesian coordinated for F_X+C18 vdW complexes molecule in singlet ground state optimized at CAM-B3LYP-D3(zero-damping)/Def2-SVP. Gas-phase.

C_{60}+C18

Atom	X	Y	Z
6	-0.288965000	0.617106000	3.085558000
6	-0.290903000	-0.834389000	3.032902000
6	-1.081996000	1.344263000	2.209098000
6	-1.085780000	-1.494033000	2.106155000
6	-0.566180000	-2.644424000	1.389972000
6	1.062665000	-1.293884000	3.283802000
6	1.561039000	-2.394052000	2.598562000
6	0.728664000	-3.084372000	1.630539000
6	0.736615000	2.960113000	1.849956000
6	1.567112000	2.199168000	2.765294000
6	-0.559422000	2.542270000	1.578219000
6	1.065759000	1.053599000	3.369128000
6	1.901013000	-0.127266000	3.491635000
6	2.926162000	2.215167000	2.256141000
6	3.725164000	1.085894000	2.373605000
6	3.201187000	-0.111340000	3.004957000
6	-0.259672000	3.057772000	-0.808401000
6	1.095131000	3.494011000	-0.524351000
6	-1.067203000	2.591429000	0.219413000
6	1.582138000	3.446552000	0.775219000
6	2.935423000	2.985969000	1.026266000
6	1.939625000	3.083520000	-1.631327000
6	3.234216000	2.643558000	-1.390757000
6	3.743257000	2.593814000	-0.032541000
6	-1.897303000	0.774014000	-1.214596000
6	-1.052700000	1.261367000	-2.290157000
6	-1.904477000	1.423727000	0.011275000

PDI+C18

Atom	X	Y	Z
8	-6.252655000	2.092367000	0.889804000
8	-6.336484000	-2.353257000	-0.019615000
7	-6.302873000	-0.121901000	0.432736000
6	-4.163604000	0.979514000	0.921337000
6	-3.456503000	2.118228000	1.233748000
6	-2.063150000	2.069508000	1.367496000
1	-1.539979000	2.994906000	1.600708000
6	-1.353357000	0.889988000	1.194462000
6	-2.072230000	-0.309647000	0.904935000
6	-1.412723000	-1.566902000	0.751404000
6	-2.173110000	-2.686817000	0.446403000
1	-1.693823000	-3.654859000	0.312099000
6	-3.562687000	-2.614553000	0.286462000
6	-4.218526000	-1.413824000	0.439185000
6	-5.693065000	-1.366408000	0.261035000
6	-3.484135000	-0.248491000	0.757177000
6	-5.635920000	1.058362000	0.756733000
8	4.955001000	-2.823798000	1.167651000
8	5.066985000	1.674412000	1.759659000
7	5.019278000	-0.582973000	1.467189000
6	2.863839000	-1.715357000	1.155510000
6	2.147137000	-2.870766000	0.943030000
6	0.752951000	-2.823920000	0.818007000
1	0.224675000	-3.759071000	0.641173000
6	0.050598000	-1.630733000	0.908823000
6	0.774092000	-0.423381000	1.152349000
6	0.116089000	0.837407000	1.286047000

