Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Endohedral Alkali Cations Promote Charge Transfer Transitions in Complexes of C_{60} with [10]Cycloparaphenylenes

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Table S1. Energetic and geometric results of the optimised minima found for the $M^+@C_{60}$ complexes. Energies (kcal mol^{-1}) relative to the most stable minimum of each case as obtained at the TPSS-D3(BJ)/def2-TZVP level. The optimisation is performed starting with the cation in three different locations inside C_{60}: R5 (with the cation close to a five-membered ring); R6 (with the cation close to a six-membered ring; C (with the cation at the centre of the fullerene). **Page S1**

Figure S1. Molecular electrostatic potential mapped onto an isosurface of isodensity 0.001 a.u calculated at the B97-D2/def2-TZVP level. **Page S2**

Figure S2. Molecular electrostatic potential at the B97-D2/def2-TZVP level in selected points. Left: along a line passing through the cation and hexagonal rings. Solid line: the same side as the cation; dotted line: the opposite side. Right: on a circumference at 10 a.u. from the centre of the carbon cage. The cation is at 180 º. **Page S2**

Figure S3. Schematic energy levels of the highest and lowest occupied molecular orbitals in monomers. CAM-B3LYP/TZVP//B97-D2/def2-TZVP. **Page S3**

Figure S4. Potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation near a hexagonal ring as found with B97-D2. **Page S5**

Figure S5. 2D potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation near a hexagonal ring as found with B97-D2. Labels correspond to the most stable structures. **Page S6**

Figure S6. Potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with TPSS-D3(BJ). **Page S7**

Figure S7. Potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with TPSS-D3(BJ). Labels correspond to the most stable structures. **Page S8**

Figure S8. Most stable structures optimised after scan of $Na^+@C_{60}\cdots$[10]CPP complex. The complexation energy for each complex is included (kcal mol^{-1}). C and R6 refer to the starting location of Na^+ cation inside C_{60}, not to the final optimised structures of the complexes. **Page S9**

Figure S9. Potential energy surface of $K^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with B97-D2. **Page S10**

Figure S10. 2D energy surface of $K^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with B97-D2. Labels correspond to the most stable structures. **Page S11**

Figure S11. Potential energy surface of $K^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation near a pentagonal ring as found with TPSS-D3(BJ). **Page S12**

Figure S12. Potential energy surface of $K^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation near a pentagonal ring as found with TPSS-D3(BJ). Labels correspond to the most stable structures. **Page S13**

Figure S13. Classification in families of the minima found of $K^+@C_{60}\cdots$[10]CPP complex. Geometry of the endofullerene: cation at the centre of the carbon cage as found with B97-D2. **Page S14**

Figure S14. Classification in families of the minima found of $K^+@C_{60}\cdots$[10]CPP complex. Geometry of the endofullerene: cation near a pentagonal ring as found with TPSS-D3(BJ).

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Figure S15. Most stable structures optimised after scan of $K^+@C_{60}\cdots$[10]CPP complex. The complexation energy for each complex is included (kcal mol^{-1}). R5 and C refer to the starting location of K^+ cation inside C_{60}, not to the final optimised structures of the complexes.

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Figure S16. Optimised most stable structures of $Li^+@C_{60}\cdots$[10]CPP complex. The complexation energy for each complex is included (kcal mol^{-1}). Top line: B97-D2. Bottom line: TPSS-D3(BJ). C and R6 refer to the starting location of Li^+ cation inside C_{60}, not to the final optimised structures of the complexes. **Page S17**

Table S2. Energetic results (kcal mol^{-1}) and point charges of the best structure found for the $M^+@C_{60}\cdots$[10]CPP complexes with TPSS-D3(BJ). $\Delta E_{complex}$ = complexation energy; E_{def} = deformation energy; ΔE_{disp}= contribution of dispersion to the total complexation energy; Q = charge of the fullerene according to Mulliken (Mull) and NBO analysis. **Page S18**

Table S3. Energetic results (kcal mol^{-1}) and point charges of the best structure found for the $M^+@C_{60}\cdots$[10]CPP complexes optimised starting from the experimental geometries of Ueno et al. (H. Ueno, T. Nishihara, Y. Segawa and K. Itami, *Angew. Chem. Int. Ed.*, 2015, **54**, 3707-3711). $\Delta E_{complex}$ = complexation energy; E_{def} = deformation energy; ΔE_{disp}= contribution of dispersion to the total complexation energy; Q = charge of the fullerene according to Mulliken (Mull) and NBO analysis. **Page S18**

Table S4. Most favourable location of the cation inside C_{60} in the endofullerene ($M^+@C_{60}$) and in the final complex with the [10]CPP ($M^+@C_{60}\cdots$[10]CPP). R5: cation on a five-membered ring of C_{60}. R6: cation on a five-membered ring of C_{60}. C: cation at the centre of the fullerene. **Page S19**

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Table S7. Distance (Å) between the cation and the barycentres of charge for the most stable $M^+@C_{60}\cdots$[10]CPP complexes. N_{tr} is the number of the transition, $R_{cat\text{-}neg}$ is the distance between the cation and the negative barycentre and $R_{cat\text{-}pos}$ is the distance between the cation and the positive barycentre. **Page S27**

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Figure S27. Difference density between the excited state and the ground state for the first 12 transitions (from left to rigth and top to bottom) in $Li^+@C_{60}\cdots$[10]CPP$\cdots BF_4^-$. CAM-B3LYP/TZVP level, using the B97-D2/def2-TZVP geometry. **Page S31**

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Figure S29. Difference density between the excited state and the ground state for the first 12 transitions (from left to right and top to bottom) in $Li^+@C_{60}\cdots$[10]CPP$\cdots TFPB^-$. CAM-B3LYP/def2-SVP level, using the B97-D2/def2-SVP geometry. **Page S32**

Geometry of the optimised complexes **Page S33**

Table S1. Energetic and geometric results of the optimised minima found for the $M^+@C_{60}$ complexes. Energies (kcal mol^{-1}) relative to the most stable minimum of each case as obtained at the TPSS-D3(BJ)/def2-TZVP level. The optimisation is performed starting with the cation in three different locations inside C_{60}: R5 (with the cation close to a five-membered ring); R6 (with the cation close to a six-membered ring; C (with the cation at the centre of the fullerene).

	R5	**R6**	**C**
	Relative Energy (kcal mol^{-1})		
$Li^+@C_{60}$	0.32	**0.00**	3.55
$Na^+@C_{60}$	- [a]	- [a]	**0.00**
$K^+@C_{60}$	**0.00**	0.18	1.77
	Distance to C_{60} centre (Å)		
$Li^+@C_{60}$	1.402	1.426	0.000
$Na^+@C_{60}$	- [a]	- [a]	0.000
$K^+@C_{60}$	0.528	0.533	0.000

[a] The three optimisations led to the same final structure (with the Na^+ cation at the centre of C_{60}) at the TPSS-D3(BJ) level.

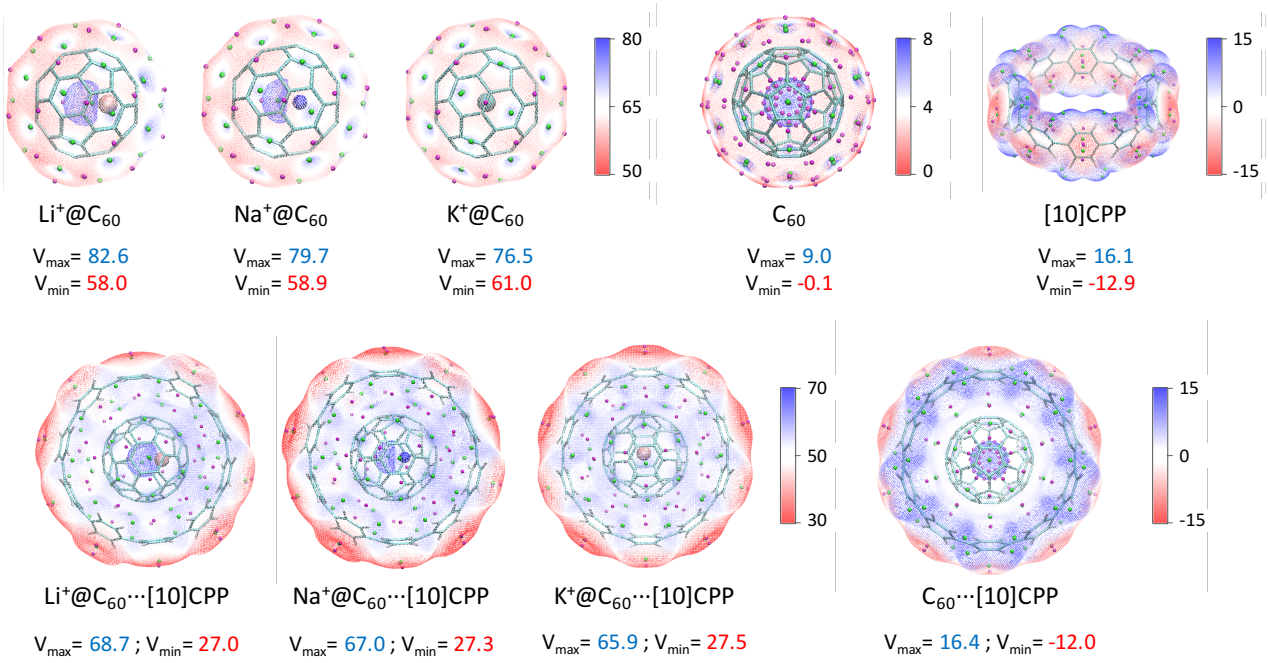
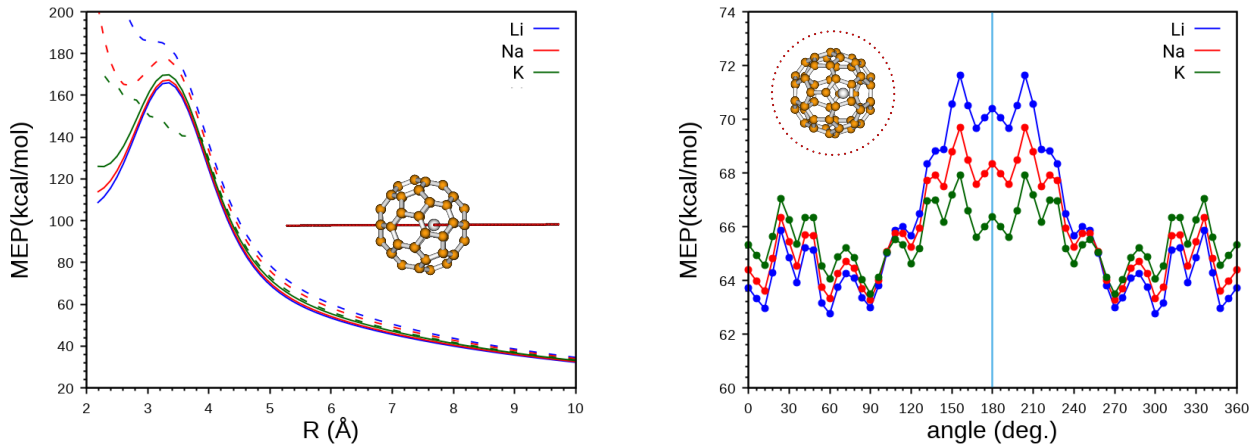


Figure S1. Molecular electrostatic potential mapped onto an isosurface of isodensity 0.001 a.u calculated at the B97-D2/def2-TZVP level. Values in kcal/mol. Green and magenta dots represent the maxima and minima onto the isosurface, respectively, as obtained using Multiwfn.[1, 2] The values of the largest and smallest of these extrema are listed below the images.

1. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.
2. T. Lu and F. Chen, *J. Mol. Graphics Modell.*, 2012, **38**, 314-323.



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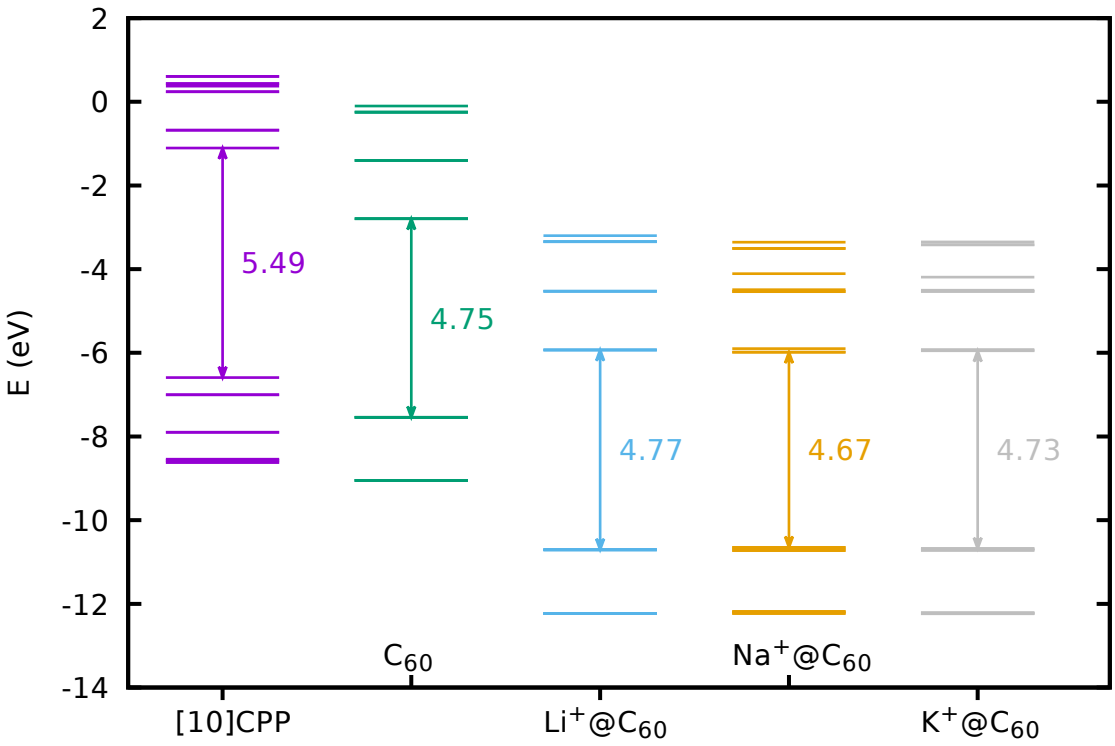


Figure S3. Schematic energy levels of the highest and lowest occupied molecular orbitals in monomers. CAM-B3LYP/TZVP//B97-D2/def2-TZVP.

Searching of the most stable structure of $M^+@C_{60}$···[10]CPP complexes

As commented in the Computational Details section, to explore the potential energy surface (PES) of the complexes and find their most stable minima, a preliminary scanning procedure was applied where the endofullerene (with fixed geometry) is rotated inside the [10]CPP ring (with fixed geometry) in all the directions changing the three Euler angles (α, β, γ) using steps of 6 degrees. Single point energy calculations were performed for each geometry at the third-order self-consistent charge density functional tight-binding level to save computation time (DFTB3 + Grimme's dispersion correction). For the [10]CPP the chosen geometry was that obtained with B3LYP (nearly equal to that obtained by B97-D2 and TPSS-D3(BJ)). For the $Na^+@C_{60}$ endofullerene, two different geometries were taken into account, specifically the most stable structure obtained by each of the two functionals. That is, the R6 found with B97-D2 (cation close to a six-membered ring), and C (cation at the centre of the cage), the only one found with TPSS-D3(BJ). For the $K^+@C_{60}$ endofullerene, a similar strategy was followed, employing C and R5 structures (cation close to a five-membered ring).

In the case of $Na^+@C_{60}$···[10]CPP complex, once the lower energy structures are found, those with the same geometry are eliminated by a comparison of structure and dispersion energy. The data of the scans are found in Figures S4-S7. The minimum energy structures from these scans are fully optimised with both functionals (B97-D2 and TPSS-D3(BJ)) and the complexation energies are obtained (Figure S8). For the $K^+@C_{60}$···[10]CPP complex the same strategy is followed (scans in Figures S9-S12). However, there is a large number of structures of similar energy, so in this case it was necessary to classify structures by families (see Figures S13-S14), to then carry out the full optimization of only the best structures of each family (with both functionals, B97-D2 and TPSS-D3(BJ)). The most favourable structures at both levels and their complexation energies are shown in Figure S15.

There are not DFTB+ parameters for the Li^+ cation. For this reason we can not perform the scan of the Euler angles and then choose a simple procedure for searching the best energy minima of the $Li^+@C_{60}$···[10]CPP complex. Thus, we opted for selecting the best structures of $Na^+@C_{60}$···[10]CPP complex, replace Na^+ with Li^+ and perform a reoptimization (without restrictions) with the two levels of calculation considered(the optimised structures and their complexation energies are shown in Figure S16). With this procedure, there is no certainty that we will find the absolute minimum energy structure. However, in light of the results obtained with the complexes including Na^+ and K^+, it does not seem that this is too relevant, since there are many minima in the PES with small energy differences (indicating a very flat PES), so finding just the best of them is not going to be very relevant when it comes to reproducing the properties of these complexes.

For the $Li^+@C_{60}$···[10]CPP complex the experimental geometry is available (H. Ueno, T. Nishihara, Y. Segawa and K. Itami, *Angew. Chem. Int. Ed.*, 2015, **54**, 3707-3711). Therefore, another option to computationally study this complex could be to use that geometry. However, if we use it as a starting point, the results lead to more unstable structures than those obtained from the previous calculations (see Table S3). This is not surprising since the experimental geometry is the one corresponding to the crystalline structure, in which, for example, the structure of the nanoring [10]CPP is very different from the one it has in the gas phase (with non-parallel phenyl rings). This results in a large deformation energy of [10]CPP (which becomes close to 3 kcal mol^{-1}), as can be seen in Table S3.

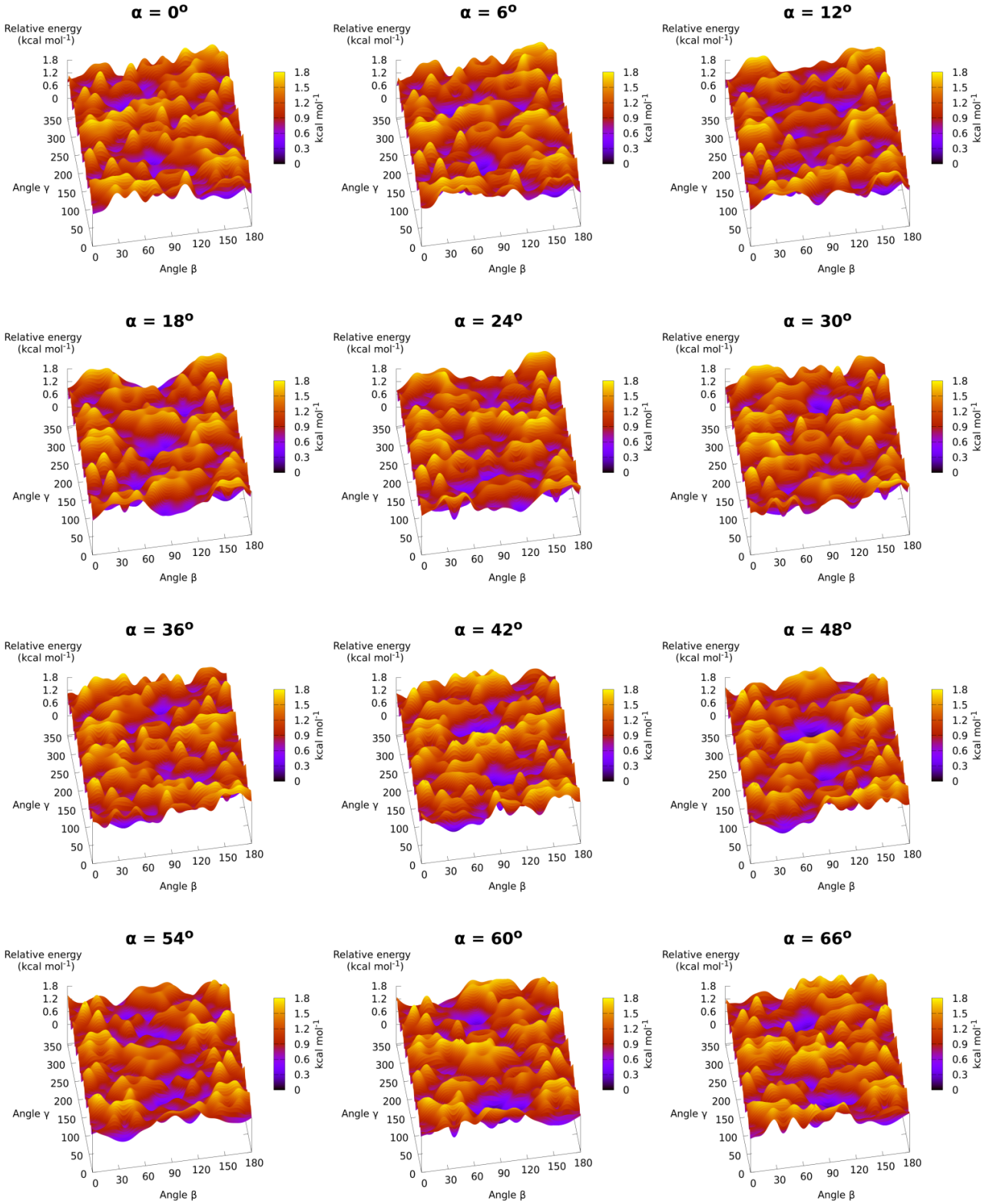
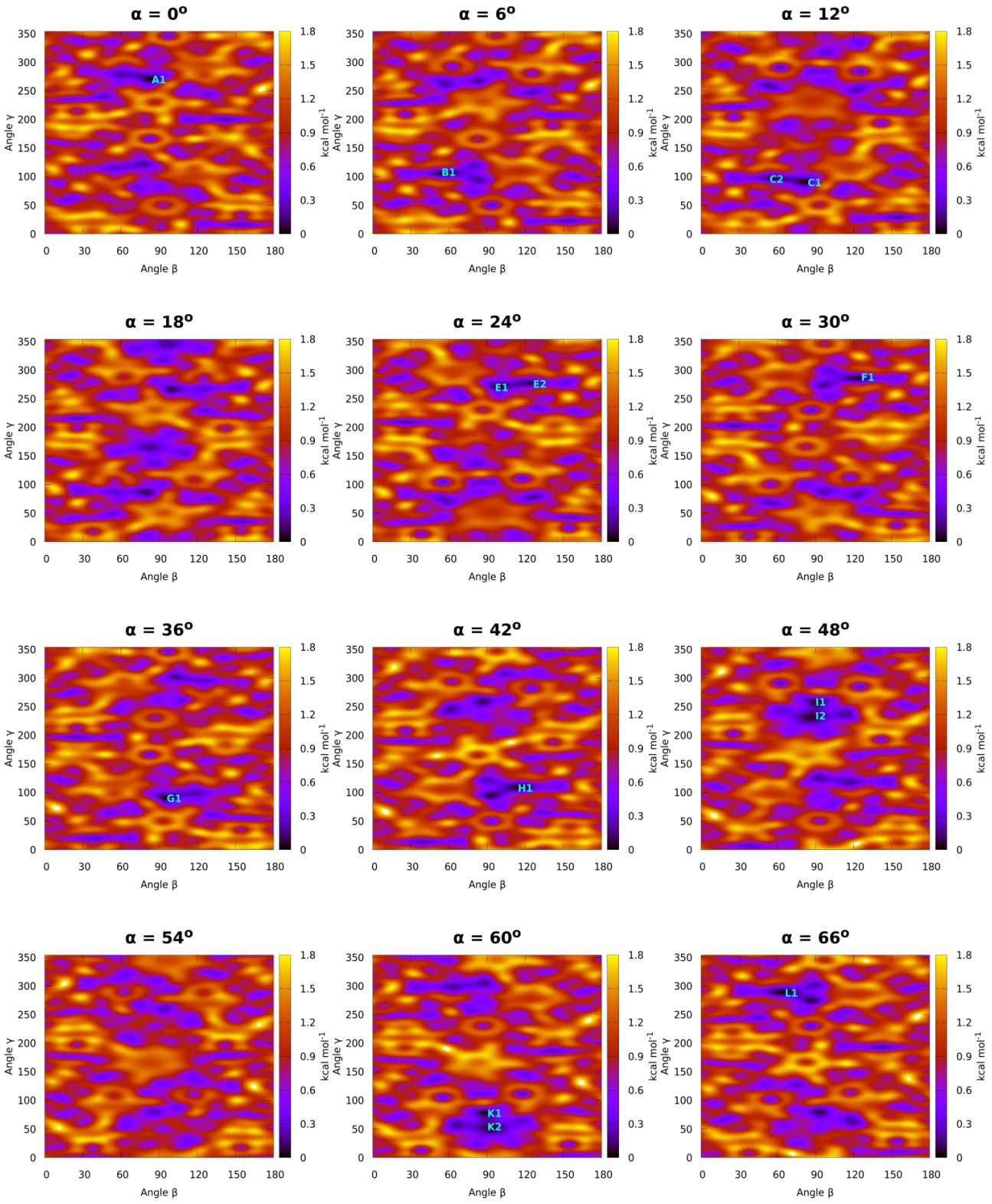


Figure S4. Potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation near a hexagonal ring as found with B97-D2.



