Supporting Information

Evaluation of Charge-Transfer Rates in Fullerene-Based Donor-Acceptor Dyads with Different Density Functional Approximations

Pau Besalú-Sala,[a] Alexander A. Voityuk,[ab]* Josep M. Luis[a]* and Miquel Solà[a]*

[a] Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, C/ M. Aurèlia Capmany, 69, 17003 Girona, Catalonia, Spain.
[b] Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Catalonia, Spain.

All necessary values to compute k_{CT} for all the systems are summarized in this supporting information, as well as the computed k_{CT}. All tables are ordered from lowest-error DFA to greatest-error DFA. Green marks on the tables highlight the (correct) negative ΔG prediction, and red marks highlight the logarithm of k_{CT} and the relative error of such value. The Cartesian coordinates for the optimized systems, as well as the optimized fragments for the calculation of λ_{int} are given at the end of this document.

Charge transfer data of C_{60}-Az

Table SI1. Marcus' equation parameters computed with different DFAs for C_{60}-Az.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
CAM-B3LYP	0.241	0.368	$5.40 \cdot 10^{-3}$	0.196	0.648	$3.55 \cdot 10^{10}$	10.55	2.42
ωB97xD	0.242	0.218	$4.97 \cdot 10^{-3}$	0.349	0.654	$1.19 \cdot 10^{8}$	8.08	-21.61
MN15	0.232	0.100	$6.72 \cdot 10^{-3}$	-0.020	0.097	$1.13 \cdot 10^{13}$	13.05	26.72
M11	0.251	0.206	$2.31 \cdot 10^{-4}$	0.466	0.852	$1.74 \cdot 10^{15}$	5.24	-49.12
LC-ωhPBE	0.262	0.257	$5.24 \cdot 10^{-3}$	0.888	1.979	$9.07 \cdot 10^{-3}$	-2.04	-119.83
LC-TPSS	0.268	0.243	$6.97 \cdot 10^{-3}$	1.004	2.296	$1.69 \cdot 10^{-5}$	-4.77	-146.33
LC-BLYP	0.266	0.108	$7.19 \cdot 10^{-3}$	1.295	2.786	$6.46 \cdot 10^{-18}$	-17.19	-266.88

Experimental $k_{CT} = 2.0 \cdot 10^{10}$ s^{-1}, experimental ΔG = -0.27 eV.

Charge transfer data of C_{60}-ZnTTP

Table SI2. Marcus' equation parameters computed with different DFAs for C_{60}-ZnTPP.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
MN15	0.270	0.298	$2.19 \cdot 10^{-6}$	-0.727	0.025	$3.16 \cdot 10^{10}$	10.50	0.42
ωB97xD	0.282	0.161	$5.84 \cdot 10^{-5}$	-0.092	0.123	$9.87 \cdot 10^{10}$	10.99	5.14
CAM-B3LYP	0.280	0.251	$9.80 \cdot 10^{-6}$	-0.420	0.012	$1.80 \cdot 10^{11}$	11.26	7.64
M11	0.290	0.219	$9.80 \cdot 10^{-6}$	-0.150	0.129	$4.28 \cdot 10^{9}$	9.63	-7.89
LC-ωhPBE	0.303	0.092	$1.45 \cdot 10^{-5}$	0.411	0.649	$4.32 \cdot 10^{4}$	4.64	-55.67
LC-TPSS	0.258	0.061	$1.83 \cdot 10^{-5}$	0.513	0.692	$3.63 \cdot 10^{2}$	2.56	-75.52
LC-BLYP	0.311	0.117	$1.69 \cdot 10^{-4}$	0.798	1.503	$6.17 \cdot 10^{3}$	-2.21	-121.13

Experimental $k_{CT} = 2.86 \cdot 10^{10}$ s^{-1}

Charge transfer data of C_{59}N-Pc

Table SI3. Marcus' equation parameters computed with different DFAs for C_{59}N-Pc.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
LC-ωhPBE	0.145	0.234	$3.81 \cdot 10^{-3}$	0.031	0.168	$1.39 \cdot 10^{12}$	12.14	0.38
LC-TPSS	0.148	0.242	$4.02 \cdot 10^{-3}$	0.065	0.207	$6.13 \cdot 10^{11}$	11.79	-2.56
M11	0.139	0.210	$9.99 \cdot 10^{-4}$	-0.078	0.073	$3.66 \cdot 10^{12}$	12.56	3.86
MN15	0.126	0.271	$2.16 \cdot 10^{-4}$	-0.757	0.129	$2.42 \cdot 10^{11}$	11.38	-5.89
LC-BLYP	0.148	0.236	$4.06 \cdot 10^{-3}$	0.119	0.253	$1.80 \cdot 10^{11}$	11.25	-6.96
ωB97xD	0.134	0.105	$5.36 \cdot 10^{-3}$	0.03	0.072	$9.69 \cdot 10^{12}$	12.99	7.35
CAM-B3LYP	0.133	0.209	$2.76 \cdot 10^{-3}$	-0.523	0.033	$3.10 \cdot 10^{13}$	13.49	11.53

Experimental $k_{CT} = 1.25 \cdot 10^{12}$ s^{-1}, experimental ΔG = -0.24 eV

Charge transfer data of C_{60}-TPA

Table SI4. Marcus' equation parameters computed with different DFAs for C_{60}-TPA.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
CAM-B3LYP	0.210	0.94	$2.13\cdot10^{-6}$	-0.956	0.038	$2.43\cdot10^{10}$	10.39	-3.64
MN15	0.188	0.968	$4.90\cdot10^{-7}$	-1.409	0.064	$4.47\cdot10^{9}$	9.65	-10.46
ωB97xD	0.219	0.822	$6.10\cdot10^{-6}$	-0.227	0.663	$2.04\cdot10^{8}$	8.31	-22.90
M11	0.213	0.821	$1.50\cdot10^{-5}$	-0.039	0.992	$2.19\cdot10^{7}$	7.34	-31.90
LC-ωhPBE	0.236	0.883	$1.51\cdot10^{-5}$	0.096	1.476	$6.33\cdot10^{5}$	5.80	-46.17
LC-TPSS	0.321	0.891	$2.08\cdot10^{-5}$	0.206	2.012	$3.06\cdot10^{4}$	4.49	-58.38
LC-BLYP	0.262	0.526	$4.72\cdot10^{-5}$	0.962	3.061	$3.30\cdot10^{-5}$	-4.48	-141.58

Experimental k_{CT} = $6.00\cdot10^{10}$ s^{-1}, experimental ΔG = -0.31 eV

Tuned LC-BLYP data of C_{60}-TPA

The tuning of LC-BLYP was done in two ways, leading to optimally-tuned LC-BLYP version 1 (OT1) and optimally tuned LC-BLYP version 2 (OT2). Both functionals are tuned by changing the parameter that governs the steepness of the transition from short-range to long-range region (*i.e.* ω parameter). In the case of OT1, we computed the ω parameter that enforces the fulfillment of Janak's theorem[1,2,3] through the minimization of

$$J^2(\omega) = \sum_{i=N}^{N+1} \left(IP^i + \varepsilon_{HOMO}^{\ i}(\omega)\right)^2, \quad (1)$$

Where IP^i is the vertical ionization potential for the neutral (*i=N*) or the anionic (*i=N+1*) system and $\varepsilon_{HOMO}^{\ i}$ is the energy of the Highest Occupied Molecular Orbital for the netural or anionic system. For simplicity, we have computed IP^i at LC-BLYP level of theory (ω=0.47 Bohr^{-1}) and we have checked that this approximation only triggers very small changes on the final result of $J^2(\omega)$, if any.

In the case of OT1,[4] we computed the ω parameter through

$$\omega_{OT2} = 0.6269\cdot A^2 - 0.4556\cdot A + 0.3791 \quad (2)$$

$$A = log\left(\frac{\alpha_{LC-BLYP}}{N}\right) \quad (3)$$

Where N is the number of electrons and $\alpha_{LC-BLYP}$ is the ZZ element of the polarizability tensor computed at LC-BLYP level of theory. Note that this approach requires a pre-alignment of the molecular inertia axis with the Z axis.

The equation used for the computation of ω_{OT2} arises from an empirical correlation (eq. 2) between the indicator A (eq. 3) and the ω that is required to reproduce CCSD(T) 2nd hyperpolarizabilities for a set of 60 molecules.

The resulting ω parameters obtained through OT1 and OT2 procedures were used, then, to compute all the variables needed in the Marcus' equation by using the ω-tailored LC-BLYP, summarized in Table SI5.

Table SI5. Marcus' equation parameters computed with OT2, OT1 and LC-BLYP for C_{60}-TPA.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
OT2	0.217	0.888	$9.36\cdot10^{-6}$	-0.148	0.916	$4.69\cdot10^{-7}$	7.67	-28.82
OT1	0.211	0.558	$6.81\cdot10^{-6}$	0.214	0.966	$6.35\cdot10^{-5}$	5.80	-46.16
LC-BLYP	0.262	0.526	$4.72\cdot10^{-5}$	0.962	1.550	$3.30\cdot10^{-5}$	-4.48	-141.58

Experimental k_{CT} = 6.00·10^{10} s^{-1}, experimental ΔG = -0.31 eV.

Table SI6. Summary of all the data recollected for **C$_{60}$-TPA**. Ordered from best to worst DFA.

DFA method	λ_{int} (eV)	λ_{ext} (eV)	$(V_{DA})^2$	ΔG (eV)	$(\lambda+\Delta G)^2$	k_{CT} (s^{-1})	log k_{CT}	Err log k_{CT} (%)
CAM-B3LYP	0.210	0.94	2.13·10^{-6}	-0.956	0.038	2.43·10^{10}	10.39	-3.64
MN15	0.188	0.968	4.90·10^{-7}	-1.409	0.064	4.47·10^{9}	9.65	-10.46
ωB97xD	0.219	0.822	6.10·10^{-6}	-0.227	0.663	2.04·10^{8}	8.31	-22.90
OT2	0.217	0.888	9.36·10^{-6}	-0.148	0.916	4.69·10^{7}	7.67	-28.82
M11	0.213	0.821	1.50·10^{-5}	-0.039	0.992	2.19·10^{7}	7.34	-31.90
OT1	0.211	0.558	6.81·10^{-6}	0.214	0.966	6.35·10^{5}	5.80	-46.16
LC-ωhPBE	0.236	0.883	1.51·10^{-5}	0.096	1.476	6.33·10^{5}	5.80	-46.17
LC-TPSS	0.321	0.891	2.08·10^{-5}	0.206	2.012	3.06·10^{4}	4.49	-58.38
LC-BLYP	0.262	0.526	4.72·10^{-5}	0.962	3.061	3.30·10^{-5}	-4.48	-141.58

Experimental k_{CT} = 6.00·10^{10} s^{-1}, experimental ΔG = -0.31 eV

Besalú-Sala, P., et al., *Phys. Chem. Chem. Phys.*, **2021**, Supporting Information

Estimation of the geometrical changes in the CS reaction

The geometrical changes arising from the charge separation (CS) can play a key role in the CT reaction. Therefore, in case that the CS geometrical changes are big, they should be taken into account in order to estimate the k_{CT}. On the contrary, if the geometrical changes are not large the CS is assumed to be a purely electronic process, simplifying a lot the calculation of the rate constants.

The evaluation of the geometry changes in donor-acceptor (D-A) dyads is usually challenging because the systems are typically very big. In order to address this problem, a commonly used strategy is to divide the molecule into D and A fragments determined by the orbitals involved in the CS, and compute the geometry differences assuming that the CS occurs locally on these fragments. The charge transfer reaction occurs when the system goes from the lowest local excited state (LES1) to the CT state. For a typical D-A dyad, the fragments would be D* and A (or D and A*) in the LES1 state, and D^+ and A^- CT state. Therefore, the geometrical differences computed are D* (D) with respect to D^+ and A (A*) with respect to A^-.

The geometric differences have been computed by means of the root mean square deviation (RMSD) of atomic positions, which is computed following equation 4

$$RMSD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\delta_i^2} \quad (4)$$

were N is the number of atoms, and δ_i is the distance between atom i in the two compared (and superimposed) structures.

For the four systems studied in this manuscript, Table SI7 summarizes the computed RMSDs

Table SI7. RMSD of the four studied systems and summary of the fragments involved. All RMSD in Angstroms.

System	C_{60}-Az	C_{60}-ZnTTP	C_{59}N-PC	C_{60}-TPA
Reaction	$C_{60}{}^{S1}+Az \rightarrow C_{60}{}^-+Az^+$	$C_{60}+ZnTTP^{S1} \rightarrow C_{60}{}^-+ZnTTP^+$	$(C_{59}N)+PC^{S1} \rightarrow C_{59}+N\text{-}PC^+$	$C_{60}{}^{S1}+TPA \rightarrow C_{60}{}^-+TPA^+$
Donor RMSD (Å)	0.020	0.087	0.062	0.017
Acceptor RMSD (Å)	0.025	0.010	0.010	0.025
Total RMSD (Å)	**0.045**	**0.097**	**0.072**	**0.042**

All RMSDs < 0.1 Å which indicates a very low geometrical change along the CT reaction for all the studied systems. Thus, treating the CT reaction as a purely electronic process is a reliable approach.

State characters of the target excited states

Table SI8. Amount of CS/CT state characters of the target excited states following Eq. 2 of the manuscript for **C$_{60}$-Az** and **C$_{60}$-ZnTTP** for all DFAs.

C$_{60}$-Az	CT	CS
CAM-B3LYP	0.463	0.468
MN15	0.488	0.496
wB97XD	0.617	0.619
M11	0.463	0.470
LC-wHPBE	0.700	0.703
LC-TPSS	0.352	0.372
LC-BLYP	0.394	0.405

C$_{60}$-ZnTTP	CT	CS
CAM-B3LYP	0.795	0.804
MN15	0.856	0.862
wB97XD	0.654	0.669
M11	0.771	0.787
LC-wHPBE	0.484	0.505
LC-TPSS	0.386	0.41
LC-BLYP	0.581	0.594

Table SI9. Amount of CS/CT state characters of the target excited states following Eq. 2 of the manuscript for **C$_{59}$N-Pc** and **C$_{60}$-TPA** for all DFAs.

C$_{59}$N-Pc	CT	CS
CAM-B3LYP	0.870	0.873
MN15	0.367	0.383
wB97XD	0.694	0.701
M11	0.588	0.596
LC-wHPBE	0.927	0.929
LC-TPSS	0.935	0.937
LC-BLYP	0.930	0.932

C$_{60}$-TPA	CT	CS
CAM-B3LYP	0.924	0.927
MN15	0.974	0.974
wB97XD	0.866	0.866
M11	0.914	0.921
LC-wHPBE	0.920	0.920
LC-TPSS	0.934	0.934
LC-BLYP	0.717	0.723
OT1	0.930	0.931
OT2	0.982	0.982

Graphical representation of the obtained results

Graphical representation of the error on the log(k_{CT})