6	-0.252300000	2.377600000	-2.091726000
6	1.107065000	2.393837000	-2.599848000
6	-0.533135000	0.111761000	-3.007859000
6	0.767306000	0.127701000	-3.494456000
6	1.605449000	1.294157000	-3.285851000
6	-1.915511000	-0.732773000	1.189653000
6	-1.908037000	-1.411762000	-0.091558000
6	-1.913635000	0.653667000	1.239906000
6	-1.899064000	-0.675053000	-1.267136000
6	-1.055765000	-1.085451000	-2.375314000
6	-1.073860000	-2.593580000	0.031276000
6	-0.267651000	-2.986553000	-1.027760000
6	-0.258369000	-2.215252000	-2.258451000
6	2.956743000	-0.616250000	-3.086187000
6	1.602360000	-1.053052000	-3.371166000
6	1.101001000	-2.198210000	-2.766561000
6	3.751420000	-1.343652000	-2.210551000
6	4.586032000	0.733662000	-1.192135000
6	3.755226000	1.494179000	-2.107600000
6	2.958694000	0.834263000	-3.033569000
6	4.584191000	-0.653781000	-1.242465000
6	4.567758000	-0.774344000	1.213998000
6	4.569666000	0.676047000	1.266625000
6	4.578568000	1.413287000	0.090246000
6	4.574853000	-1.424510000	-0.012703000
6	2.927399000	-3.056451000	0.806965000
6	2.920057000	-2.376714000	2.089442000
6	3.722065000	-1.261076000	2.288441000
6	3.736482000	-2.590879000	-0.220685000
6	1.931669000	-2.958579000	-1.850696000
6	1.085965000	-3.445753000	-0.776249000
6	1.572954000	-3.494127000	0.523292000
6	3.227426000	-2.540700000	-1.578960000
6	-4.458011000	-0.566699000	-3.657176000
6	-4.457866000	0.783704000	-3.646047000
6	-4.455844000	1.919212000	-3.164588000
6	-4.450807000	2.947665000	-2.289384000
6	-4.448781000	3.508508000	-1.190963000
6	-4.449901000	3.732035000	0.140898000
6	-4.448680000	3.454043000	1.342530000
6	-4.446112000	2.768842000	2.506242000
6	-4.443452000	1.783379000	3.247881000
6	-4.438394000	0.510658000	3.699390000
6	-4.438083000	-0.720995000	3.635073000
6	-4.442000000	-1.986415000	3.163488000
6	-4.443971000	-2.889090000	2.323049000
6	-4.445148000	-3.555114000	1.148247000
6	-4.446375000	-3.705732000	-0.075883000
6	-4.445931000	-3.460605000	-1.403933000
6	-4.448990000	-2.788372000	-2.437949000
6	-4.455241000	-1.746236000	-3.296797000
6	0.885232000	1.973257000	1.494566000
1	0.411358000	2.949236000	1.581006000
6	2.280988000	1.911165000	1.593634000
6	2.933139000	0.703573000	1.483057000
6	4.413113000	0.667750000	1.591689000
6	2.189347000	-0.478300000	1.264394000
6	4.340911000	-1.784140000	1.263031000
1	-4.003171000	3.053533000	1.362061000
1	2.873883000	2.811732000	1.756536000
1	2.688781000	-3.814329000	0.864657000
1	-4.148038000	-3.500886000	0.038118000
6	-7.747440000	-0.016791000	0.270039000
1	-8.134655000	-1.006988000	0.015740000
1	-8.203522000	0.347698000	1.200141000
1	-7.982837000	0.704627000	-0.523673000
6	6.472313000	-0.671440000	1.529011000
1	6.868823000	0.335762000	1.681359000
1	6.773574000	-1.333712000	2.351229000
1	6.857834000	-1.099600000	0.593900000
6	-1.358542000	3.274968000	-1.746140000
6	-2.134254000	2.212057000	-2.052302000
6	-2.403928000	1.038720000	-2.316463000
6	-2.285492000	-0.284781000	-2.559949000
6	-1.708843000	-1.365572000	-2.697266000
6	-0.747617000	-2.312561000	-2.764836000
6	0.392291000	-2.781806000	-2.731103000
6	1.732678000	-2.911822000	-2.623855000
6	2.901237000	-2.560897000	-2.446690000
6	4.002536000	-1.817797000	-2.204124000
6	4.661560000	-0.805602000	-1.956775000
6	5.015114000	0.467925000	-1.678876000
6	4.860634000	1.669607000	-1.450685000
6	4.284107000	2.874886000	-1.253925000
6	3.366360000	3.693514000	-1.170219000
6	2.136165000	4.251714000	-1.174134000
6	0.909536000	4.314760000	-1.283496000
6	-0.385256000	3.986787000	-1.488480000