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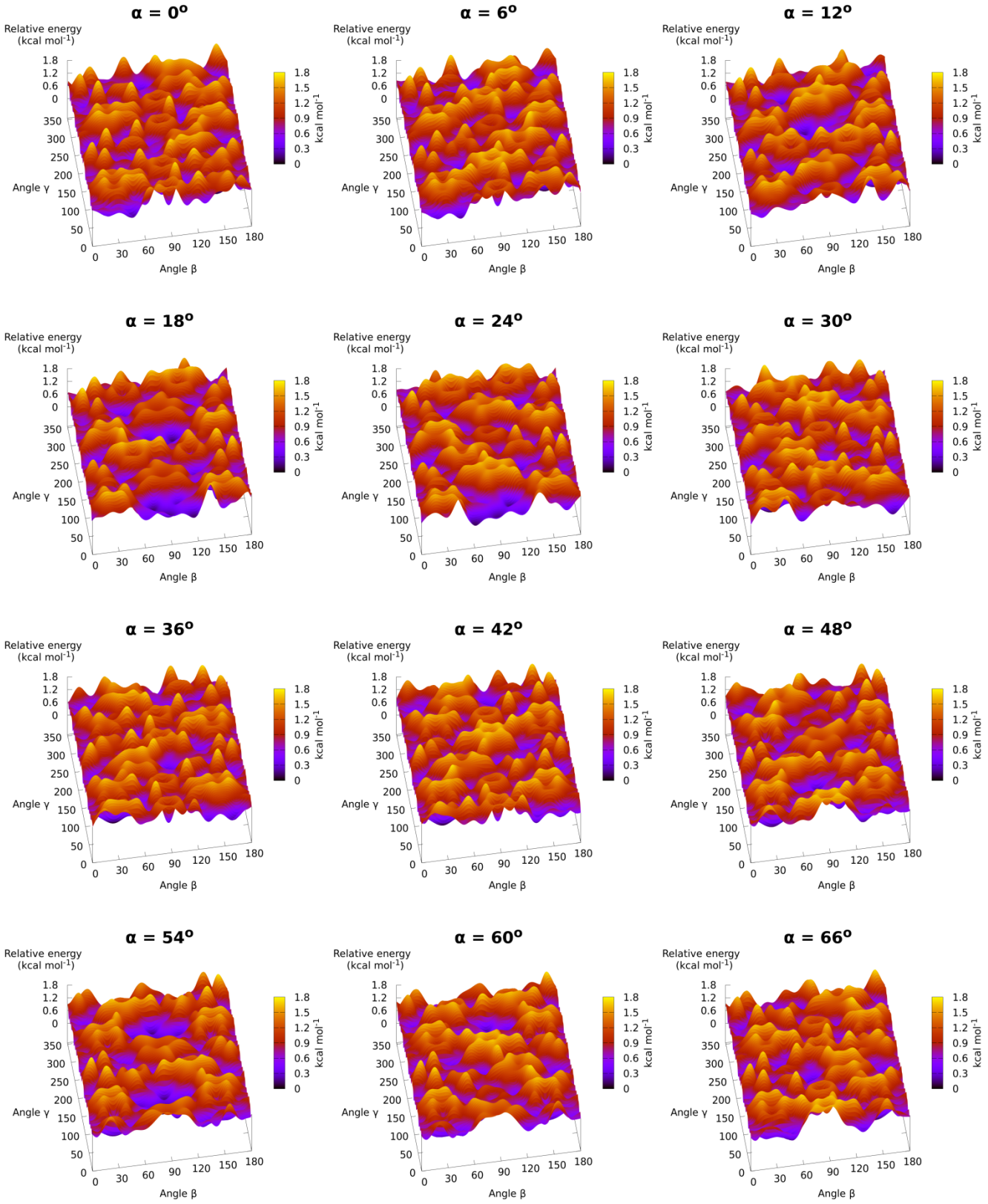
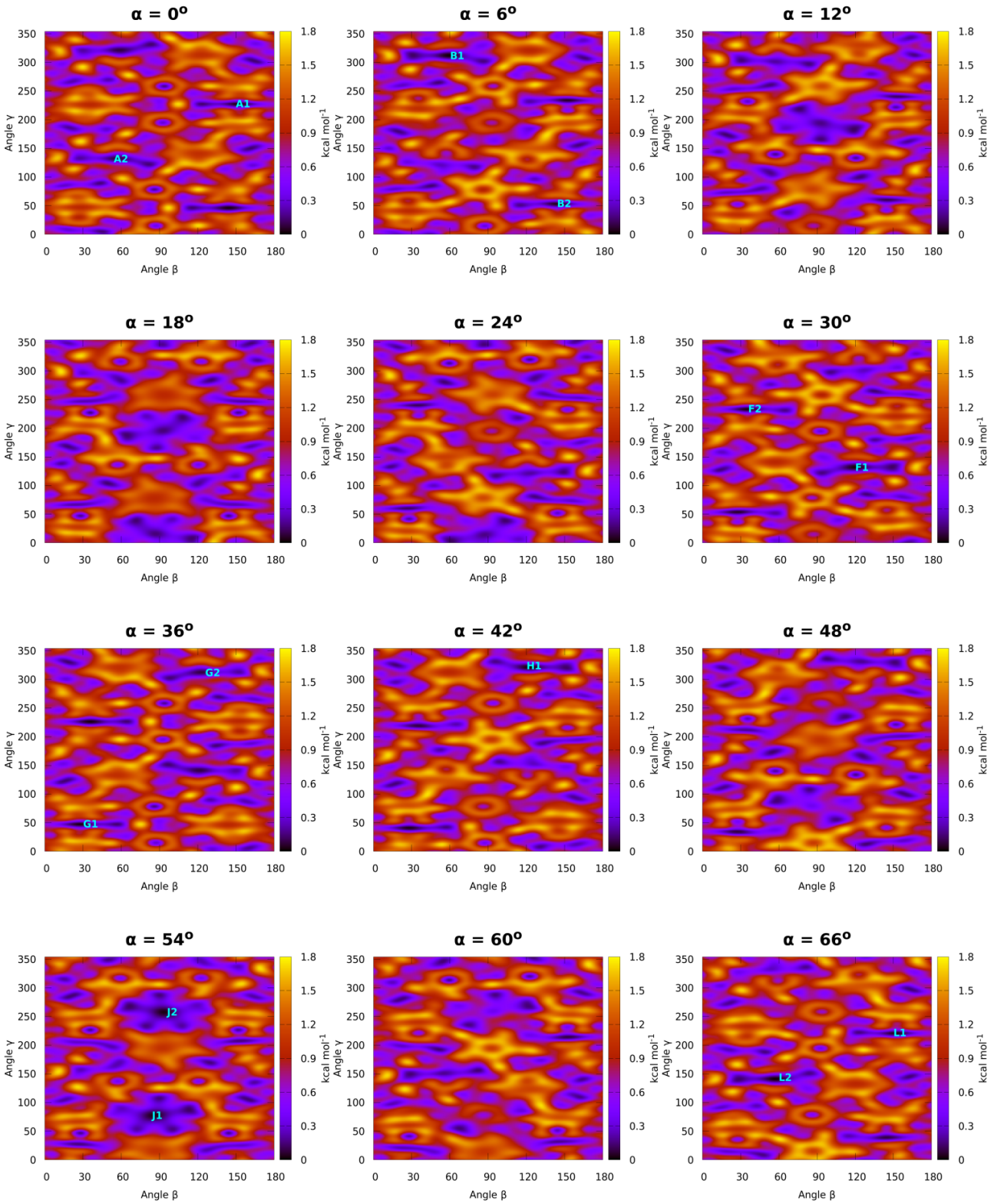


Figure S6. Potential energy surface of $Na^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with TPSS-D3(BJ).



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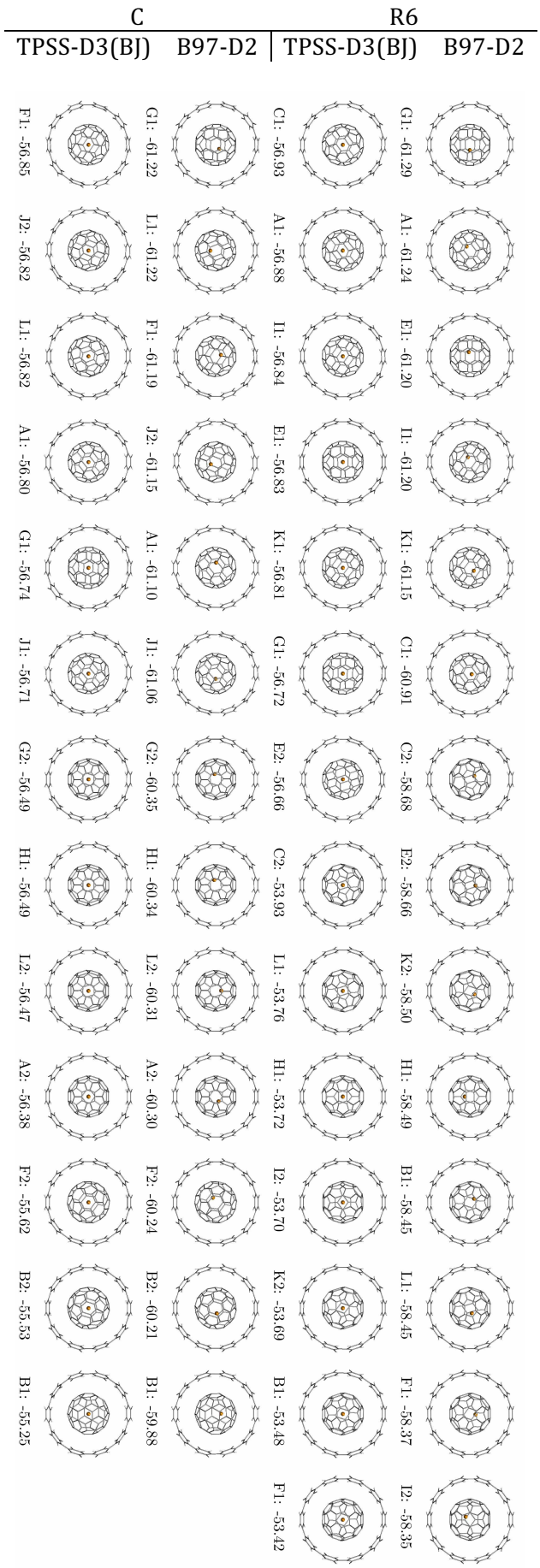


Figure S8. Most stable structures optimised after scan of $Na^+@C_{60}\cdots$[10]CPP complex. The complexation energy for each complex is included (kcal mol^{-1}). C and R6 refer to the starting location of Na^+ cation inside C_{60}, not to the final optimised structures of the complexes.

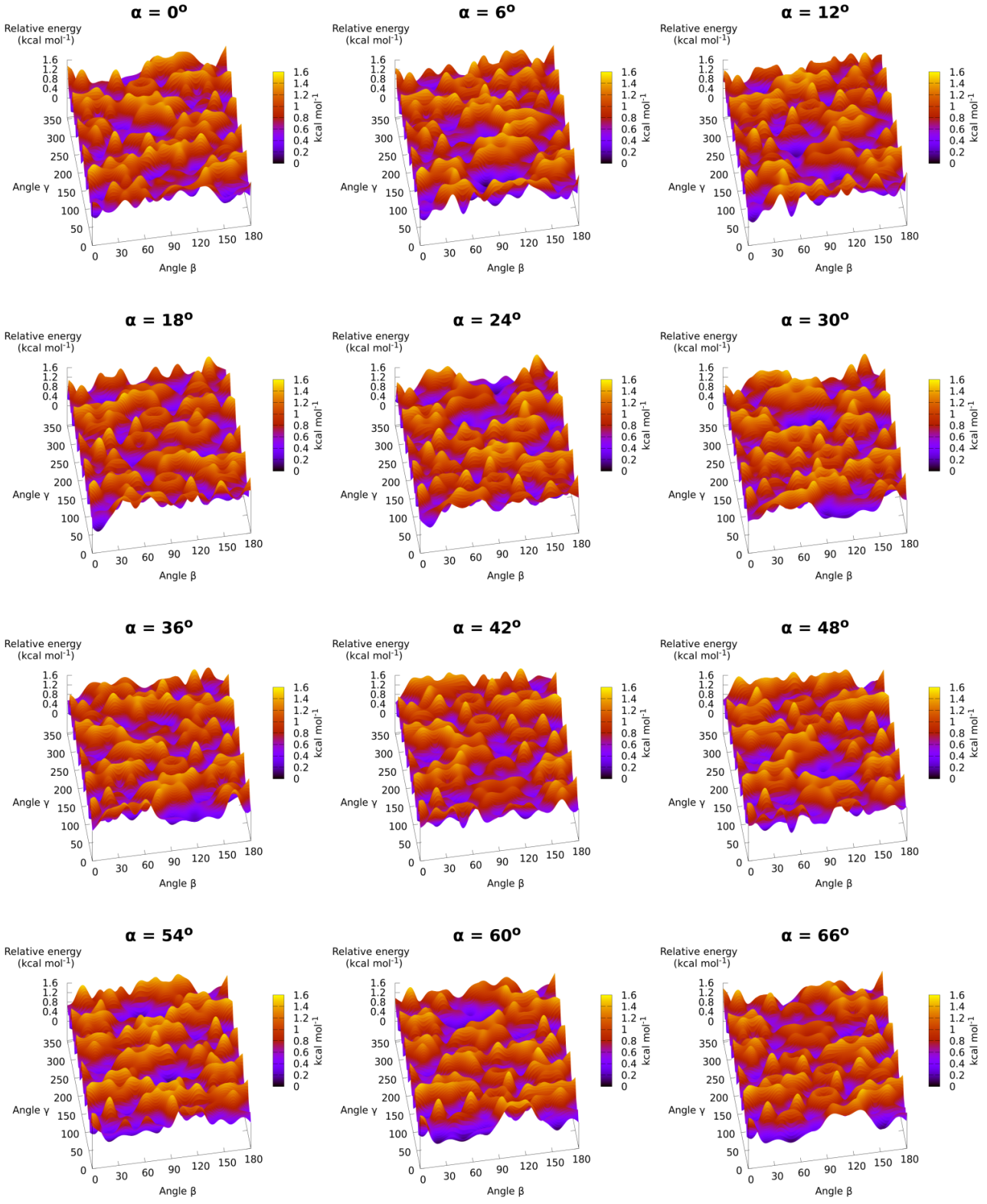
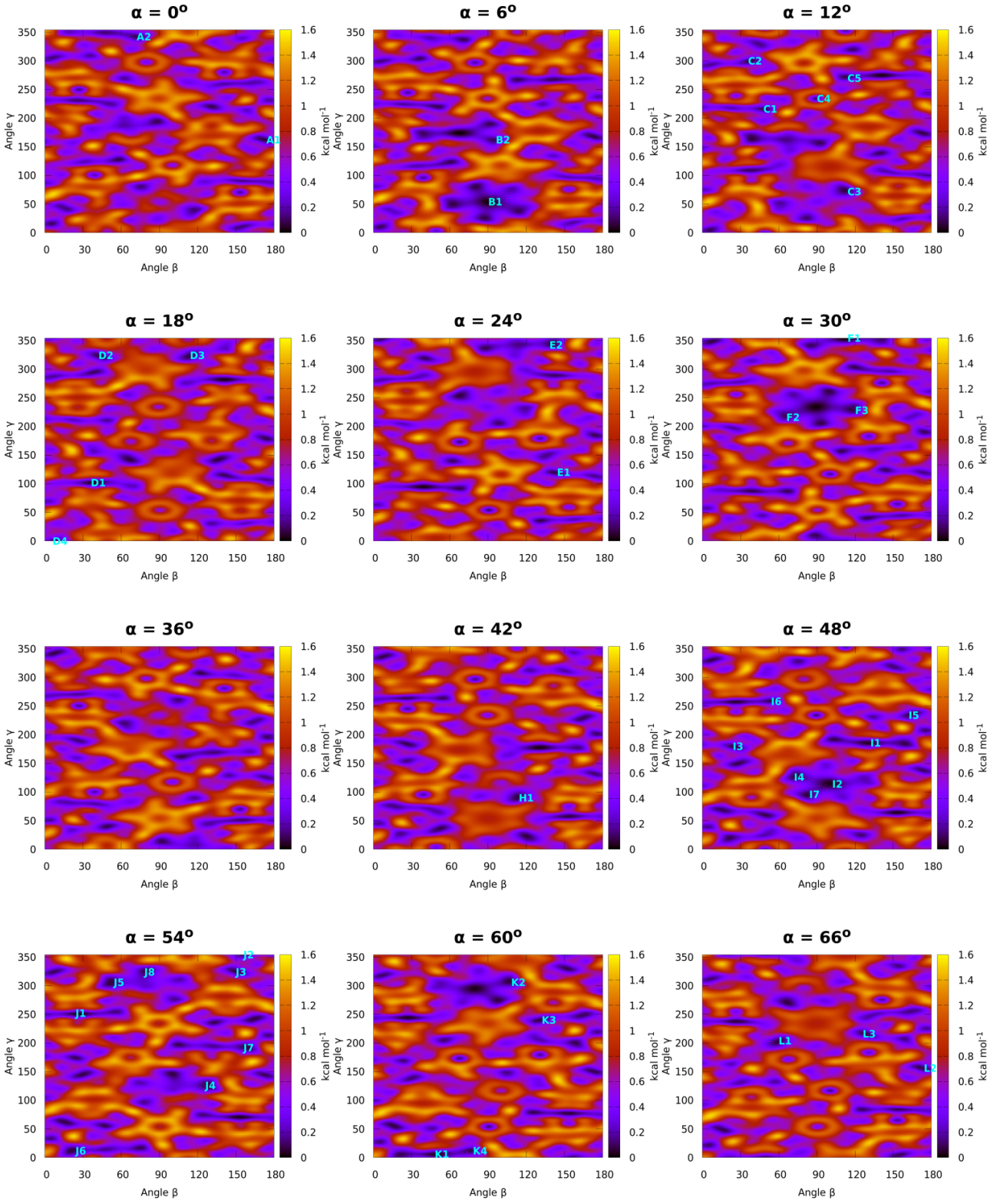


Figure S9. Potential energy surface of $K^+@C_{60}\cdots$[10]CPP complex obtained with DFTB3+D by changing the orientation of the fullerene inside [10]CPP. Geometry of the endofullerene: cation at the centre of the carbon cage as found with B97-D2.



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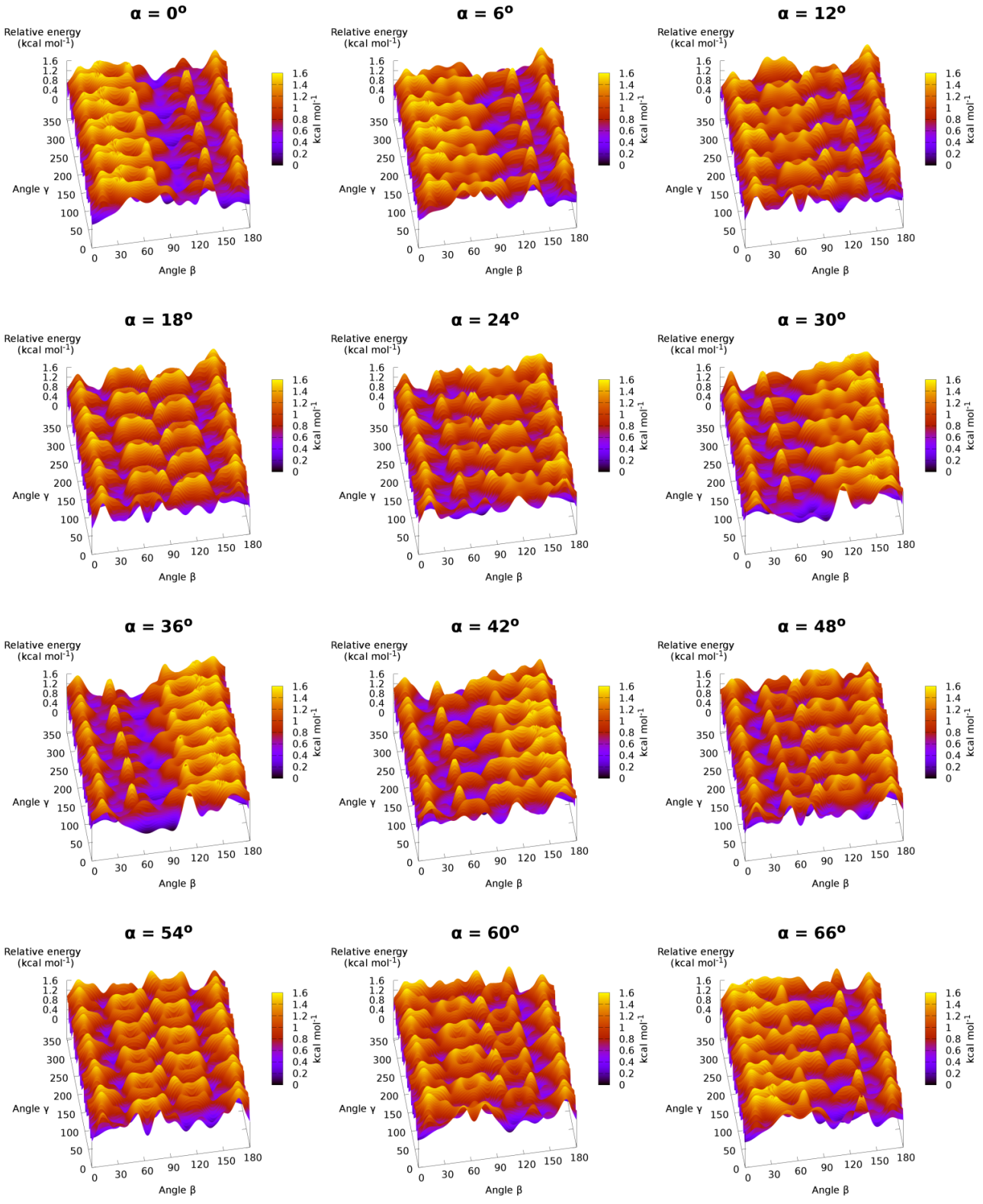

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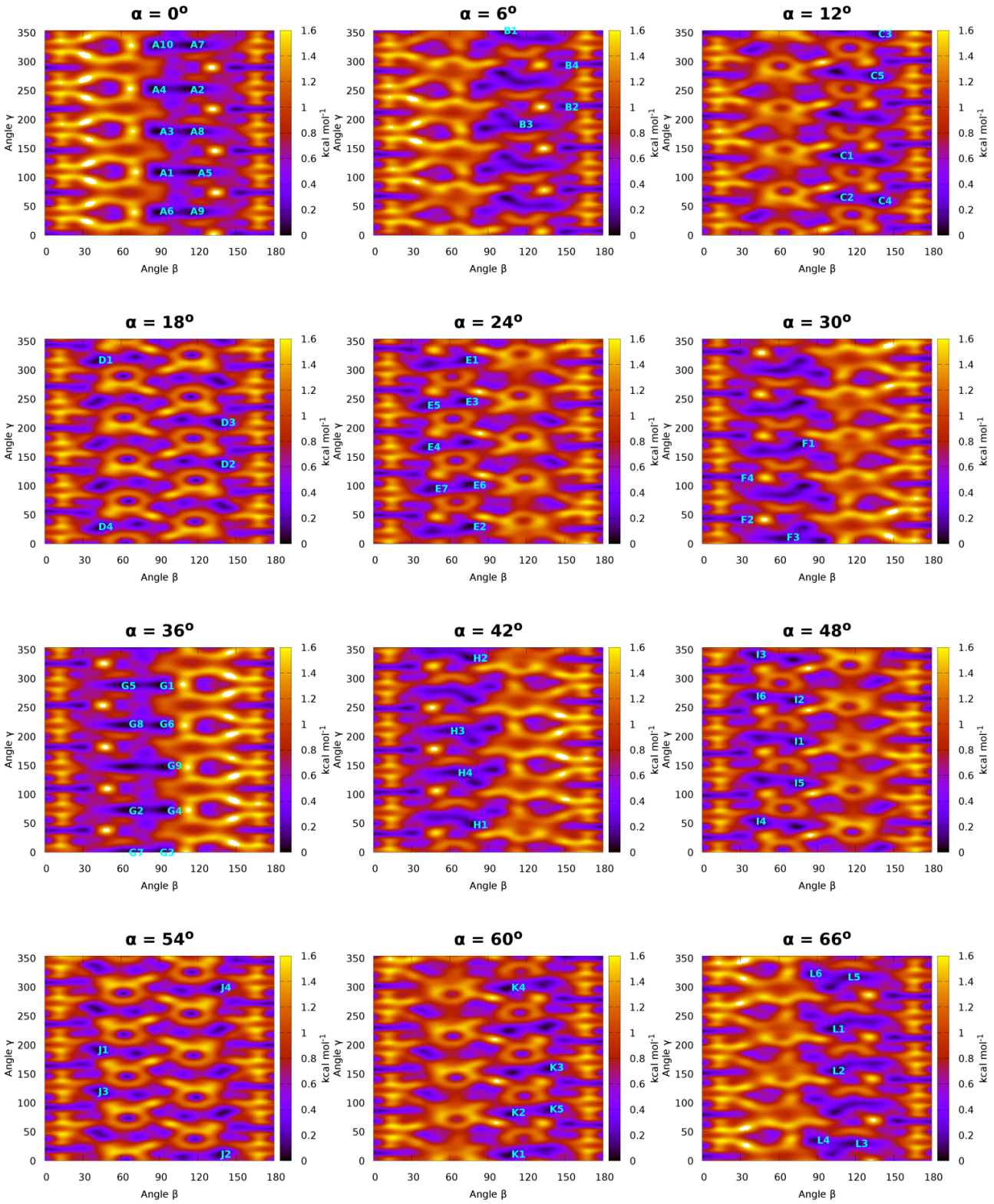