Figure SI1. Mean absolute percentage errors in the log(k_{CT}) for each DFA.
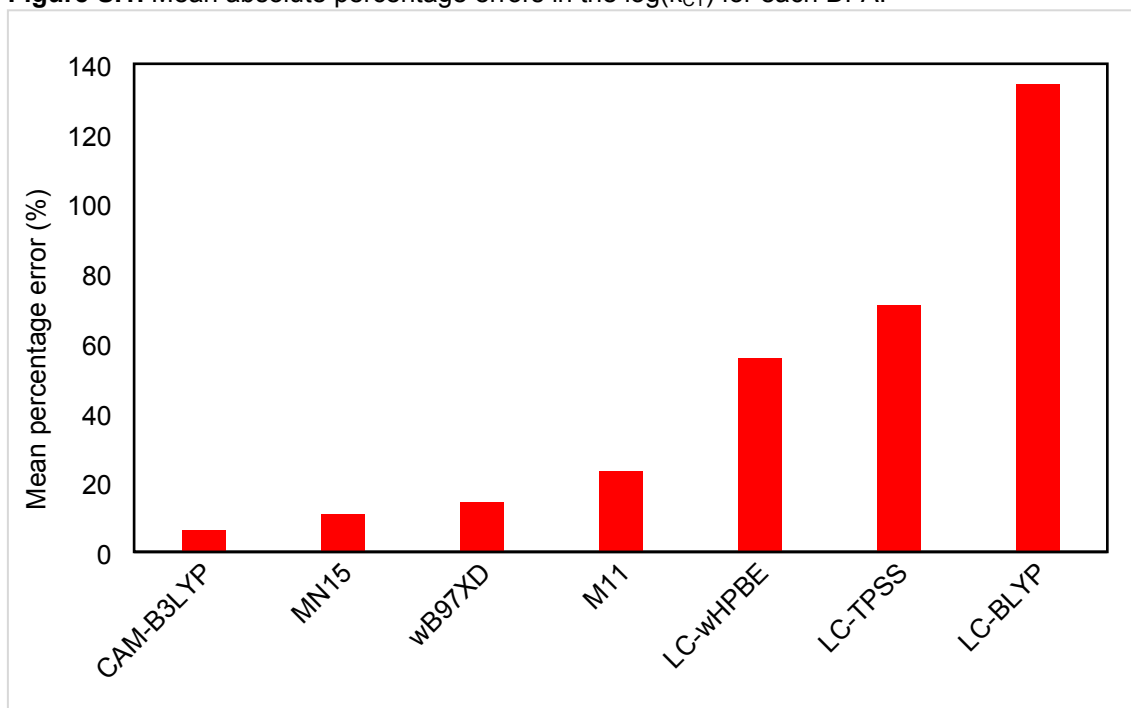
Figure SI2. Mean percentage errors in the log(k_{CT}) for each DFA.
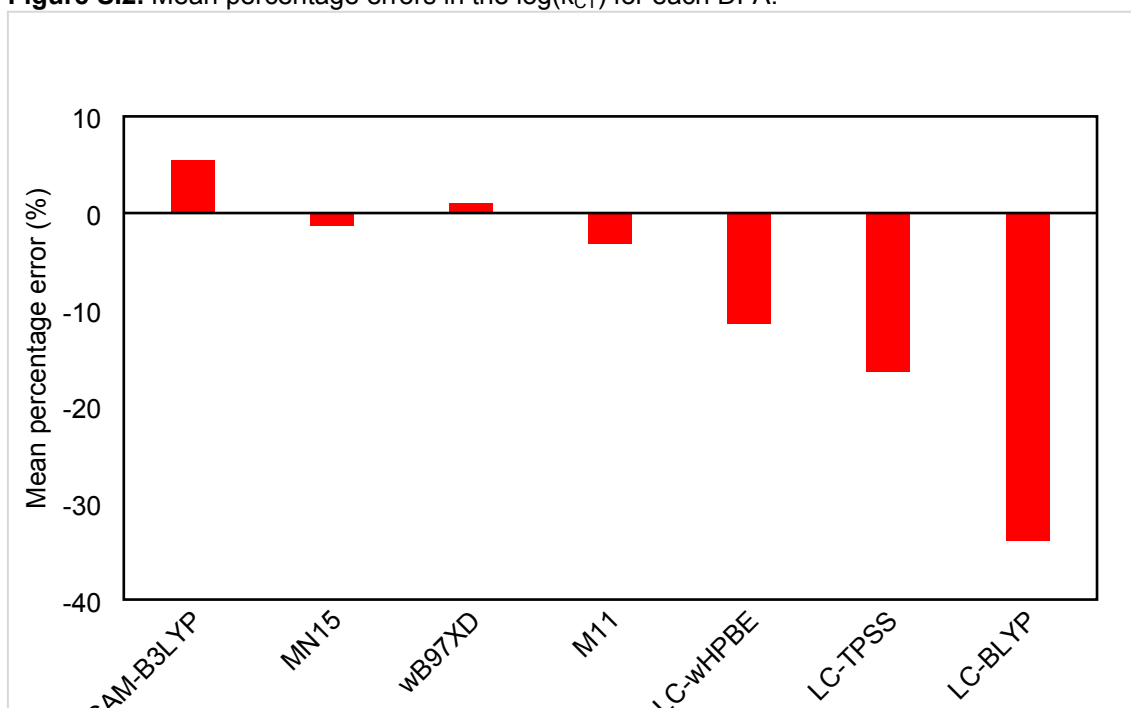
Figure SI3. Absolute percentage errors in the log(k$_{CT}$) for each DFA and for each system.
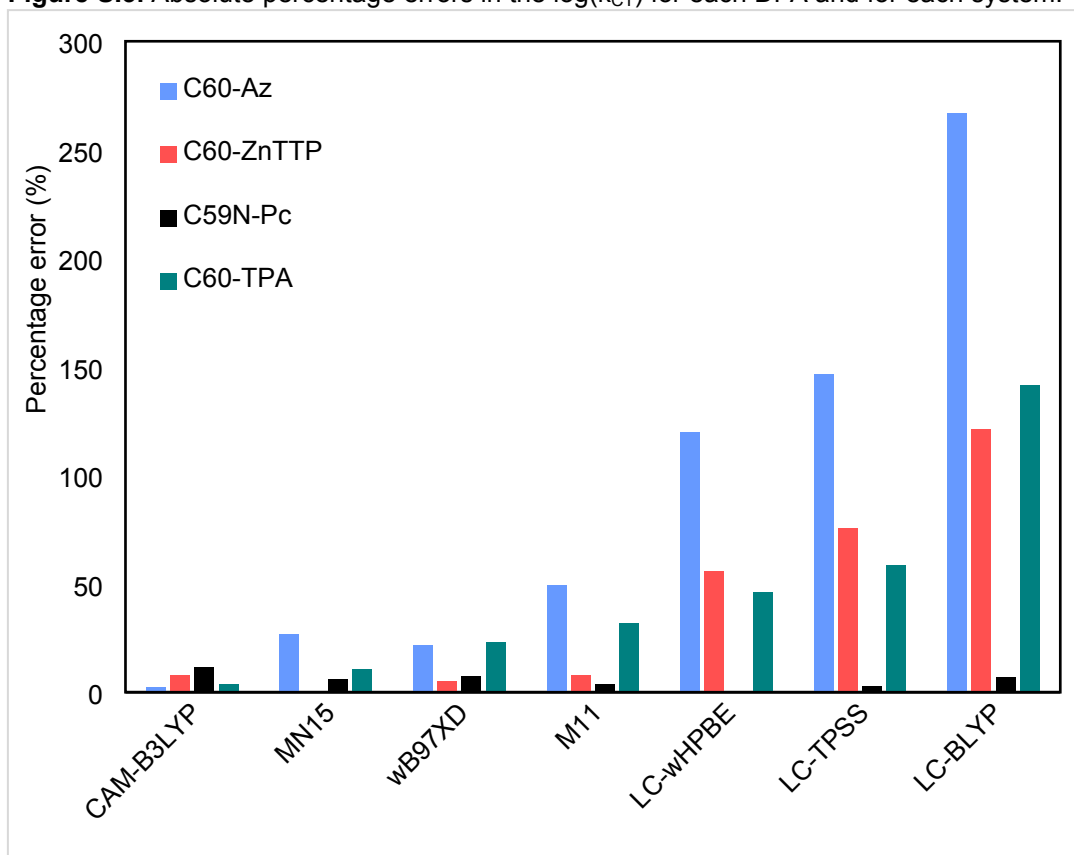
Graphical representation of the reorganization energy, λ

Figure SI4. Internal reorganization energy by DFA and system.
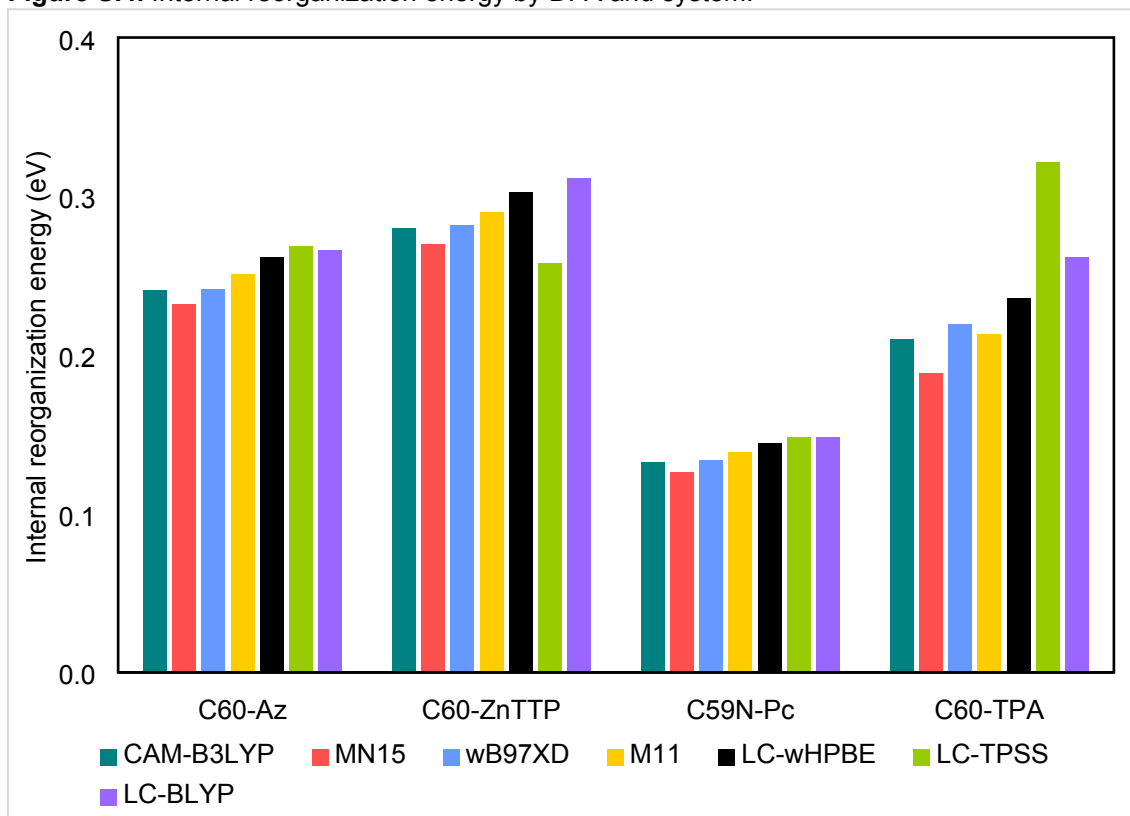
Figure SI5. External reorganization energy by DFA and system.
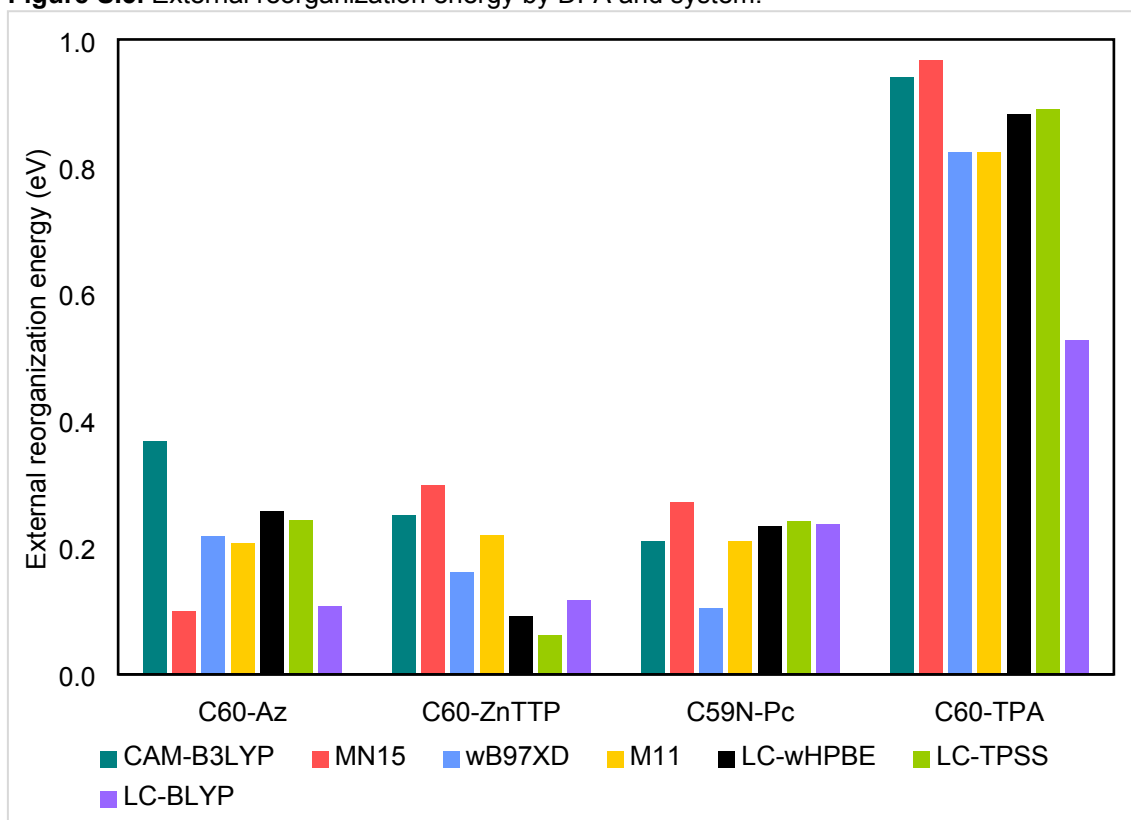
Figure SI6. Total reorganization energy by DFA and system.
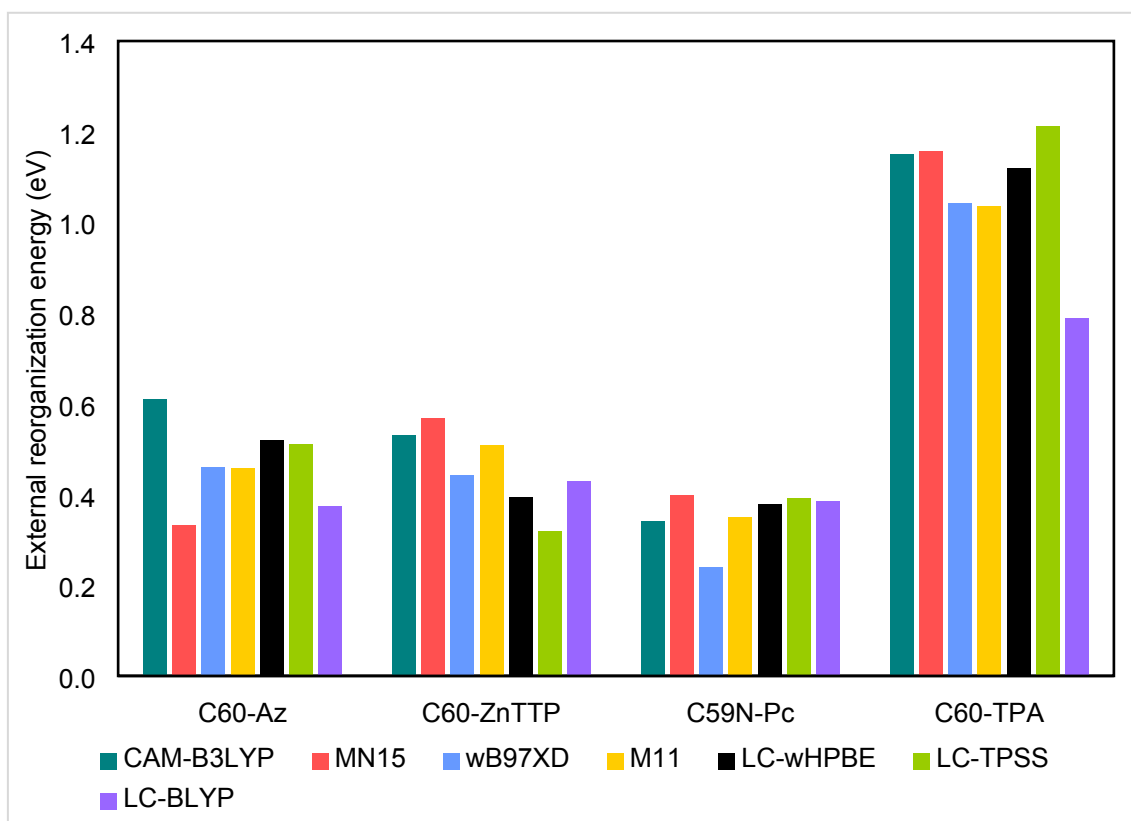
Graphical representation of the electronic coupling squared, V^2_{DA}

Figure SI7. Electronic coupling squared (V^2_{DA}) for **C_{60}-Az** and **$C_{59}N$-Pc**.
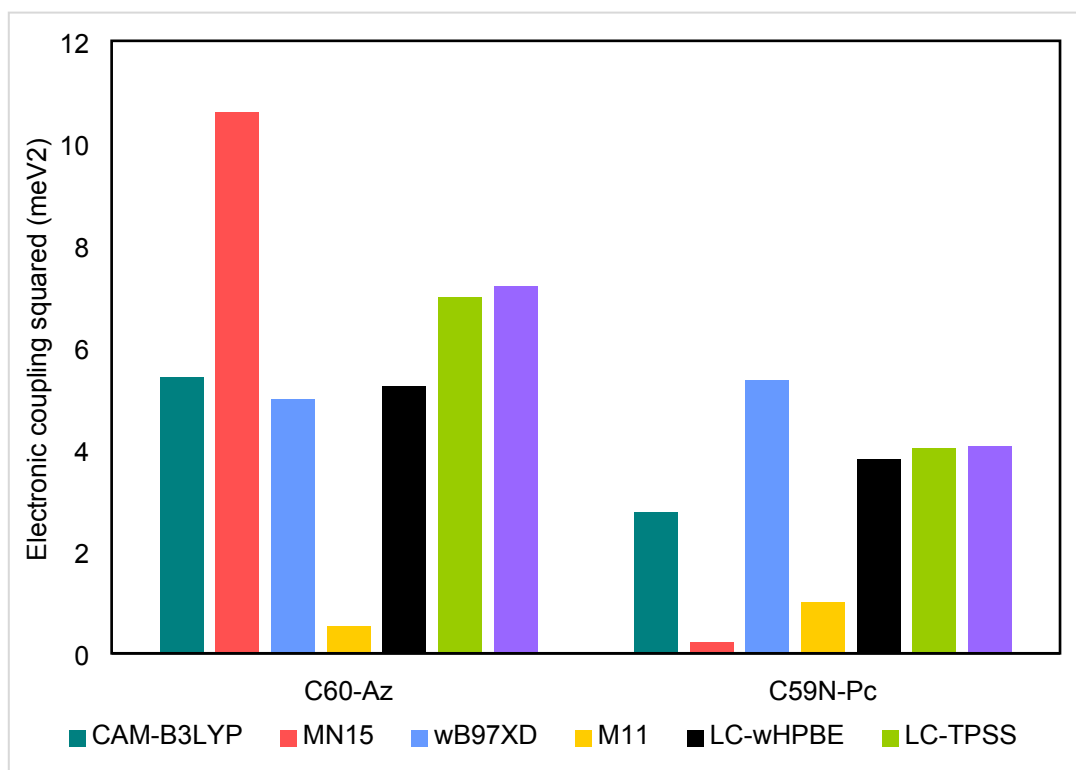
Figure SI8. Electronic coupling squared (V^2_{DA}) for **C_{60}-ZnTTP** and **C_{60}-TPA**.
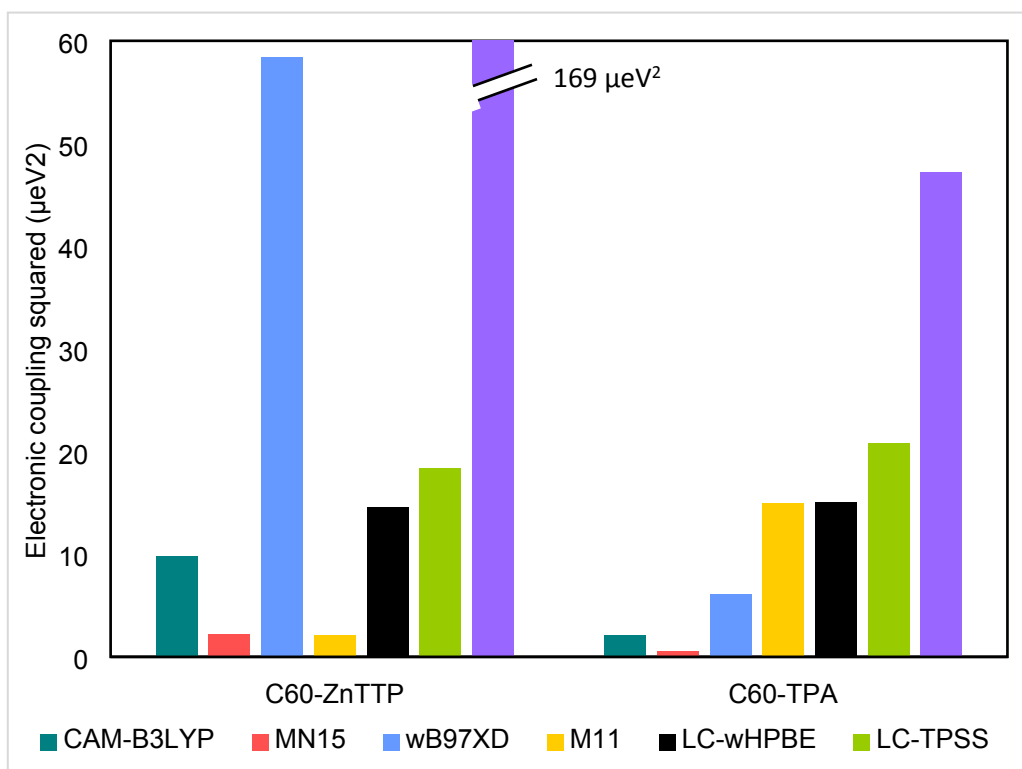
Graphical representation of the ΔG° and (λ+ΔG°)²

Figure SI9. ΔG° for all methods and systems.