NTDA+C18

Atom	X	Y	Z
6	-7.396939000	-0.348541000	-1.225615000
6	-6.062737000	0.333805000	-1.263880000
6	-4.819106000	-0.368292000	-1.250914000
6	-3.717051000	0.451112000	-1.276437000
6	-2.300687000	0.088942000	-1.222247000
6	-1.308688000	1.030652000	-1.116888000
6	0.083209000	0.712682000	-1.069452000
6	1.090033000	1.738237000	-0.985976000
7	0.855335000	3.038809000	-0.948419000
16	2.295763000	3.791004000	-0.860051000
7	3.265942000	2.484782000	-0.870144000
6	2.498240000	1.407438000	-0.940741000
6	2.936504000	0.025831000	-0.963684000
6	4.349677000	-0.337735000	-0.860923000
6	5.458405000	0.471218000	-0.913993000
6	6.693325000	-0.229647000	-0.760929000
6	8.034369000	0.440102000	-0.788157000
6	6.488920000	-1.570404000	-0.585662000
16	4.824067000	-1.994481000	-0.602536000
6	1.944416000	-0.915412000	-1.058777000
6	0.552685000	-0.596117000	-1.111561000
6	-0.451778000	-1.620779000	-1.218764000
7	-0.213259000	-2.920353000	-1.288115000
16	-1.649189000	-3.672384000	-1.414508000
7	-2.623483000	-2.369573000	-1.384791000
6	-1.859730000	-1.291611000	-1.275586000
16	-4.209576000	2.120473000	-1.336931000
6	-5.872097000	1.686906000	-1.309424000
1	-8.221277000	0.377550000	-1.236375000
1	-7.497841000	-0.964216000	-0.318237000
1	-7.523054000	-1.019793000	-2.089172000
1	-4.732909000	-1.451454000	-1.213213000
1	-1.560713000	2.091113000	-1.064212000
1	5.383309000	1.547095000	-1.053600000
1	8.848625000	-0.283711000	-0.646570000
1	8.200198000	0.954630000	-1.747387000
1	8.112677000	1.199332000	0.005444000
1	2.195479000	-1.976619000	-1.093875000
1	-6.638699000	2.460158000	-1.332986000
1	7.247101000	-2.339082000	-0.442157000
6	-1.682701000	-3.644365000	2.065583000
6	-0.343400000	-3.814835000	2.108861000
6	0.844744000	-3.490020000	2.161829000
6	1.983690000	-2.767699000	2.234368000
6	2.688865000	-1.759222000	2.311060000
6	3.084134000	-0.470055000	2.387484000
6	2.956495000	0.755281000	2.424660000
6	2.412975000	1.992095000	2.431100000
6	1.523835000	2.846053000	2.406090000
6	0.318852000	3.454378000	2.353541000

ZnPc+C18

Atom	X	Y	Z
6	3.263389000	-1.163586000	-0.492050000
6	3.954657000	-2.446422000	-0.379687000
6	5.291588000	-2.775222000	-0.171938000
1	6.042736000	-1.991006000	-0.065790000
6	5.620205000	-4.124491000	-0.104206000
6	4.637885000	-5.120909000	-0.240864000
6	3.302961000	-4.792268000	-0.448568000
1	2.529325000	-5.554419000	-0.554179000
6	2.974335000	-3.441168000	-0.516255000
6	1.702595000	-2.747125000	-0.706014000
6	1.683989000	2.756149000	-0.707666000
6	2.950886000	3.458827000	-0.517405000
6	3.270362000	4.812136000	-0.449937000
1	2.491649000	5.569014000	-0.556139000
6	4.602915000	5.149847000	-0.241671000
6	5.591890000	4.160125000	-0.104181000
6	5.272444000	2.808660000	-0.171678000
1	6.028808000	2.029568000	-0.064856000
6	3.937851000	2.470760000	-0.380037000
6	3.255377000	1.183255000	-0.492472000
6	-2.209901000	1.164472000	-1.170479000
6	-2.903397000	2.446592000	-1.279735000
6	-4.246926000	2.773360000	-1.439243000
1	-5.000150000	1.988271000	-1.519045000
6	-4.581606000	4.122484000	-1.477621000
6	-3.597827000	5.119823000	-1.363109000
6	-2.255069000	4.792505000	-1.210283000
1	-1.480521000	5.555315000	-1.117278000
6	-1.921040000	3.441698000	-1.170113000
6	-0.644967000	2.749134000	-0.999731000
6	-0.626394000	-2.756056000	-0.998072000
6	-1.897834000	-3.457346000	-1.167475000
6	-2.222735000	-4.810393000	-1.206373000
1	-1.443000000	-5.567865000	-1.113015000
6	-3.563326000	-5.146920000	-1.358332000
6	-4.553844000	-4.156347000	-1.473304000
6	-4.228256000	-2.804947000	-1.436302000
1	-4.986817000	-2.025070000	-1.516518000
6	-2.886913000	-2.468971000	-1.277596000
6	-2.202034000	-1.182117000	-1.169642000
7	1.934502000	-1.405981000	-0.684080000
7	3.860404000	0.011881000	-0.411894000
7	1.924968000	1.416578000	-0.685191000
7	0.516971000	3.359394000	-0.860548000
7	-0.879495000	1.405533000	-1.003221000
7	-2.810634000	-0.010882000	-1.236867000
7	-0.869970000	-1.414075000	-1.002656000
7	0.539670000	-3.358295000	-0.858600000
30	0.525704000	0.000497000	-0.804775000
1	-3.856240000	-6.198525000	-1.388464000