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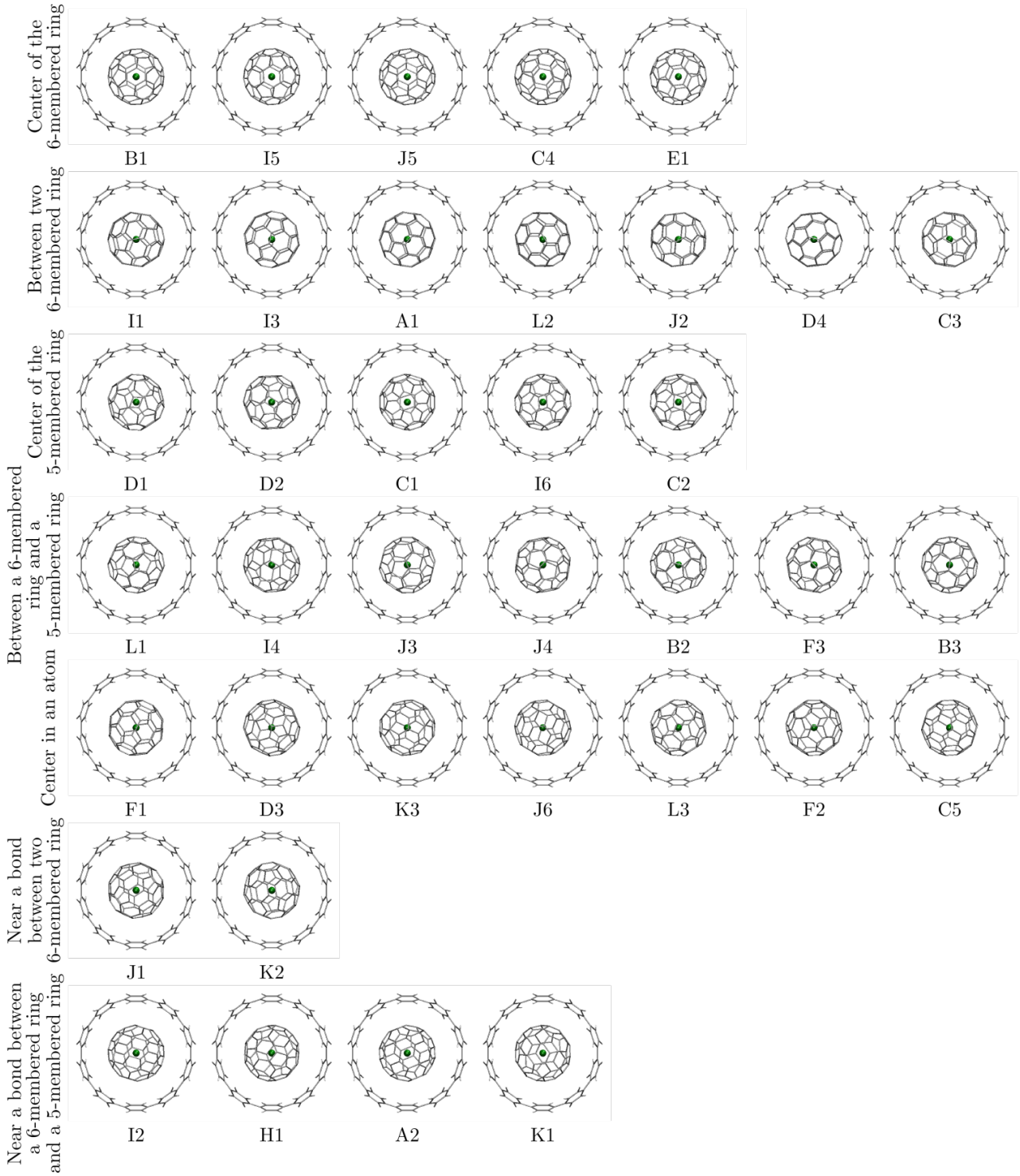
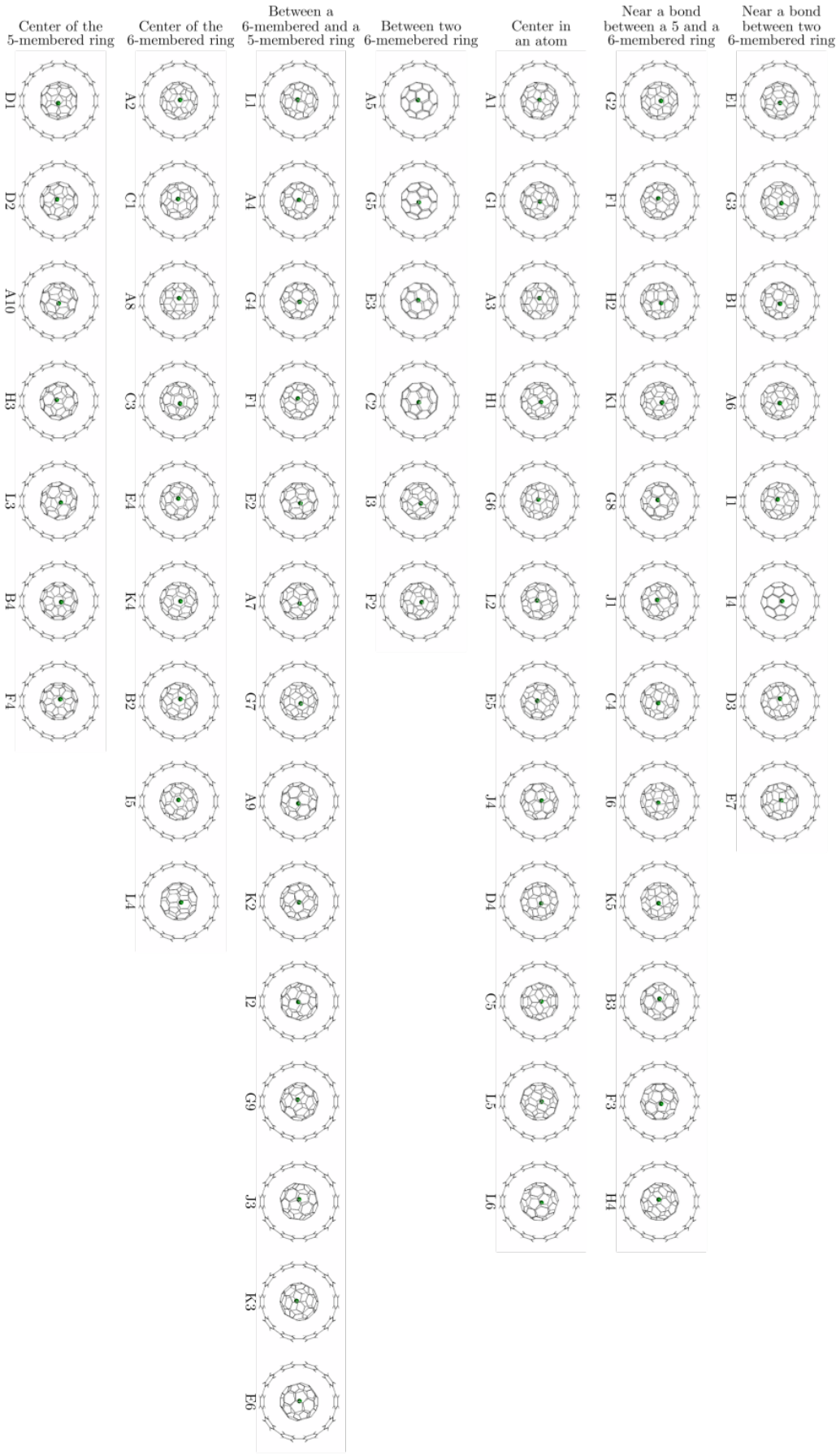


Figure S13. Classification in families of the minima found of $K^+@C_{60}\cdots$[10]CPP complex. Geometry of the endofullerene: cation at the centre of the carbon cage as found with B97-D2.



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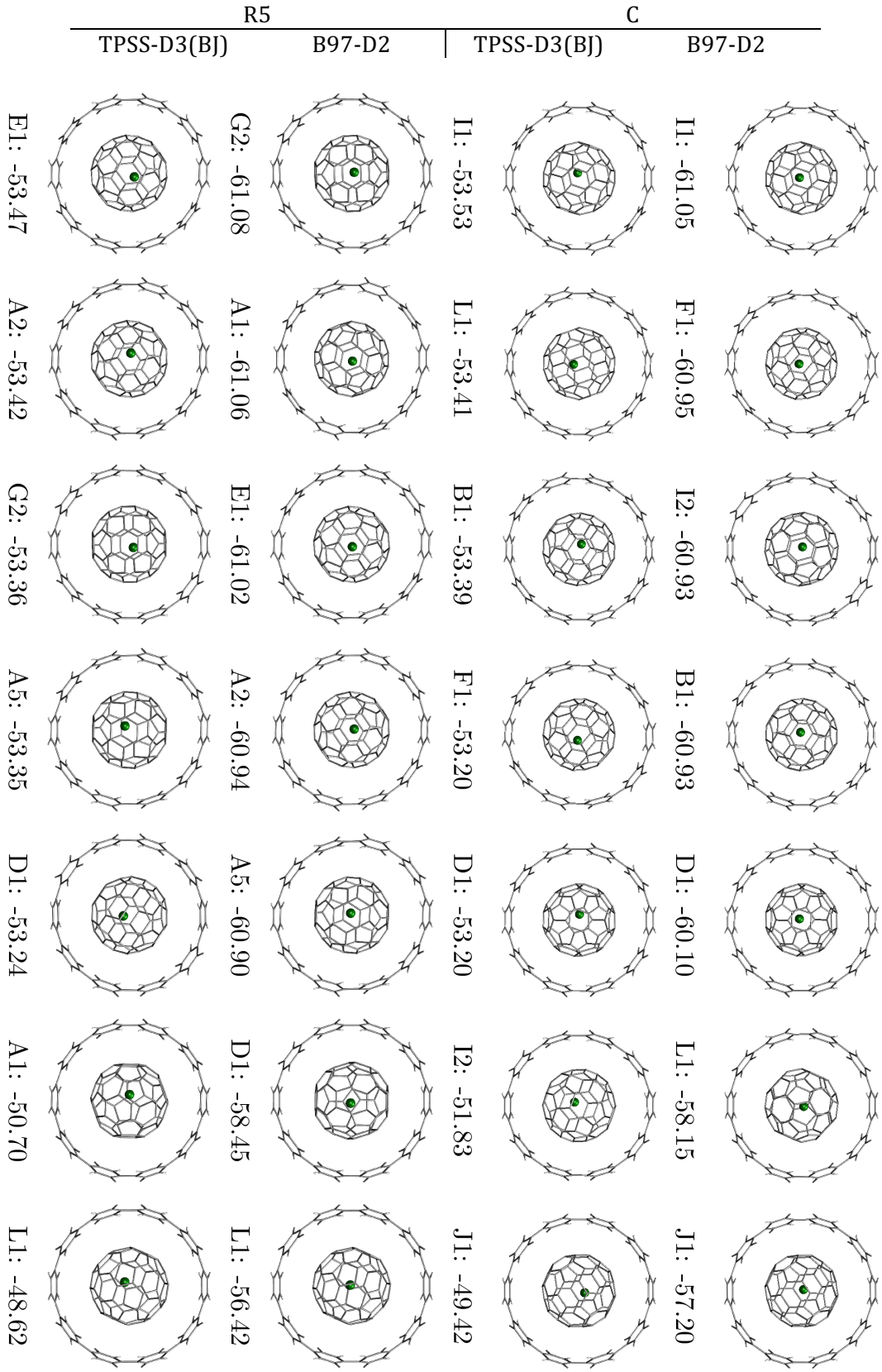

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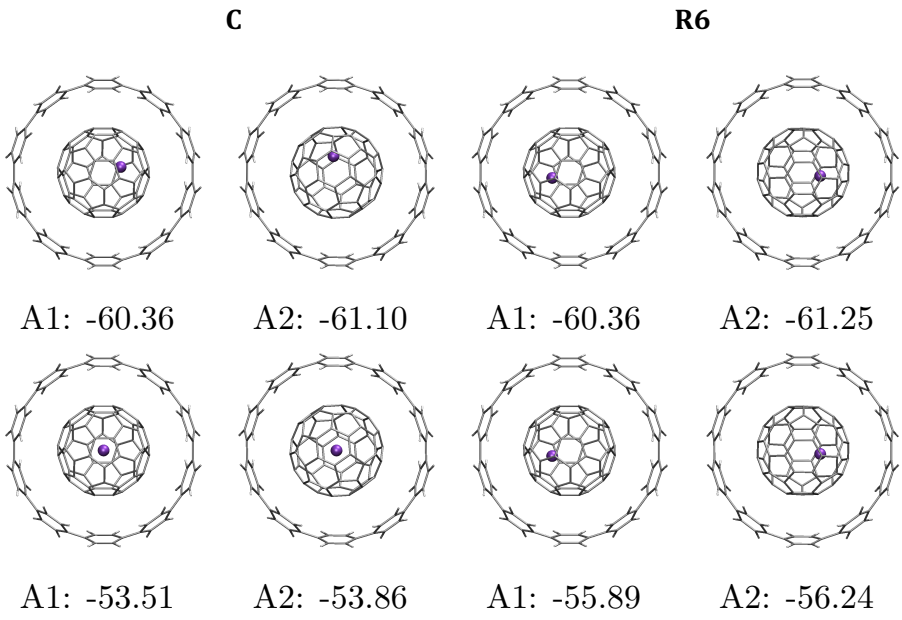

Figure S16. Optimised most stable structures of $Li^+@C_{60}\cdots$[10]CPP complex. The complexation energy for each complex is included (kcal mol^{-1}). Top line: B97-D2. Bottom line: TPSS-D3(BJ). C and R6 refer to the starting location of Li^+ cation inside C_{60}, not to the final optimised structures of the complexes.

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$M^+@C_{60}$	$\Delta E_{complex}$	$\Delta E_{def,fullerene}$	$\Delta E_{def,[10]CPP}$	ΔE_{disp}	$Q_{fuller,Mull}$	$Q_{fuller,NBO}$
C_{60}(5)	-46.71	0.21	0.19	-66.88	-0.047	-0.051
C_{60}(6)	-45.56	0.16	0.46	-66.52	-0.053	-0.092
$Li^+@C_{60}$(5)	-55.89	0.10	0.37	-65.70	0.805	0.899
$Li^+@C_{60}$(6)	-56.24	0.12	0.56	-65.58	0.758	0.824
$Na^+@C_{60}$(5)	-56.49	0.42	0.39	-66.98	0.802	0.895
$Na^+@C_{60}$(6)	-56.93	0.27	0.68	-66.75	0.756	0.821
$K^+@C_{60}$(5)	-53.20	0.22	0.41	-63.29	0.799	0.896
$K^+@C_{60}$(6)	-53.53	0.16	0.65	-63.18	0.751	0.825

Table S3. Energetic results (kcal mol^{-1}) and point charges of the best structure found for the $M^+@C_{60}\cdots$[10]CPP complexes optimised starting from the experimental geometries of Ueno et al. (H. Ueno, T. Nishihara, Y. Segawa and K. Itami, *Angew. Chem. Int. Ed.*, 2015, **54**, 3707-3711). $\Delta E_{complex}$ = complexation energy; E_{def} = deformation energy; ΔE_{disp}= contribution of dispersion to the total complexation energy; Q = charge of the fullerene according to Mulliken (Mull) and NBO analysis.

		B97-D2				
$M^+@C_{60}$	$\Delta E_{complex}$	$\Delta E_{def,fullerene}$	$\Delta E_{def,[10]CPP}$	ΔE_{disp}	$Q_{fuller,Mull}$	$Q_{fuller,NBO}$
C_{60}(5)	-58.57	0.06	2.87	-84.35	0.762	0.823
C_{60}(6)	-58.70	0.11	2.81	-83.58	0.746	0.814
		TPSS-D3(BJ)				
$M^+@C_{60}$	$\Delta E_{complex}$	$\Delta E_{def,fullerene}$	$\Delta E_{def,[10]CPP}$	ΔE_{disp}	$Q_{fuller,Mull}$	$Q_{fuller,NBO}$
C_{60}(5)	-53.63	0.33	2.97	-64.90	0.772	0.827
C_{60}(6)	-55.87	0.36	0.72	-65.70	0.760	0.824

Structures of the most favourable complexes

Figures S8, S15, and S16 show the best minima for the three complexes $M^+@C_{60}\cdots$[10]CPP ($M=Na^+$, K^+, Li^+) obtained with the B97-D2 and TPSS-D3(BJ) functionals. To analyse and discuss the geometry of the most favourable structures, different aspects have been taken into account.

First, the final location of the cation within C_{60} is observed. Figure S17 details the place of the cation within the complex for the most stable structures of each case, and reflects the fact that the structures found for each cation are very similar, since the distances shown are very similar for all the structures of the same cation. The only exception is the TPSS-D3(BJ) structures with the Li^+ cation, because this is the only case where two types of structures can be found (C and R6). In an approximate way, all the information of Figure S17 is summarized in Tables S4 and S5. Using the B97-D2 method the final structure of the endofullerene is always R6 for the complexes that include Li^+ or Na^+, in such a way that although even if we start from a centred position of the cation it moves towards one of the six-membered ring of C_{60}. When the TPSS-D3(BJ) functional is used, the results are slightly different, and Li^+ remains at the centre when starting from a central position (although this structure is worse than the R6). Using this functional, the final position of the Na^+ cation is always at the centre. As for the complexes that include K^+ cation, using both functionals the final structure of the endofullerene is always R6, in such a way that although even if we start from a C or R5 location it moves towards one of the six-membered ring of C_{60}. If the results of Table S5 are compared with those of the endofullerenes ($M^+@C_{60}$) discussed in of the manuscript (Table 1), it can be observed that the complexation process with [10]CPP does not cause a perceptible displacement of Li^+ and Na^+ cations; the K^+ cation does undergo a small displacement (0.3 Å away from the centre). In summary, only the location of the K^+ cation undergoes a significant change when the endofullerene joins the CNR: it moves a little towards the inner surface of the fullerene and points to a six-membered ring.

Table S4. Most favourable location of the cation inside C_{60} in the endofullerene ($M^+@C_{60}$) and in the final complex with [10]CPP ($M^+@C_{60}\cdots$[10]CPP). R5: cation on a five-membered ring of C_{60}. R6: cation on a six-membered ring of C_{60}. C: cation at the centre of the fullerene.

	B97-D2		**TPSS-D3(BJ)**	
	$M^+@C_{60}$	**$M^+@C_{60}\cdots$[10]CPP**	**$M^+@C_{60}$**	**$M^+@C_{60}\cdots$[10]CPP**
Li^+	R6	R6	R6	R6
Na^+	R6	R6	C	C
K^+	C	R6	R5	R6

Table S5. Distance (Å) between the cation and the centre of C_{60} and between the cation and the nearest six-membered ring of C_{60} in the final $M^+@C_{60}\cdots$[10]CPP complex.

	B97-D2		**TPSS-D3(BJ)**	
	centre	**6 ring**	**centre**	**6 ring**
Li^+	1.4	1.9	1.3 [0.0][a]	1.8 [3.3][a]
Na^+	0.9	2.4	0.0	3.3
K^+	0.3	3.0	0.6	2.7

[a] In square brackets the values of the C type structures (A1, A2 of figure S16).

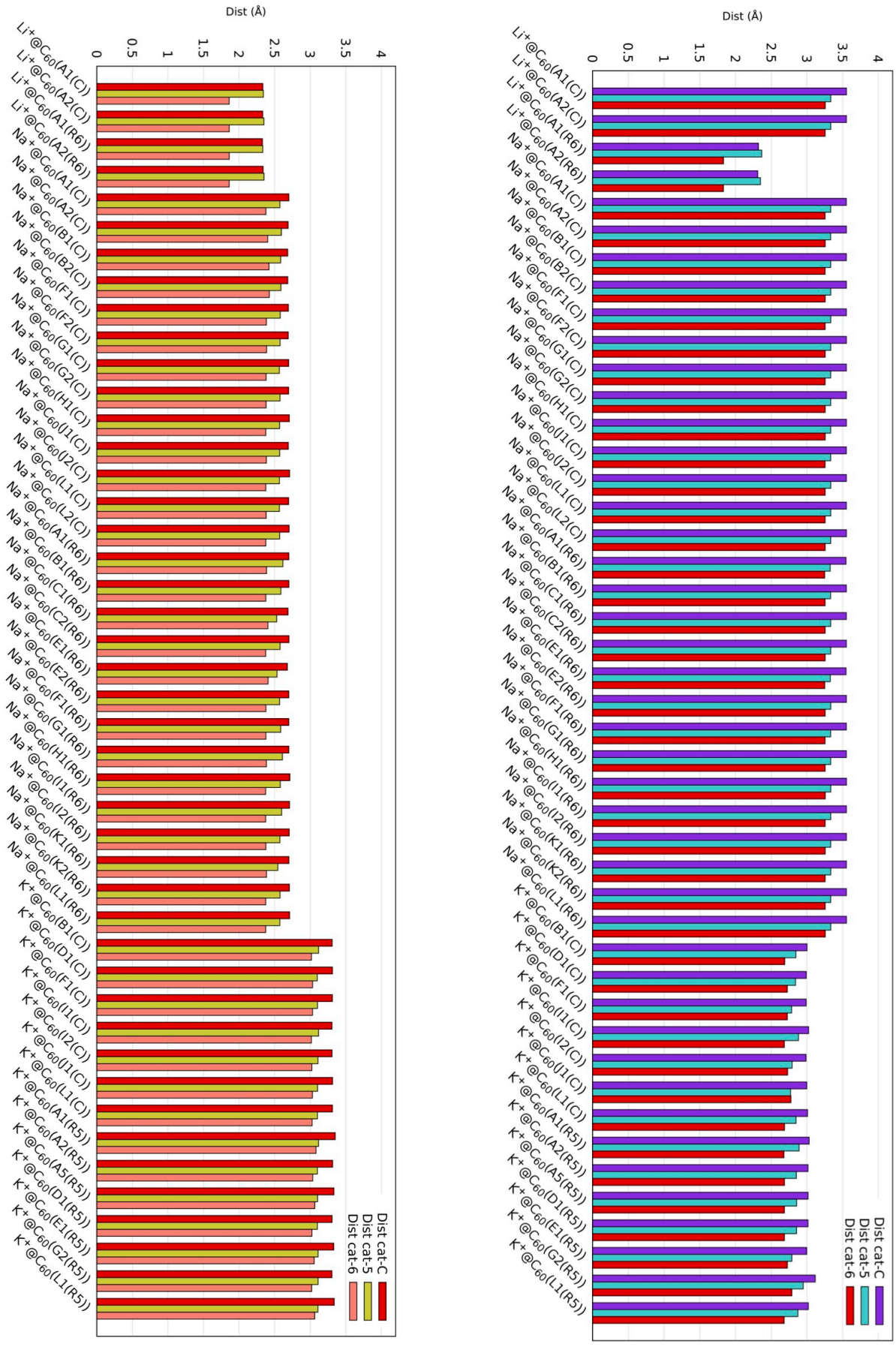


Figure S17. Distance from the cation to the nearest carbon of the fullerene (Dist cat-C), to the nearest centre of the 5 membered ring (Dist cat-5) and to the nearest centre of the 6 membered ring (Dist cat-6). Left: B97-D2. Right: TPSS-D3(BJ).

Secondly two main different spatial arrangements of the fullerene are obtained (Figure S18). In the first one ($C_{60}(5)$), the axis that goes through the centre of a 5-membered top and bottom rings of C_{60} is placed perpendicularly to the CNR, and in the second one ($C_{60}(6)$), the axis goes through the centre of a 6-membered top and bottom rings of C_{60}.