Figure SI10. (λ+ΔG°)² for all methods and systems.

Cartesian coordinates of the optimized systems

All systems were optimized at B3LYP-D3(BJ)/6-311G(d,p) level of theory.

C$_{60}$-Az

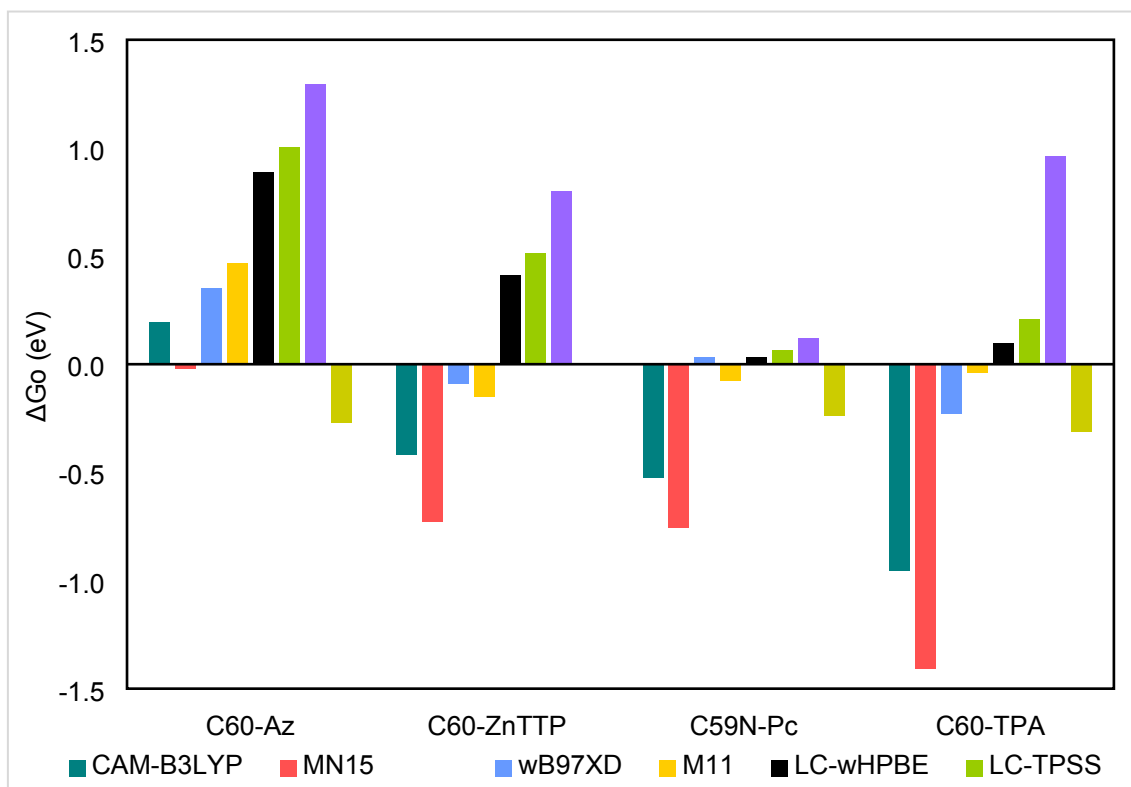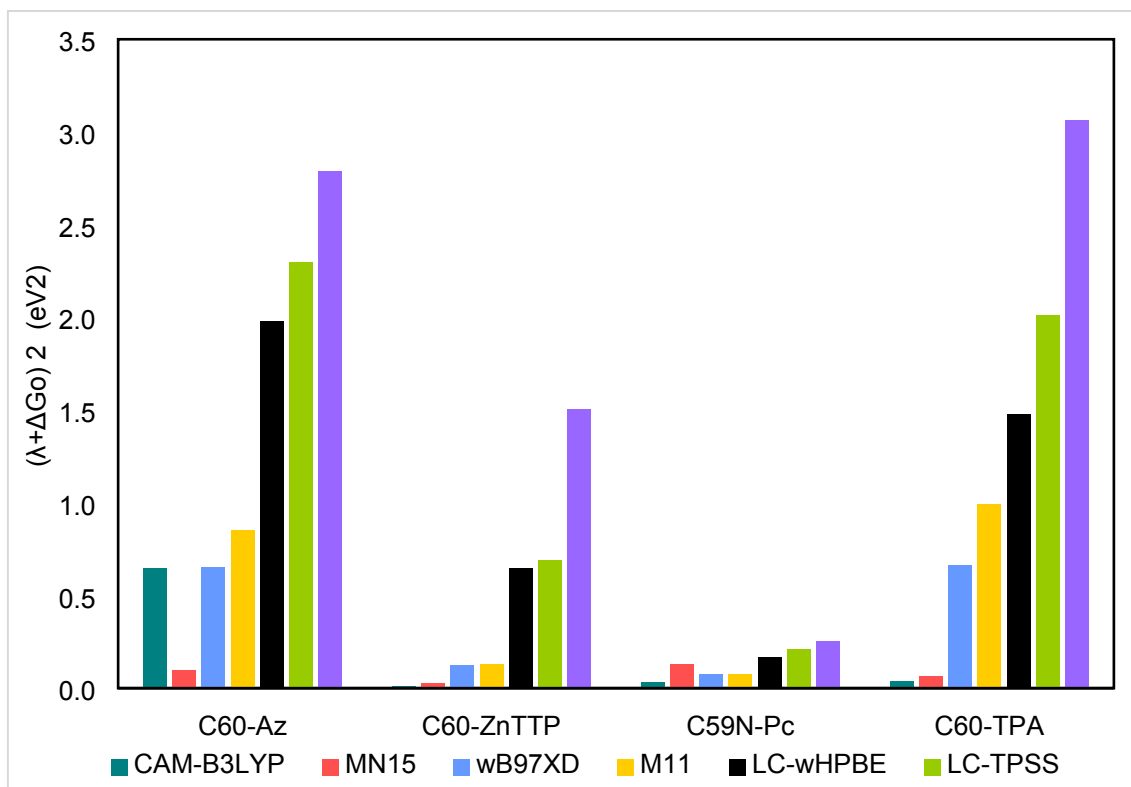|			
6	-5.308103000	1.577832000	0.945578000
6	-4.617818000	2.686958000	0.307047000
6	-4.666759000	2.478076000	-1.129059000
6	-5.388576000	1.242009000	-1.379525000
6	-5.783561000	0.685596000	-0.096774000
6	-5.756991000	-0.692663000	0.101550000
6	-5.253638000	-1.237544000	1.347071000
6	-4.799261000	-0.384095000	2.349608000
6	-4.827060000	1.055270000	2.143159000
6	-3.633211000	1.616361000	2.751225000
6	-2.973507000	2.677544000	2.141272000
6	-3.475992000	3.226677000	0.893638000
6	-2.332178000	3.579516000	0.067705000
6	-2.380943000	3.374901000	-1.309367000
6	-3.571332000	2.816601000	-1.919766000
6	-3.153192000	1.934243000	-2.999988000
6	-3.849377000	0.752411000	-3.241715000
6	-4.988551000	0.398345000	-2.411896000
6	-4.966380000	-1.040355000	-2.209318000
6	-5.339192000	-1.575163000	-0.978475000
6	-4.578363000	-2.664759000	-0.399321000
6	-4.518375000	-2.453621000	1.038218000
6	-3.352535000	-2.754999000	1.735655000
6	-2.875142000	-1.865738000	2.779702000
6	-3.590799000	-0.707186000	3.085517000
6	-2.872465000	0.519991000	3.329447000
6	-1.478073000	0.522590000	3.252710000
6	-0.789074000	1.631719000	2.618742000
6	-1.520952000	2.692720000	2.080087000
6	-1.127916000	3.248366000	0.807827000
6	-0.023839000	2.713749000	0.141621000
6	-0.077219000	2.503896000	-1.294354000
6	-1.225180000	2.833546000	-2.007422000
6	-1.704783000	1.948251000	-3.056768000
6	-1.006181000	0.780768000	-3.356765000
6	-1.732726000	-0.453452000	-3.609871000
6	-3.124046000	-0.466478000	-3.552504000
6	-3.815107000	-1.575382000	-2.914161000
6	-3.084852000	-2.623388000	-2.359923000
6	-3.474312000	-3.180893000	-1.073998000
6	-2.264578000	-3.508927000	-0.343074000
6	-2.200392000	-3.292156000	1.034558000
6	-1.005532000	-2.741544000	1.637198000
6	-1.428880000	-1.845329000	2.734147000
6	-0.744275000	-0.681958000	2.978042000
6	0.622940000	-0.336589000	2.375951000
6	0.372923000	1.114237000	1.951692000
6	0.731161000	1.628868000	0.729626000
6	1.154898000	0.731374000	-0.366867000
6	0.650797000	1.285905000	-1.602902000
6	0.200621000	0.446713000	-2.623027000
6	0.221074000	-0.981632000	-2.417951000
6	-0.972410000	-1.546043000	-3.027950000
6	-1.633588000	-2.606675000	-2.418017000
6	-1.133935000	-3.151968000	-1.166193000
6	-0.002069000	-2.594540000	-0.568379000
6	0.067844000	-2.405410000	0.853553000
6	1.080539000	-1.308335000	1.189564000
6	1.201186000	-0.626978000	-0.177401000
6	0.692074000	-1.491653000	-1.206247000
6	2.419018000	-1.978673000	1.695860000

6	1.760833000	-0.464273000	3.427079000
7	2.390083000	-1.728822000	3.137198000
6	3.611446000	-2.008152000	3.865585000
1	3.412095000	-1.955050000	4.938736000
1	3.952743000	-3.019216000	3.633691000
1	4.428443000	-1.310184000	3.623145000
6	5.591067000	2.455257000	-0.031623000
6	4.500627000	2.084491000	0.770803000
6	3.969584000	0.834484000	1.053051000
6	6.408961000	1.559040000	-0.720262000
6	4.325194000	-0.435215000	0.619024000
6	6.351583000	0.164637000	-0.821023000
6	5.470525000	-0.760423000	-0.283046000
1	3.965151000	2.898203000	1.244288000
1	3.111249000	0.872386000	1.706657000
1	7.219736000	1.994049000	-1.286756000
1	7.129467000	-0.250019000	-1.449751000
6	3.666493000	-1.647188000	0.903829000
6	4.369998000	-2.667078000	0.227511000
1	4.074024000	-3.706515000	0.264817000
6	5.462421000	-2.168395000	-0.492755000
6	6.413420000	-3.007009000	-1.338040000
6	6.021768000	-4.494546000	-1.267215000
1	6.066980000	-4.871943000	-0.242445000
1	5.012455000	-4.661575000	-1.651551000
1	6.712107000	-5.086852000	-1.872889000
6	7.862327000	-2.885365000	-0.816166000
1	8.530305000	-3.521528000	-1.404694000
1	8.241481000	-1.864436000	-0.869339000
1	7.918423000	-3.204218000	0.227548000
6	6.342273000	-2.581291000	-2.821793000
1	6.993318000	-3.217545000	-3.428963000
1	5.320658000	-2.680544000	-3.196444000
1	6.649801000	-1.546388000	-2.974512000
6	5.859336000	3.973717000	-0.139631000
6	6.140338000	4.546510000	1.267217000
1	6.339049000	5.619613000	1.199525000
1	5.297536000	4.406097000	1.945586000
1	7.014512000	4.064783000	1.712536000
6	4.613590000	4.660320000	-0.744467000
1	4.790052000	5.735221000	-0.839978000
1	4.396843000	4.259627000	-1.737816000
1	3.724734000	4.520917000	-0.127427000
6	7.061888000	4.321055000	-1.032052000
1	6.920600000	3.979633000	-2.060288000
1	7.183268000	5.406291000	-1.060054000
1	7.992772000	3.895988000	-0.648784000
1	2.300781000	-3.058541000	1.564772000
1	1.354440000	-0.464045000	4.442094000
1	2.443136000	0.398692000	3.360202000

C$_{60}$-ZnTTP

6	-0.659508000	1.087065000	-3.178859000
6	0.067829000	2.320657000	-3.423926000
6	1.331579000	2.250506000	-2.718139000
6	1.379080000	0.950295000	-2.024591000
6	0.144556000	0.250148000	-2.321115000
6	-0.485885000	-0.516751000	-1.342226000
6	-1.925757000	-0.502683000	-1.199223000
6	-2.690541000	0.275278000	-2.042156000
6	-2.045708000	1.107677000	-3.024444000

6	-2.769736000	2.363883000	-3.111385000	6	4.716384000	2.075834000	-1.698738000
6	-2.073945000	3.547096000	-3.360738000	8	4.257261000	1.544374000	-2.669347000
6	-0.628463000	3.523437000	-3.519450000	8	6.031846000	2.247506000	-1.449435000
6	-0.093587000	4.704918000	-2.887646000	6	-5.954037000	-1.583473000	1.034287000
6	1.112272000	4.620709000	-2.189686000	1	-5.419885000	-0.692072000	1.350706000
6	1.863173000	3.388885000	-2.141589000	1	-7.014300000	-1.348815000	0.913583000
6	2.622243000	3.365997000	-0.853386000	6	-5.789651000	-2.664309000	2.070174000
6	2.667000000	1.963593000	-0.112234000	1	-6.288376000	-2.328771000	2.988019000
6	1.957322000	0.834191000	-0.777092000	1	-6.265534000	-3.590809000	1.730729000
6	1.277576000	0.083861000	0.248046000	6	6.977549000	1.452956000	-2.192230000
6	0.101751000	-0.612237000	-0.026577000	1	6.597266000	1.264059000	-3.196196000
6	-0.972876000	-0.632712000	0.953295000	1	7.885366000	2.054698000	-2.234897000
6	-2.228491000	-0.579090000	0.242993000	6	7.209842000	0.164675000	-1.423145000
6	-3.277133000	0.131465000	0.784399000	1	8.165424000	-0.289290000	-1.692852000
6	-4.252629000	0.881878000	-0.055738000	1	7.227359000	0.397064000	-0.356034000
6	-3.943217000	0.955799000	-1.596888000	6	4.085945000	-2.753288000	-1.464969000
6	-3.872760000	2.330913000	-2.184761000	6	-0.604089000	-3.624523000	-2.550182000
6	-4.182952000	3.466459000	-1.460950000	6	-1.645873000	-3.810971000	2.210986000
6	-3.456989000	4.695418000	-1.692520000	6	2.781150000	-1.961870000	3.162338000
6	-2.427875000	4.743455000	-2.633898000	7	-0.754840000	-3.656475000	-0.083149000
6	-1.203940000	5.466214000	-2.337263000	7	1.643520000	-3.153943000	-1.627500000
6	-1.061258000	6.121832000	-1.119196000	7	3.083367000	-2.504116000	0.770817000
6	0.194763000	6.047359000	-0.398407000	7	0.675510000	-2.940421000	2.319428000
6	1.255769000	5.305533000	-0.919653000	6	3.554640000	-2.142978000	2.004931000
6	2.091550000	4.511182000	-0.060011000	6	4.164355000	-2.573323000	-0.076576000
6	1.801294000	4.417635000	1.285503000	6	2.875358000	-2.899658000	-2.174032000
6	1.857734000	3.120124000	1.984493000	6	0.749345000	-3.271369000	-2.666182000
6	2.189041000	1.963509000	1.302062000	6	1.437278000	-2.342424000	3.296949000
6	1.436016000	0.760486000	1.521790000	6	-0.545140000	-3.233937000	2.873213000
6	0.413991000	0.719806000	2.468740000	6	-1.738018000	-3.980367000	0.822608000
6	-0.816394000	0.003584000	2.178417000	6	-1.276730000	-3.850379000	-1.337573000
6	-1.910347000	0.760476000	2.733660000	6	4.995125000	-2.021818000	1.949662000
6	-3.111185000	0.837757000	2.027810000	6	5.371556000	-2.325178000	0.678096000
6	-3.826272000	2.096323000	1.940650000	6	2.744034000	-2.797300000	-3.610413000
6	-4.464485000	2.182959000	0.648868000	6	1.433609000	-3.009212000	-3.910622000
6	-4.483201000	3.390191000	-0.020737000	6	-2.632774000	-4.341096000	-1.218560000
6	-3.932536000	4.574214000	0.606584000	6	-2.905723000	-4.442158000	0.109346000
6	-3.303512000	5.383229000	-0.421259000	6	0.646493000	-2.212122000	4.498176000
6	-2.136662000	6.086463000	-0.141370000	6	-0.562869000	-2.787252000	4.245939000
6	-1.535020000	6.000007000	1.181263000	1	5.628086000	-1.772614000	2.785881000
6	-0.094589000	5.974871000	1.016161000	1	6.371118000	-2.364957000	0.280957000
6	0.691296000	5.165283000	1.838306000	1	3.543741000	-2.559077000	-4.291578000
6	0.063452000	4.357460000	2.867740000	1	0.967756000	-2.980071000	-4.881353000
6	0.782891000	3.097039000	2.955192000	1	-3.288393000	-4.566122000	-2.042512000
6	0.080953000	1.915697000	3.207100000	1	-3.824073000	-4.771671000	0.563172000
6	-1.362863000	1.948784000	3.370906000	1	0.971468000	-1.739028000	5.409856000
6	-2.047292000	3.156317000	3.283449000	1	-1.404530000	-2.871558000	4.913828000
6	-3.306235000	3.232138000	2.564120000	6	5.324125000	-2.853201000	-2.294112000
6	-3.360507000	4.502858000	1.877486000	6	6.287265000	-1.830697000	-2.413563000
6	-2.136280000	5.225369000	2.168895000	6	5.506247000	-4.010252000	-3.060734000
6	-1.318463000	4.389719000	3.034018000	1	4.779183000	-4.805675000	-2.955388000
6	-5.165676000	0.218144000	-1.080792000	6	7.332006000	-1.955641000	-3.333189000
6	3.929901000	2.666723000	-0.560722000	6	6.570681000	-4.158586000	-3.943319000
6	-6.521958000	0.823422000	-1.306746000	1	8.032933000	-1.146411000	-3.482566000
8	-6.761690000	1.995205000	-1.415041000	1	6.679763000	-5.070802000	-4.516572000
8	-7.458486000	-0.145066000	-1.353664000	6	7.474211000	-3.115003000	-4.090897000
6	-8.807299000	0.302314000	-1.598617000	1	8.293958000	-3.190995000	-4.795647000
1	-9.133851000	0.969331000	-0.800266000	6	-1.383866000	-3.784046000	-3.811761000
1	-8.858922000	0.828364000	-2.551732000	6	-1.047526000	-4.772155000	-4.744738000
1	-9.409729000	-0.601777000	-1.623191000	6	-2.470539000	-2.945938000	-4.078814000
6	4.795654000	3.235065000	0.549133000	1	-0.214970000	-5.433926000	-4.537462000
8	5.067753000	4.395338000	0.689462000	1	-2.753636000	-2.189372000	-3.362181000
8	5.213580000	2.244227000	1.353545000	6	-1.779448000	-4.914509000	-5.919657000
6	6.067729000	2.645318000	2.439270000	6	-3.203410000	-3.089748000	-5.252631000
1	6.987560000	3.084989000	2.051311000	1	-1.510895000	-5.688066000	-6.630177000
1	5.557641000	3.376933000	3.066903000	1	-4.046432000	-2.433542000	-5.434020000
1	6.273127000	1.734721000	2.995440000	6	-2.859006000	-4.071606000	-6.178123000
6	-5.136683000	-1.301043000	-1.254057000	1	-3.430157000	-4.184383000	-7.092582000
8	-4.849342000	-1.796600000	-2.307750000	6	-2.722676000	-4.366136000	3.087918000
8	-5.444201000	-2.085726000	-0.209214000	6	-2.364318000	-5.412444000	3.945334000