6	-0.908126000	3.549341000	2.283542000
6	-2.224361000	3.256392000	2.203653000
6	-3.232865000	2.550169000	2.139687000
6	-4.058173000	1.482310000	2.083058000
6	-4.368264000	0.289992000	2.046898000
6	-4.285681000	-1.058066000	2.021878000
6	-3.740199000	-2.163629000	2.018619000
6	-2.807734000	-3.140581000	2.033873000
1	-5.596893000	-4.457602000	-1.591059000
1	-5.626605000	4.416629000	-1.596056000
1	-3.897827000	6.169399000	-1.394295000
1	6.628433000	4.462698000	0.059316000
1	4.890796000	6.201662000	-0.182353000
1	4.932909000	-6.170732000	-0.181379000
1	6.658855000	-4.420005000	0.058825000
6	-2.735034000	3.487983000	2.121477000
6	-1.419666000	3.759260000	2.264891000
6	-0.216009000	3.521154000	2.385835000
6	0.958524000	2.864375000	2.499350000
6	1.718958000	1.896307000	2.575588000
6	2.198968000	0.635693000	2.613785000
6	2.178558000	-0.597998000	2.612415000
6	1.761516000	-1.881029000	2.581169000
6	0.968528000	-2.822183000	2.500675000
6	-0.170714000	-3.539408000	2.392240000
6	-1.382187000	-3.732324000	2.268673000
6	-2.710008000	-3.530621000	2.125419000
6	-3.751870000	-2.884104000	1.998285000
6	-4.626523000	-1.861676000	1.881072000
6	-5.011087000	-0.691843000	1.820485000
6	-5.046532000	0.658397000	1.816451000
6	-4.620317000	1.813401000	1.882137000
6	-3.799951000	2.880526000	1.993250000

ZnP+C18

Atom	X	Y	Z
30	1.067210000	-0.000503000	-0.861921000
6	3.444036000	2.355994000	-0.141827000
6	-1.161566000	2.482528000	-1.628148000
6	-1.287831000	-2.355705000	-1.652286000
6	3.324223000	-2.484917000	-0.186901000
7	-0.878957000	0.053630000	-1.487836000
7	1.134556000	2.046366000	-0.896440000
7	3.020634000	-0.054648000	-0.254101000
7	1.030397000	-2.047327000	-0.925020000
6	3.762697000	-1.173665000	-0.013405000
6	3.816755000	1.021940000	0.008043000
6	2.205612000	2.827187000	-0.573133000
6	0.118533000	2.883286000	-1.250318000
6	2.062726000	-2.886152000	-0.621564000
6	-0.028376000	-2.826248000	-1.286007000
6	-1.677887000	-1.021910000	-1.741570000
6	-1.620156000	1.171938000	-1.732252000
6	5.081914000	-0.792189000	0.435916000
6	5.115286000	0.567288000	0.449562000
6	1.857082000	4.219754000	-0.736373000
6	0.564542000	4.254633000	-1.157004000
6	-2.952617000	0.790705000	-2.144679000
6	-2.988591000	-0.567608000	-2.149757000
6	1.644174000	-4.256613000	-0.806480000

TTF+C18

Atom	X	Y	Z
16	-1.362351000	-1.368547000	1.480936000
6	-0.975114000	-2.984847000	0.926871000
6	0.239147000	-0.704349000	1.107246000
16	1.449617000	-1.931925000	0.693064000
6	0.286816000	-3.238037000	0.572447000
16	2.083652000	1.312142000	0.747458000
6	1.498487000	2.962995000	0.676490000
6	0.497681000	0.617707000	1.129906000
16	-0.737725000	1.823309000	1.536963000
6	0.232093000	3.192025000	1.031431000
1	-1.775834000	-3.724599000	0.928550000
1	0.652075000	-4.211175000	0.243475000
1	-0.231473000	4.178204000	1.062206000
1	2.204868000	3.737179000	0.375998000
6	-3.686390000	-1.226136000	4.544069000
6	-3.907739000	0.105683000	4.583935000
6	-3.645661000	1.310530000	4.601723000
6	-2.991749000	2.492564000	4.605944000
6	-2.030127000	3.263791000	4.578029000
6	-0.772545000	3.752581000	4.510933000
6	0.455690000	3.701496000	4.411353000
6	1.718055000	3.239976000	4.283774000
6	2.611398000	2.396115000	4.178718000
6	3.283419000	1.228551000	4.094094000