For the three cations the most favourable arrangement is which we call $C_{60}(6)$. This does not mean that the $C_{60}(5)$ arrangement is not found; in all cases (figures S8, S15 and S16) both types of structures are obtained (although always the best one corresponds to a $C_{60}(6)$ kind, though by a narrow energy margin). It is striking that for the endofullerenes studied in the present work the most favourable arrangement is the $C_{60}(6)$ in all cases, while for pristine C_{60} the contrary occurs; that is, the most favourable arrangement is the $C_{60}(5)$. In our previous work we demonstrated that the preference for the $C_{60}(5)$ arrangement is based on the good match between the fullerene and the carbon nanoring, the structure allowing the ten rings of [10]CPP to be directly faced to the six-membered rings of the fullerene (I. González-Veloso, J. Rodríguez-Otero and E. M. Cabaleiro-Lago, *Phys. Chem. Chem. Phys.*, 2016, **18**, 31670-31679). Therefore, it seems evident that in $M^+@C_{60}\cdots$[10]CPP complexes the cation causes the natural preference towards the $C_{60}(5)$ arrangement to be overcome.

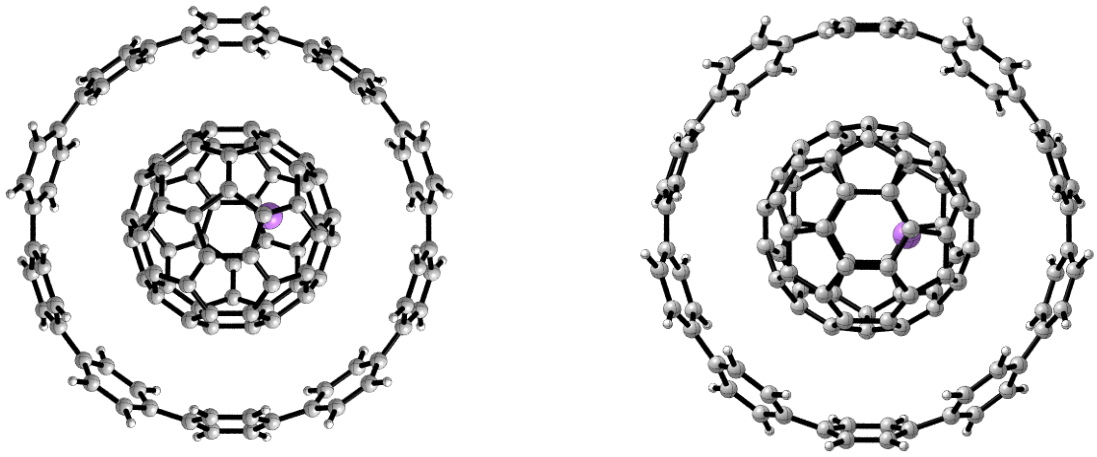
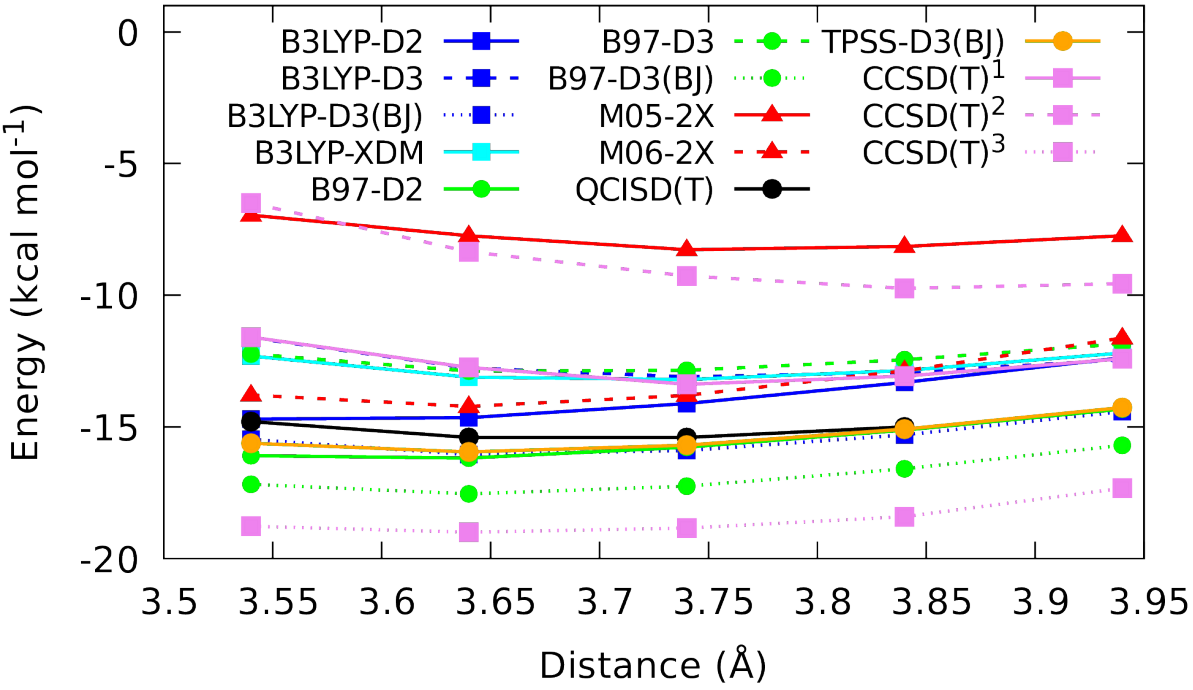


Figure S18. Main orientations of the fullerene inside the nanoring. Left: $C_{60}(5)$. Right: $C_{60}(6)$.

Finally, and with the aim of completely describing the geometry of the complexes, it is necessary to know how the cation is located with respect to the CNR that "catches" the endofullerene. In all cases, the cation is placed inside the fullerene pointing towards the external nanoring, as expected from an electrostatic point of view: the cation is oriented towards the inner side of the [10]CPP which presents a significantly negative MEP (see Fig. S1).



[1] DLPNO-CCSD(D)/def2-SVP and default cutoffs.
[2] DLPNO-CCSD(T)/def2-SVP and tight cutoffs.
[3] DLPNO-CCSD(T)/def2-TZVP and default cutoffs.

Figure S19. Interaction energy for the corannulene dimer as a function of the intermolecular distance. QCISD(T) benchmark values obtained by T. Janowski and P. Pulay. (*Chem. Phys. Lett.*, 2011, **512**, 155–160). Data for B3LYP, B97, M05-2X and M06-2X are taken from M. R. Kennedy, L. A. Burns, and C. D. Sherrill, *J. Phys. Chem. A*, 2012 **116**, 11920–11926.

Using QCISD(T) values as a reference, B97-D2 and TPSS-D3(BJ) produce a very slight overestimation of the interaction energy. DLPNO-CCSD(T)/def2-SVP produces reasonable results (although with a significant underestimation) probably due to the cancellation of errors for using a small basis and using the default cutoffs. The use of def2-TZVP basis and tight PNOs would be prohibitive for systems of the size of those studied in the present work.

Table S6. Contributions to the interaction energy obtained by Local Energy Decomposition (LED) analysis based on DLPNO-CCSD(T) with the def2-SVP basis set for the most stable compounds using the B97-D2 geometry.

	C_{60}	$Li^+@C_{60}$	$Na^+@C_{60}$	$K^+@C_{60}$
E_{disp}	-22.18	-18.89	-19.05	-18.64
E_{CT}	-6.71	-8.78	-8.74	-8.52
E_{Elec}	-97.46	-134.11	-133.87	-131.94
E_{Exch}	-44.19	-53.01	-53.01	-52.34
E_{IWP}	-57.12	-63.67	-63.61	-63.84
E_{IT}	-4.90	-4.35	-4.37	-4.27
$E_{prep, HF}$	174.51	208.42	208.52	205.61
$E_{prep, corr}$	12.21	18.29	18.41	18.06
$\Delta E_{def,fuller}$	0.30	0.29	0.25	0.26
$\Delta E_{def,[10]CPP}$	1.34	2.59	2.57	2.62
$\Delta E_{complex}$	-44.21	-53.22	-52.9	-52.98

E_{Disp}: genuine dispersion; E_{CT}: charge transfer contribution; E_{Elec}: electrostatic interaction; E_{Exch}: inter-fragment exchange; E_{IWP}: contribution from weak pairs; E_{IT}: contribution of triple excitations; $E_{prep,HF}$: HF contribution to preparation energy at the HF level; $E_{prep,corr}$: correlation contribution to preparation energy.

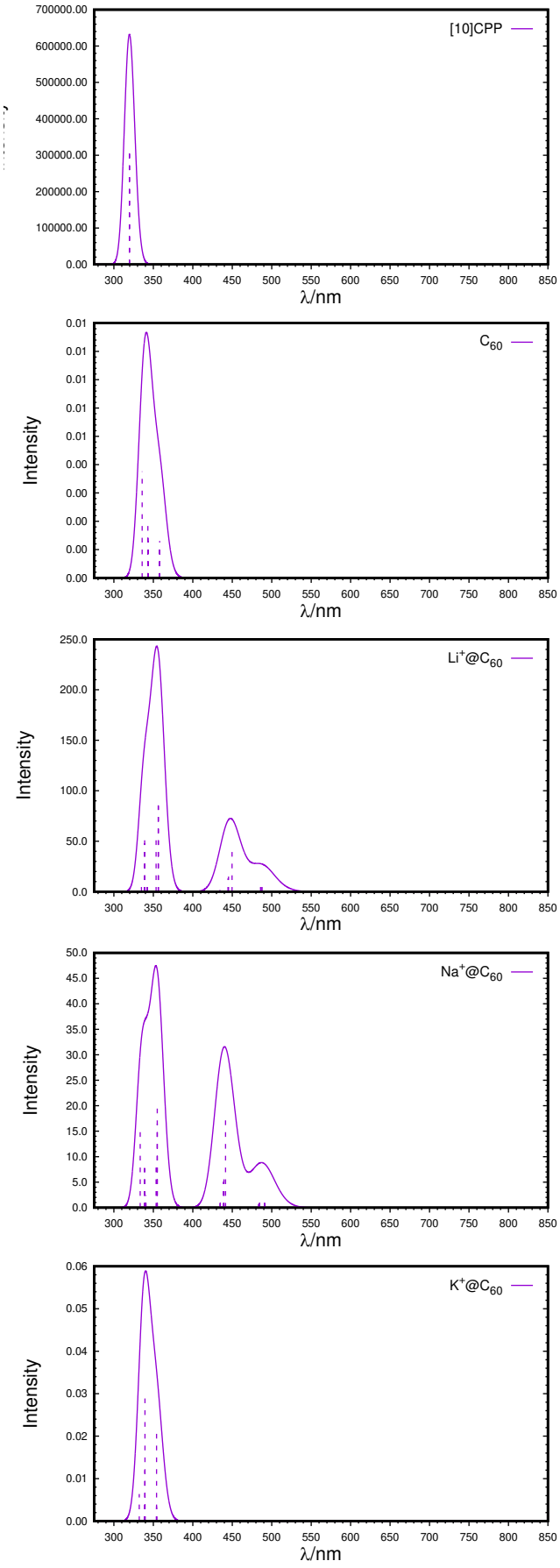


Figure S20. Absorption spectra for the monomers obtained at the CAM-B3LYP/TZVP level, using B97-D2 geometries.

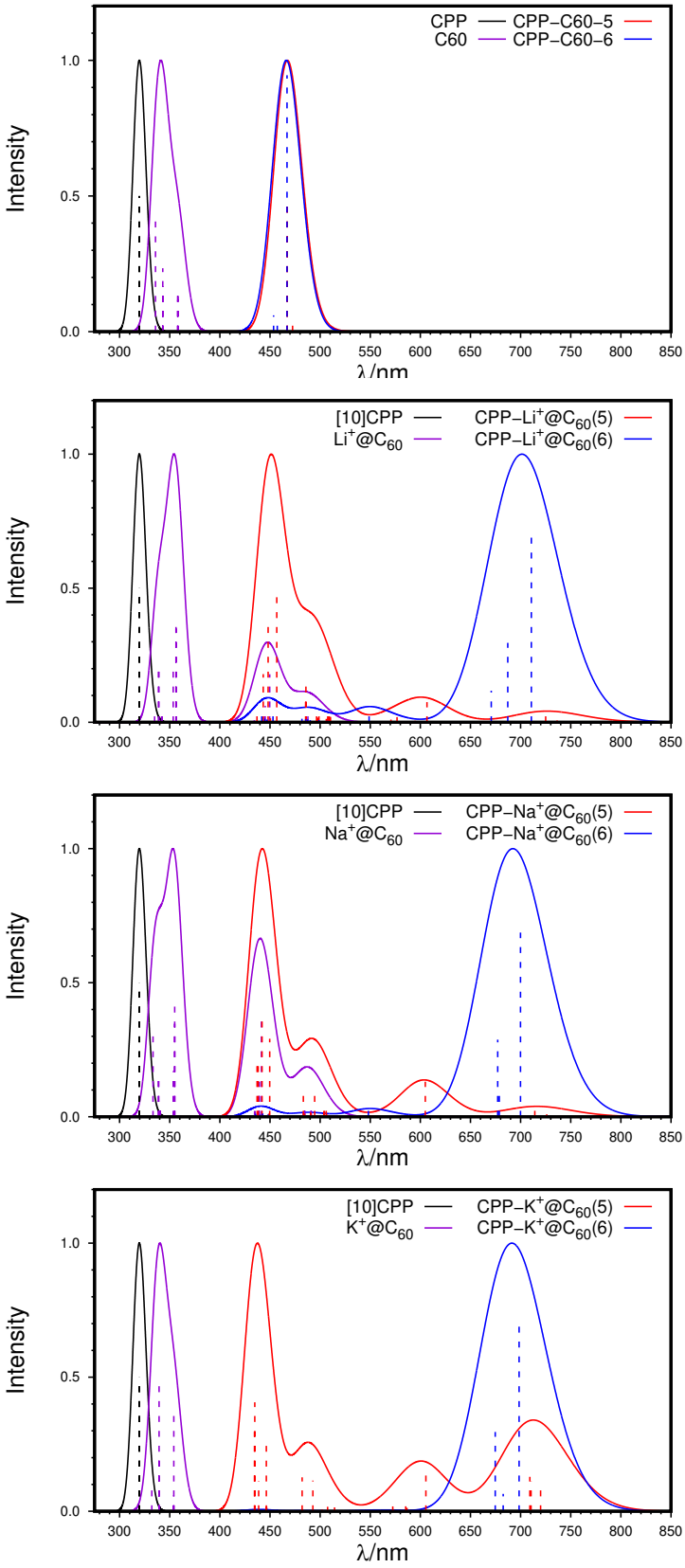


Figure S21. Normalised absorption spectra for the $M^+@C_{60}\cdots$[10]CPP complexes obtained at the CAM-B3LYP/TZVP level, using B97-D2 geometries.

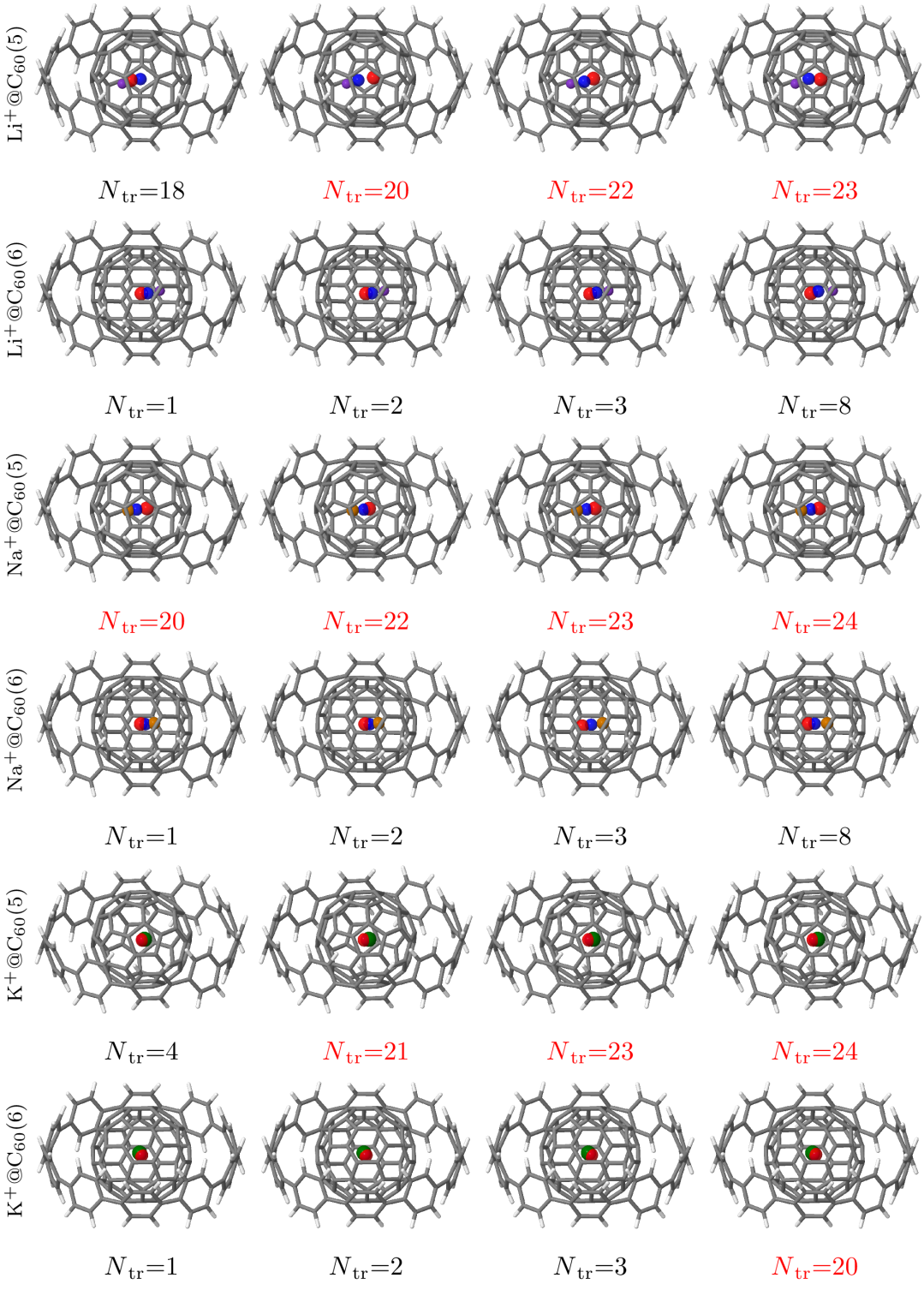


Figure S22. Position of the barycentres (blue and red dots) of charge for the transitions of $M^+@C_{60}\cdots$[10]CPP complexes shown in Figure 4. N_{tr} is the number of the transition and the red colour corresponds to intrafullerene transitions.

Table S7. Distance (Å) between the cation and the barycentres of charge for the most stable $M^+@C_{60}\cdots$[10]CPP complexes. N_{tr} is the number of the transition, $R_{cat\text{-}neg}$ is the distance between the cation and the negative barycentre and $R_{cat\text{-}pos}$ is the distance between the cation and the positive barycentre. Intrafullerene transitions in bold.

	N_{tr}	$R_{cat\text{-}neg}$ (Å)	$R_{cat\text{-}pos}$ (Å) (Å)	N_{tr}	$R_{cat\text{-}neg}$ (Å)	$R_{cat\text{-}pos}$ (Å)
$Li^+@C_{60}(5)$	18	1.365	0.681	**20**	**0.890**	**2.045**
	22	**0.965**	**1.712**	**23**	**1.063**	**1.879**
$Li^+@C_{60}(6)$	1	0.969	1.405	2	0.969	1.404
	3	0.932	1.401	8	1.107	1.651
$Na^+@C_{60}(5)$	**20**	**0.602**	**1.363**	**22**	**0.822**	**1.21**
	23	**0.706**	**1.304**	**24**	**0.706**	**1.302**
$Na^+@C_{60}(6)$	1	0.642	0.962	2	0.642	0.962
	3	0.845	1.510	8	0.907	1.36
$K^+@C_{60}(5)$	**4**	**0.160**	**0.228**	**21**	**0.183**	**0.352**
	23	**0.211**	**0.349**	**24**	**0.209**	**0.349**
$K^+@C_{60}(6)$	1	0.176	0.274	2	0.176	0.274
	3	0.183	0.309	**20**	**0.180**	**0.339**

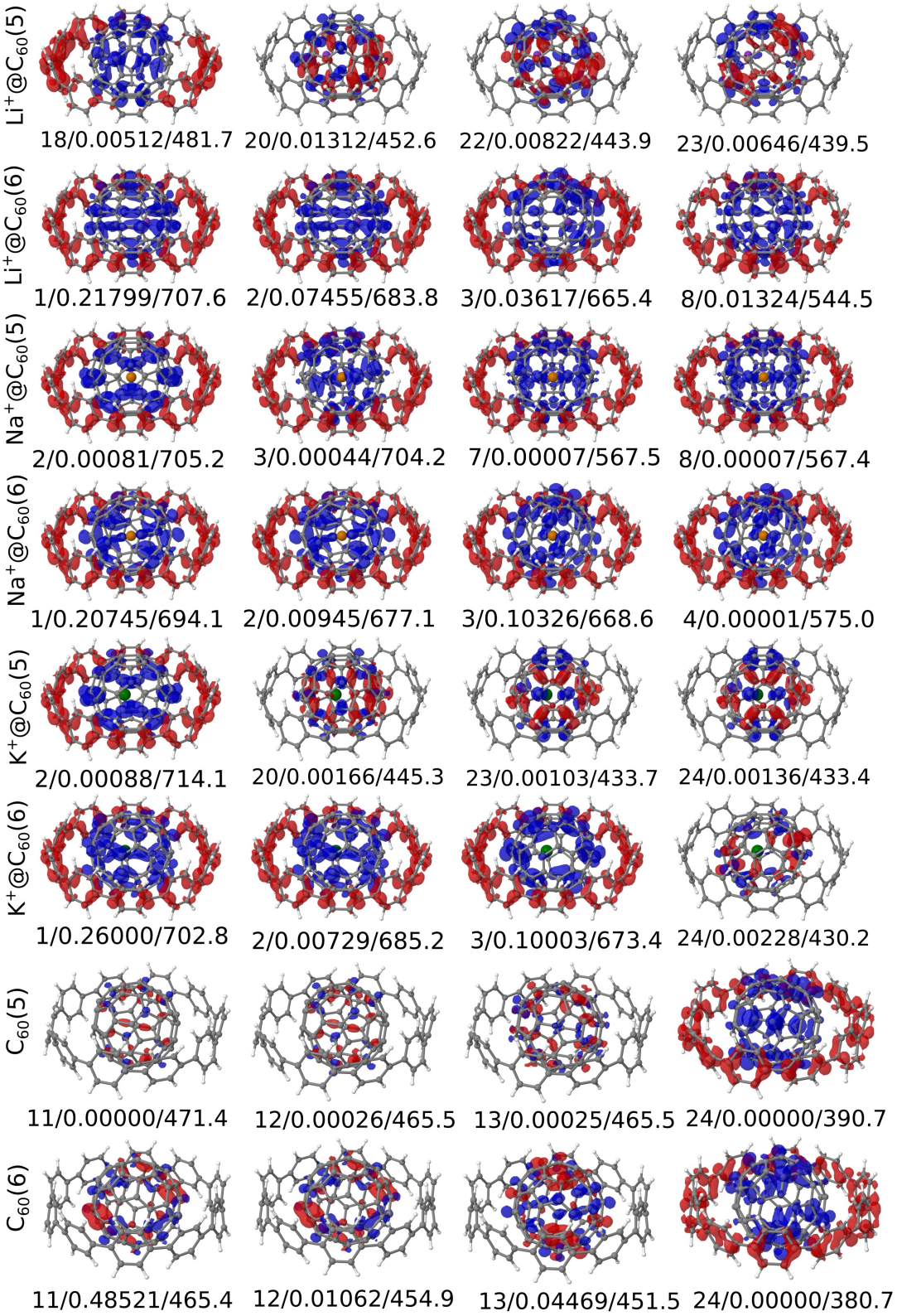


Figure S23. Difference density between the excited state and the ground state for the four most intense transitions in the most stable complexes (with TPSS-D3(BJ)) obtained at the CAM-B3LYP/TZVP level. Each of the rows corresponds to one of the fullerenes. The numbers are the number of the transition/oscillator strength*100/wavelength (nm). Surface corresponds to −0.001 a.u.(red) and 0.001 a.u.(blue).