6	-4.060476000	-3.925967000	3.112749000
1	-1.336396000	-5.752771000	3.922926000
6	-3.278367000	-6.024409000	4.796068000
6	-4.984077000	-4.541754000	3.963433000
1	-2.964036000	-6.836965000	5.439337000
1	-6.010886000	-4.206941000	3.990823000
6	-4.594589000	-5.583993000	4.799790000
1	-5.328365000	-6.044460000	5.450940000
6	3.443162000	-1.302000000	4.323675000
6	3.868079000	0.028084000	4.210213000
6	3.644941000	-1.971533000	5.535050000
1	3.716079000	0.552302000	3.275008000
1	3.331210000	-3.004632000	5.624930000
6	4.463740000	0.675128000	5.288843000
6	4.250104000	-1.326672000	6.610514000
1	4.766527000	1.711506000	5.193308000
1	4.405076000	-1.861692000	7.540448000
6	4.656992000	0.000289000	6.492437000
1	5.120375000	0.504841000	7.332299000
30	1.152204000	-3.042763000	0.340350000
8	-4.403077000	-2.881366000	2.296109000
8	6.129234000	-0.740493000	-1.606221000

$C_{59}N$-Pc

7	2.132303000	1.645298000	-2.629747000
7	1.374674000	-0.967597000	-3.541201000
7	-1.400664000	-0.239027000	-3.575904000
7	-0.665602000	2.364033000	-2.695343000
6	2.122625000	2.853032000	-1.971142000
6	3.301384000	0.944436000	-2.399423000
6	2.653087000	-1.187653000	-3.122568000
6	0.793337000	-2.194138000	-3.694639000
6	-1.462723000	-1.592265000	-3.823444000
6	-2.643625000	0.289941000	-3.287100000
6	-2.014542000	2.404090000	-2.512294000
6	-0.145273000	3.440629000	-2.033328000
6	3.409073000	2.976002000	-1.315331000
6	4.146584000	1.800815000	-1.580656000
6	2.924184000	-2.620943000	-2.994209000
6	1.740120000	-3.273248000	-3.374606000
6	-2.865189000	-1.956248000	-3.763875000
6	-3.598226000	-0.799789000	-3.419002000
6	-2.400827000	3.561029000	-1.701412000
6	-1.209636000	4.244817000	-1.411395000
6	3.832003000	3.920661000	-0.381720000
6	5.344123000	1.533446000	-0.890886000
6	3.987871000	-3.298416000	-2.411342000
6	1.582460000	-4.650981000	-3.179174000
6	-3.465223000	-3.210641000	-3.844375000
6	-4.963946000	-0.881674000	-3.098759000
6	-3.607754000	3.891673000	-1.098348000
6	-1.189568000	5.308985000	-0.499112000
6	5.020936000	3.663260000	0.285273000
6	5.754873000	2.491147000	0.038383000
6	3.841285000	-4.670908000	-2.226323000
6	2.662884000	-5.329029000	-2.599922000
6	-4.822599000	-3.283317000	-3.564698000
6	-5.551431000	-2.144282000	-3.185226000
6	-3.595651000	4.948452000	-0.190394000
6	-2.413010000	5.638537000	0.101057000
1	3.227077000	4.792096000	-0.169184000
1	4.869541000	-2.765283000	-2.081525000
1	-2.876480000	-4.086176000	-4.084647000
1	-4.503421000	3.320766000	-1.302640000
1	5.384526000	4.367323000	1.024622000
1	6.672355000	2.313900000	0.587104000
1	4.640784000	-5.238835000	-1.765701000
1	2.571368000	-6.395731000	-2.430980000
1	-5.332031000	-4.238194000	-3.618367000
1	-6.603967000	-2.240730000	-2.945886000
1	-4.512327000	5.234883000	0.311916000
1	-2.435016000	6.458296000	0.809755000
7	3.545180000	-0.310936000	-2.678431000
7	-0.488689000	-2.461461000	-3.917649000
7	-2.919435000	1.489030000	-2.841217000
7	1.130948000	3.682985000	-1.768408000
1	1.326830000	1.242320000	-3.092650000
1	-0.539143000	0.286574000	-3.489446000
6	6.107380000	0.277458000	-1.082973000
6	6.349519000	-0.561008000	0.006348000
6	6.557884000	-0.087349000	-2.352689000
6	7.023903000	-1.774067000	-0.159080000
6	7.242330000	-1.282237000	-2.554914000
6	7.456678000	-2.107836000	-1.444689000
1	5.971302000	-0.269189000	0.976035000
1	6.348193000	0.574274000	-3.179952000
1	7.972621000	-3.047921000	-1.591795000
6	0.051941000	6.040396000	-0.152051000
6	0.468361000	6.133111000	1.171236000
6	0.827032000	6.624413000	-1.161601000
6	1.660845000	6.788981000	1.510567000
6	2.008317000	7.289535000	-0.864856000
6	2.406426000	7.357283000	0.481165000
1	-0.130417000	5.656810000	1.937863000
1	0.487554000	6.529906000	-2.182276000
1	3.329005000	7.866780000	0.719318000
6	-5.729245000	0.295779000	-2.617289000
6	-5.937457000	1.396399000	-3.438413000
6	-6.190891000	0.317659000	-1.296911000
6	-6.588737000	2.538567000	-2.964455000
6	-6.840489000	1.438784000	-0.786135000
6	-7.027099000	2.535471000	-1.640216000
1	-5.557904000	1.365338000	-4.451419000
1	-5.995005000	-0.542691000	-0.672346000
1	-7.516617000	3.415306000	-1.248383000
6	0.325763000	-5.375113000	-3.503983000
6	-0.098957000	-5.529734000	-4.826463000
6	-0.452349000	-5.908897000	-2.476164000
6	-1.272437000	-6.219535000	-5.104843000
6	-1.651057000	-6.577233000	-2.740142000
6	-2.048222000	-6.737303000	-4.067977000
1	0.492908000	-5.106951000	-5.628787000
1	-0.132937000	-5.769537000	-1.448956000
1	-1.591079000	-6.348065000	-6.133009000
1	-2.971569000	-7.261691000	-4.291965000
6	7.243074000	-2.758136000	0.998778000
6	7.754251000	-1.716128000	-3.935296000
6	2.098668000	6.849957000	2.979671000
6	2.888723000	7.931272000	-1.945548000
6	-7.301863000	1.531619000	0.674468000
6	-6.773128000	3.742545000	-3.897796000
6	6.321816000	-3.978243000	0.781351000
1	6.557659000	-4.485106000	-0.157627000
1	6.440818000	-4.699362000	1.595663000
1	5.273772000	-3.672980000	0.744988000
6	8.713010000	-3.223187000	1.034207000
1	8.868786000	-3.908097000	1.872450000
1	9.001480000	-3.748451000	0.121936000
1	9.386017000	-2.371089000	1.159057000
6	6.913508000	-2.132933000	2.363457000
1	7.119389000	-2.855903000	3.156732000
1	7.521374000	-1.244170000	2.552914000
1	5.862812000	-1.852925000	2.441178000
6	9.292542000	-1.827268000	-3.889326000
1	9.619569000	-2.563509000	-3.151825000
1	9.681719000	-2.131538000	-4.865485000
1	9.741363000	-0.866371000	-3.624933000
6	7.150583000	-3.086320000	-4.308511000

1	7.527545000	-3.409957000	-5.283010000
1	7.408783000	-3.857038000	-3.579238000
1	6.061641000	-3.030272000	-4.364058000
6	7.370423000	-0.713997000	-5.034926000
1	7.739645000	-1.070117000	-5.999870000
1	6.286189000	-0.601317000	-5.111963000
1	7.807785000	0.271367000	-4.855518000
6	4.295314000	7.297105000	-1.908734000
1	4.774979000	7.430073000	-0.936730000
1	4.243788000	6.225366000	-2.112124000
1	4.937217000	7.758996000	-2.664563000
6	2.313234000	7.729200000	-3.355666000
1	2.976302000	8.190826000	-4.091624000
1	2.224657000	6.668634000	-3.603623000
1	1.327938000	8.190329000	-3.460161000
6	3.000686000	9.446445000	-1.676700000
1	3.621750000	9.923600000	-2.440587000
1	2.013581000	9.915392000	-1.694535000
1	3.450737000	9.649995000	-0.702661000
6	1.045186000	7.635595000	3.788414000
1	0.949499000	8.656568000	3.410045000
1	0.063049000	7.161900000	3.729264000
1	1.332742000	7.684813000	4.842863000
6	2.206300000	5.417323000	3.538081000
1	2.542978000	5.436269000	4.578792000
1	1.246794000	4.901424000	3.510058000
1	2.916467000	4.822584000	2.957996000
6	3.459771000	7.539530000	3.157015000
1	3.730208000	7.547549000	4.215742000
1	4.250936000	7.013604000	2.615806000
1	3.438762000	8.576541000	2.812676000
6	-7.425014000	4.938173000	-3.186540000
1	-7.525899000	5.769833000	-3.888116000
1	-8.423982000	4.695516000	-2.815080000
1	-6.817677000	5.285572000	-2.346614000
6	-7.673807000	3.326561000	-5.079508000
1	-7.818575000	4.168884000	-5.762442000
1	-7.233203000	2.504302000	-5.647174000
1	-8.654406000	3.000675000	-4.722897000
6	-5.398097000	4.196236000	-4.433360000
1	-4.890290000	3.398076000	-4.977259000
1	-5.522646000	5.042265000	-5.115524000
1	-4.744630000	4.507663000	-3.616193000
6	-8.792315000	1.923272000	0.732811000
1	-9.407935000	1.180626000	0.218745000
1	-9.125688000	1.984451000	1.772768000
1	-8.977855000	2.892836000	0.267002000
6	-7.129870000	0.200564000	1.422539000
1	-7.490336000	0.305992000	2.448774000
1	-7.699108000	-0.602968000	0.947192000
1	-6.082227000	-0.097732000	1.473803000
6	-6.455346000	2.605550000	1.392011000
1	-6.748181000	2.684792000	2.443178000
1	-5.393240000	2.354893000	1.349686000
1	-6.587754000	3.586570000	0.930051000
6	-2.536671000	-7.009738000	-1.595635000
1	-3.137262000	-7.878056000	-1.883579000
1	-1.914910000	-7.316973000	-0.748466000
6	-3.443861000	-5.846597000	-1.161867000
1	-2.830157000	-4.953531000	-1.034486000
1	-4.158238000	-5.613287000	-1.954458000
6	-4.176613000	-6.097928000	0.142530000
1	-4.998289000	-6.811579000	0.044076000
1	-3.503746000	-6.459956000	0.922639000
8	-4.708343000	-4.816304000	0.564389000
6	-4.959380000	-4.659700000	1.876803000
8	-4.987914000	-5.557663000	2.677971000
6	-5.090904000	-3.189798000	2.216872000
1	-5.655274000	-2.663584000	1.445909000
1	-5.598547000	-3.096923000	3.176416000

6	-3.386713000	-0.230030000	1.589422000
6	-2.886147000	-1.089878000	0.533641000
6	-2.918561000	-2.448790000	0.991156000
6	-3.685890000	-2.542839000	2.327233000
6	-3.742415000	-1.049184000	2.713467000
6	-3.485835000	-0.597215000	3.983373000
6	-2.907187000	0.711089000	4.199074000
6	-2.600633000	1.528045000	3.109476000
6	-2.851947000	1.048164000	1.770865000
6	-1.768106000	1.509746000	0.913775000
6	-1.281342000	0.678263000	-0.083460000
6	-1.859059000	-0.640692000	-0.297780000
6	-0.793743000	-1.543731000	-0.663288000
6	-0.807539000	-2.853796000	-0.187961000
6	-1.891338000	-3.294966000	0.658532000
6	-1.338217000	-4.225583000	1.650966000
6	-1.794342000	-4.125981000	2.953186000
6	-2.585952000	-2.783813000	4.608101000
6	-2.938651000	-1.505576000	4.999829000
6	-2.011695000	-0.755393000	5.814301000
6	-1.994422000	0.617177000	5.322480000
6	-0.806485000	1.342269000	5.312839000
6	-0.479880000	2.187797000	4.172914000
6	-1.359627000	2.283399000	3.095230000
6	-0.843261000	2.274574000	1.735283000
6	0.529206000	2.175185000	1.515204000
6	1.034454000	1.309996000	0.462259000
6	0.146681000	0.579209000	-0.317693000
6	0.448734000	-0.795997000	-0.674143000
6	1.621820000	-1.388563000	-0.219653000
6	1.609589000	-2.760556000	0.263017000
6	0.416308000	-3.477160000	0.281628000
6	0.087145000	-4.321284000	1.425182000
6	0.988991000	-4.413532000	2.495838000
6	0.480911000	-4.384519000	3.843665000
6	-0.892626000	-4.255171000	4.064187000
6	-1.391756000	-3.407689000	5.108358000
6	-0.515471000	-2.693106000	5.927963000
6	-0.825154000	-1.333054000	6.286960000
6	0.413232000	-0.576273000	6.260853000
6	0.425012000	0.734154000	5.790720000
6	1.506661000	1.190471000	4.938129000
6	0.947576000	2.090863000	3.940915000
6	1.443235000	2.081872000	2.639258000
6	2.519942000	1.174203000	2.275409000
6	2.263495000	0.692513000	0.929474000
6	2.549934000	-0.628660000	0.592901000
6	3.108126000	-1.528762000	1.588453000
6	2.536690000	-2.848275000	1.380463000
6	2.226254000	-3.652725000	2.474025000
6	2.485334000	-3.170165000	3.823937000
6	1.400640000	-3.625823000	4.677138000
6	0.915323000	-2.802396000	5.690977000
6	1.491766000	-1.484733000	5.898884000
6	2.527139000	-1.045902000	5.079207000
6	2.538287000	0.322068000	4.590149000
6	3.051607000	0.310176000	3.230325000
6	3.355386000	-1.066854000	2.878679000
6	3.033206000	-1.905877000	4.019998000
7	-2.873067000	-3.307972000	3.334767000

C$_{60}$-TPA (properly oriented for OT2 calculation)

6	1.086332756	3.175907430	-4.334875490
6	2.342476559	2.440163624	-4.318661770
6	2.519159381	1.346270265	-5.162304700
6	3.176481999	0.148809288	-4.670085650
6	3.631223490	0.094799510	-3.355084175