6	0.348983000	-4.219727000	-1.218391000
1	5.875785000	-1.488634000	0.700153000
1	5.942306000	1.218513000	0.727116000
1	2.527119000	5.056332000	-0.546173000
1	-0.048383000	5.125415000	-1.383005000
1	-3.750347000	1.487885000	-2.393773000
1	-3.822039000	-1.219635000	-2.404125000
1	2.272554000	-5.128732000	-0.634685000
1	-0.308321000	-5.054747000	-1.454349000
1	4.199749000	3.106721000	0.095779000
1	-1.874412000	3.273283000	-1.867040000
1	-2.041362000	-3.105776000	-1.897489000
1	4.042546000	-3.276292000	0.034197000
6	-1.912648000	3.701890000	1.594223000
6	-0.639496000	3.493726000	1.991207000
6	0.363050000	2.843285000	2.294487000
6	1.213279000	1.825634000	2.543593000
6	1.586973000	0.655523000	2.650671000
6	1.607132000	-0.693784000	2.656456000
6	1.170409000	-1.839882000	2.530714000
6	0.352868000	-2.886815000	2.292698000
6	-0.682441000	-3.476650000	1.976757000
6	-1.948187000	-3.731836000	1.582103000
6	-3.098564000	-3.486203000	1.211938000
6	-4.219338000	-2.826272000	0.847945000
6	-4.949838000	-1.860308000	0.614058000
6	-5.413617000	-0.600035000	0.470709000
6	-5.379232000	0.632589000	0.483988000
6	-4.958307000	1.908829000	0.616528000
6	-4.174941000	2.827796000	0.868481000
6	-3.076288000	3.527762000	1.224154000
6	3.441334000	0.005997000	4.056875000
6	3.213766000	-1.323433000	4.032466000
6	2.558523000	-2.368126000	4.036636000
6	1.536866000	-3.249363000	4.082843000
6	0.372163000	-3.644706000	4.171179000
6	-0.972686000	-3.669473000	4.291176000
6	-2.108766000	-3.201176000	4.395984000
6	-3.134791000	-2.327716000	4.489618000

BDT+C18

Atom	X	Y	Z
6	-5.348305000	0.085728000	2.369632000
6	-3.880103000	0.370666000	2.345645000
6	-3.177467000	1.182183000	3.191362000
6	-1.786944000	1.241058000	2.893759000
6	-1.428942000	0.464750000	1.824122000
6	-0.062691000	0.284155000	1.298580000
6	0.560869000	-0.974929000	1.222847000
6	0.019536000	-2.263789000	1.581256000
6	0.915865000	-3.266706000	1.432606000
16	2.466373000	-2.739548000	0.857830000
6	1.915460000	-1.078982000	0.804678000
6	2.691690000	0.025893000	0.445447000
6	4.090349000	-0.141035000	0.013522000
6	4.576127000	-0.972142000	-0.960365000
6	5.993683000	-0.911871000	-1.094898000
6	6.585490000	-0.042941000	-0.221564000
6	8.039215000	0.277250000	-0.074197000
16	5.395689000	0.712928000	0.784421000

PNTCN+C18

Atom	X	Y	Z
6	3.691401000	-2.979910000	0.663864000
6	2.683757000	-3.853920000	0.448528000
6	1.525896000	-4.275963000	0.409733000
6	0.181792000	-4.366738000	0.516603000
6	-0.967232000	-4.000089000	0.773101000
6	-2.031524000	-3.258304000	1.150554000
6	-2.633309000	-2.259416000	1.550316000
6	-2.915690000	-1.010554000	1.979977000
6	-2.684094000	0.151592000	2.319065000
6	-2.046751000	1.305779000	2.612019000
6	-1.093232000	2.075567000	2.746807000
6	0.154411000	2.592557000	2.781158000
6	1.382914000	2.619611000	2.678132000
6	2.668814000	2.266432000	2.461392000
6	3.611046000	1.531723000	2.157698000
6	4.328694000	0.461475000	1.753400000
6	4.525496000	-0.690612000	1.361951000
6	4.323860000	-1.963868000	0.958958000