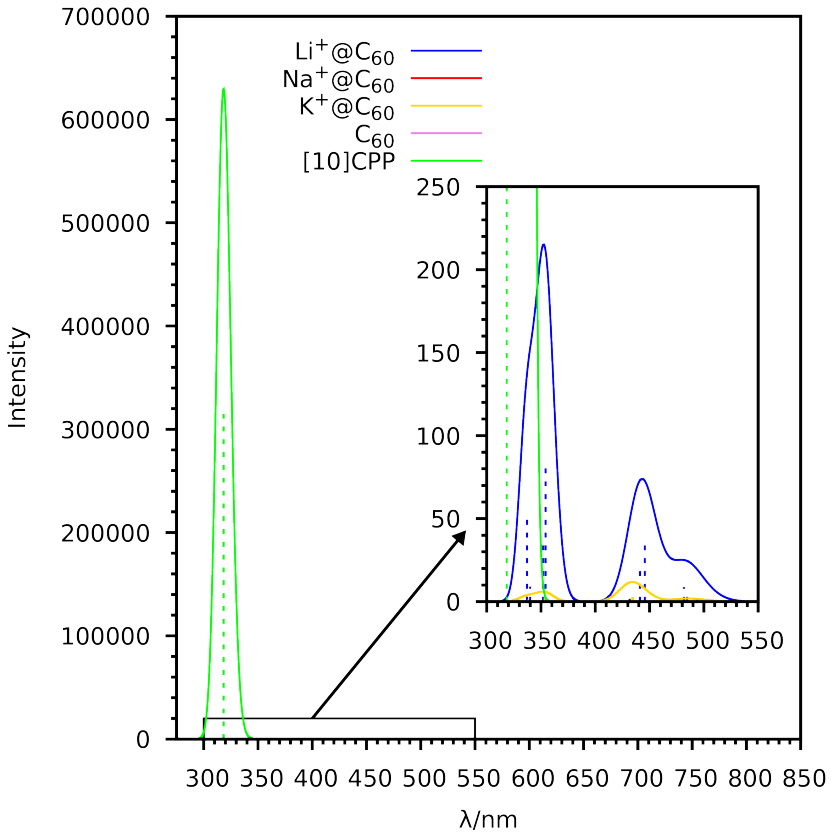


Figure S24. Absorption spectra for the monomers (fullerene, cationic endofullerenes, [10]CPP) obtained at the CAM-B3LYP/TZVP level, with TPSS-D3(BJ) geometries.

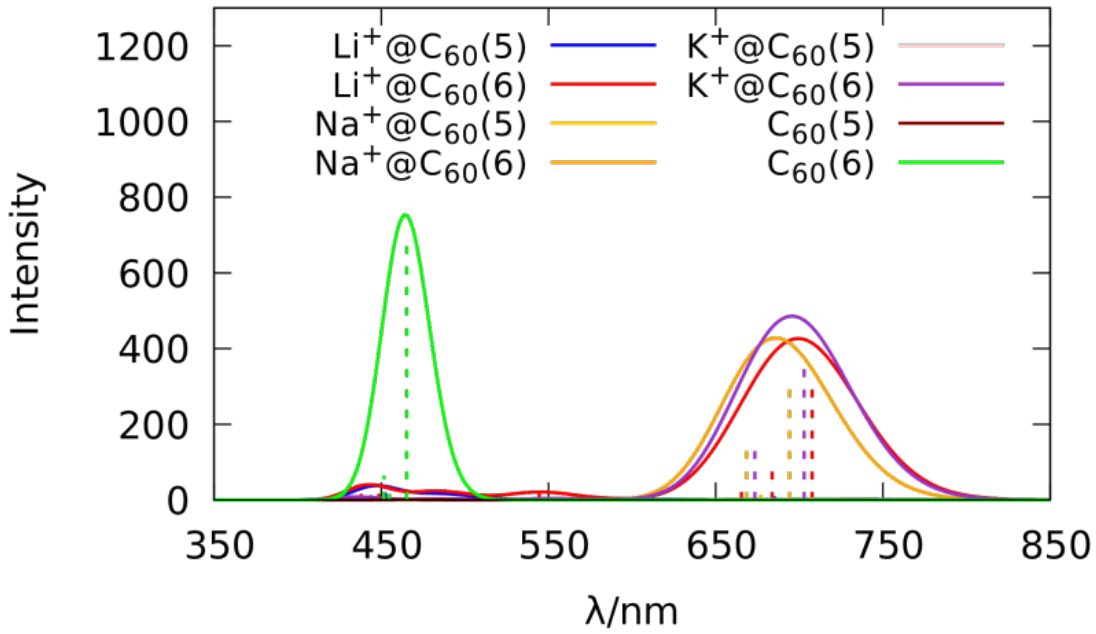


Figure S25. Absorption spectra for the $M^+@C_{60}\cdots$[10]CPP complexes obtained at the CAM-B3LYP/TZVP level, using TPSS-D3(BJ) geometries.

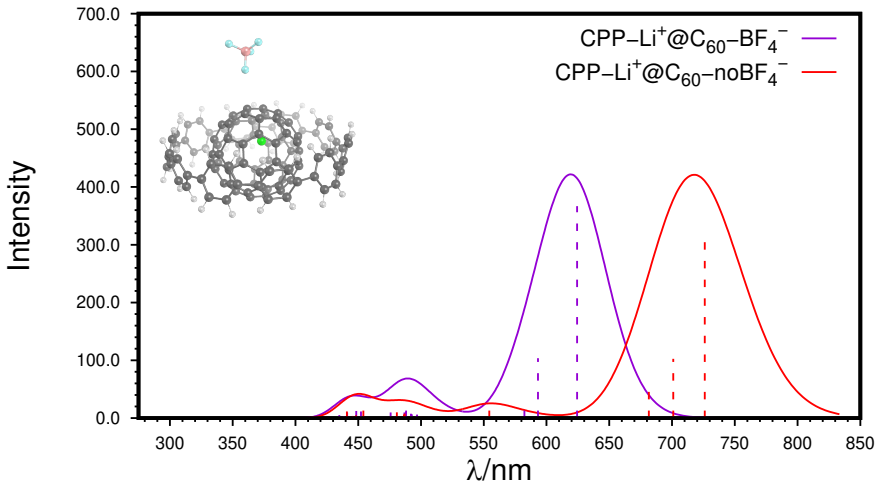


Figure S26. Absorption spectra for the $Li^+@C_{60}\cdots$[10]CPP$\cdots BF_4^-$ complex obtained at the CAM-B3LYP/TZVP level, using the B97-D2/def2-TZVP geometry. The red line corresponds to the complex without the anion but keeping the same geometry for the rest of the complex.

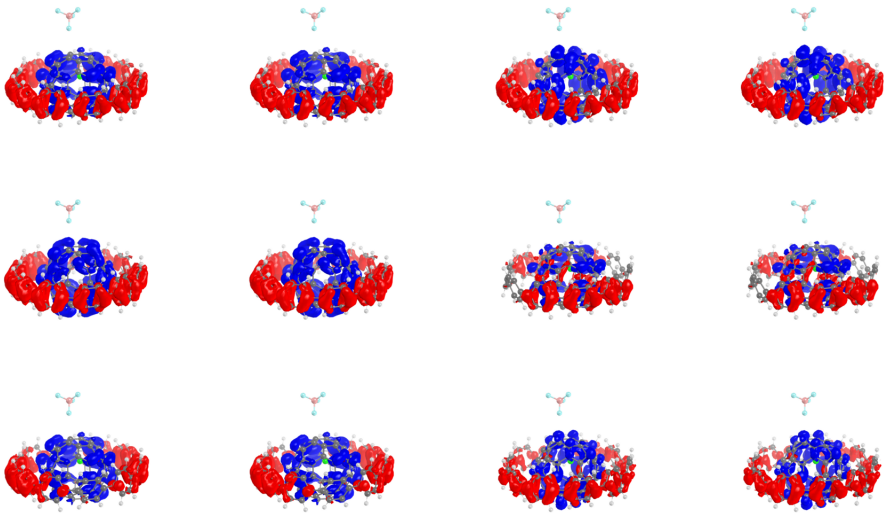


Figure S27. Difference density between the excited state and the ground state for the first 12 transitions (from left to rigth and top to bottom) in $Li^+@C_{60}\cdots$[10]CPP$\cdots BF_4^-$. CAM-B3LYP/TZVP level, using the B97-D2/def2-TZVP geometry.

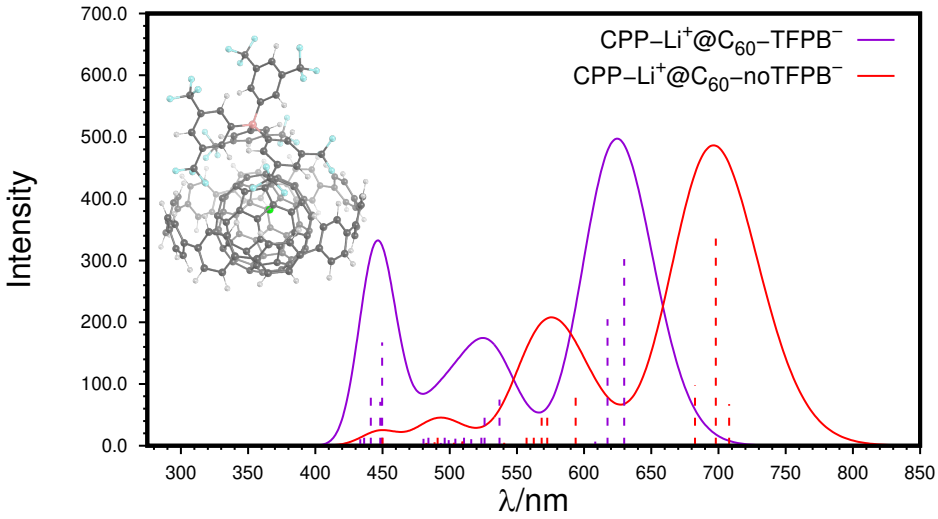


Figure S28. Absorption spectra for the $Li^{+}@C_{60}\cdots$[10]CPP$\cdots TFPB^{-}$ complex obtained at the CAM-B3LYP/def2-SVP level, using the B97-D2/def2-SVP geometry. The red line corresponds to the complex without the anion but keeping the same geometry for the rest of the complex.

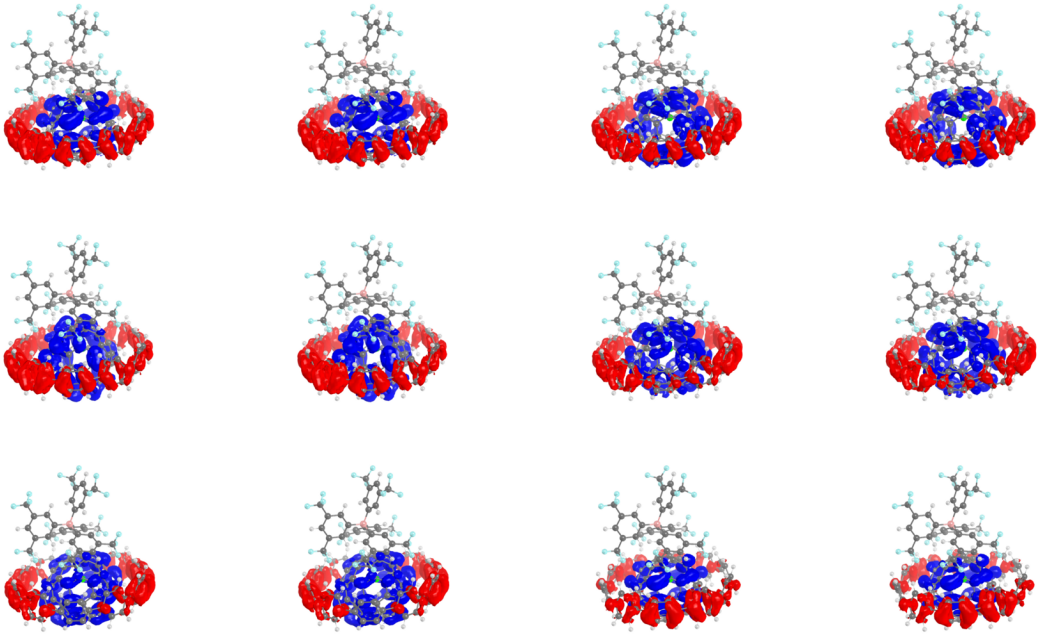


Figure S29. Difference density between the excited state and the ground state for the first 12 transitions (from left to right and top to bottom) in $Li^{+}@C_{60}\cdots$[10]CPP$\cdots TFPB^{-}$. CAM-B3LYP/def2-SVP level, using the B97-D2/def2-SVP geometry.

Geometry of the optimised complexes

$Li^+@C_{60}(5)\cdots[10]CPP$ (B97-D2)

C	0.789122	0.936151	3.327634
C	-0.662476	0.930001	3.356485
C	-1.106487	-0.451235	3.333885
C	0.070175	-1.299142	3.292589
C	1.242014	-0.441989	3.288098
C	2.355177	-0.789818	2.517014
C	2.342576	-2.009340	1.728536
C	1.216098	-2.837564	1.738190
C	0.057600	-2.472499	2.533001
C	0.741285	-3.430097	0.502394
C	1.413690	-3.173556	-0.694348
C	2.586408	-2.318488	-0.703964
C	3.042154	-1.744706	0.484921
C	0.656182	-2.911688	-1.903051
C	1.362160	-1.895272	-2.661573
C	2.555293	-1.528074	-1.919742
C	2.980422	-0.196066	-1.900595
C	2.232099	0.815947	-2.625335
C	1.088072	0.460433	-3.345691
C	0.644359	-0.921484	-3.362277
C	2.246594	2.035243	-1.836725
C	1.114226	2.854649	-1.794341
C	-0.076412	2.480609	-2.536308
C	-0.088790	1.308582	-3.298221
C	-0.806713	-0.926906	-3.324361
C	-1.259485	0.450811	-3.284779
C	-2.378847	0.798333	-2.520254
C	-2.365521	2.015444	-1.732096
C	-1.234361	2.839787	-1.738601
C	-1.488999	-1.908889	-2.597696
C	-0.743283	-2.919982	-1.873189
C	-3.066282	1.751577	-0.490473
C	-3.530802	0.372838	-0.510961
C	-3.100069	-0.220626	-1.771357
C	-2.660348	-1.555385	-1.809103
C	-2.601053	2.322900	0.697454
C	-1.432618	3.183425	0.691177
C	-0.759304	3.437271	-0.505251
C	0.691332	3.445872	-0.539412
C	3.456265	0.398548	-0.665935
C	3.003282	1.776155	-0.626511
C	2.594981	2.345824	0.581705
C	1.418543	3.193602	0.625909
C	3.485913	-0.363464	0.504514
C	-2.633441	-2.351512	-0.588522
C	-3.049780	-1.781039	0.626804
C	-3.506419	-0.395084	0.666345
C	-0.709577	-3.431202	0.533128
C	-1.442451	-3.186260	-0.631139
C	-2.570011	1.531732	1.912025
C	-3.006406	0.201697	1.896397
C	0.719616	2.928132	1.869523
C	-0.678228	2.925494	1.902849
C	-1.132892	-2.839033	1.787111
C	-2.272878	-2.027750	1.832591
C	-1.381251	1.904675	2.658309
C	-2.255712	-0.808636	2.618404
C	3.061918	0.227368	1.759610
C	2.625374	1.555402	1.797637
C	1.466254	1.915142	2.594404
Li	-1.343215	-0.422583	-0.197344
C	6.656333	-2.896360	0.899858
C	7.083002	-1.573045	0.913153
C	6.890569	-0.736066	-0.204144
C	6.425619	-1.338809	-1.388280
C	5.999819	-2.660516	-1.401670
C	6.018432	-3.442843	-0.231547
C	6.887344	0.734737	-0.096688
C	7.020167	1.573233	-1.221316
C	6.473545	1.333889	1.108034
C	6.585577	2.893570	-1.186956
C	6.038715	2.652232	1.142093
C	5.997388	3.435846	-0.026667
C	5.154772	-4.635453	-0.150782
C	4.460148	-4.899563	1.044760
C	4.779970	-5.374116	-1.290847
C	3.334842	-5.713227	1.056707
C	3.653366	-6.189014	-1.278912
C	2.850322	-6.302686	-0.126343
C	1.446647	-6.751157	-0.184376
C	0.738660	-7.163654	0.962296
C	0.697002	-6.517197	-1.352893
C	-0.651621	-7.159233	0.987915
C	-0.691336	-6.513036	-1.327516
C	-1.399041	-6.743353	-0.132381
C	5.126651	4.625581	-0.066243
C	4.790923	5.353483	1.092826
C	4.388736	4.899340	-1.233400
C	3.664609	6.168323	1.127861
C	3.263898	5.712817	-1.198419
C	2.821555	6.293534	0.005376
C	1.422656	6.747753	0.115605
C	0.674462	7.162344	-1.004612
C	0.715314	6.518895	1.311218
C	-0.715776	7.163970	-0.979288
C	-0.673134	6.521494	1.336971
C	-1.423305	6.752939	0.168269
C	-2.798366	-6.290573	-0.022592
C	-3.640485	-6.163637	-1.145730
C	-3.245487	-5.716510	1.182800
C	-4.768332	-5.350969	-1.109983
C	-4.372556	-4.906063	1.218939
C	-5.108546	-4.628064	0.051187
C	-5.981658	-3.439991	0.013703
C	-6.560548	-2.892921	1.176648
C	-6.037065	-2.660905	-1.157916
C	-6.995756	-1.572590	1.209773

C	-6.472366	-1.342718	-1.125075
C	-6.873263	-0.737091	0.081243
C	-2.826324	6.302023	0.111016
C	-3.627644	6.182837	1.264428
C	-3.314251	5.717777	-1.073360
C	-4.753103	5.366270	1.275699
C	-4.439037	4.903324	-1.062648
C	-5.131163	4.632803	0.133192
C	-5.996014	3.440867	0.210642
C	-6.625345	2.891046	-0.924330
C	-5.993022	2.662408	1.383893
C	-7.054185	1.568437	-0.937474
C	-6.422342	1.341707	1.371235
C	-6.875213	0.734122	0.184425
H	6.768638	-3.500953	1.796654
H	7.521980	-1.164499	1.820177
H	6.277119	-0.730532	-2.276369
H	5.529598	-3.051463	-2.299999
H	7.418570	1.168108	-2.148394
H	6.371123	0.724381	2.001817
H	6.652374	3.498769	-2.087808
H	5.607966	3.038246	2.062006
H	4.728043	-4.361216	1.949885
H	5.347528	-5.263982	-2.211688
H	2.753082	-5.789487	1.971345
H	3.359424	-6.703259	-2.190772
H	1.285859	-7.439032	1.860559
H	1.205708	-6.212517	-2.263461
H	-1.166487	-7.432690	1.905686
H	-1.230286	-6.205795	-2.219639
H	5.389964	5.236022	1.992549
H	4.623473	4.369332	-2.152442
H	3.403675	6.673884	2.054501
H	2.650561	5.796178	-2.091461
H	1.189075	7.434368	-1.922882
H	1.254761	6.211570	2.202906
H	-1.262962	7.437177	-1.878296
H	-1.180374	6.216324	2.248209
H	-3.377817	-6.666581	-2.073146
H	-2.635447	-5.804701	2.077669
H	-5.366602	-5.233733	-2.010226
H	-4.611953	-4.383884	2.141374
H	-6.620841	-3.494270	2.080456
H	-5.619155	-3.051173	-2.081923
H	-7.387789	-1.166008	2.138866
H	-6.382731	-0.738934	-2.024110
H	-3.332736	6.693652	2.177864
H	-2.735562	5.799454	-1.989394
H	-5.318382	5.253120	2.197685
H	-4.708988	4.371117	-1.970767
H	-6.729880	3.492601	-1.823974
H	-5.533934	3.055603	2.286950
H	-7.486830	1.159474	-1.847317
H	-6.287504	0.738685	2.265073

$Li^+@C_{60}$(6)···[10]CPP (B97-D2)

C	-1.465567	0.437793	-3.222626
C	-0.721689	1.675125	-3.067719
C	-1.425844	2.504286	-2.105652
C	-2.604312	1.779560	-1.666566
C	-2.628135	0.501945	-2.356960
C	-3.061880	-0.646960	-1.688166
C	-3.490004	-0.563275	-0.305297
C	-3.465655	0.665348	0.357401
C	-3.015176	1.858745	-0.333971
C	-2.996966	0.737638	1.727874
C	-2.575337	-0.422125	2.385445
C	-2.602280	-1.699524	1.695081
C	-3.049616	-1.767283	0.373915
C	-1.386038	-0.386356	3.215932
C	-0.676466	-1.639691	3.038784
C	-1.428076	-2.451537	2.099433
C	-0.751230	-3.249891	1.172694
C	0.700809	-3.263004	1.151988
C	1.427700	-2.487808	2.062412
C	0.723304	-1.658429	3.022185
C	1.129977	-3.345330	-0.229494
C	2.269241	-2.652229	-0.651675
C	3.037896	-1.855020	0.291567
C	2.620935	-1.773642	1.631139
C	1.466784	-0.423076	3.178356
C	2.643104	-0.488870	2.324153
C	3.079657	0.666149	1.651827
C	3.512577	0.581960	0.263006
C	3.491911	-0.654751	-0.403779
C	0.780551	0.786200	3.342338
C	-0.670333	0.806191	3.366819
C	3.052092	1.783510	-0.416590
C	2.347662	2.609493	0.543894
C	2.358829	1.918985	1.819032
C	1.234377	1.978042	2.650642
C	2.595035	1.713191	-1.735337
C	2.568100	0.436258	-2.424963
C	3.000059	-0.723392	-1.771318
C	2.257499	-1.959001	-1.926105
C	-1.220658	-3.323987	-0.196932
C	-0.058040	-3.383099	-1.063464
C	-0.066757	-2.717830	-2.291431
C	1.110570	-1.989944	-2.728406
C	-2.346551	-2.595206	-0.588049
C	0.063777	2.735925	2.247519
C	0.054825	3.398669	1.017886
C	1.217216	3.333627	0.151795
C	-2.255796	1.975728	1.883745
C	-1.113811	2.010543	2.689721
C	1.425158	2.469136	-2.145915
C	0.747349	3.264675	-1.217849
C	0.666605	-0.788627	-3.410281
C	1.382993	0.403409	-3.261900
C	-2.265496	2.668299	0.607300

C	-1.133255	3.368750	0.183951
C	0.676356	1.659299	-3.089452
C	-0.704593	3.286370	-1.198350
C	-2.356448	-1.902528	-1.864263
C	-1.238474	-1.964211	-2.701957
C	-0.784718	-0.772214	-3.393779
Li	1.323219	-0.268064	0.381182
C	6.528069	-2.879601	1.085571
C	6.956133	-1.558192	1.081246
C	6.818010	-0.750463	-0.066894
C	6.412736	-1.391819	-1.254463
C	5.986782	-2.714920	-1.250396
C	5.940891	-3.460810	-0.058001
C	6.815526	0.722248	0.002865
C	6.939188	1.531403	-1.145611
C	6.419745	1.361239	1.195003
C	6.507726	2.851871	-1.143934
C	5.990237	2.682862	1.196757
C	5.931068	3.430740	0.006166
C	5.082067	-4.657580	0.021382
C	4.362513	-4.910026	1.204901
C	4.743711	-5.421693	-1.113774
C	3.249515	-5.739463	1.205454
C	3.631067	-6.255428	-1.112291
C	2.802367	-6.359966	0.022840
C	1.408273	-6.835375	-0.054805
C	0.684021	-7.227962	1.089370
C	0.677665	-6.640183	-1.242012
C	-0.705610	-7.224358	1.093991
C	-0.712107	-6.635164	-1.236904
C	-1.435634	-6.825678	-0.044493
C	5.072042	4.628177	-0.061355
C	4.738552	5.383011	1.081723
C	4.348955	4.892906	-1.239935
C	3.627596	6.218611	1.091818
C	3.237642	5.724584	-1.228945
C	2.795015	6.335409	-0.039409
C	1.403493	6.817001	0.047745
C	0.673712	7.213813	-1.091484
C	0.679251	6.627614	1.239915
C	-0.715931	7.221225	-1.086347
C	-0.710546	6.634213	1.244815
C	-1.441373	6.830331	0.057710
C	-2.826466	-6.342498	0.044001
C	-3.661222	-6.228249	-1.085486
C	-3.261955	-5.723497	1.231779
C	-4.769761	-5.389284	-1.075650
C	-4.370233	-4.887857	1.242168
C	-5.096631	-4.627680	0.064755
C	-5.954858	-3.429984	-0.004587
C	-6.535938	-2.853517	1.144047
C	-6.006964	-2.680567	-1.194393
C	-6.969696	-1.533879	1.144741
C	-6.438458	-1.359737	-1.193340
C	-6.841961	-0.723897	-0.002663
C	-2.837023	6.359471	-0.019763
C	-3.663371	6.252249	1.116662
C	-3.286654	5.742618	-1.203269
C	-4.776692	5.419526	1.117541
C	-4.399791	4.913362	-1.202908
C	-5.116626	4.657525	-0.018647
C	-5.973442	3.459371	0.060801
C	-6.563362	2.879576	-1.081609
C	-6.011502	2.710700	1.251760
C	-6.989928	1.557590	-1.077548
C	-6.436452	1.387644	1.255559
C	-6.846873	0.748952	0.068941
H	6.601607	-3.457968	2.003169
H	7.357751	-1.129127	1.995809
H	6.312568	-0.815102	-2.169635
H	5.564734	-3.131494	-2.161015
H	7.331598	1.104198	-2.065038
H	6.330863	0.783473	2.110720
H	6.570102	3.430744	-2.061989
H	5.577090	3.097015	2.112460
H	4.601193	-4.354189	2.107471
H	5.331041	-5.321559	-2.023290
H	2.648019	-5.808433	2.107616
H	3.367381	-6.791538	-2.020739
H	1.217839	-7.482131	2.001834
H	1.199181	-6.357271	-2.152518
H	-1.234670	-7.475897	2.009847
H	-1.238219	-6.348223	-2.143383
H	5.329135	5.274851	1.988156
H	4.582049	4.344347	-2.148318
H	3.369024	6.747151	2.006112
H	2.633254	5.801466	-2.128355
H	1.202492	7.463170	-2.008136
H	1.204215	6.340974	2.147170
H	-1.249111	7.475363	-1.999071
H	-1.232400	6.351616	2.155127
H	-3.406454	-6.761479	-1.998224
H	-2.654144	-5.797684	2.129208
H	-5.363004	-5.282436	-1.980479
H	-4.598481	-4.332485	2.147557
H	-6.599934	-3.433501	2.061355
H	-5.584297	-3.091954	-2.107061
H	-7.365451	-1.106977	2.062865
H	-6.340647	-0.778959	-2.106113
H	-3.397451	6.784800	2.026600
H	-2.685783	5.811111	-2.105839
H	-5.362148	5.316468	2.027876
H	-4.638035	4.357392	-2.105323
H	-6.638639	3.458469	-1.998750
H	-5.582548	3.124831	2.160237
H	-7.391653	1.127979	-1.991845
H	-6.327583	0.807997	2.167858