6	3.444912732	1.236962977	-2.473974631	6	-3.229309290	-1.036843811	-3.290861303
6	2.811970405	2.383212362	-2.948308782	6	-2.919761055	-0.544475564	-4.620562963
6	1.843572882	3.077296598	-2.114453278	6	-1.992777251	-1.216041719	-5.413885435
6	0.780843515	3.573092552	-2.974543395	6	-1.335192549	-2.411293003	-4.910208396
6	-0.537412309	3.569663111	-2.525395058	6	-1.622627122	-2.873855608	-3.629688947
6	-1.607454641	3.163086250	-3.422667762	6	-0.557502757	-3.363934875	-2.773361632
6	-1.312905041	2.778242352	-4.727985828	6	-0.852903707	-2.974888032	-1.411031517
6	0.062199202	2.785454389	-5.194150255	6	0.159071201	-2.595772731	-0.566128157
6	0.246196102	1.640208111	-6.069529486	6	-0.001570923	-1.601719368	0.586092016
6	1.447243815	0.936691199	-6.053849767	6	-0.036439723	-2.307528146	1.968817161
6	1.441158358	-0.515107225	-6.110749382	1	0.469542041	-3.274620192	1.947057510
6	2.509450841	-1.002664239	-5.256478853	1	0.468644750	-1.667822759	2.710107177
6	2.325130971	-2.158772020	-4.502802341	7	-1.455744899	-2.459614091	2.231268531
6	2.796814400	-2.211781293	-3.129934401	6	-1.815424510	-3.044980237	3.529290240
6	3.435740406	-1.111235664	-2.569552418	1	-1.377958095	-4.046550588	3.562341793
6	3.128747849	-0.707639963	-1.206568376	1	-2.902095031	-3.167900522	3.536186392
6	3.136768141	0.733941870	-1.147665341	6	-1.375050511	-2.242806913	4.734603071
6	2.195764629	1.390001133	-0.352081155	6	-0.116510777	-2.435561561	5.311318017
6	1.539303814	2.585707109	-0.848975353	6	0.334821834	-1.633146030	6.351279525
6	0.165952255	2.579011430	-0.378152466	1	1.317604706	-1.791101789	6.776424151
6	-0.850996201	3.069830694	-1.199056518	1	0.529303045	-3.221542677	4.933533966
6	-2.103068190	2.356825994	-1.274150185	6	-2.183207618	-1.228908155	5.257833570
6	-2.578831089	2.411663896	-2.647255520	1	-3.175766925	-1.072459216	4.847970061
6	-3.216001208	1.310081904	-3.207685183	6	-1.752731649	-0.429276576	6.307571455
6	-2.912589348	0.909119054	-4.570527484	1	-2.396209871	0.345078693	6.705011382
6	-1.979795237	1.626745438	-5.314415857	6	-0.478695854	-0.613129643	6.859703358
6	-1.015864968	0.924004165	-6.142616785	7	-0.026711679	0.217291960	7.909329018
6	-1.023992822	-0.467903476	-6.190920632	6	0.744429887	-0.325283710	8.967650217
6	0.232166766	-1.203634302	-6.174653543	6	1.852800864	0.369846890	9.464911778
6	0.038409132	-2.405784406	-5.387744591	6	2.599649571	-0.161605679	10.510110606
6	1.062049348	-2.876813248	-4.569177730	6	2.266657645	-1.396854405	11.062323079
6	0.758408746	-3.372609630	-3.239293373	6	1.168064440	-2.093424522	10.562458758
6	1.821398981	-2.961790600	-2.354651207	6	0.404499010	-1.561328056	9.529886405
6	1.510556443	-2.562565015	-1.053578869	1	-0.456119873	-2.097775732	9.150751570
6	2.178950934	-1.415176688	-0.467782723	1	0.893035107	-3.051644916	10.988084732
6	1.242214608	-0.737818902	0.385125469	1	2.854987079	-1.810917172	11.872153216
6	1.238319552	0.635123412	0.427812820	1	3.455114725	0.388176754	10.885402980
6	-0.039295469	1.383338722	0.411288467	1	2.118464048	1.325101423	9.030300469
6	-1.237862009	0.714731796	0.353231644	6	-0.321410526	1.604317878	7.889718591
6	-1.386997421	-0.790523252	0.567591865	6	-0.697642061	2.263353743	9.065542421
6	-2.014540729	-1.151939623	1.941103830	1	-0.764554783	1.702595946	9.989224753
1	-3.104731018	-1.186746245	1.896143493	6	-0.976696053	3.625105786	9.044539759
1	-1.721873522	-0.389042693	2.680068501	1	-1.266505281	4.122798362	9.962816736
6	-2.309558065	-1.149125247	-0.598872955	6	-0.903021630	4.344945418	7.853594928
6	-2.129663843	-2.227071689	-1.427684522	1	-1.128117303	5.404443651	7.839699149
6	-2.587095062	-2.174900898	-2.799704146	6	-0.535715336	3.688010322	6.680819754
6	-2.270153509	1.190766154	-0.525187963	1	-0.466439929	4.237517087	5.749061400
6	-2.932824260	0.040068118	-1.111063657	6	-0.237005016	2.330415082	6.695963776
6	-3.408153230	0.101186668	-2.422275011	1	0.060263665	1.824097711	5.786324857

Cartesian coordinates of the optimized fragments for the calculation of λ_{int}

All systems were optimized at B3LYP-D3(BJ)/6-311G(d,p) level of theory.

C_{60}-Az Donor N electron system

6	-2.216215000	-0.006471000	-0.000169000
6	-2.014938000	1.385836000	-0.000127000
6	-0.839589000	2.123023000	-0.000104000
6	-1.201698000	-0.963840000	-0.000384000
6	0.487072000	1.705708000	-0.000056000
6	0.193047000	-0.826962000	-0.000411000
6	0.995789000	0.300506000	-0.000102000
1	-2.913768000	1.990188000	-0.000103000
1	-0.972894000	3.202814000	-0.000125000
1	-1.524656000	-1.994840000	-0.000569000
1	0.716098000	-1.775506000	-0.000678000
6	1.605972000	2.540798000	0.000024000
6	2.756740000	1.735062000	0.000055000
1	3.766181000	2.120120000	0.000101000
6	2.418410000	0.370335000	-0.000002000
6	3.416208000	-0.781511000	0.000069000
6	4.859035000	-0.243981000	0.000492000
1	5.059719000	0.363671000	-0.885468000
1	5.059209000	0.363569000	0.886635000
1	5.564061000	-1.079239000	0.000628000
6	3.247106000	-1.650154000	-1.266540000
1	3.991195000	-2.452681000	-1.277585000
1	2.259711000	-2.108619000	-1.327860000
1	3.385202000	-1.042977000	-2.164484000
6	3.246543000	-1.650554000	1.266309000
1	3.990686000	-2.453030000	1.277435000
1	3.384188000	-1.043662000	2.164518000
1	2.259157000	-2.109112000	1.327050000
6	-3.693531000	-0.468568000	0.000071000
6	-4.397800000	0.074556000	-1.263224000
1	-5.440970000	-0.253578000	-1.279582000
1	-4.389987000	1.164745000	-1.303090000
1	-3.908213000	-0.297494000	-2.166730000
6	-4.397163000	0.074380000	1.263826000
1	-5.440333000	-0.253729000	1.280666000
1	-3.907112000	-0.297824000	2.167016000
1	-4.389261000	1.164562000	1.303827000
6	-3.859808000	-1.997232000	-0.000005000
1	-3.417691000	-2.457391000	0.886906000
1	-4.925140000	-2.239568000	0.000246000
1	-3.418142000	-2.457247000	-0.887218000
1	1.581679000	3.621250000	0.000123000

C_{60}-Az Donor N-1 electron system

6	-2.229941000	-0.009223000	-0.000071000
6	-2.007828000	1.381178000	-0.000087000
6	-0.823421000	2.112812000	-0.000067000
6	-1.210090000	-0.966160000	-0.000192000
6	0.487029000	1.660375000	-0.000026000
6	0.186137000	-0.835956000	-0.000175000
6	0.971198000	0.302377000	-0.000027000
1	-2.900670000	1.993234000	-0.000104000
1	-0.944283000	3.192063000	-0.000088000
1	-1.539866000	-1.995305000	-0.000347000
1	0.712770000	-1.780068000	-0.000336000
6	1.645876000	2.520726000	-0.000022000
6	2.788278000	1.738139000	0.000028000
1	3.796752000	2.119139000	0.000030000
6	2.442288000	0.369749000	-0.000025000
6	3.419297000	-0.778390000	0.000033000
6	4.868479000	-0.258820000	0.000110000

1	5.083909000	0.339595000	-0.888025000
1	5.083726000	0.339828000	0.888132000
1	5.555244000	-1.106466000	0.000289000
6	3.219564000	-1.639424000	-1.274183000
1	3.962962000	-2.439151000	-1.279535000
1	2.234778000	-2.102918000	-1.329988000
1	3.362486000	-1.038720000	-2.174712000
6	3.219402000	-1.639390000	1.274234000
1	3.962730000	-2.439181000	1.279657000
1	3.362311000	-1.038677000	2.174761000
1	2.234562000	-2.102779000	1.329988000
6	-3.702850000	-0.460439000	0.000040000
6	-4.393558000	0.096526000	-1.267416000
1	-5.435990000	-0.227338000	-1.281166000
1	-4.389942000	1.187369000	-1.303576000
1	-3.911175000	-0.276699000	-2.173784000
6	-4.393407000	0.097291000	1.267245000
1	-5.435887000	-0.226410000	1.281229000
1	-3.911018000	-0.275515000	2.173782000
1	-4.389589000	1.188157000	1.302797000
6	-3.869013000	-1.988155000	0.000479000
1	-3.435824000	-2.452058000	0.890266000
1	-4.933551000	-2.225906000	0.000459000
1	-3.435659000	-2.452576000	-0.888959000
1	1.606573000	3.601074000	-0.000038000

C_{60}-Az Acceptor N electron system

6	-2.765922000	2.601535000	0.860106000
6	-2.849063000	2.601546000	-0.591667000
6	-3.594771000	1.423725000	-0.997969000
6	-3.974222000	0.695956000	0.201236000
6	-3.460856000	1.423895000	1.349082000
6	-2.962239000	0.727963000	2.447630000
6	-1.749576000	1.177217000	3.102926000
6	-1.082376000	2.307572000	2.637415000
6	-1.602852000	3.035272000	1.490733000
6	-0.472339000	3.484470000	0.696862000
6	-0.552150000	3.485337000	-0.691291000
6	-1.765644000	3.035912000	-1.350952000
6	-1.379357000	2.307767000	-2.549268000
6	-2.094923000	1.176984000	-2.935017000
6	-3.225377000	0.727852000	-2.146423000
6	-3.225363000	-0.728068000	-2.146373000
6	-3.594738000	-1.423864000	-0.997867000
6	-3.974205000	-0.696019000	0.201285000
6	-3.460823000	-1.423864000	1.349183000
6	-2.962222000	-0.727839000	2.447682000
6	-1.749548000	-1.177020000	3.103005000
6	-0.994682000	0.000122000	3.502146000
6	0.393252000	0.000136000	3.404174000
6	1.091513000	1.176294000	2.917580000
6	0.366380000	2.311016000	2.549893000
6	0.741393000	3.030764000	1.357130000
6	1.819487000	2.575408000	0.595944000
6	1.737420000	2.578794000	-0.852980000
6	0.578389000	3.031661000	-1.485504000
6	0.070196000	2.310638000	-2.627209000
6	0.748789000	1.176107000	-3.075247000
6	-0.000455000	-0.000124000	-3.478224000
6	-1.390260000	-0.000136000	-3.417478000
6	-2.094899000	-1.177233000	-2.934936000
6	-1.379301000	-2.307967000	-2.549096000
6	-1.765578000	-3.036037000	-1.350732000

6	-2.849006000	-2.601641000	-0.591479000
6	-2.765866000	-2.601525000	0.860295000
6	-1.602780000	-3.035186000	1.490951000
6	-1.082326000	-2.307394000	2.637581000
6	0.366436000	-2.310816000	2.550056000
6	1.091538000	-1.176040000	2.917646000
6	2.224237000	-0.739784000	2.129675000
6	2.224239000	0.740002000	2.129644000
6	2.587944000	1.431208000	1.002196000
6	3.268293000	0.803284000	-0.216577000
6	2.458643000	1.438056000	-1.346055000
6	1.963932000	0.740197000	-2.420842000
6	1.963961000	-0.740321000	-2.420808000
6	0.748815000	-1.176308000	-3.075177000
6	0.070246000	-2.310817000	-2.627044000
6	0.578455000	-3.031747000	-1.485283000
6	-0.552076000	-3.485389000	-0.691040000
6	-0.472256000	-3.484419000	0.697110000
6	0.741465000	-3.030641000	1.357350000
6	1.819558000	-2.575311000	0.596147000
6	2.588021000	-1.431075000	1.002310000
6	3.268338000	-0.803231000	-0.216537000
6	2.458649000	-1.438088000	-1.345943000
6	1.737470000	-2.578805000	-0.852778000
6	4.781403000	-1.143030000	-0.278364000
6	4.781393000	1.143025000	-0.278336000
7	5.416751000	-0.000007000	0.350058000
6	6.865990000	0.000025000	0.266374000
1	7.263056000	0.883196000	0.771126000
1	7.262940000	-0.884062000	0.769602000
1	7.230984000	0.000883000	-0.776531000
1	5.014109000	-2.070301000	0.247441000
1	5.014102000	2.070404000	0.247298000
1	5.085428000	1.257242000	-1.335215000
1	5.085382000	-1.257325000	-1.335240000

C$_{60}$-Az Acceptor N+1 electron system

6	-2.785993000	2.605734000	0.844128000
6	-2.859082000	2.604795000	-0.600020000
6	-3.598250000	1.425232000	-1.014425000
6	-3.986329000	0.696023000	0.181719000
6	-3.476667000	1.426675000	1.330780000
6	-2.983963000	0.725577000	2.431325000
6	-1.766849000	1.170102000	3.094863000
6	-1.100270000	2.304408000	2.625859000
6	-1.614623000	3.035830000	1.487212000
6	-0.477890000	3.473347000	0.697318000
6	-0.548330000	3.473681000	-0.691845000
6	-1.762668000	3.033823000	-1.360669000
6	-1.369506000	2.305023000	-2.547431000
6	-2.081252000	1.170127000	-2.945741000
6	-3.222298000	0.726379000	-2.159726000
6	-3.222298000	-0.726513000	-2.159685000
6	-3.598245000	-1.425299000	-1.014342000
6	-3.986326000	-0.696023000	0.181759000
6	-3.476662000	-1.426606000	1.330862000
6	-2.983961000	-0.725442000	2.431367000
6	-1.766845000	-1.169924000	3.094928000
6	-1.022312000	0.000102000	3.508692000
6	0.383666000	0.000102000	3.418887000
6	1.075689000	1.169536000	2.927982000
6	0.355097000	2.307955000	2.547725000
6	0.738978000	3.031579000	1.367888000
6	1.827662000	2.578434000	0.605563000
6	1.755147000	2.582064000	-0.837926000
6	0.590496000	3.034846000	-1.483719000
6	0.086627000	2.306925000	-2.615599000
6	0.763757000	1.168765000	-3.067573000

6	0.024533000	-0.000102000	-3.486277000
6	-1.383625000	-0.000102000	-3.432551000
6	-2.081251000	-1.170303000	-2.945676000
6	-1.369498000	-2.305171000	-2.547295000
6	-1.762660000	-3.033905000	-1.360493000
6	-2.859076000	-2.604837000	-0.599869000
6	-2.785986000	-2.605692000	0.844279000
6	-1.614612000	-3.035744000	1.487386000
6	-1.100264000	-2.304256000	2.625991000
6	0.355105000	-2.307805000	2.547857000
6	1.075689000	-1.169357000	2.928040000
6	2.219687000	-0.737817000	2.143776000
6	2.219703000	0.737953000	2.143752000
6	2.590077000	1.433904000	1.020311000
6	3.275278000	0.803195000	-0.195294000
6	2.471233000	1.441118000	-1.328140000
6	1.983819000	0.736521000	-2.405548000
6	1.983831000	-0.736658000	-2.405521000
6	0.763763000	-1.168944000	-3.067513000
6	0.086634000	-2.307077000	-2.615465000
6	0.590501000	-3.034928000	-1.483542000
6	-0.548323000	-3.473723000	-0.691645000
6	-0.477877000	-3.473305000	0.697517000
6	0.738991000	-3.031500000	1.368064000
6	1.827672000	-2.578392000	0.605721000
6	2.590112000	-1.433845000	1.020405000
6	3.275289000	-0.803197000	-0.195257000
6	2.471216000	-1.441184000	-1.328047000
6	1.755153000	-2.582105000	-0.837769000
6	4.786238000	-1.143792000	-0.258245000
6	4.786232000	1.143773000	-0.258251000
7	5.437590000	-0.000006000	0.357829000
6	6.879212000	0.000020000	0.228380000
1	7.295151000	0.884485000	0.717815000
1	7.295156000	-0.884585000	0.717556000
1	7.213216000	0.000175000	-0.827528000
1	5.018084000	-2.069364000	0.271823000
1	5.018102000	2.069364000	0.271776000
1	5.088686000	1.263397000	-1.315837000
1	5.088694000	-1.263438000	-1.315828000

C$_{60}$-ZnTTP Donor N electron system

6	2.574046000	-0.577469000	1.894857000
6	1.729656000	-0.473299000	3.145410000
8	1.486257000	0.551815000	3.741114000
8	1.282269000	-1.674517000	3.543809000
6	0.525467000	-1.681296000	4.773341000
1	1.096966000	-1.207515000	5.570998000
1	-0.418001000	-1.152073000	4.639385000
1	0.351916000	-2.731187000	4.996139000
6	3.953506000	-1.155172000	2.189783000
8	4.263542000	-2.279689000	1.907032000
8	4.862490000	-0.378456000	2.829654000
6	4.652237000	1.009122000	3.150328000
1	3.597090000	1.252522000	3.259439000
1	5.141088000	1.151895000	4.115332000
6	5.310686000	1.904965000	2.128517000
1	5.379371000	2.922769000	2.532781000
1	6.319392000	1.538115000	1.911085000
8	4.512707000	1.897245000	0.951411000
6	4.078075000	2.630880000	-1.243053000
6	4.447827000	3.377439000	-2.360067000
6	4.925692000	2.638009000	-0.121014000
1	3.790736000	3.367398000	-3.221483000
6	5.627592000	4.118518000	-2.384888000
6	6.109256000	3.378260000	-0.136615000
1	5.894615000	4.688145000	-3.266411000
1	6.764725000	3.391075000	0.722493000