6	2.062175000	1.282527000	0.500809000
6	2.601143000	2.572356000	0.138620000
6	1.707636000	3.575450000	0.296656000
16	0.161444000	3.048029000	0.885476000
6	0.710039000	1.387071000	0.925286000
16	-2.828348000	-0.325444000	1.154673000
1	-5.884691000	0.662100000	1.601356000
1	-5.564573000	-0.977561000	2.193673000
1	-5.762026000	0.363093000	3.349017000
1	-3.646560000	1.716558000	4.018409000
1	-1.060927000	1.819907000	3.464786000
1	-1.000713000	-2.410243000	1.930815000
1	3.929455000	-1.601150000	-1.571489000
1	6.560965000	-1.494458000	-1.821793000
1	8.409788000	0.035216000	0.933938000
1	8.241890000	1.344601000	-0.253024000
1	8.624665000	-0.305027000	-0.798840000
1	3.615588000	2.718359000	-0.227320000
1	1.869419000	4.632647000	0.089696000
1	0.748977000	-4.324641000	1.631555000
6	-5.594723000	-2.000426000	-0.811035000
6	-6.026738000	-0.849378000	-0.905989000
6	-5.986598000	0.485788000	-1.104519000
6	-5.585261000	1.630586000	-1.325625000
6	-4.709860000	2.614891000	-1.622613000
6	-3.674513000	3.217485000	-1.914541000
6	-2.370111000	3.385512000	-2.219207000
6	-1.181522000	3.158391000	-2.454995000
6	-0.061597000	2.422551000	-2.617433000
6	0.720161000	1.471748000	-2.685756000
6	1.122181000	0.185243000	-2.621670000
6	1.137904000	-1.037946000	-2.467473000
6	0.650318000	-2.261562000	-2.174113000
6	-0.096379000	-3.188270000	-1.852431000
6	-1.247652000	-3.787742000	-1.483527000
6	-2.423035000	-3.997946000	-1.174822000
6	-3.715480000	-3.690626000	-0.934350000
6	-4.775884000	-3.074129000	-0.806904000
6	-0.637583000	1.982678000	-0.788680000
6	-0.564331000	-0.720946000	-1.548308000
1	-0.664461000	3.032696000	-0.487543000
1	-0.536139000	-1.774262000	-1.838316000
6	0.597062000	1.386707000	-1.067133000
6	-1.837679000	1.273269000	-0.894225000
6	-1.800073000	-0.118518000	-1.289155000
6	0.635829000	-0.007041000	-1.457245000
6	1.813110000	2.106426000	-0.990861000
6	-3.091998000	1.869881000	-0.621168000
6	-3.020860000	-0.826232000	-1.397573000
6	1.889015000	-0.596301000	-1.752714000
1	1.784305000	3.155891000	-0.687615000
1	-3.118736000	2.918467000	-0.314446000
1	-2.992818000	-1.878207000	-1.691401000
1	1.919457000	-1.649319000	-2.043848000
6	3.026274000	1.520094000	-1.296336000
6	-4.274444000	1.161897000	-0.725155000
6	-4.237768000	-0.228993000	-1.128113000
6	3.065119000	0.127704000	-1.693989000
6	4.265879000	2.247541000	-1.228189000
6	-5.552507000	1.756632000	-0.436578000
6	-5.480356000	-0.948726000	-1.219569000
6	4.341051000	-0.455058000	-2.014888000
1	4.234180000	3.294723000	-0.918507000
1	-5.578199000	2.805732000	-0.132517000
1	-5.449200000	-1.998224000	-1.521709000
1	4.368781000	-1.505318000	-2.313347000
6	5.446526000	1.651680000	-1.539066000
6	-6.699104000	1.035018000	-0.535049000
6	-6.662477000	-0.343858000	-0.933705000
6	5.484411000	0.275313000	-1.942923000
1	6.379103000	2.216867000	-1.482301000
1	-7.661582000	1.499558000	-0.310692000
1	-7.597576000	-0.903296000	-1.004901000
1	6.444821000	-0.182478000	-2.188658000

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