$Li^+@C_{60}$(5)···[10]CPP (TPSS-D3(BJ))

C	0.792314	0.938097	3.329556
C	-0.660672	0.933825	3.361660
C	-1.105967	-0.450064	3.344868
C	0.072431	-1.300217	3.298943
C	1.245137	-0.441858	3.290806
C	2.357067	-0.789975	2.520814
C	2.344254	-2.011510	1.732137
C	1.219861	-2.839624	1.743688
C	0.060518	-2.474874	2.541874
C	0.744564	-3.435303	0.505684
C	1.415417	-3.178750	-0.692197
C	2.588683	-2.321174	-0.702272
C	3.044366	-1.747501	0.485801
C	0.658712	-2.919824	-1.906442
C	1.364172	-1.898910	-2.665153
C	2.557770	-1.530406	-1.920797
C	2.983248	-0.200161	-1.902404
C	2.234677	0.813031	-2.628768
C	1.092378	0.458478	-3.349419
C	0.648171	-0.925350	-3.366967
C	2.249447	2.034092	-1.839625
C	1.118792	2.852976	-1.797869
C	-0.073189	2.480598	-2.542303
C	-0.085143	1.309193	-3.304209
C	-0.805095	-0.931044	-3.332971
C	-1.258763	0.451713	-3.294138
C	-2.377562	0.805915	-2.531978
C	-2.367481	2.027684	-1.741488
C	-1.233365	2.845689	-1.744914
C	-1.484350	-1.916824	-2.608316
C	-0.739687	-2.933475	-1.880428
C	-3.066251	1.765616	-0.492634
C	-3.506877	0.377712	-0.508194
C	-3.081590	-0.216353	-1.768618
C	-2.644368	-1.549977	-1.806089
C	-2.602654	2.331687	0.699116
C	-1.429567	3.189656	0.691248
C	-0.756913	3.440638	-0.506837
C	0.695564	3.445777	-0.540745
C	3.460634	0.395644	-0.665847
C	3.007519	1.775141	-0.627133
C	2.599949	2.344856	0.580353
C	1.422052	3.194046	0.624064
C	3.489828	-0.364746	0.504583
C	-2.614716	-2.343117	-0.584405
C	-3.024351	-1.770245	0.629213
C	-3.478164	-0.386907	0.667961
C	-0.708572	-3.440080	0.537549
C	-1.437224	-3.199118	-0.631592
C	-2.571547	1.538813	1.919964
C	-3.004736	0.208286	1.910415
C	0.722598	2.929641	1.870460
C	-0.673409	2.929632	1.905173
C	-1.132635	-2.845371	1.797208
C	-2.269571	-2.031125	1.847635
C	-1.378430	1.909759	2.664738
C	-2.257261	-0.808030	2.636334
C	3.065508	0.227557	1.761779
C	2.629990	1.554235	1.798960
C	1.469392	1.915176	2.596683
Li	-1.340981	-0.431573	-0.242626
C	6.636401	-2.889686	0.905516
C	7.062677	-1.567627	0.918802
C	6.881354	-0.735008	-0.200784
C	6.426013	-1.339968	-1.384977
C	6.000402	-2.660372	-1.398340
C	6.009880	-3.438890	-0.228120
C	6.878219	0.736366	-0.099418
C	7.001151	1.570489	-1.225661
C	6.473109	1.337662	1.104701
C	6.567170	2.889647	-1.191500
C	6.039295	2.654943	1.138688
C	5.990170	3.434614	-0.029751
C	5.145671	-4.631594	-0.153704
C	4.456556	-4.902579	1.040976
C	4.765184	-5.360354	-1.295508
C	3.332610	-5.715725	1.052491
C	3.639552	-6.174354	-1.284120
C	2.844061	-6.297300	-0.130150
C	1.440678	-6.747250	-0.182195
C	0.734554	-7.149392	0.966425
C	0.691741	-6.522584	-1.350326
C	-0.654365	-7.147107	0.992113
C	-0.695269	-6.521163	-1.325009
C	-1.401348	-6.744250	-0.130191
C	5.119352	4.624336	-0.063690
C	4.778936	5.343426	1.096671
C	4.385986	4.902704	-1.230005
C	3.653587	6.157211	1.132027
C	3.262188	5.715196	-1.194698
C	2.817165	6.289600	0.008466
C	1.417961	6.743357	0.113481
C	0.670660	7.147012	-1.008287
C	0.712268	6.521454	1.308645
C	-0.718187	7.148962	-0.982405
C	-0.674629	6.523966	1.334803
C	-1.424000	6.748660	0.167005
C	-2.800978	-6.291607	-0.025817
C	-3.636073	-6.156089	-1.150254
C	-3.250253	-5.722986	1.178711
C	-4.761581	-5.342367	-1.114522
C	-4.374590	-4.911123	1.214741
C	-5.105248	-4.627327	0.047712
C	-5.976986	-3.438059	0.015779
C	-6.545221	-2.888328	1.179883
C	-6.039156	-2.662659	-1.155243
C	-6.979122	-1.568955	1.212900
C	-6.472397	-1.345046	-1.122262
C	-6.865044	-0.737607	0.083280
C	-2.827296	6.298182	0.115724

C	-3.620868	6.169781	1.270539
C	-3.319799	5.722614	-1.068295
C	-4.745982	5.354980	1.281090
C	-4.444038	4.909853	-1.058223
C	-5.130633	4.632530	0.136624
C	-5.995145	3.439731	0.207726
C	-6.612740	2.886566	-0.929217
C	-5.998480	2.664378	1.380346
C	-7.038490	1.564266	-0.942624
C	-6.424245	1.344020	1.367298
C	-6.867753	0.734141	0.180788
H	6.748318	-3.491075	1.803275
H	7.499254	-1.161368	1.826766
H	6.285528	-0.734255	-2.275030
H	5.537692	-3.053686	-2.298392
H	7.397671	1.167663	-2.153327
H	6.377263	0.730546	1.999733
H	6.633296	3.491768	-2.093237
H	5.615766	3.043862	2.059611
H	4.728545	-4.370463	1.947490
H	5.329901	-5.250775	-2.216956
H	2.754969	-5.798858	1.968093
H	3.346937	-6.685202	-2.197096
H	1.279515	-7.421768	1.865730
H	1.199927	-6.223343	-2.261952
H	-1.166131	-7.418149	1.911157
H	-1.235203	-6.221870	-2.218260
H	5.375623	5.226814	1.996847
H	4.624218	4.377372	-2.149815
H	3.394149	6.660259	2.059218
H	2.651585	5.803799	-2.088034
H	1.182458	7.416870	-1.927580
H	1.252557	6.220332	2.200923
H	-1.263012	7.420733	-1.882048
H	-1.181840	6.224858	2.246990
H	-3.375361	-6.656656	-2.078347
H	-2.643270	-5.817233	2.074016
H	-5.356931	-5.224759	-2.015469
H	-4.616895	-4.393093	2.137753
H	-6.605758	-3.487008	2.084242
H	-5.629809	-3.056767	-2.080496
H	-7.369866	-1.164556	2.142236
H	-6.389961	-0.743525	-2.022485
H	-3.326230	6.675824	2.185391
H	-2.745081	5.810878	-1.985164
H	-5.307516	5.241339	2.204004
H	-4.718953	4.384585	-1.967870
H	-6.718130	3.484889	-1.829678
H	-5.547525	3.060900	2.284899
H	-7.468392	1.156799	-1.853204
H	-6.295773	0.743221	2.262551

$Li^+@C_{60}$(6)···[10]CPP (TPSS-D3(BJ))

C	-1.463860	0.437783	-3.224552
C	-0.719738	1.676673	-3.069311
C	-1.424625	2.506219	-2.105413
C	-2.604624	1.780204	-1.666177
C	-2.628214	0.501578	-2.358276
C	-3.061990	-0.646105	-1.690915
C	-3.491762	-0.563044	-0.305571
C	-3.467544	0.663667	0.357681
C	-3.015667	1.858834	-0.334729
C	-2.997364	0.735289	1.730675
C	-2.575982	-0.423228	2.387295
C	-2.602895	-1.701812	1.695202
C	-3.049801	-1.768827	0.374868
C	-1.386727	-0.387747	3.220967
C	-0.678215	-1.645211	3.046352
C	-1.428784	-2.456701	2.101334
C	-0.753340	-3.255558	1.174280
C	0.701207	-3.273031	1.154958
C	1.423392	-2.498864	2.070470
C	0.720268	-1.667282	3.036095
C	1.132168	-3.355365	-0.233042
C	2.269616	-2.663438	-0.661063
C	3.017244	-1.848557	0.287056
C	2.603714	-1.769097	1.625482
C	1.462520	-0.425764	3.191768
C	2.627594	-0.486879	2.319478
C	3.063312	0.667000	1.648595
C	3.493890	0.583535	0.259722
C	3.469952	-0.649881	-0.407032
C	0.780304	0.786088	3.352747
C	-0.672653	0.804903	3.373225
C	3.056857	1.795613	-0.420575
C	2.353508	2.623779	0.547184
C	2.360207	1.930272	1.826954
C	1.235999	1.982711	2.659569
C	2.600873	1.719273	-1.739995
C	2.573781	0.438126	-2.433221
C	3.003320	-0.724821	-1.784732
C	2.262918	-1.967283	-1.939785
C	-1.222562	-3.327343	-0.199316
C	-0.058459	-3.388317	-1.068690
C	-0.065793	-2.721212	-2.295517
C	1.113829	-1.993801	-2.736921
C	-2.346052	-2.597576	-0.589888
C	0.062873	2.739388	2.253189
C	0.055194	3.401120	1.023213
C	1.220426	3.341238	0.154473
C	-2.255647	1.975203	1.887554
C	-1.116003	2.010784	2.694186
C	1.426908	2.474296	-2.148760
C	0.749783	3.268272	-1.219104
C	0.669119	-0.787391	-3.415390
C	1.384590	0.404743	-3.268350
C	-2.264949	2.669085	0.609244
C	-1.133866	3.368933	0.186612
C	0.676558	1.661997	-3.092926
C	-0.704293	3.287277	-1.198612
C	-2.355192	-1.903186	-1.867693

C	-1.238123	-1.964334	-2.704230
C	-0.783583	-0.770567	-3.396007
Li	1.323020	-0.263614	0.425505
C	6.511065	-2.874596	1.089410
C	6.935615	-1.553407	1.084781
C	6.805129	-0.750737	-0.064707
C	6.409384	-1.394227	-1.251532
C	5.987057	-2.717178	-1.247329
C	5.935926	-3.459444	-0.055384
C	6.802281	0.722053	-0.000651
C	6.917174	1.526336	-1.150397
C	6.416805	1.363026	1.191085
C	6.489274	2.846555	-1.148343
C	5.990804	2.684537	1.193362
C	5.925550	3.429045	0.003334
C	5.079581	-4.658011	0.019119
C	4.365967	-4.916799	1.202292
C	4.736275	-5.413167	-1.117641
C	3.253929	-5.745382	1.202196
C	3.624258	-6.245251	-1.116879
C	2.802409	-6.357329	0.019433
C	1.407650	-6.830766	-0.052921
C	0.684763	-7.211914	1.093053
C	0.677867	-6.643250	-1.239128
C	-0.703386	-7.206996	1.098399
C	-0.710547	-6.637453	-1.233457
C	-1.432497	-6.819095	-0.041463
C	5.069102	4.628350	-0.059457
C	4.730358	5.374328	1.084907
C	4.352464	4.899445	-1.237990
C	3.620609	6.209196	1.094764
C	3.242457	5.730752	-1.227232
C	2.795291	6.333513	-0.037894
C	1.403038	6.813151	0.044176
C	0.673851	7.198588	-1.096393
C	0.680308	6.631385	1.235816
C	-0.714342	7.205036	-1.090928
C	-0.708137	6.637112	1.241054
C	-1.438129	6.824570	0.054809
C	-2.823702	-6.337125	0.041965
C	-3.651934	-6.217145	-1.088667
C	-3.262978	-5.724803	1.229132
C	-4.760161	-5.380211	-1.079062
C	-4.370847	-4.890790	1.239288
C	-5.092277	-4.626720	0.062191
C	-5.949671	-3.428450	-0.002612
C	-6.517656	-2.848385	1.147802
C	-6.009277	-2.683105	-1.192050
C	-6.947719	-1.529015	1.149003
C	-6.436953	-1.362247	-1.190353
C	-6.829039	-0.724038	0.000185
C	-2.833978	6.354299	-0.017333
C	-3.654199	6.241171	1.119945
C	-3.286840	5.743970	-1.200280
C	-4.767066	5.410251	1.120559
C	-4.399367	4.916035	-1.200206
C	-5.111497	4.656136	-0.016535
C	-5.967158	3.457149	0.058305
C	-6.544977	2.874013	-1.085612
C	-6.011608	2.712371	1.248890
C	-6.968408	1.552465	-1.081646
C	-6.433047	1.389435	1.252387
C	-6.833626	0.748682	0.066211
H	6.584906	-3.449538	2.007954
H	7.333419	-1.124621	1.999966
H	6.316910	-0.820061	-2.168234
H	5.574041	-3.137589	-2.159312
H	7.304811	1.099667	-2.070872
H	6.336570	0.787247	2.107977
H	6.551019	3.422187	-2.067263
H	5.587682	3.102623	2.110771
H	4.609566	-4.367175	2.106477
H	5.320513	-5.313036	-2.027944
H	2.656349	-5.820942	2.105429
H	3.361670	-6.777394	-2.026701
H	1.216210	-7.465350	2.005930
H	1.198645	-6.368194	-2.151440
H	-1.229538	-7.456604	2.015296
H	-1.236509	-6.358020	-2.141340
H	5.317065	5.265703	1.992619
H	4.590603	4.356743	-2.147641
H	3.362995	6.734467	2.009981
H	2.642634	5.814524	-2.128153
H	1.199625	7.446777	-2.013934
H	1.205394	6.352927	2.144536
H	-1.245308	7.457563	-2.004211
H	-1.229263	6.362274	2.153138
H	-3.398267	-6.747856	-2.001883
H	-2.658576	-5.803750	2.127503
H	-5.350366	-5.274727	-1.984831
H	-4.603614	-4.340035	2.145366
H	-6.581315	-3.425233	2.065910
H	-5.597086	-3.098350	-2.106720
H	-7.338848	-1.102777	2.068201
H	-6.347976	-0.783937	-2.104657
H	-3.390139	6.771494	2.030489
H	-2.689056	5.817529	-2.103521
H	-5.350155	5.308657	2.031391
H	-4.641611	4.364568	-2.103319
H	-6.620534	3.449791	-2.003481
H	-5.591722	3.130110	2.158911
H	-7.366730	1.123714	-1.996583
H	-6.331901	0.812133	2.166090

$Na^+@C_{60}$(5)···[10]CPP (B97-D2)

C	0.781306	0.932724	3.323761
C	-0.670305	0.925645	3.351558
C	-1.114849	-0.455026	3.328462
C	0.062337	-1.301776	3.288053
C	1.234474	-0.445031	3.284302
C	2.348816	-0.792189	2.514257

C	2.336675	-2.011239	1.725309
C	1.209027	-2.838316	1.733340
C	0.049620	-2.474026	2.527403
C	0.734503	-3.431291	0.498070
C	1.407782	-3.174812	-0.697892
C	2.579999	-2.319571	-0.706777
C	3.036921	-1.746468	0.482298
C	0.650584	-2.913278	-1.906955
C	1.356766	-1.896636	-2.665015
C	2.549217	-1.528808	-1.922511
C	2.975322	-0.197011	-1.903161
C	2.226828	0.814923	-2.627546
C	1.081911	0.458913	-3.346825
C	0.638336	-0.922757	-3.364685
C	2.240668	2.033966	-1.838769
C	1.107416	2.852180	-1.796308
C	-0.083136	2.478434	-2.538389
C	-0.095537	1.306170	-3.299451
C	-0.812888	-0.928402	-3.327770
C	-1.266313	0.448618	-3.287146
C	-2.385157	0.794385	-2.521706
C	-2.372092	2.011194	-1.733881
C	-1.241619	2.835972	-1.740788
C	-1.494248	-1.908299	-2.599454
C	-0.748256	-2.919923	-1.876033
C	-3.075573	1.746762	-0.493046
C	-3.535014	0.367779	-0.513217
C	-3.100672	-0.222983	-1.769280
C	-2.658643	-1.551330	-1.806000
C	-2.610127	2.317728	0.694120
C	-1.440473	3.177225	0.687793
C	-0.766396	3.432879	-0.507641
C	0.683928	3.442575	-0.541160
C	3.451058	0.397198	-0.668082
C	2.997374	1.774753	-0.628312
C	2.589088	2.344338	0.579974
C	1.411720	3.191348	0.624006
C	3.480834	-0.365119	0.502177
C	-2.631596	-2.344111	-0.589533
C	-3.051566	-1.778806	0.620916
C	-3.512227	-0.398287	0.661440
C	-0.716376	-3.433167	0.529290
C	-1.447955	-3.185311	-0.633980
C	-2.580094	1.526911	1.908457
C	-3.019145	0.197691	1.893432
C	0.712421	2.924676	1.866902
C	-0.685868	2.919451	1.898499
C	-1.141047	-2.841500	1.782482
C	-2.281583	-2.031042	1.827880
C	-1.389530	1.898874	2.653135
C	-2.264900	-0.812262	2.614272
C	3.056037	0.225320	1.757447
C	2.619304	1.553527	1.795864
C	1.459286	1.912452	2.592157
Na	-0.908390	-0.189373	-0.011867
C	6.660943	-2.897716	0.897885
C	7.088235	-1.574645	0.909585
C	6.892785	-0.737831	-0.207303
C	6.424878	-1.340229	-1.390444
C	5.998919	-2.662048	-1.402385
C	6.020056	-3.443960	-0.231966
C	6.888628	0.732711	-0.098665
C	7.021982	1.572879	-1.221914
C	6.473185	1.329462	1.106694
C	6.586622	2.892910	-1.185481
C	6.036976	2.647335	1.142778
C	5.996649	3.432708	-0.024872
C	5.156469	-4.636368	-0.149363
C	4.461615	-4.898538	1.046536
C	4.781987	-5.376662	-1.288407
C	3.335712	-5.711610	1.059379
C	3.655101	-6.191110	-1.275437
C	2.851133	-6.302162	-0.123174
C	1.447092	-6.749809	-0.182024
C	0.737548	-7.161850	0.963770
C	0.698854	-6.515779	-1.351483
C	-0.652802	-7.157993	0.986897
C	-0.689666	-6.511264	-1.328285
C	-1.399065	-6.741773	-0.134158
C	5.125349	4.621965	-0.064105
C	4.789954	5.350838	1.094476
C	4.387238	4.894635	-1.231402
C	3.663915	6.166255	1.128818
C	3.262663	5.708525	-1.197082
C	2.820657	6.290441	0.006302
C	1.421699	6.744842	0.116067
C	0.674055	7.159179	-1.004572
C	0.713594	6.516039	1.311252
C	-0.716286	7.160444	-0.980331
C	-0.674852	6.518216	1.335816
C	-1.424478	6.749210	0.166696
C	-2.798687	-6.289331	-0.025330
C	-3.640335	-6.161464	-1.148725
C	-3.246305	-5.715925	1.180245
C	-4.768883	-5.349578	-1.112373
C	-4.373253	-4.905503	1.216695
C	-5.109714	-4.627663	0.049265
C	-5.983739	-3.440167	0.013095
C	-6.561996	-2.894287	1.176964
C	-6.039868	-2.659969	-1.157644
C	-6.997057	-1.573990	1.212041
C	-6.475642	-1.342069	-1.123022
C	-6.875928	-0.737769	0.084091
C	-2.827970	6.299419	0.108915
C	-3.629390	6.180518	1.262236
C	-3.316892	5.716415	-1.075721
C	-4.755790	5.365370	1.273112
C	-4.442263	4.902764	-1.065078
C	-5.134184	4.631962	0.130723
C	-5.999038	3.440067	0.209213
C	-6.627905	2.888654	-0.925033
C	-5.995748	2.663093	1.383415

C	-7.057683	1.566367	-0.935530
C	-6.424505	1.342354	1.372836
C	-6.878181	0.733394	0.187194
H	6.774774	-3.501991	1.794709
H	7.529791	-1.165538	1.815128
H	6.274501	-0.731906	-2.278297
H	5.526914	-3.053689	-2.299472
H	7.421573	1.169285	-2.149183
H	6.371304	0.717959	1.999173
H	6.654140	3.500057	-2.084987
H	5.604954	3.031415	2.062972
H	4.730243	-4.359195	1.950910
H	5.349984	-5.268137	-2.209224
H	2.753977	-5.786847	1.974168
H	3.361553	-6.706905	-2.186509
H	1.283354	-7.436836	1.863105
H	1.209064	-6.211495	-2.261352
H	-1.169220	-7.432243	1.903544
H	-1.227094	-6.203661	-2.221323
H	5.389382	5.234162	1.994056
H	4.621921	4.363619	-2.149896
H	3.403463	6.673709	2.054585
H	2.649789	5.792157	-2.090374
H	1.189314	7.431919	-1.922262
H	1.252610	6.210164	2.203869
H	-1.262877	7.433756	-1.879663
H	-1.182886	6.214321	2.247023
H	-3.377098	-6.663396	-2.076649
H	-2.636442	-5.804624	2.075161
H	-5.366987	-5.231850	-2.012703
H	-4.611678	-4.382519	2.138889
H	-6.621271	-3.496495	2.080212
H	-5.621185	-3.048173	-2.082174
H	-7.387885	-1.168006	2.141954
H	-6.385909	-0.737163	-2.021175
H	-3.334393	6.690572	2.175948
H	-2.738936	5.798685	-1.992169
H	-5.321362	5.252912	2.194845
H	-4.713111	4.371322	-1.973357
H	-6.731462	3.488084	-1.826228
H	-5.536588	3.057888	2.285689
H	-7.490457	1.155929	-1.844540
H	-6.288046	0.740266	2.267069

$Na^{+}@C_{60}$(6)···[10]CPP (B97-D2)