6	6.454229000	4.114336000	-1.269245000
1	7.376379000	4.683673000	-1.268760000
6	-1.393375000	1.483301000	2.427815000
6	-2.820915000	1.554588000	2.926906000
8	-3.162848000	1.576545000	4.079203000
8	-3.659271000	1.542571000	1.873958000
6	-5.054258000	1.336055000	2.158483000
1	-5.212350000	0.281245000	2.385960000
1	-5.370770000	1.958489000	2.994615000
1	-5.576822000	1.600879000	1.243649000
6	-1.093391000	0.104848000	1.891241000
8	-0.271335000	-0.130680000	1.033044000
8	-1.812899000	-0.835518000	2.503336000
6	-1.773766000	-2.184440000	1.974408000
1	-1.409576000	-2.154003000	0.953297000
1	-1.081191000	-2.769033000	2.583360000
6	-3.176629000	-2.744383000	2.068320000
1	-3.164218000	-3.779129000	1.714608000
1	-3.518058000	-2.728975000	3.107396000
8	-4.088209000	-1.956124000	1.290989000
6	-4.330461000	-2.474629000	-1.042707000
6	-4.774465000	-2.601288000	0.281358000
6	-5.068385000	-3.090172000	-2.054929000
1	-4.726497000	-2.992583000	-3.078500000
6	-5.924264000	-3.327703000	0.581037000
6	-6.217894000	-3.819807000	-1.761427000
1	-6.247733000	-3.396711000	1.613011000
1	-6.778752000	-4.289930000	-2.560340000
6	-6.644804000	-3.939437000	-0.441201000
1	-7.540475000	-4.502372000	-0.206067000
6	-3.077274000	-1.708814000	-1.310858000
6	1.656703000	-2.887104000	-1.479351000
6	2.803065000	1.851959000	-1.248355000
6	-1.936007000	3.024354000	-1.167638000
7	1.847960000	-0.422410000	-1.383766000
7	-0.623729000	-1.923938000	-1.481394000
7	-2.128702000	0.567588000	-1.315537000
7	0.341745000	2.062002000	-1.235595000
6	-2.663057000	1.830223000	-1.290119000
6	-3.178021000	-0.313531000	-1.334232000
6	-1.889700000	-2.446956000	-1.395501000
6	0.253711000	-2.979171000	-1.460106000
6	-0.534609000	3.111482000	-1.117086000
6	1.608652000	2.580159000	-1.152762000
6	2.897974000	0.459577000	-1.376053000
6	2.381457000	-1.685466000	-1.471847000
6	-4.106491000	1.740653000	-1.354431000
6	-4.423712000	0.418429000	-1.360811000
6	-1.810714000	-3.888252000	-1.319668000
6	-0.489205000	-4.216546000	-1.358247000
6	3.824298000	-1.590934000	-1.542200000
6	4.140714000	-0.270370000	-1.484553000
6	0.211024000	4.337066000	-0.918612000
6	1.531069000	4.009889000	-0.947059000
1	-4.778986000	2.581986000	-1.384583000
1	-5.404174000	-0.029164000	-1.396417000
1	-2.655161000	-4.554662000	-1.245413000
1	-0.052579000	-5.200404000	-1.311167000
1	4.498011000	-2.427131000	-1.622472000
1	5.121881000	0.174769000	-1.516537000
1	-0.223293000	5.311879000	-0.769601000
1	2.377523000	4.666799000	-0.829850000
6	2.431280000	-4.162610000	-1.484039000
6	2.343183000	-5.044012000	-2.567740000
6	3.256061000	-4.496383000	-0.403106000
1	1.715439000	-4.783135000	-3.411716000
1	3.343213000	-3.819233000	0.437901000
6	3.061637000	-6.235993000	-2.571979000
6	3.972436000	-5.690280000	-0.409775000
1	2.988712000	-6.905369000	-3.421642000

1	4.606591000	-5.934308000	0.434762000
6	3.877397000	-6.563470000	-1.490990000
1	4.437888000	-7.491357000	-1.493827000
6	-2.711738000	4.293924000	-1.048777000
6	-3.523382000	4.524165000	0.068258000
6	-2.640185000	5.275399000	-2.043046000
1	-3.581953000	3.764263000	0.837283000
1	-2.020471000	5.099455000	-2.914272000
6	-4.242255000	5.709903000	0.189144000
6	-3.362200000	6.459613000	-1.923792000
1	-4.860928000	5.876462000	1.063705000
1	-3.301028000	7.207808000	-2.705811000
6	-4.164121000	6.681277000	-0.806440000
1	-4.724675000	7.604168000	-0.712920000
30	-0.134205000	0.065376000	-1.252317000
1	-1.209508000	2.191718000	1.619754000
1	-0.700263000	1.679376000	3.247766000
1	2.643864000	0.406516000	1.439229000
1	2.093782000	-1.258696000	1.199676000

C$_{60}$- ZnTTP Donor N-1 electron system

6	2.229534000	-0.205978000	2.068017000
6	1.733111000	-0.148628000	3.497722000
8	0.790072000	-0.761938000	3.929018000
8	2.490681000	0.669897000	4.251665000
6	2.074011000	0.818759000	5.623627000
1	1.067910000	1.236859000	5.661800000
1	2.084035000	-0.145755000	6.131488000
1	2.791013000	1.500923000	6.072803000
6	3.054615000	-1.460594000	1.817923000
8	2.550160000	-2.488265000	1.448449000
8	4.392639000	-1.433879000	2.020089000
6	5.087321000	-0.279262000	2.520226000
1	4.435543000	0.347878000	3.125379000
1	5.875971000	-0.675046000	3.161976000
6	5.727253000	0.514977000	1.404759000
1	6.344061000	1.300951000	1.854949000
1	6.360579000	-0.126496000	0.783525000
8	4.688320000	1.080486000	0.606913000
6	3.997275000	2.062377000	-1.418399000
6	4.271411000	2.868214000	-2.527540000
6	5.024772000	1.826133000	-0.484611000
1	3.484680000	3.036726000	-3.252503000
6	5.534563000	3.412670000	-2.730771000
6	6.294175000	2.366541000	-0.688284000
1	5.730176000	4.019530000	-3.605437000
1	7.089027000	2.186051000	0.021329000
6	6.543378000	3.154741000	-1.809488000
1	7.534245000	3.567103000	-1.956158000
6	-1.958153000	1.467345000	2.118755000
6	-0.802556000	2.446843000	2.183330000
8	0.360787000	2.165764000	2.319823000
8	-1.276586000	3.696332000	2.104030000
6	-0.306923000	4.759781000	2.230970000
1	0.057899000	4.804697000	3.257597000
1	0.523314000	4.590206000	1.548947000
1	-0.844617000	5.668216000	1.973196000
6	-1.512341000	0.031836000	2.031339000
8	-0.835873000	-0.413888000	1.121745000
8	-1.974758000	-0.672266000	3.047704000
6	-1.785970000	-2.109665000	3.067797000
1	-1.050074000	-2.387574000	2.316893000
1	-1.412790000	-2.350026000	4.060327000
6	-3.139199000	-2.734902000	2.796285000
1	-3.069982000	-3.827556000	2.845291000
1	-3.878826000	-2.385648000	3.524392000
8	-3.480389000	-2.304388000	1.487298000
6	-4.746298000	-2.207056000	-0.453127000

6	-4.663414000	-2.615702000	0.893946000
6	-5.919228000	-2.433193000	-1.163205000
1	-5.978420000	-2.124769000	-2.200260000
6	-5.731967000	-3.261476000	1.505416000
6	-6.997961000	-3.075750000	-0.554127000
1	-5.667863000	-3.583666000	2.536377000
1	-7.905018000	-3.260037000	-1.115329000
6	-6.897434000	-3.487121000	0.770449000
1	-7.731054000	-3.990360000	1.245063000
6	-3.520023000	-1.558327000	-0.997162000
6	1.043774000	-3.185745000	-1.535880000
6	2.663134000	1.418345000	-1.284341000
6	-1.950489000	3.043995000	-1.257040000
7	1.494946000	-0.762571000	-1.284702000
7	-1.122492000	-2.009463000	-1.391201000
7	-2.391929000	0.618997000	-1.226331000
7	0.228237000	1.856357000	-1.217231000
6	-2.806492000	1.927871000	-1.246251000
6	-3.512577000	-0.148850000	-1.095924000
6	-2.417890000	-2.406001000	-1.195295000
6	-0.366073000	-3.144893000	-1.441203000
6	-0.539345000	2.992732000	-1.214226000
6	1.537033000	2.263723000	-1.184119000
6	2.620227000	0.013661000	-1.388854000
6	1.887783000	-2.054831000	-1.510413000
6	-4.247062000	1.980173000	-1.163371000
6	-4.681540000	0.693193000	-1.034073000
6	-2.487001000	-3.846676000	-1.147503000
6	-1.216070000	-4.306462000	-1.300423000
6	3.305202000	-2.095026000	-1.776469000
6	3.758064000	-0.815338000	-1.698329000
6	0.311145000	4.153338000	-1.136426000
6	1.597436000	3.701446000	-1.108290000
1	-4.841814000	2.877899000	-1.188427000
1	-5.695859000	0.346084000	-0.926388000
1	-3.387840000	-4.422502000	-1.012977000
1	-0.878931000	-5.328970000	-1.294638000
1	3.869124000	-2.980226000	-2.014840000
1	4.760636000	-0.461122000	-1.869004000
1	-0.031084000	5.173927000	-1.101573000
1	2.499732000	4.285501000	-1.040260000
6	1.685483000	-4.514690000	-1.658711000
6	1.355461000	-5.367515000	-2.722096000
6	2.629652000	-4.931419000	-0.707771000
1	0.639665000	-5.040798000	-3.466696000
1	2.867155000	-4.280224000	0.124290000
6	1.966986000	-6.609799000	-2.840165000
6	3.220235000	-6.185209000	-0.821960000
1	1.720697000	-7.253588000	-3.675903000
1	3.934845000	-6.508416000	-0.074482000
6	2.896511000	-7.023540000	-1.887134000
1	3.366461000	-7.995753000	-1.975667000
6	-2.576077000	4.395738000	-1.293326000
6	-3.282585000	4.889225000	-0.191083000
6	-2.453588000	5.189034000	-2.439305000
1	-3.353202000	4.291624000	0.707906000
1	-1.911504000	4.807568000	-3.296290000
6	-3.853956000	6.157490000	-0.236465000
6	-3.037097000	6.451389000	-2.485331000
1	-4.391364000	6.534888000	0.625410000
1	-2.946926000	7.052352000	-3.382153000
6	-3.736322000	6.939172000	-1.383693000
1	-4.187119000	7.923541000	-1.419070000
30	-0.445617000	-0.090806000	-1.065474000
1	-2.587996000	1.616381000	2.995772000
1	-2.560692000	1.691777000	1.236792000
1	2.764887000	0.702349000	1.817040000
1	1.354605000	-0.298974000	1.435832000

C$_{60}$- ZnTTP Acceptor N electron system

6	-1.131363000	-2.811212000	-1.841704000
6	-0.629197000	-1.946919000	-2.896542000
6	0.822803000	-1.962371000	-2.836736000
6	1.218060000	-2.836719000	-1.745189000
6	0.010231000	-3.361200000	-1.130229000
6	-0.048326000	-3.536934000	0.249005000
6	-1.251151000	-3.170864000	0.977709000
6	-2.344404000	-2.644370000	0.296384000
6	-2.283363000	-2.460677000	-1.143926000
6	-2.983716000	-1.229838000	-1.469773000
6	-2.502919000	-0.401946000	-2.479959000
6	-1.300010000	-0.768237000	-3.208543000
6	-0.548677000	0.446991000	-3.474712000
6	0.841770000	0.432083000	-3.417873000
6	1.542092000	-0.798784000	-3.091622000
6	2.688677000	-0.457924000	-2.266192000
6	3.067256000	-1.295034000	-1.221015000
6	2.315857000	-2.510287000	-0.954752000
6	2.254773000	-2.693809000	0.485533000
6	1.098264000	-3.196338000	1.074441000
6	0.603886000	-2.619211000	2.313128000
6	-0.848023000	-2.603434000	2.253443000
6	-1.555099000	-1.533575000	2.793659000
6	-2.696766000	-0.983703000	2.081935000
6	-3.082680000	-1.526827000	0.860735000
6	-3.478090000	-0.652733000	-0.231079000
6	-3.470570000	0.727660000	-0.054764000
6	-2.968261000	1.592159000	-1.109358000
6	-2.494806000	1.039488000	-2.295477000
6	-1.287072000	1.564138000	-2.910459000
6	-0.603909000	2.619095000	-2.313135000
6	0.847940000	2.603570000	-2.253484000
6	1.555139000	1.533549000	-2.793844000
6	2.696731000	0.983783000	-2.082259000
6	3.082820000	1.526924000	-0.860653000
6	3.478176000	0.652665000	0.231082000
6	3.470677000	-0.727745000	0.054912000
6	2.968192000	-1.592192000	1.109362000
6	2.494761000	-1.039487000	2.295670000
6	1.287018000	-1.564193000	2.910434000
6	0.548603000	-0.446908000	3.474678000
6	-0.841842000	-0.431941000	3.417846000
6	-1.542176000	0.798732000	3.091553000
6	-2.688638000	0.457924000	2.266126000
6	-3.067205000	1.295012000	1.220990000
6	-2.316001000	2.510277000	0.954826000
6	-2.254653000	2.693889000	-0.485484000
6	-1.098276000	3.196302000	-1.074360000
6	0.048334000	3.536916000	-0.248983000
6	1.251182000	3.170835000	-0.977699000
6	2.344603000	2.644445000	-0.296382000
6	2.283181000	2.460634000	1.143947000
6	2.983832000	1.229777000	1.469873000
6	2.502896000	0.401924000	2.479843000
6	1.299984000	0.768178000	3.208643000
6	0.629133000	1.946775000	2.896464000
6	-0.822759000	1.962529000	2.836831000
6	-1.218057000	2.836769000	1.745210000
6	-0.010248000	3.361106000	1.130221000
6	1.131388000	2.811240000	1.841704000

C$_{60}$- ZnTTP Acceptor N+1 electron system

6	-2.120441000	1.414268000	-2.471749000
6	-1.234027000	2.520039000	-2.153999000
6	0.069032000	2.246933000	-2.746106000
6	-0.004823000	0.970259000	-3.411933000
6	-1.355252000	0.448325000	-3.237542000
6	-1.557659000	-0.915415000	-3.043524000
6	-2.538524000	-1.370357000	-2.070198000
6	-3.272277000	-0.441947000	-1.329993000
6	-3.061224000	0.978693000	-1.533041000
6	-3.153207000	1.635368000	-0.244031000
6	-2.302748000	2.701965000	0.058909000
6	-1.322233000	3.150953000	-0.916432000
6	-0.114918000	3.543290000	-0.204851000
6	1.141184000	3.274972000	-0.774613000
6	1.232616000	2.620666000	-2.056236000
6	2.363948000	1.705113000	-2.017129000
6	2.292839000	0.472980000	-2.660444000
6	1.084609000	0.088294000	-3.378420000
6	0.874673000	-1.324525000	-3.179730000
6	-0.427318000	-1.829404000	-3.014991000
6	-0.694765000	-2.834495000	-2.016097000
6	-1.998471000	-2.553087000	-1.426382000
6	-2.212742000	-2.767257000	-0.067653000
6	-2.979252000	-1.802638000	0.704464000
6	-3.496439000	-0.664796000	0.087487000
6	-3.422078000	0.621104000	0.759192000
6	-2.833200000	0.712722000	2.019832000
6	-1.945809000	1.822247000	2.332322000
6	-1.688221000	2.794452000	1.369338000
6	-0.337560000	3.319361000	1.202088000
6	0.694760000	2.834510000	2.016107000
6	1.998490000	2.553113000	1.426389000
6	2.212724000	2.767255000	0.067650000
6	2.979284000	1.802660000	-0.704470000
6	3.496433000	0.664798000	-0.087489000
6	3.422095000	-0.621113000	-0.759204000
6	2.833193000	-0.712738000	-2.019829000
6	1.945828000	-1.822277000	-2.332348000
6	1.688198000	-2.794441000	-1.369330000
6	0.337551000	-3.319369000	-1.202077000
6	0.114916000	-3.543290000	0.204858000
6	-1.141196000	-3.274986000	0.774606000
6	-1.232622000	-2.620697000	2.056235000
6	-2.363953000	-1.705132000	2.017143000
6	-2.292812000	-0.472983000	2.660416000
6	-1.084598000	-0.088294000	3.378425000
6	-0.874672000	1.324534000	3.179726000
6	0.427325000	1.829419000	3.015019000
6	1.557665000	0.915425000	3.043531000
6	2.538518000	1.370361000	2.070201000
6	3.272262000	0.441948000	1.329991000
6	3.061221000	-0.978689000	1.533034000
6	3.153208000	-1.635367000	0.244021000
6	2.302751000	-2.701975000	-0.058908000
6	1.322221000	-3.150915000	0.916440000
6	1.234041000	-2.520075000	2.154038000
6	-0.069036000	-2.246929000	2.746082000
6	0.004817000	-0.970266000	3.411935000
6	1.355256000	-0.448326000	3.237544000
6	2.120420000	-1.414248000	2.471726000

C$_{59}$-Pc Donor N electron system

7	-1.706687000	0.770832000	0.521776000
7	-1.421564000	-1.982354000	0.616952000
7	1.396042000	-1.794724000	0.815230000
7	1.114834000	0.949183000	0.534336000
6	-1.532331000	2.131177000	0.424226000
6	-3.035316000	0.409922000	0.533284000
6	-2.771850000	-1.900608000	0.453528000
6	-1.076871000	-3.292260000	0.481065000
6	1.216016000	-3.152610000	0.886243000
6	2.721165000	-1.436556000	0.885244000
6	2.472702000	0.850286000	0.515659000
6	0.797371000	2.251672000	0.283349000
6	-2.863104000	2.710488000	0.420377000
6	-3.794292000	1.650049000	0.498908000
6	-3.342649000	-3.225337000	0.178446000
6	-2.247964000	-4.103075000	0.124154000
6	2.531175000	-3.728491000	1.093081000
6	3.468976000	-2.671603000	1.082479000
6	3.083059000	2.148060000	0.213637000
6	2.013001000	3.041755000	0.038706000
6	-3.277270000	4.035993000	0.303440000
6	-5.176287000	1.891423000	0.460954000
6	-4.638061000	-3.666240000	-0.059210000
6	-2.396243000	-5.441080000	-0.255240000
6	2.927762000	-5.059265000	1.195302000
6	4.846272000	-2.930819000	1.158378000
6	4.404436000	2.557391000	0.080458000
6	2.229851000	4.381854000	-0.297096000
6	-4.644800000	4.273743000	0.253027000
6	-5.574757000	3.221330000	0.326390000
6	-4.805687000	-5.020862000	-0.352597000
6	-3.708940000	-5.886260000	-0.461922000
6	4.290708000	-5.314174000	1.272495000
6	5.230044000	-4.269383000	1.244738000
6	4.629073000	3.901721000	-0.216049000
6	3.564158000	4.794019000	-0.400341000
1	-2.549871000	4.834336000	0.233621000
1	-5.474570000	-2.980071000	-0.018747000
1	2.191606000	-5.852811000	1.178127000
1	5.218895000	1.855252000	0.207351000
1	-5.007710000	5.290752000	0.158898000
1	-6.635126000	3.443323000	0.294355000
1	-5.801394000	-5.407454000	-0.537345000
1	-3.869662000	-6.915931000	-0.760740000
1	4.642554000	-6.336612000	1.346237000
1	6.287336000	-4.500664000	1.301799000
1	5.645153000	4.264132000	-0.323502000
1	3.769907000	5.826303000	-0.659443000
7	-3.527326000	-0.807804000	0.486739000
7	0.116926000	-3.837007000	0.695620000
7	3.217559000	-0.231927000	0.729702000
7	-0.414186000	2.800931000	0.288734000
1	-0.951310000	0.097188000	0.553245000
1	0.658799000	-1.124634000	0.635240000
6	-6.148862000	0.771723000	0.565771000
6	-6.886679000	0.371682000	-0.546685000
6	-6.264733000	0.072234000	1.767107000
6	-7.726712000	-0.742940000	-0.482013000
6	-7.104788000	-1.033575000	1.874361000
6	-7.819024000	-1.421217000	0.735880000
1	-6.762469000	0.918393000	-1.470976000
1	-5.667318000	0.395269000	2.607527000
1	-8.465363000	-2.287783000	0.799847000
6	-8.513851000	-1.257791000	-1.694893000
6	-8.059263000	-2.697903000	-2.016535000
1	-8.243298000	-3.373668000	-1.178435000
1	-8.602676000	-3.083723000	-2.884101000
1	-6.990174000	-2.725543000	-2.241220000

6	-10.021941000	-1.254150000	-1.369646000
1	-10.596515000	-1.621276000	-2.225212000
1	-10.251516000	-1.891204000	-0.513112000
1	-10.363719000	-0.242706000	-1.135603000
6	-8.288598000	-0.393782000	-2.945201000
1	-8.870305000	-0.796306000	-3.778252000
1	-8.608157000	0.639040000	-2.784693000
1	-7.238231000	-0.386038000	-3.246463000
6	-7.251101000	-1.837671000	3.173357000
6	-8.723154000	-1.797217000	3.633611000
1	-9.390980000	-2.227975000	2.884512000
1	-8.847347000	-2.364297000	4.560919000
1	-9.043065000	-0.767939000	3.815204000
6	-6.828966000	-3.300463000	2.921732000
1	-6.936157000	-3.887548000	3.838592000
1	-7.441501000	-3.771667000	2.150045000
1	-5.787240000	-3.354415000	2.599115000
6	-6.374423000	-1.277342000	4.303873000
1	-6.509324000	-1.880846000	5.204934000
1	-5.314292000	-1.304624000	4.040386000
1	-6.642073000	-0.246754000	4.550457000
6	1.089320000	5.293212000	-0.580844000
6	0.313768000	5.072472000	-1.713317000
6	0.741568000	6.312879000	0.308477000
6	-0.827145000	5.835976000	-1.972548000
6	-0.391264000	7.093886000	0.086802000
6	-1.157465000	6.836801000	-1.059665000
1	0.595749000	4.268154000	-2.380785000
1	1.348543000	6.453876000	1.191897000
1	-2.041592000	7.433703000	-1.232594000
6	-0.844538000	8.190609000	1.059916000
6	-2.250385000	7.841980000	1.594747000
1	-2.983786000	7.781084000	0.787742000
1	-2.239425000	6.879331000	2.112137000
1	-2.590330000	8.606531000	2.299542000
6	0.103279000	8.332655000	2.260698000
1	-0.256941000	9.126321000	2.920094000
1	0.154049000	7.411320000	2.846077000
1	1.116163000	8.595727000	1.945523000
6	-0.896031000	9.544714000	0.322122000
1	-1.220314000	10.337116000	1.003259000
1	0.090482000	9.809396000	-0.066889000
1	-1.591638000	9.519667000	-0.519113000
6	-1.664734000	5.541002000	-3.224187000
6	-0.818969000	5.859007000	-4.474986000
1	-0.523413000	6.911407000	-4.484783000
1	0.090597000	5.255257000	-4.503366000
1	-1.390765000	5.653323000	-5.384928000
6	-2.069255000	4.051191000	-3.243273000
1	-2.658265000	3.834860000	-4.139360000
1	-1.199042000	3.392827000	-3.249647000
1	-2.671624000	3.800475000	-2.368391000
6	-2.950134000	6.381202000	-3.277184000
1	-3.517533000	6.124719000	-4.175263000
1	-3.590693000	6.186859000	-2.412956000
1	-2.735830000	7.452243000	-3.316551000
6	5.837339000	-1.825917000	1.111321000
6	5.904124000	-0.900258000	2.145034000
6	6.646135000	-1.668041000	-0.017973000
6	6.752805000	0.207464000	2.070054000
6	7.494704000	-0.569427000	-0.135786000
6	7.530036000	0.352442000	0.920672000
1	5.260111000	-1.037712000	3.003754000
1	6.556835000	-2.390552000	-0.817367000
1	8.181506000	1.210161000	0.832527000
6	6.800038000	1.204449000	3.236096000
6	7.640972000	2.447537000	2.906101000
1	7.625263000	3.134996000	3.755335000
1	8.685256000	2.193698000	2.707491000
1	7.242728000	2.981540000	2.039285000

6	7.424182000	0.499229000	4.458908000
1	7.471541000	1.183593000	5.311300000
1	6.836398000	-0.372075000	4.756132000
1	8.438380000	0.158945000	4.233964000
6	5.373652000	1.675829000	3.590413000
1	4.729484000	0.845279000	3.883146000
1	5.411743000	2.378341000	4.427927000
1	4.904640000	2.178616000	2.743094000
6	8.352604000	-0.321847000	-1.383501000
6	9.840967000	-0.265188000	-0.981226000
1	10.152517000	-1.206785000	-0.521986000
1	10.466202000	-0.089403000	-1.861588000
1	10.035356000	0.536773000	-0.266130000
6	8.180205000	-1.428843000	-2.435776000
1	8.802306000	-1.205973000	-3.306238000
1	8.489095000	-2.402652000	-2.047221000
1	7.145936000	-1.512489000	-2.776909000
6	7.942044000	1.023258000	-2.020678000
1	8.536076000	1.215261000	-2.918967000
1	6.886949000	1.014011000	-2.302965000
1	8.095836000	1.857261000	-1.332732000
1	2.067268000	-8.235374000	-1.273327000
6	-1.204376000	-6.279410000	-0.542942000
6	-0.946638000	-7.484682000	0.112803000
6	-0.283531000	-5.815079000	-1.485907000
6	0.229490000	-8.181736000	-0.155844000
6	0.899089000	-6.496340000	-1.762373000
6	1.150547000	-7.688512000	-1.078644000
1	-1.646617000	-7.855052000	0.852720000
1	-0.490470000	-4.883420000	-2.000677000
1	0.433467000	-9.111288000	0.363636000
6	1.874296000	-5.911678000	-2.760309000
1	2.618497000	-6.663008000	-3.041167000
1	1.324137000	-5.660886000	-3.675066000
6	2.577072000	-4.642352000	-2.238961000
1	1.849075000	-4.000269000	-1.745407000
1	3.332868000	-4.907559000	-1.497322000
6	3.219430000	-3.861817000	-3.375009000
1	3.950366000	-4.467147000	-3.912953000
1	2.453677000	-3.518169000	-4.074901000
8	3.978317000	-2.709164000	-2.932305000
6	3.267427000	-1.610356000	-2.581851000
8	2.063393000	-1.598573000	-2.491556000
6	4.170763000	-0.433072000	-2.339331000
1	4.919198000	-0.363577000	-3.129364000
1	3.573903000	0.474745000	-2.295045000
1	4.688466000	-0.556092000	-1.387211000

C$_{59}$-Pc Donor N-1 electron system

7	-1.733881000	0.747251000	0.371840000
7	-1.445164000	-2.004132000	0.585087000
7	1.366146000	-1.801063000	0.666275000
7	1.075742000	0.937210000	0.365805000
6	-1.564985000	2.089525000	0.119673000
6	-3.063044000	0.376983000	0.327294000
6	-2.791003000	-1.932306000	0.385172000
6	-1.099984000	-3.316687000	0.474024000
6	1.191254000	-3.149856000	0.848440000
6	2.685956000	-1.432373000	0.756959000
6	2.432447000	0.834461000	0.305679000
6	0.764212000	2.240977000	0.112024000
6	-2.897981000	2.645075000	-0.066363000
6	-3.828306000	1.597937000	0.104245000
6	-3.359163000	-3.265551000	0.142187000
6	-2.263384000	-4.142562000	0.124004000
6	2.508925000	-3.704213000	1.129318000
6	3.438908000	-2.644990000	1.073517000
6	3.042525000	2.124586000	-0.038367000

6	1.980253000	3.039221000	-0.115562000	6	1.085316000	5.369157000	-0.431570000
6	-3.293621000	3.924397000	-0.430347000	6	0.698418000	6.003954000	-1.609144000
6	-5.201677000	1.803562000	-0.071567000	6	0.392823000	5.623179000	0.752516000
6	-4.651813000	-3.708142000	-0.076362000	6	-0.399547000	6.869562000	-1.628386000
6	-2.407135000	-5.495033000	-0.185017000	6	-0.695912000	6.492181000	0.778137000
6	2.902789000	-5.019499000	1.316768000	6	-1.076704000	7.097371000	-0.425943000
6	4.812271000	-2.878984000	1.203702000	1	1.238528000	5.785509000	-2.522180000
6	4.351283000	2.496992000	-0.292050000	1	0.714075000	5.122136000	1.656671000
6	2.191385000	4.381878000	-0.429752000	1	-1.921120000	7.767942000	-0.425577000
6	-4.661209000	4.131793000	-0.624497000	6	-1.422039000	6.758844000	2.104321000
6	-5.587843000	3.098347000	-0.453562000	6	-2.670785000	7.635024000	1.920458000
6	-4.820081000	-5.082344000	-0.305043000	1	-2.421423000	8.623381000	1.527486000
6	-3.729708000	-5.949639000	-0.363388000	1	-3.395487000	7.168834000	1.247117000
6	4.272753000	-5.260006000	1.439446000	1	-3.161235000	7.779599000	2.885710000
6	5.201014000	-4.217419000	1.374025000	6	-1.865384000	5.423467000	2.738916000
6	4.572144000	3.835009000	-0.647203000	1	-2.363139000	5.610441000	3.694195000
6	3.521482000	4.749436000	-0.714915000	1	-2.566112000	4.895426000	2.088482000
1	-2.564726000	4.713834000	-0.565082000	1	-1.018910000	4.761065000	2.929293000
1	-5.489739000	-3.022391000	-0.064366000	6	-0.452149000	7.483013000	3.061981000
1	2.173337000	-5.819196000	1.330185000	1	-0.943619000	7.690379000	4.016647000
1	5.162449000	1.783569000	-0.218076000	1	0.435315000	6.878999000	3.263046000
1	-5.015673000	5.114779000	-0.910362000	1	-0.121875000	8.432281000	2.633290000
1	-6.642736000	3.298633000	-0.597750000	6	-0.834514000	7.509870000	-2.953260000
1	-5.815895000	-5.475284000	-0.470680000	6	0.339673000	8.318696000	-3.543107000
1	-3.891237000	-6.994531000	-0.600453000	1	0.647407000	9.111263000	-2.856626000
1	4.627116000	-6.273522000	1.583104000	1	1.208539000	7.687322000	-3.739529000
1	6.257279000	-4.435954000	1.474445000	1	0.043028000	8.781210000	-4.488292000
1	5.579496000	4.170913000	-0.862071000	6	-1.238822000	6.393253000	-3.939897000
1	3.726990000	5.782881000	-0.967218000	1	-1.556156000	6.825293000	-4.892899000
7	-3.548731000	-0.840563000	0.344055000	1	-0.409562000	5.711524000	-4.139711000
7	0.098811000	-3.847805000	0.713061000	1	-2.067978000	5.803747000	-3.539037000
7	3.181003000	-0.239561000	0.545447000	6	-2.031939000	8.456994000	-2.780963000
7	-0.453873000	2.770058000	0.011434000	1	-2.296105000	8.890724000	-3.747965000
1	-0.977428000	0.094319000	0.538153000	1	-2.914025000	7.932848000	-2.403569000
1	0.633489000	-1.153274000	0.406108000	1	-1.802983000	9.280369000	-2.099949000
6	-6.181569000	0.714674000	0.145340000	6	5.801585000	-1.778817000	1.139682000
6	-6.968471000	0.254873000	-0.910718000	6	5.768300000	-0.753853000	2.078698000
6	-6.268621000	0.109783000	1.400966000	6	6.726388000	-1.739300000	0.090919000
6	-7.822342000	-0.836680000	-0.736119000	6	6.635535000	0.338181000	1.984443000
6	-7.130776000	-0.961650000	1.619606000	6	7.586871000	-0.653422000	-0.052554000
6	-7.885382000	-1.418647000	0.533678000	6	7.520985000	0.368974000	0.906543000
1	-6.872293000	0.730593000	-1.876763000	1	5.049232000	-0.811364000	2.885108000
1	-5.647580000	0.488274000	2.200093000	1	6.722436000	-2.542222000	-0.633314000
1	-8.550990000	-2.259050000	0.684157000	1	8.189697000	1.211253000	0.803464000
6	-8.659011000	-1.424762000	-1.879740000	6	6.605712000	1.428405000	3.064498000
6	-8.229792000	-2.890115000	-2.110991000	6	7.461895000	2.646626000	2.684613000
1	-8.390925000	-3.501623000	-1.220288000	1	7.384069000	3.405780000	3.465994000
1	-8.808039000	-3.330683000	-2.927553000	1	8.518735000	2.389235000	2.584039000
1	-7.169990000	-2.946238000	-2.374258000	1	7.124624000	3.098447000	1.747576000
6	-10.153885000	-1.378551000	-1.500387000	6	7.157805000	0.825574000	4.374250000
1	-10.761738000	-1.795061000	-2.308045000	1	7.156862000	1.576552000	5.169163000
1	-10.361444000	-1.953636000	-0.595863000	1	6.553028000	-0.021023000	4.707240000
1	-10.477175000	-0.349574000	-1.325181000	1	8.182808000	0.472680000	4.237038000
6	-8.470377000	-0.654374000	-3.195388000	6	5.160926000	1.917333000	3.298162000
1	-9.087839000	-1.105571000	-3.975212000	1	4.499966000	1.110166000	3.618982000
1	-8.773409000	0.391182000	-3.098032000	1	5.150848000	2.681148000	4.080064000
1	-7.432638000	-0.683296000	-3.537574000	1	4.742774000	2.355056000	2.390064000
6	-7.268948000	-1.646960000	2.985540000	6	8.569243000	-0.530113000	-1.223911000
6	-8.728009000	-1.516920000	3.470688000	6	10.008215000	-0.421732000	-0.677680000
1	-9.427063000	-1.992281000	2.779564000	1	10.268251000	-1.307847000	-0.093575000
1	-8.846458000	-1.993099000	4.447772000	1	10.720161000	-0.335159000	-1.502842000
1	-9.012385000	-0.466106000	3.565214000	1	10.133509000	0.452276000	-0.035474000
6	-6.901056000	-3.139751000	2.852436000	6	8.500784000	-1.739625000	-2.169400000
1	-7.015996000	-3.643365000	3.815984000	1	9.213854000	-1.605746000	-2.985803000
1	-7.540574000	-3.653161000	2.131198000	1	8.759289000	-2.668440000	-1.654670000
1	-5.864411000	-3.257715000	2.528270000	1	7.508621000	-1.857870000	-2.612333000
6	-6.347586000	-1.021092000	4.043786000	6	8.229027000	0.739571000	-2.034118000
1	-6.476676000	-1.541902000	4.995181000	1	8.915113000	0.845215000	-2.878632000
1	-5.294650000	-1.103117000	3.760978000	1	7.210394000	0.688552000	-2.427382000
1	-6.579909000	0.033670000	4.210389000	1	8.310509000	1.641264000	-1.423418000

1	1.978888000	-8.436299000	-1.076511000
6	-1.227276000	-6.356519000	-0.424522000
6	-1.022346000	-7.559209000	0.257029000
6	-0.276667000	-5.934552000	-1.358661000
6	0.136013000	-8.294528000	0.022718000
6	0.883310000	-6.664352000	-1.609899000
6	1.084332000	-7.849335000	-0.898376000
1	-1.748178000	-7.898587000	0.986450000
1	-0.452963000	-5.015309000	-1.906301000
1	0.301636000	-9.220894000	0.559972000
6	1.874264000	-6.150350000	-2.630158000
1	2.596093000	-6.932461000	-2.879612000
1	1.328013000	-5.927722000	-3.554166000
6	2.612790000	-4.877193000	-2.169359000
1	1.918156000	-4.217458000	-1.652277000
1	3.406645000	-5.133704000	-1.464020000
6	3.196483000	-4.127814000	-3.357472000
1	3.858135000	-4.764512000	-3.945050000
1	2.393210000	-3.758498000	-3.999542000
8	4.035472000	-3.002679000	-2.991635000
6	3.419228000	-1.881935000	-2.565856000
8	2.235517000	-1.819766000	-2.319444000
6	4.388968000	-0.739379000	-2.434850000
1	5.152291000	-0.790508000	-3.210145000
1	3.843543000	0.200563000	-2.492187000
1	4.881922000	-0.791693000	-1.462733000