C	-1.457537	0.437108	-3.218537
C	-0.712377	1.673103	-3.062346
C	-1.416611	2.503361	-2.101721
C	-2.596480	1.780066	-1.663572
C	-2.621029	0.502304	-2.354007
C	-3.055724	-0.646235	-1.685235
C	-3.484771	-0.562222	-0.302442
C	-3.459999	0.666527	0.360235
C	-3.007709	1.859487	-0.331038
C	-2.991430	0.738577	1.730898
C	-2.569425	-0.421537	2.388197
C	-2.597066	-1.699026	1.697813
C	-3.045329	-1.766665	0.376792
C	-1.381151	-0.387153	3.219963
C	-0.672465	-1.641188	3.043298
C	-1.424344	-2.452546	2.103654
C	-0.747282	-3.250789	1.177113
C	0.704789	-3.265824	1.156797
C	1.430106	-2.488214	2.064470
C	0.726558	-1.659903	3.025225
C	1.135190	-3.347614	-0.224085
C	2.273914	-2.653630	-0.645130
C	3.034275	-1.850627	0.295931
C	2.614334	-1.767909	1.627695
C	1.471201	-0.424721	3.179689
C	2.639762	-0.489412	2.318894
C	3.084819	0.660592	1.653863
C	3.524130	0.576858	0.269578
C	3.497445	-0.656968	-0.396168
C	0.787139	0.783749	3.346849
C	-0.664088	0.804378	3.370448
C	3.067347	1.778989	-0.410208
C	2.358248	2.603817	0.549503
C	2.368527	1.913420	1.824345
C	1.243119	1.973768	2.654679
C	2.607014	1.708195	-1.728107
C	2.579157	0.431979	-2.418135
C	3.011674	-0.727197	-1.764558
C	2.264216	-1.961415	-1.919202
C	-1.216261	-3.323504	-0.192592
C	-0.052549	-3.383328	-1.058023
C	-0.060638	-2.718967	-2.286243
C	1.117686	-1.992158	-2.721719
C	-2.342182	-2.594906	-0.584652
C	0.072878	2.731414	2.250642
C	0.064644	3.394977	1.022118
C	1.227694	3.328088	0.157340
C	-2.248811	1.975540	1.886860
C	-1.106285	2.008315	2.692709
C	1.435810	2.463282	-2.137777
C	0.757679	3.259865	-1.211763
C	0.674405	-0.790812	-3.403148
C	1.392293	0.399570	-3.253380
C	-2.257341	2.668344	0.610639
C	-1.123447	3.366811	0.188073
C	0.686091	1.654922	-3.081210
C	-0.694200	3.283639	-1.193686
C	-2.350671	-1.902396	-1.860699
C	-1.231664	-1.964872	-2.697043
C	-0.776694	-0.773176	-3.388035
Na	0.904608	-0.057177	0.102724
C	6.529284	-2.880256	1.085744
C	6.958718	-1.559331	1.080675
C	6.821089	-0.751891	-0.067561
C	6.414985	-1.393054	-1.254779
C	5.987779	-2.715685	-1.250089

C	5.941564	-3.461121	-0.057504
C	6.817968	0.720854	0.002862
C	6.940434	1.530555	-1.145371
C	6.422391	1.359193	1.195362
C	6.508221	2.850694	-1.142796
C	5.992335	2.680664	1.198140
C	5.932064	3.428820	0.007912
C	5.081347	-4.656784	0.022003
C	4.360092	-4.907502	1.204724
C	4.743924	-5.421111	-1.113228
C	3.247283	-5.737112	1.204563
C	3.631120	-6.254588	-1.112700
C	2.802075	-6.359238	0.022062
C	1.408625	-6.836231	-0.055601
C	0.685492	-7.230772	1.088558
C	0.677216	-6.640434	-1.242159
C	-0.704176	-7.226712	1.094768
C	-0.712501	-6.635754	-1.235768
C	-1.434924	-6.826986	-0.042768
C	5.071809	4.625451	-0.059868
C	4.738128	5.381394	1.082378
C	4.348740	4.889124	-1.238757
C	3.627327	6.217285	1.091273
C	3.237576	5.721068	-1.229046
C	2.794956	6.333154	-0.040160
C	1.403318	6.814485	0.047022
C	0.673142	7.212346	-1.091592
C	0.679556	6.624110	1.239372
C	-0.716533	7.219812	-1.085670
C	-0.710189	6.630941	1.245103
C	-1.441430	6.827965	0.058459
C	-2.825354	-6.342969	0.046081
C	-3.659764	-6.229658	-1.083821
C	-3.260589	-5.722368	1.233112
C	-4.768004	-5.390359	-1.075407
C	-4.368904	-4.886663	1.242155
C	-5.095338	-4.628144	0.064353
C	-5.954157	-3.430998	-0.005709
C	-6.536163	-2.855069	1.142638
C	-6.005927	-2.681430	-1.195461
C	-6.969462	-1.535294	1.143782
C	-6.436848	-1.360365	-1.193998
C	-6.840653	-0.724939	-0.003174
C	-2.836971	6.356776	-0.018990
C	-3.664413	6.251220	1.116841
C	-3.285512	5.738401	-1.202119
C	-4.778419	5.419313	1.117430
C	-4.399104	4.909769	-1.201907
C	-5.117654	4.656284	-0.018195
C	-5.975284	3.458709	0.061337
C	-6.565071	2.878975	-1.081196
C	-6.013428	2.710194	1.252366
C	-6.990591	1.556607	-1.077322
C	-6.436892	1.386622	1.255824
C	-6.846323	0.747821	0.068881
H	6.601382	-3.457991	2.003833
H	7.360117	-1.129980	1.995173
H	6.313204	-0.816200	-2.169685
H	5.563715	-3.131836	-2.159911
H	7.332027	1.103901	-2.065376
H	6.332003	0.780554	2.110305
H	6.569738	3.430206	-2.060516
H	5.578155	3.093466	2.114049
H	4.596807	-4.349571	2.106472
H	5.332351	-5.321154	-2.021968
H	2.643909	-5.804485	2.105642
H	3.368048	-6.790649	-2.021395
H	1.220468	-7.486029	2.000027
H	1.197992	-6.356784	-2.152827
H	-1.232271	-7.478704	2.011099
H	-1.239541	-6.348461	-2.141532
H	5.328424	5.273976	1.989077
H	4.582180	4.339570	-2.146390
H	3.368829	6.747256	2.004767
H	2.633664	5.797691	-2.128850
H	1.201467	7.462571	-2.008320
H	1.205100	6.336645	2.146067
H	-1.250393	7.475058	-1.997746
H	-1.231762	6.347959	2.155531
H	-3.404585	-6.763966	-1.995748
H	-2.652856	-5.795626	2.130768
H	-5.360592	-5.284046	-1.980712
H	-4.597675	-4.330141	2.146751
H	-6.601303	-3.435806	2.059421
H	-5.584383	-3.093333	-2.108410
H	-7.365952	-1.108727	2.061736
H	-6.339566	-0.779359	-2.106698
H	-3.399272	6.784851	2.026416
H	-2.683776	5.805922	-2.104248
H	-5.365314	5.317915	2.027059
H	-4.637238	4.352801	-2.103741
H	-6.641170	3.458225	-1.998043
H	-5.586241	3.125192	2.161333
H	-7.392562	1.126840	-1.991422
H	-6.328334	0.806979	2.168183

$Na^+@C_{60}$(5)···[10]CPP (TPSS-D3(BJ))

C	0.799181	0.939896	3.322019
C	-0.655657	0.938771	3.354016
C	-1.104483	-0.445430	3.337485
C	0.072879	-1.299593	3.295195
C	1.249433	-0.443514	3.285500
C	2.364260	-0.796191	2.517973
C	2.349519	-2.020450	1.730088
C	1.218506	-2.843054	1.739445
C	0.057440	-2.474508	2.536946
C	0.741187	-3.440637	0.501054
C	1.416038	-3.189674	-0.697111
C	2.592789	-2.333902	-0.706780
C	3.051883	-1.759875	0.482165
C	0.659484	-2.929294	-1.912893

C	1.369412	-1.911509	-2.674300
C	2.564622	-1.543533	-1.928610
C	2.995898	-0.213101	-1.912660
C	2.249464	0.802390	-2.641923
C	1.102596	0.448132	-3.359616
C	0.653779	-0.936081	-3.376033
C	2.266473	2.026287	-1.853777
C	1.134786	2.847131	-1.813289
C	-0.059387	2.477217	-2.559015
C	-0.074779	1.302286	-3.317244
C	-0.801040	-0.937264	-3.343856
C	-1.251347	0.446152	-3.307425
C	-2.366219	0.798820	-2.540009
C	-2.351522	2.023143	-1.752179
C	-1.220526	2.845771	-1.761546
C	-1.483370	-1.913776	-2.611267
C	-0.738921	-2.930393	-1.881990
C	-3.053968	1.762622	-0.504262
C	-3.502696	0.378511	-0.520821
C	-3.077877	-0.217862	-1.778731
C	-2.645080	-1.547418	-1.813682
C	-2.594850	2.336630	0.684709
C	-1.418014	3.192359	0.675076
C	-0.743173	3.443234	-0.523083
C	0.711398	3.443953	-0.555123
C	3.473765	0.383941	-0.674276
C	3.023134	1.766724	-0.637881
C	2.615838	2.340074	0.569940
C	1.438692	3.194015	0.612095
C	3.500521	-0.375860	0.498713
C	-2.618037	-2.337605	-0.591933
C	-3.025351	-1.764219	0.615884
C	-3.476001	-0.381284	0.652197
C	-0.713433	-3.441463	0.533155
C	-1.440775	-3.191594	-0.634054
C	-2.566618	1.546224	1.906562
C	-2.997886	0.215810	1.890555
C	0.736923	2.932953	1.860078
C	-0.661427	2.931890	1.890873
C	-1.136784	-2.844503	1.791295
C	-2.268483	-2.023623	1.831745
C	-1.371349	1.914166	2.652266
C	-2.251376	-0.799675	2.619805
C	3.075806	0.220478	1.756654
C	2.643016	1.549985	1.791694
C	1.481458	1.916413	2.589392
Na	-0.000835	0.001346	-0.011036
C	6.609715	-2.890807	0.916318
C	7.033738	-1.568238	0.930113
C	6.865731	-0.739426	-0.194389
C	6.426730	-1.350205	-1.381942
C	6.002720	-2.671123	-1.395541
C	5.997325	-3.445610	-0.222407
C	6.859848	0.732013	-0.096286
C	6.976425	1.564196	-1.224704
C	6.459647	1.336303	1.108113
C	6.540063	2.882652	-1.191770
C	6.024098	2.652934	1.141043
C	5.967403	3.429959	-0.028975
C	5.134568	-4.639499	-0.152228
C	4.450400	-4.921025	1.043003
C	4.749336	-5.359910	-1.297803
C	3.326073	-5.733524	1.052385
C	3.623445	-6.173483	-1.288352
C	2.831211	-6.304433	-0.132969
C	1.427250	-6.752579	-0.184060
C	0.721997	-7.153719	0.965453
C	0.676802	-6.526882	-1.351139
C	-0.666787	-7.149473	0.993083
C	-0.710195	-6.523059	-1.323644
C	-1.414869	-6.744585	-0.127686
C	5.095292	4.618624	-0.062012
C	4.754837	5.336464	1.099140
C	4.361560	4.898932	-1.227846
C	3.629619	6.150453	1.135766
C	3.238010	5.711780	-1.191325
C	2.792509	6.284298	0.012799
C	1.393358	6.738145	0.118914
C	0.644923	7.141156	-1.002360
C	0.688476	6.517891	1.315019
C	-0.743893	7.144849	-0.974773
C	-0.698506	6.521336	1.342531
C	-1.449108	6.745053	0.175182
C	-2.813608	-6.289786	-0.021079
C	-3.653222	-6.161708	-1.142857
C	-3.255621	-5.711032	1.181262
C	-4.778364	-5.347501	-1.107582
C	-4.379172	-4.898088	1.216473
C	-5.115731	-4.624215	0.050962
C	-5.988173	-3.435900	0.015271
C	-6.567698	-2.891494	1.175945
C	-6.037951	-2.656921	-1.153725
C	-7.004520	-1.573247	1.208975
C	-6.474000	-1.340361	-1.120693
C	-6.881358	-0.739120	0.082757
C	-2.853019	6.296412	0.124468
C	-3.644779	6.165337	1.280171
C	-3.348227	5.725518	-1.060720
C	-4.770636	5.351721	1.289923
C	-4.472665	4.913127	-1.051103
C	-5.156229	4.631607	0.144416
C	-6.018750	3.437515	0.214908
C	-6.637624	2.886438	-0.922082
C	-6.017069	2.659711	1.385750
C	-7.061788	1.563839	-0.937413
C	-6.441453	1.338986	1.370718
C	-6.887349	0.732115	0.183840
H	6.711532	-3.487762	1.818090
H	7.458143	-1.159192	1.842537
H	6.298949	-0.749771	-2.277478
H	5.554621	-3.068265	-2.301251
H	7.369843	1.160663	-2.153299

H	6.370567	0.732371	2.005963
H	6.601811	3.482527	-2.095211
H	5.606421	3.043361	2.063964
H	4.727077	-4.399312	1.954114
H	5.310034	-5.244136	-2.220950
H	2.753848	-5.825143	1.970484
H	3.327534	-6.676939	-2.204264
H	1.267476	-7.427622	1.864010
H	1.183527	-6.229865	-2.264354
H	-1.177768	-7.420287	1.912552
H	-1.251218	-6.222747	-2.215895
H	5.352463	5.219949	1.998654
H	4.600133	4.376260	-2.149108
H	3.371153	6.652824	2.063548
H	2.628379	5.803012	-2.085103
H	1.155297	7.410794	-1.922487
H	1.229263	6.219055	2.207845
H	-1.289511	7.417163	-1.873717
H	-1.204875	6.225697	2.256364
H	-3.396936	-6.669149	-2.068487
H	-2.643227	-5.797775	2.073665
H	-5.378787	-5.235332	-2.005827
H	-4.615788	-4.370318	2.135371
H	-6.634602	-3.493769	2.077419
H	-5.614490	-3.046038	-2.074612
H	-7.403815	-1.171236	2.135721
H	-6.379918	-0.733903	-2.016383
H	-3.348757	6.668559	2.196107
H	-2.776328	5.817224	-1.978965
H	-5.331282	5.235586	2.213026
H	-4.750000	4.391500	-1.962046
H	-6.744796	3.486375	-1.821251
H	-5.563246	3.054338	2.289714
H	-7.491708	1.156985	-1.848227
H	-6.308591	0.735339	2.263390

$Na^+@C_{60}$(6)···[10]CPP (TPSS-D3(BJ))

C	-1.055495	0.292489	-3.387052
C	0.133015	1.131089	-3.372604
C	-0.190451	2.358229	-2.660612
C	-1.580420	2.278360	-2.234934
C	-2.114868	1.000546	-2.684191
C	-3.011563	0.293115	-1.876388
C	-3.409759	0.835042	-0.584362
C	-2.895701	2.061376	-0.153284
C	-1.961513	2.797114	-0.994174
C	-2.479944	2.230166	1.230953
C	-2.595055	1.163203	2.128230
C	-3.131329	-0.113491	1.679241
C	-3.529224	-0.274764	0.349411
C	-1.523201	0.892398	3.075333
C	-1.396795	-0.550902	3.211641
C	-2.389870	-1.172910	2.349581
C	-2.076213	-2.349805	1.662695
C	-0.762661	-2.957407	1.814927
C	0.191025	-2.359274	2.645282
C	-0.132451	-1.132112	3.357176
C	-0.364668	-3.499247	0.523388
C	0.969788	-3.421764	0.114778
C	1.962231	-2.798418	0.979037
C	1.580981	-2.279486	2.219720
C	1.056009	-0.293562	3.371599
C	2.115329	-1.001674	2.668875
C	3.012015	-0.294234	1.861147
C	3.410265	-0.836165	0.569235
C	2.896451	-2.062612	0.138172
C	0.934618	1.094180	3.240144
C	-0.380577	1.698607	3.089168
C	3.529706	0.273624	-0.364552
C	3.203227	1.500283	0.348353
C	2.882771	1.148805	1.723476
C	1.867473	1.831059	2.401602
C	3.131900	0.112389	-1.694378
C	2.595713	-1.164358	-2.143441
C	2.480711	-2.231392	-1.246155
C	1.290550	-3.070600	-1.260577
C	-2.492610	-2.518306	0.278720
C	-1.435074	-3.229119	-0.425153
C	-1.128220	-2.893671	-1.746582
C	0.261727	-2.811095	-2.171886
C	-3.202851	-1.501469	-0.363555
C	1.128850	2.892573	1.731366
C	1.435654	3.227967	0.409942
C	2.493155	2.517173	-0.293925
C	-1.289832	3.069371	1.245362
C	-0.261070	2.810003	2.156654
C	2.390440	1.171815	-2.364771
C	2.076818	2.348771	-1.677929
C	0.381196	-1.699724	-3.104477
C	1.523858	-0.893498	-3.090633
C	-0.969126	3.420497	-0.129939
C	0.365279	3.498135	-0.538582
C	1.397431	0.549822	-3.226929
C	0.763244	2.956349	-1.830176
C	-2.882406	-1.149983	-1.738746
C	-1.866911	-1.832161	-2.416856
C	-0.934063	-1.095310	-3.255477
Na	0.000301	0.000207	-0.007881
C	6.628696	-2.919859	1.078753
C	7.035133	-1.591913	1.079388
C	6.864225	-0.779179	-0.056777
C	6.441328	-1.409479	-1.239904
C	6.032531	-2.734448	-1.239656
C	6.029331	-3.494607	-0.056736
C	6.845369	0.693606	0.018466
C	6.954006	1.505017	-1.127239
C	6.454427	1.321964	1.212723
C	6.514301	2.821072	-1.119730
C	6.012428	2.638239	1.219937
C	5.943827	3.391489	0.034000
C	5.179137	-4.696938	0.018224

C	4.489198	-4.980262	1.209306
C	4.807007	-5.424046	-1.127958
C	3.361774	-5.790436	1.209655
C	3.679974	-6.234221	-1.127546
C	2.872724	-6.354979	0.019110
C	1.462973	-6.781212	-0.054497
C	0.727259	-7.160848	1.082898
C	0.741136	-6.555912	-1.240107
C	-0.661147	-7.132401	1.080790
C	-0.645269	-6.530169	-1.243029
C	-1.378696	-6.726496	-0.060086
C	5.073165	4.579478	-0.023931
C	4.697522	5.294195	1.129348
C	4.379827	4.873986	-1.212075
C	3.576351	6.111882	1.133431
C	3.259402	5.693837	-1.208283
C	2.774938	6.256369	-0.015527
C	1.378594	6.725964	0.053615
C	0.661238	7.132071	-1.087260
C	0.645385	6.527902	1.236405
C	-0.727145	7.160044	-1.089451
C	-0.740900	6.553141	1.233393
C	-1.462539	6.779649	0.047913
C	-2.775024	-6.256246	0.008964
C	-3.577279	-6.112676	-1.139556
C	-3.259295	-5.692866	1.201413
C	-4.698575	-5.295000	-1.135558
C	-4.379777	-4.873073	1.205107
C	-5.073701	-4.579256	0.017208
C	-5.944761	-3.391485	-0.040806
C	-6.514986	-2.821020	1.113081
C	-6.013954	-2.638447	-1.226893
C	-6.954783	-1.505024	1.120610
C	-6.456065	-1.322153	-1.219661
C	-6.846489	-0.693811	-0.025228
C	-2.872051	6.353318	-0.025747
C	-3.678430	6.231719	1.121420
C	-3.361119	5.789079	-1.216416
C	-4.805403	5.421675	1.121880
C	-4.488561	4.978981	-1.216018
C	-5.178194	4.695629	-0.024738
C	-6.028572	3.493604	0.050227
C	-6.628865	2.919562	-1.085120
C	-6.030704	2.733127	1.232924
C	-7.035983	1.591821	-1.085766
C	-6.440075	1.408406	1.233133
C	-6.864643	0.778911	0.050188
H	6.732384	-3.504964	1.988052
H	7.448168	-1.166542	1.989516
H	6.311166	-0.821818	-2.143257
H	5.593250	-3.147083	-2.142553
H	7.345615	1.084906	-2.049059
H	6.374569	0.738400	2.124895
H	6.572235	3.400920	-2.036188
H	5.601920	3.045232	2.138747
H	4.758068	-4.457319	2.122087
H	5.376784	-5.311523	-2.045773
H	2.781444	-5.878540	2.123054
H	3.392000	-6.738922	-2.045163
H	1.248637	-7.435427	1.995401
H	1.271616	-6.276037	-2.144939
H	-1.195256	-7.386211	1.991906
H	-1.160919	-6.231543	-2.150408
H	5.264070	5.172701	2.047893
H	4.646850	4.360604	-2.130519
H	3.291098	6.610983	2.054921
H	2.682802	5.795523	-2.122635
H	1.195479	7.385852	-1.998324
H	1.161061	6.227995	2.143345
H	-1.248659	7.434401	-2.001944
H	-1.271333	6.271686	2.137778
H	-3.293289	-6.613227	-2.060628
H	-2.682841	-5.794268	2.115849
H	-5.266050	-5.174914	-2.053714
H	-4.646717	-4.359292	2.123331
H	-6.572567	-3.400746	2.029632
H	-5.603798	-3.045490	-2.145872
H	-7.345840	-1.084567	2.042537
H	-6.376395	-0.738339	-2.131724
H	-3.389188	6.735061	2.039379
H	-2.780620	5.877070	-2.129759
H	-5.374250	5.307807	2.040106
H	-4.757469	4.455887	-2.128723
H	-6.732583	3.504916	-1.994304
H	-5.590000	3.145180	2.135400
H	-7.449730	1.166753	-1.995725
H	-6.308831	0.820272	2.136016

$K^+@C_{60}$(5)···[10]CPP (B97-D2)

C	-3.074552	-0.163633	-1.765068
C	-3.486996	0.436458	-0.510472
C	-3.013215	1.807379	-0.490547
C	-1.236891	0.466224	-3.288444
C	-0.815082	-0.922303	-3.326844
C	-1.517482	-1.888084	-2.598209
C	-2.669451	-1.502090	-1.803163
C	-3.476743	-0.326313	0.659687
C	-3.055410	-1.714150	0.621007
C	-2.659198	-2.293715	-0.587094
C	-2.543870	2.369918	0.698848
C	-2.532473	1.578616	1.914575
C	-0.047052	1.297298	-3.295059
C	-0.674247	3.442186	-0.503144
C	-1.354952	3.201823	0.692613
C	0.635900	-0.948888	-3.356995
C	1.110390	0.422831	-3.337679
C	-1.501746	-3.167946	-0.629790
C	-0.795496	-2.918025	-1.872380
C	0.775955	3.415446	-0.533691
C	1.187844	2.814191	-1.788208
C	-1.335148	1.921784	2.660427

C	-0.607126	2.925228	1.904634
C	0.603020	-2.942787	-1.901092
C	1.331465	-1.939613	-2.656910
C	2.303452	1.971741	-1.829506
C	2.262711	0.753205	-2.617591
C	0.790910	2.899237	1.875080
C	1.497043	3.148813	0.632616
C	-1.114121	-0.440358	3.340476
C	-0.639692	0.931405	3.360947
C	-1.191598	-2.833324	1.792314
C	-0.779951	-3.434186	0.537138
C	2.529504	-1.597437	-1.911641
C	2.985835	-0.275407	-1.891930
C	0.005510	-2.488593	2.537651
C	0.043346	-1.314946	3.297503
C	0.811030	0.904660	3.330645
C	1.512502	1.869026	2.600322
C	2.653956	2.274434	0.589593
C	3.051531	1.695835	-0.617871
C	2.664104	1.483000	1.805268
C	1.233030	-0.483581	3.291313
C	-0.009138	2.469495	-2.533714
C	-1.160336	2.857385	-1.738728
C	-2.307314	2.056865	-1.733035
C	-2.345277	0.838450	-2.521400
C	-2.990385	0.257198	1.895716
C	-2.267159	-0.771310	2.621641
C	-2.307224	-1.990176	1.833187
C	3.473081	0.308235	-0.656380
C	3.071379	0.145537	1.768120
C	3.483759	-0.454620	0.513573
C	2.540910	-2.388829	-0.696118
C	1.351314	-3.219641	-0.689227
C	3.008987	-1.825396	0.493282
C	0.670534	-3.461104	0.506808
C	1.156667	-2.876661	1.742855
C	2.341179	-0.855939	2.523992
C	2.302556	-2.074398	1.735459
K	-0.116223	-0.216225	-0.047762
C	6.619366	-2.921606	0.944361
C	7.048653	-1.599196	0.956653
C	6.869063	-0.765580	-0.165297
C	6.414790	-1.372034	-1.351772
C	5.985713	-2.692726	-1.364199
C	5.990989	-3.471116	-0.191102
C	6.870322	0.705310	-0.061373
C	7.010547	1.541248	-1.187248
C	6.458400	1.309557	1.141679
C	6.586444	2.865026	-1.155203
C	6.034715	2.631652	1.173301
C	6.001024	3.413640	0.003305
C	5.125913	-4.662777	-0.114777
C	4.423134	-4.925653	1.076370
C	4.757163	-5.400856	-1.257123
C	3.295423	-5.736160	1.080494
C	3.628570	-6.213084	-1.252878
C	2.816997	-6.323992	-0.105899
C	1.412267	-6.767838	-0.172842
C	0.695887	-7.177253	0.969551
C	0.670511	-6.528601	-1.345162
C	-0.694436	-7.165259	0.987343
C	-0.717973	-6.515109	-1.327101
C	-1.433512	-6.742835	-0.136089
C	5.137244	4.607931	-0.040256
C	4.802568	5.340221	1.116541
C	4.403705	4.882608	-1.210001
C	3.680468	6.161065	1.146610
C	3.283549	5.702614	-1.179958
C	2.841239	6.287870	0.021578
C	1.444638	6.749682	0.127083
C	0.705350	7.175366	-0.994786
C	0.730479	6.519564	1.318373
C	-0.684890	7.188048	-0.975727
C	-0.658173	6.533431	1.337611
C	-1.400330	6.775841	0.166224
C	-2.831051	-6.282967	-0.032303
C	-3.667238	-6.151077	-1.159013
C	-3.278783	-5.704924	1.170861
C	-4.790146	-5.331422	-1.128153
C	-4.399472	-4.885602	1.201512
C	-5.128983	-4.604263	0.030706
C	-5.992002	-3.409069	-0.011502
C	-6.574255	-2.858308	1.147726
C	-6.028714	-2.627994	-1.182115
C	-6.998139	-1.534324	1.178852
C	-6.451649	-1.305888	-1.151197
C	-6.860176	-0.699359	0.051817
C	-2.804779	6.331120	0.098944
C	-3.617077	6.220109	1.245397
C	-3.281734	5.742407	-1.087501
C	-4.745288	5.407134	1.248961
C	-4.408913	4.931388	-1.084065
C	-5.113082	4.668910	0.106273
C	-5.978816	3.477511	0.181399
C	-6.604792	2.927534	-0.955131
C	-5.977214	2.699606	1.354833
C	-7.034138	1.605169	-0.968158
C	-6.406716	1.379035	1.341875
C	-6.858082	0.771812	0.154583
H	6.723162	-3.522849	1.844459
H	7.481118	-1.188767	1.865969
H	6.277666	-0.767398	-2.244172
H	5.524383	-3.086316	-2.265906
H	7.407449	1.132370	-2.113182
H	6.349124	0.702739	2.036544
H	6.659535	3.468861	-2.056409
H	5.606300	3.023137	2.092114
H	4.686691	-4.388617	1.983748
H	5.331872	-5.292475	-2.173684
H	2.707154	-5.811139	1.991184
H	3.339864	-6.727110	-2.166483
H	1.236512	-7.457021	1.870554