C_{59}-Pc Acceptor N electron system

6	2.634975000	2.179368000	-0.735086000
6	2.634867000	2.186281000	0.714816000
6	3.191091000	0.947404000	1.179441000
6	3.778900000	0.156425000	-0.000552000
6	3.191245000	0.936155000	-1.188030000
6	2.651000000	0.318471000	-2.286874000
6	1.564064000	0.929366000	-3.016979000
6	1.050347000	2.160127000	-2.604787000
6	1.602620000	2.804257000	-1.438280000
6	0.513337000	3.441266000	-0.710820000
6	0.513282000	3.448059000	0.678479000
6	1.602513000	2.817842000	1.411985000
6	1.050064000	2.184661000	2.584419000
6	1.563760000	0.957854000	3.008227000
6	2.650760000	0.340073000	2.284036000
6	2.437840000	-1.114603000	2.303010000
6	2.690318000	-1.826950000	1.144703000
6	2.690422000	-1.837777000	-1.127190000
6	2.437984000	-1.136306000	-2.292073000
6	1.211146000	-1.401795000	-3.004224000
6	0.671490000	-0.124964000	-3.456755000
6	-0.703149000	0.090411000	-3.467237000
6	-1.240913000	1.370457000	-3.028797000
6	-0.382636000	2.384400000	-2.609684000
6	-0.716329000	3.178280000	-1.437739000
6	-1.895455000	2.928037000	-0.740804000
6	-1.895525000	2.934975000	0.713048000
6	-0.716571000	3.192048000	1.407771000
6	-0.382940000	2.409088000	2.587170000
6	-1.241214000	1.399067000	3.015662000
6	-0.703503000	0.123195000	3.466120000
6	0.671134000	-0.092263000	3.457721000
6	1.210818000	-1.373286000	3.017289000
6	0.331679000	-2.388337000	2.614351000
6	0.650773000	-3.166819000	1.446066000
6	1.818825000	-2.891799000	0.730698000
6	1.818909000	-2.898619000	-0.703264000
6	0.650970000	-3.180448000	-1.416157000
6	0.331975000	-2.412986000	-2.591749000
6	-1.099948000	-2.176047000	-2.590389000
6	-1.610520000	-0.955442000	-3.023979000
6	-2.696574000	-0.323562000	-2.299384000
6	-2.471082000	1.114537000	-2.306779000
6	-2.791240000	1.874724000	-1.184127000
6	-3.348977000	1.233501000	-0.005966000
6	-2.791345000	1.885813000	1.166104000
6	-2.471301000	1.136252000	2.295922000
6	-2.696808000	-0.301805000	2.302069000
6	-1.610782000	-0.926799000	3.032628000
6	-1.100190000	-2.151428000	2.610649000
6	-1.664146000	-2.805461000	1.438515000
6	-0.575320000	-3.437986000	0.712703000
6	-0.575231000	-3.444548000	-0.680347000
6	-1.664022000	-2.818978000	-1.412222000
6	-2.704023000	-2.209992000	-0.717265000
6	-3.234918000	-0.936524000	-1.171188000
6	-3.562228000	-0.142403000	0.000519000
6	-3.235091000	-0.925405000	1.179659000
6	-2.704071000	-2.203080000	0.737774000
7	3.305802000	-1.269902000	0.006218000
1	4.873053000	0.153408000	-0.000498000

C_{59}-Pc Acceptor N+1 electron system

6	2.607084000	2.239930000	-0.700554000
6	2.600779000	2.233760000	0.744002000
6	3.175486000	1.003601000	1.201787000
6	3.781805000	0.232722000	0.018595000
6	3.186681000	1.013349000	-1.163878000
6	2.662616000	0.389871000	-2.269922000
6	1.558486000	0.981112000	-2.999437000
6	1.021121000	2.199999000	-2.572618000
6	1.558744000	2.850079000	-1.408898000
6	0.445967000	3.446840000	-0.678188000
6	0.440000000	3.440708000	0.711513000
6	1.545148000	2.838522000	1.447509000
6	0.996182000	2.177688000	2.600051000
6	1.529475000	0.955254000	3.021294000
6	2.640956000	0.369931000	2.297779000
6	2.457837000	-1.083849000	2.303923000
6	2.725660000	-1.783615000	1.140193000
6	2.736522000	-1.773378000	-1.130166000
6	2.479582000	-1.064609000	-2.290362000
6	1.254400000	-1.343301000	-3.014245000
6	0.697823000	-0.083262000	-3.462625000
6	-0.697620000	0.109896000	-3.479151000
6	-1.255151000	1.365212000	-3.024025000
6	-0.421714000	2.398583000	-2.583291000
6	-0.776026000	3.176296000	-1.416747000
6	-1.962962000	2.901008000	-0.719312000
6	-1.969141000	2.894332000	0.725322000
6	-0.789749000	3.163201000	1.436271000
6	-0.446530000	2.376541000	2.599949000
6	-1.284355000	1.339578000	3.024389000
6	-0.731216000	0.080328000	3.473694000
6	0.664367000	-0.112777000	3.467832000
6	1.225252000	-1.368877000	3.013583000
6	0.371496000	-2.403820000	2.587669000
6	0.712403000	-3.170723000	1.427557000
6	1.886305000	-2.865689000	0.710416000
6	1.892265000	-2.858990000	-0.716904000
6	0.726226000	-3.157339000	-1.447656000
6	0.396418000	-2.381913000	-2.604964000
6	-1.046077000	-2.170118000	-2.605940000
6	-1.576415000	-0.953914000	-3.037512000
6	-2.687329000	-0.355142000	-2.312781000
6	-2.488912000	1.082966000	-2.305663000
6	-2.828780000	1.830353000	-1.178927000
6	-3.382789000	1.165375000	-0.010717000

6	-2.840098000	1.819889000	1.168272000
6	-2.510791000	1.063755000	2.291829000
6	-2.709164000	-0.374948000	2.284678000
6	-1.605617000	-0.979773000	3.015333000
6	-1.071075000	-2.192358000	2.578129000
6	-1.617856000	-2.848751000	1.406882000
6	-0.508152000	-3.442528000	0.679604000
6	-0.502279000	-3.436590000	-0.713501000
6	-1.604258000	-2.837300000	-1.445964000
6	-2.671691000	-2.259375000	-0.745957000
6	-3.220755000	-0.993516000	-1.193611000
6	-3.570665000	-0.214151000	-0.017520000
6	-3.231808000	-1.003010000	1.155376000
6	-2.677880000	-2.265415000	0.701644000
7	3.340200000	-1.202620000	0.010276000
1	4.877225000	0.248473000	0.023843000

6	0.866844000	3.030133000	1.374841000
6	0.472804000	2.310506000	2.562248000
6	-0.977111000	2.307170000	2.626042000
6	-1.651814000	1.176957000	3.080807000
6	-0.903525000	0.000039000	3.492070000
6	0.486232000	0.000038000	3.417902000
6	1.192022000	-1.176435000	2.943168000
6	2.337162000	-0.739949000	2.172281000
6	2.716551000	-1.428979000	1.047139000
6	3.412927000	-0.799732000	-0.158330000
6	4.955250000	1.142138000	-0.188141000
1	5.177864000	2.062087000	0.350732000
1	5.260407000	1.269547000	-1.230334000
6	4.955242000	-1.142137000	-0.188141000
1	5.177869000	-2.062094000	0.350715000
1	5.260389000	-1.269535000	-1.230339000
7	5.654420000	-0.000002000	0.371928000
1	5.559355000	-0.000001000	1.384134000

C₆₀-TPA Donor N electron system

6	-3.043180000	0.727826000	-2.191742000
6	-3.043180000	-0.727875000	-2.191726000
6	-3.430907000	-1.423683000	-1.049372000
6	-2.691458000	-2.601329000	-0.631077000
6	-1.596119000	-3.035544000	-1.372967000
6	-1.190622000	-2.307480000	-2.565083000
6	-1.900030000	-1.176973000	-2.962372000
6	-1.187706000	-0.000038000	-3.433396000
6	-1.900030000	1.176907000	-2.962398000
6	-1.190622000	2.307423000	-2.565134000
6	-1.596119000	3.035513000	-1.373033000
6	-2.691459000	2.601314000	-0.631135000
6	-3.430908000	1.423660000	-1.049403000
6	-3.829478000	0.695971000	0.143571000
6	-3.829478000	-0.695969000	0.143587000
6	-3.334513000	-1.423688000	1.299611000
6	-2.631663000	-2.601319000	0.821872000
6	-1.478962000	-3.035023000	1.471088000
6	-0.336110000	-3.484445000	0.695471000
6	-0.393404000	-3.484861000	-0.693870000
6	0.749725000	-3.031713000	-1.470300000
6	0.259984000	-2.310703000	-2.620398000
6	0.945836000	-1.176342000	-3.057840000
6	0.203147000	-0.000038000	-3.472863000
6	0.945836000	1.176274000	-3.057865000
6	0.259984000	2.310645000	-2.620448000
6	0.749726000	3.031681000	-1.470367000
6	-0.393404000	3.484845000	-0.693946000
6	-0.336111000	3.484461000	0.695395000
6	-1.478963000	3.035056000	1.471021000
6	-2.631664000	2.601337000	0.821815000
6	-3.334513000	1.423716000	1.299579000
6	-2.854158000	0.727839000	2.406167000
6	-2.854158000	-0.727786000	2.406183000
6	-1.651814000	-1.176889000	3.080833000
6	-0.977110000	-2.307112000	2.626093000
6	0.472805000	-2.310448000	2.562299000
6	0.866845000	-3.030102000	1.374908000
6	1.956525000	-2.576166000	0.630588000
6	1.897848000	-2.578909000	-0.818929000
6	2.625056000	-1.435373000	-1.297773000
6	2.150526000	-0.739786000	-2.383910000
6	2.150526000	0.739732000	-2.383924000
6	2.625060000	1.435345000	-1.297805000
6	3.412926000	0.799729000	-0.158346000
6	2.716547000	1.429002000	1.047106000
6	2.337162000	0.739999000	2.172265000
6	1.192023000	1.176501000	2.943142000
6	1.897848000	2.578891000	-0.818987000
6	1.956523000	2.576179000	0.630531000

C₆₀-TPA Donor N-1 electron system

6	-3.045387000	0.724884000	-2.193443000
6	-3.045384000	-0.724702000	-2.193503000
6	-3.429912000	-1.420699000	-1.047311000
6	-2.684287000	-2.588531000	-0.632804000
6	-1.595591000	-3.025674000	-1.380852000
6	-1.196952000	-2.304838000	-2.578601000
6	-1.905100000	-1.175932000	-2.973369000
6	-1.195401000	0.000144000	-3.449731000
6	-1.905102000	1.176180000	-2.973272000
6	-1.196955000	2.305053000	-2.578408000
6	-1.595595000	3.025788000	-1.380599000
6	-2.684291000	2.588582000	-0.632588000
6	-3.429914000	1.420783000	-1.047193000
6	-3.829387000	0.694247000	0.147585000
6	-3.829385000	-0.694262000	0.147527000
6	-3.331171000	-1.420755000	1.304197000
6	-2.622397000	-2.588346000	0.827885000
6	-1.474515000	-3.025311000	1.481483000
6	-0.328934000	-3.454422000	0.703656000
6	-0.388356000	-3.454854000	-0.702269000
6	0.746810000	-3.019356000	-1.477055000
6	0.255283000	-2.304389000	-2.634957000
6	0.936646000	-1.174297000	-3.074801000
6	0.194800000	0.000146000	-3.494573000
6	0.936645000	1.174555000	-3.074704000
6	0.255281000	2.304609000	-2.634763000
6	0.746806000	3.019481000	-1.476803000
6	-0.388360000	3.454912000	-0.701980000
6	-0.328938000	3.454362000	0.703945000
6	-1.474518000	3.025185000	1.481735000
6	-2.622401000	2.588276000	0.828102000
6	-3.331172000	1.420643000	1.304315000
6	-2.851308000	0.724551000	2.413710000
6	-2.851308000	-0.724756000	2.413650000
6	-1.649112000	-1.176026000	3.095127000
6	-0.976568000	-2.304712000	2.641779000
6	0.474843000	-2.304204000	2.575816000
6	0.867680000	-3.018105000	1.379897000
6	1.958893000	-2.562793000	0.631066000
6	1.898454000	-2.565096000	-0.823361000
6	2.620973000	-1.429321000	-1.297227000
6	2.139721000	-0.731549000	-2.390969000
6	2.139720000	0.731751000	-2.390910000
6	2.620969000	1.429431000	-1.297108000
6	3.409114000	0.794303000	-0.160703000
6	2.714954000	1.423433000	1.041995000
6	2.331774000	0.731752000	2.176410000
6	1.190969000	1.174432000	2.958942000

6	1.898449000	2.565165000	-0.823146000
6	1.958891000	2.562742000	0.631280000
6	0.867676000	3.017991000	1.380149000
6	0.474841000	2.303989000	2.576008000
6	-0.976571000	2.304491000	2.641972000
6	-1.649113000	1.175765000	3.095225000
6	-0.902278000	-0.000147000	3.510762000
6	0.487184000	-0.000144000	3.439538000
6	1.190972000	-1.174679000	2.958845000
6	2.331778000	-0.731932000	2.176352000
6	2.714953000	-1.423517000	1.041876000
6	3.409112000	-0.794286000	-0.160766000
6	4.964029000	1.144805000	-0.191196000
1	5.186012000	2.060507000	0.353715000
1	5.257757000	1.281633000	-1.234674000
6	4.964035000	-1.144788000	-0.191269000
1	5.186008000	-2.060520000	0.353595000
1	5.257770000	-1.281558000	-1.234752000
7	5.652451000	-0.000008000	0.355465000
1	5.625750000	-0.000041000	1.370319000

C$_{60}$-TPA Acceptor N electron system

6	-3.888678000	-0.015548000	0.007695000
6	-3.163751000	-0.895077000	-0.801436000
6	-1.774436000	-0.887391000	-0.818095000
1	-1.231522000	-1.572091000	-1.457539000
1	-3.695392000	-1.592296000	-1.440688000
6	-3.166597000	0.867271000	0.816090000
1	-3.700776000	1.553882000	1.464733000
6	-1.777415000	0.872323000	0.823920000
1	-1.236559000	1.555453000	1.466784000
6	-1.063702000	-0.003717000	-0.000090000
7	0.354821000	0.000412000	-0.001783000
6	1.062004000	-1.225561000	0.001130000
6	2.220891000	-1.380611000	-0.769955000
6	2.913649000	-2.585580000	-0.758382000
6	2.456761000	-3.659439000	0.003287000
6	1.298310000	-3.510034000	0.763211000
6	0.608608000	-2.303240000	0.772131000
1	-0.285615000	-2.186794000	1.371025000
1	0.933998000	-4.334406000	1.365629000
1	2.995478000	-4.599269000	0.004173000
1	3.808988000	-2.689114000	-1.360765000
1	2.572090000	-0.552094000	-1.371668000
6	1.054502000	1.230552000	-0.003653000
6	2.214943000	1.390849000	0.764159000
1	2.573278000	0.563003000	1.362555000
6	2.900080000	2.600137000	0.753625000
1	3.796684000	2.707647000	1.353428000
6	2.434094000	3.673217000	-0.003655000
1	2.966966000	4.616372000	-0.003705000
6	1.274203000	3.518582000	-0.760270000
1	0.902814000	4.342243000	-1.359334000
6	0.592006000	2.307522000	-0.770258000
1	-0.303241000	2.187108000	-1.366808000
6	-5.395934000	0.000909000	-0.011829000
1	-5.801835000	-0.984449000	-0.251509000
1	-5.802765000	0.308518000	0.954289000
1	-5.773572000	0.702406000	-0.763872000

C$_{60}$-TPA Acceptor N+1 electron system

6	-3.871605000	0.075758000	-0.026444000
6	-3.147886000	-0.720331000	-0.954391000
6	-1.750306000	-0.714755000	-0.943704000
1	-1.187826000	-1.310772000	-1.653872000
1	-3.682327000	-1.317700000	-1.686327000
6	-3.160214000	0.828445000	0.894440000
1	-3.705635000	1.425513000	1.621903000
6	-1.753415000	0.824148000	0.930801000
1	-1.207178000	1.393393000	1.670829000
6	-1.046719000	0.048797000	-0.016964000
7	0.372114000	0.027212000	-0.002794000
6	1.011317000	-1.234534000	0.023142000
6	2.066320000	-1.515059000	-0.878901000
6	2.683667000	-2.774839000	-0.838379000
6	2.262166000	-3.751602000	0.050493000
6	1.190035000	-3.478687000	0.929878000
6	0.582637000	-2.221471000	0.910410000
1	-0.237945000	-1.989730000	1.579889000
1	0.846103000	-4.234312000	1.627772000
1	2.745767000	-4.723429000	0.063981000
1	3.492637000	-2.990511000	-1.531242000
1	2.372732000	-0.760148000	-1.590379000
6	1.109895000	1.219608000	-0.001306000
6	2.420890000	1.250549000	0.505043000
1	2.849201000	0.345522000	0.912804000
6	3.154887000	2.443575000	0.485950000
1	4.170557000	2.446511000	0.869424000
6	2.589500000	3.619444000	-0.004971000
1	3.159564000	4.543368000	-0.007498000
6	1.282086000	3.595731000	-0.491349000
1	0.826700000	4.503993000	-0.873634000
6	0.545946000	2.404580000	-0.504027000
1	-0.458123000	2.378616000	-0.904130000
6	-5.377340000	0.079034000	-0.051666000
1	-5.787318000	-0.927406000	0.110184000
1	-5.786945000	0.734453000	0.722078000
1	-5.765936000	0.421818000	-1.020544000

References

[1] Janak, J. F. *Phys. Rev. B*, **1978**, 18, 7165-7168.

[2] Karolewski, A.; Kronik, L. and Kümmel, S. *J. Chem. Phys.*, **2013**, 138, 204115.

[3] Stein, T.; Kronik, L. and Baer, R. *J. Am. Chem. Soc.*, **2009**, 131, 2818–2820.

[4] Besalú-Sala, P.; Sitkiewicz, S. P.; Salvador, P.; Matito, E. and Luis, J. M. *Phys. Chem. Chem. Phys.*, **2020**, 22, 11871-11880.

[5] Martínez, J. P.; Solà, M. and Voityuk, A. A. *J. Comput. Chem.*, **2016**, 37, 1396-1405.