H	1.186444	-6.226532	-2.252529
H	-1.215833	-7.436771	1.902037
H	-1.250057	-6.202184	-2.221304
H	5.399363	5.222530	2.017827
H	4.638368	4.349357	-2.127138
H	3.419210	6.670703	2.070917
H	2.672970	5.788099	-2.074657
H	1.226734	7.448233	-1.908992
H	1.263859	6.203612	2.210988
H	-1.226358	7.470273	-1.875335
H	-1.173676	6.228610	2.244475
H	-3.403288	-6.655656	-2.085192
H	-2.672245	-5.795356	2.067915
H	-5.384151	-5.210510	-2.030698
H	-4.637562	-4.358666	2.121498
H	-6.645709	-3.460301	2.050429
H	-5.603696	-3.020529	-2.101752
H	-7.392981	-1.124567	2.105415
H	-6.344974	-0.700966	-2.047443
H	-3.328970	6.734424	2.159145
H	-2.692418	5.817463	-1.997309
H	-5.320491	5.298912	2.165354
H	-4.671108	4.393967	-1.991351
H	-6.706414	3.528490	-1.855525
H	-5.518660	3.093501	2.257923
H	-7.464409	1.195053	-1.878512
H	-6.272433	0.775343	2.235362

$K^+@C_{60}$(6)···[10]CPP (B97-D2)

C	-3.499930	0.489953	0.352370
C	-3.048437	0.609124	1.725378
C	-2.375022	1.886728	1.867432
C	-2.676240	1.613593	-1.681752
C	-2.627403	0.325458	-2.351248
C	-3.008393	-0.833659	-1.667610
C	-3.454008	-0.749443	-0.290255
C	-2.570773	-0.516394	2.404226
C	-2.525755	-1.805099	1.735478
C	-2.959378	-1.918963	0.412445
C	-1.241367	1.991535	2.681112
C	-0.742698	0.823319	3.384257
C	-1.532291	2.391409	-2.123293
C	-0.130003	3.414360	0.998933
C	-0.098640	2.770411	2.239095
C	-1.455476	0.307993	-3.205996
C	-0.778224	1.583984	-3.065365
C	-2.206132	-2.724843	-0.529448
C	-2.238519	-2.054495	-1.816547
C	1.043001	3.397842	0.143354
C	0.591433	3.280442	-1.229615
C	0.707279	0.879837	3.376850
C	1.106011	2.082763	2.669410
C	-1.108708	-2.070823	-2.640784
C	-0.709974	-0.867613	-3.348144
C	1.317883	2.502283	-2.137275
C	0.619534	1.638241	-3.072233
C	2.235284	2.065200	1.844067
C	2.202405	2.735331	0.556501
C	0.775012	-1.572305	3.091899
C	1.452160	-0.296121	3.232337
C	-0.594457	-3.267488	1.256764
C	-1.046043	-3.385640	-0.116175
C	0.739955	-0.811269	-3.355583
C	1.392596	0.418801	-3.219961
C	0.856491	-3.210065	1.249138
C	1.529303	-2.379651	2.150407
C	2.624710	-0.314039	2.378245
C	3.006179	0.844938	1.695138
C	2.956130	1.929614	-0.384829
C	2.522553	1.816040	-1.707669
C	3.451590	0.760940	0.318020
C	2.673329	-1.602323	1.709246
C	-0.859765	3.223115	-1.222216
C	-1.306497	3.306549	0.155297
C	-2.407380	2.556884	0.580136
C	-3.104666	1.693643	-0.354532
C	-1.395057	-0.407293	3.247493
C	-0.622471	-1.627286	3.100021
C	-1.321250	-2.491379	2.165580
C	2.568141	0.528149	-2.377134
C	3.495972	-0.478013	-0.324628
C	3.044399	-0.596929	-1.697341
C	1.238050	-1.979450	-2.653016
C	0.095685	-2.758451	-2.211297
C	2.370621	-1.874309	-1.839151
C	0.127006	-3.401920	-0.971537
C	1.303016	-3.294053	-0.128103
C	3.100456	-1.681674	0.381941
C	2.403246	-2.544547	-0.552644
K	-0.120770	0.224194	0.031201
C	6.530439	-2.818569	1.004940
C	6.970234	-1.500811	1.002853
C	6.830872	-0.687464	-0.140635
C	6.407486	-1.319117	-1.326886
C	5.970540	-2.637867	-1.325198
C	5.931075	-3.390247	-0.136753
C	6.845757	0.785237	-0.067376
C	6.968296	1.593820	-1.216349
C	6.463757	1.425645	1.127643
C	6.543181	2.916227	-1.212341
C	6.041062	2.749522	1.132208
C	5.976291	3.496513	-0.058671
C	5.073199	-4.587648	-0.059259
C	4.377423	-4.865543	1.132513
C	4.719953	-5.336807	-1.200450
C	3.273384	-5.707064	1.139901
C	3.616154	-6.181366	-1.192465
C	2.810525	-6.314713	-0.043784
C	1.423369	-6.812415	-0.104251
C	0.721305	-7.220691	1.048259
C	0.673334	-6.630399	-1.281675

C	-0.667955	-7.243298	1.071057
C	-0.715978	-6.653454	-1.259027
C	-1.420276	-6.858445	-0.057565
C	5.112225	4.690381	-0.122498
C	4.791750	5.452995	1.018803
C	4.367823	4.938006	-1.291508
C	3.672616	6.277774	1.040149
C	3.249006	5.759368	-1.269721
C	2.820783	6.376228	-0.078220
C	1.423828	6.837485	0.028043
C	0.671315	7.218536	-1.101883
C	0.719372	6.640010	1.230669
C	-0.717894	7.197523	-1.078644
C	-0.670129	6.618650	1.253758
C	-1.420419	6.794879	0.075652
C	-2.817697	-6.398948	0.049092
C	-3.668124	-6.298342	-1.070227
C	-3.247380	-5.784957	1.241580
C	-4.785841	-5.471823	-1.049259
C	-4.365106	-4.961850	1.263113
C	-5.106363	-4.710420	0.092901
C	-5.966997	-3.514221	0.028633
C	-6.538627	-2.935414	1.180782
C	-6.024654	-2.764844	-1.161111
C	-6.963903	-1.612911	1.184894
C	-6.447447	-1.441113	-1.156476
C	-6.837382	-0.802914	0.037376
C	-2.807666	6.296799	0.016158
C	-3.614020	6.164297	1.164418
C	-3.270190	5.687639	-1.166928
C	-4.718460	5.320266	1.172464
C	-4.374569	4.846908	-1.159521
C	-5.072040	4.570545	0.031714
C	-5.931636	3.374120	0.108312
C	-6.524814	2.800189	-1.035610
C	-5.977999	2.623654	1.297766
C	-6.962594	1.481893	-1.034190
C	-6.413167	1.304142	1.298864
C	-6.827336	0.669774	0.110839
H	6.605734	-3.400768	1.919922
H	7.380757	-1.078693	1.916698
H	6.302029	-0.736875	-2.237830
H	5.536853	-3.045556	-2.234260
H	7.351648	1.163968	-2.138356
H	6.374730	0.847199	2.042909
H	6.600282	3.494663	-2.131069
H	5.633866	3.165414	2.049870
H	4.625984	-4.321187	2.039340
H	5.290124	-5.218230	-2.118495
H	2.689905	-5.796066	2.051964
H	3.342542	-6.705697	-2.104782
H	1.271060	-7.466245	1.953538
H	1.176499	-6.336909	-2.198986
H	-1.180013	-7.504632	1.993874
H	-1.258865	-6.375767	-2.158616
H	5.397723	5.356558	1.916408
H	4.590841	4.381743	-2.197687
H	3.423076	6.810955	1.954329
H	2.628943	5.822222	-2.159704
H	1.183226	7.475743	-2.025834
H	1.262152	6.366759	2.131628
H	-1.267296	7.440062	-1.984856
H	-1.173306	6.330778	2.172779
H	-3.417673	-6.830476	-1.984801
H	-2.628609	-5.850880	2.132326
H	-5.390390	-5.372831	-1.947577
H	-4.589254	-4.407159	2.170049
H	-6.599849	-3.515537	2.098227
H	-5.612599	-3.179277	-2.077281
H	-7.351573	-1.184629	2.105887
H	-6.353535	-0.861416	-2.070449
H	-3.340985	6.689150	2.076587
H	-2.686570	5.775109	-2.078952
H	-5.289121	5.202985	2.090354
H	-4.622432	4.302280	-2.066295
H	-6.596583	3.380872	-1.951782
H	-5.550103	3.032992	2.208828
H	-7.367869	1.058021	-1.949495
H	-6.312413	0.723276	2.211246

$K^+@C_{60}$(5)···[10]CPP (TPSS-D3(BJ))

C	-3.065120	-0.145304	-1.772090
C	-3.479925	0.458640	-0.517526
C	-2.997618	1.828613	-0.499022
C	-1.220842	0.475195	-3.294409
C	-0.803214	-0.917065	-3.332554
C	-1.508814	-1.877826	-2.600958
C	-2.659404	-1.483686	-1.805395
C	-3.472063	-0.302645	0.656084
C	-3.051441	-1.692054	0.620277
C	-2.652427	-2.273208	-0.586572
C	-2.525310	2.389980	0.690915
C	-2.518527	1.600744	1.909923
C	-0.026351	1.304838	-3.305798
C	-0.650503	3.456765	-0.511047
C	-1.333015	3.219107	0.685350
C	0.650673	-0.950216	-3.365990
C	1.130631	0.423477	-3.348402
C	-1.499674	-3.155794	-0.627919
C	-0.791946	-2.913213	-1.873845
C	0.803123	3.430040	-0.540844
C	1.214882	2.824415	-1.798727
C	-1.320810	1.942589	2.659344
C	-0.588031	2.944983	1.902788
C	0.606244	-2.945115	-1.902055
C	1.340896	-1.942568	-2.661648
C	2.325143	1.974725	-1.835951
C	2.281464	0.751191	-2.624761
C	0.810247	2.915339	1.875733
C	1.520718	3.161929	0.628892
C	-1.109960	-0.421985	3.343687

C	-0.630063	0.950971	3.363700
C	-1.193566	-2.816849	1.796639
C	-0.781855	-3.424839	0.540874
C	2.541353	-1.601908	-1.911891
C	3.001106	-0.281421	-1.893457
C	0.005527	-2.478435	2.548229
C	0.046340	-1.303996	3.307752
C	0.824139	0.919376	3.338592
C	1.529249	1.880649	2.606504
C	2.676629	2.279248	0.588885
C	3.071591	1.696506	-0.618243
C	2.682554	1.487720	1.809998
C	1.241805	-0.474375	3.302870
C	0.014644	2.479262	-2.546340
C	-1.137723	2.869058	-1.748367
C	-2.287555	2.072835	-1.742101
C	-2.329479	0.852920	-2.529466
C	-2.982509	0.281227	1.893085
C	-2.262669	-0.749278	2.622062
C	-2.305553	-1.969262	1.834707
C	3.488491	0.303769	-0.654044
C	3.082551	0.148455	1.774562
C	3.494859	-0.456555	0.517691
C	2.548598	-2.393459	-0.690806
C	1.353860	-3.223956	-0.684025
C	3.015697	-1.829397	0.499257
C	0.671881	-3.461510	0.513379
C	1.158989	-2.875141	1.753399
C	2.347386	-0.851910	2.534448
C	2.305980	-2.075258	1.745619
K	-0.563652	0.034101	-0.012241
C	6.585934	-2.921040	0.950480
C	7.014928	-1.599950	0.967631
C	6.857166	-0.769812	-0.157331
C	6.420606	-1.378077	-1.347085
C	5.991206	-2.697210	-1.364048
C	5.978153	-3.473366	-0.192085
C	6.860090	0.701882	-0.059942
C	6.989048	1.532134	-1.188611
C	6.459338	1.311224	1.141805
C	6.563769	2.854321	-1.159453
C	6.035539	2.631959	1.171155
C	5.990555	3.408154	-0.000017
C	5.114264	-4.667058	-0.127716
C	4.423253	-4.948498	1.063549
C	4.735480	-5.387961	-1.275167
C	3.299483	-5.761816	1.067039
C	3.610352	-6.202964	-1.271636
C	2.811886	-6.334650	-0.120456
C	1.408189	-6.784133	-0.177454
C	0.697567	-7.181890	0.970133
C	0.662140	-6.560469	-1.347696
C	-0.691326	-7.171812	0.993888
C	-0.725024	-6.550593	-1.324140
C	-1.434500	-6.764624	-0.129546
C	5.128334	4.604234	-0.038600
C	4.788238	5.326600	1.120063
C	4.403558	4.891092	-1.208495
C	3.670326	6.150854	1.150131
C	3.287387	5.714620	-1.178548
C	2.840019	6.291290	0.022905
C	1.442841	6.753402	0.123167
C	0.699638	7.158346	-1.001068
C	0.732657	6.539305	1.317338
C	-0.689324	7.165706	-0.978611
C	-0.654551	6.547251	1.339888
C	-1.400338	6.768917	0.169037
C	-2.830932	-6.300333	-0.028483
C	-3.662590	-6.161906	-1.155040
C	-3.277093	-5.721617	1.172503
C	-4.779933	-5.336871	-1.125576
C	-4.393222	-4.897773	1.202065
C	-5.118943	-4.612614	0.032261
C	-5.982424	-3.417313	-0.007251
C	-6.556693	-2.863274	1.151701
C	-6.030510	-2.642644	-1.179413
C	-6.984623	-1.541899	1.179633
C	-6.457010	-1.322668	-1.151285
C	-6.857645	-0.712290	0.050088
C	-2.804183	6.319666	0.111983
C	-3.602031	6.186466	1.263563
C	-3.294736	5.750905	-1.076359
C	-4.728553	5.373415	1.266406
C	-4.420138	4.939696	-1.073649
C	-5.110310	4.655977	0.117678
C	-5.976184	3.463418	0.180805
C	-6.580885	2.909879	-0.962988
C	-5.995870	2.689064	1.354002
C	-7.010385	1.588934	-0.980066
C	-6.426037	1.370088	1.337203
C	-6.856666	0.759690	0.146274
H	6.681137	-3.518985	1.852325
H	7.435732	-1.193153	1.882672
H	6.298502	-0.775998	-2.242284
H	5.545288	-3.091188	-2.272210
H	7.383971	1.124488	-2.114788
H	6.360711	0.709585	2.040182
H	6.634637	3.452092	-2.063658
H	5.616762	3.027048	2.091674
H	4.693506	-4.425248	1.975676
H	5.300773	-5.271872	-2.195481
H	2.722042	-5.852638	1.981928
H	3.320346	-6.706894	-2.189219
H	1.239170	-7.456421	1.870857
H	1.172271	-6.268256	-2.260569
H	-1.205756	-7.439150	1.912556
H	-1.261760	-6.251707	-2.219384
H	5.379345	5.205306	2.023310
H	4.642190	4.366087	-2.128481
H	3.411482	6.655803	2.076389
H	2.683634	5.810754	-2.075828
H	1.214235	7.425431	-1.919676

H	1.269132	6.241766	2.213161
H	-1.230329	7.438245	-1.880259
H	-1.164543	6.255557	2.252999
H	-3.405048	-6.669317	-2.080323
H	-2.672881	-5.817481	2.069562
H	-5.372161	-5.217541	-2.028365
H	-4.631933	-4.372385	2.121872
H	-6.626675	-3.460446	2.056385
H	-5.613633	-3.038829	-2.100423
H	-7.380630	-1.134556	2.105465
H	-6.362254	-0.722538	-2.051155
H	-3.310396	6.687687	2.182105
H	-2.719146	5.844206	-1.992193
H	-5.292927	5.256634	2.187179
H	-4.693297	4.420878	-1.987479
H	-6.673224	3.506630	-1.865930
H	-5.555652	3.084571	2.264280
H	-7.428576	1.181624	-1.896084
H	-6.310180	0.770111	2.234671

$K^+@C_{60}$(6)···[10]CPP (TPSS-D3(BJ))

C	-2.834168	1.792782	-1.155447
C	-3.298075	0.417902	-1.236176
C	-3.540330	-0.054571	0.115608
C	-1.765583	2.997867	0.715525
C	-0.739408	3.478937	-0.197407
C	-0.780337	3.114702	-1.546545
C	-1.846009	2.252176	-2.032036
C	-2.754432	-0.449276	-2.190857
C	-1.726194	0.027345	-3.100735
C	-1.281068	1.351106	-3.023522
C	-3.231820	-1.374093	0.461821
C	-2.667009	-2.273904	-0.528881
C	-1.133140	2.713615	1.995754
C	-2.295406	-0.615221	2.618387
C	-2.596347	-1.659465	1.737808
C	0.529166	3.485095	0.516537
C	0.285598	3.011844	1.871005
C	0.135678	1.653509	-3.152183
C	0.445912	2.742196	-2.238461
C	-1.031230	-0.607375	3.335706
C	-0.571016	0.769959	3.417903
C	-1.682865	-3.111858	0.133804
C	-1.640396	-2.733081	1.534402
C	1.663050	2.744793	-1.549624
C	1.705094	3.124985	-0.145235
C	0.792850	1.057349	3.296149
C	1.229613	2.201073	2.509401
C	-0.422646	-2.729969	2.222913
C	-0.111943	-1.644604	3.140401
C	-0.261692	-2.997419	-1.878985
C	-0.504808	-3.468976	-0.526264
C	0.592840	-0.761190	-3.425837
C	1.055139	0.616387	-3.348390
C	2.688253	2.281759	0.518222
C	2.456209	1.829272	1.818978
C	1.576098	-1.606374	-2.764728
C	1.157236	-2.706278	-2.007234
C	0.763393	-3.470422	0.185671
C	0.804210	-3.106858	1.534971
C	1.307202	-1.346240	3.017841
C	1.749391	-0.021175	3.092377
C	1.873342	-2.249214	2.025906
C	1.791472	-2.995753	-0.728516
C	-1.551793	1.613440	2.752367
C	-2.617305	0.755837	2.258113
C	-3.225074	1.030194	1.029960
C	-2.790733	2.172470	0.244862
C	-2.433885	-1.820314	-1.830778
C	-1.207464	-2.189471	-2.518431
C	-0.771382	-1.048711	-3.304296
C	2.776688	0.456413	2.179222
C	2.858613	-1.788604	1.146388
C	3.319249	-0.409987	1.225405
C	3.253308	1.380744	-0.474129
C	2.620900	1.668053	-1.753501
C	3.561687	0.062962	-0.128380
C	2.323967	0.624236	-2.636137
C	2.646715	-0.749369	-2.275620
C	2.815949	-2.169586	-0.257839
C	3.250201	-1.023888	-1.045366
K	-0.529405	-0.150561	-0.122710
C	6.617173	-2.934130	1.125021
C	7.047145	-1.616572	1.203648
C	6.939331	-0.749953	0.099691
C	6.573249	-1.321876	-1.130615
C	6.143601	-2.639834	-1.209424
C	6.060278	-3.446769	-0.061722
C	6.914267	0.716750	0.252105
C	7.085552	1.594707	-0.833705
C	6.441305	1.268216	1.455901
C	6.635155	2.907091	-0.771876
C	5.993888	2.579178	1.518326
C	5.994842	3.402652	0.379218
C	5.174314	-4.625989	-0.069471
C	4.428732	-4.928221	1.083794
C	4.833998	-5.309210	-1.251321
C	3.295487	-5.724895	1.018349
C	3.697641	-6.105023	-1.317600
C	2.850480	-6.257799	-0.203996
C	1.448010	-6.697169	-0.329948
C	0.687597	-7.110434	0.781208
C	0.753272	-6.468365	-1.529750
C	-0.699693	-7.107437	0.744252
C	-0.634803	-6.463257	-1.566390
C	-1.396928	-6.690728	-0.405848
C	5.119051	4.589027	0.349465
C	4.701847	5.244235	1.524138
C	4.465608	4.938896	-0.844102
C	3.575064	6.054129	1.533572
C	3.337051	5.747624	-0.834386

C	2.808783	6.249328	0.368745
C	1.405042	6.697260	0.415888
C	0.709383	7.114276	-0.734961
C	0.641505	6.467213	1.574724
C	-0.677790	7.115701	-0.774397
C	-0.746215	6.471795	1.535990
C	-1.439325	6.702546	0.335811
C	-2.800314	-6.241434	-0.356882
C	-3.569635	-6.048861	-1.520418
C	-3.327285	-5.738184	0.846434
C	-4.696284	-5.238550	-1.510552
C	-4.456015	-4.929410	0.856599
C	-5.111399	-4.580575	-0.336504
C	-5.988109	-3.394488	-0.366311
C	-6.624401	-2.896620	0.786218
C	-5.995089	-2.573621	-1.507628
C	-7.075566	-1.584447	0.847120
C	-6.443331	-1.262506	-1.445964
C	-6.909234	-0.707853	-0.240732
C	-2.842452	6.264840	0.209981
C	-3.688389	6.113663	1.324622
C	-3.290208	5.733099	-1.011718
C	-4.825252	5.318411	1.260668
C	-4.424659	4.937863	-1.075185
C	-5.168328	4.635772	0.079391
C	-6.054649	3.456650	0.073087
C	-6.615882	2.945091	-1.112131
C	-6.134872	2.648581	1.220247
C	-7.044986	1.627101	-1.191182
C	-6.564431	1.330625	1.141309
C	-6.933494	0.759187	-0.088537
H	6.665484	-3.559347	2.011999
H	7.423118	-1.238945	2.150189
H	6.497936	-0.693149	-2.012664
H	5.744644	-3.004437	-2.151108
H	7.531977	1.232229	-1.755271
H	6.305893	0.627125	2.321354
H	6.739828	3.542864	-1.646375
H	5.521286	2.927593	2.431377
H	4.667119	-4.433756	2.020365
H	5.438934	-5.177045	-2.143753
H	2.679660	-5.831524	1.905991
H	3.439391	-6.578223	-2.260651
H	1.189731	-7.394394	1.701469
H	1.300811	-6.167564	-2.417939
H	-1.250587	-7.389631	1.636761
H	-1.130715	-6.160793	-2.483634
H	5.240709	5.079536	2.452614
H	4.765824	4.471584	-1.777070
H	3.258504	6.504684	2.469682
H	2.790538	5.890056	-1.761396
H	1.261695	7.397076	-1.626294
H	1.136158	6.161796	2.491445
H	-1.178437	7.398756	-1.695723
H	-1.294656	6.168267	2.422526
H	-3.255973	-6.502988	-2.455817
H	-2.780311	-5.880842	1.773245
H	-5.237614	-5.077171	-2.438228
H	-4.756070	-4.462858	1.790124
H	-6.725897	-3.530711	1.662329
H	-5.529952	-2.924856	-2.423578
H	-7.519336	-1.220955	1.769511
H	-6.316011	-0.624368	-2.314946
H	-3.428163	6.587210	2.266833
H	-2.676263	5.840276	-1.900527
H	-5.428217	5.186581	2.154464
H	-4.666400	4.445059	-2.011787
H	-6.668626	3.571805	-1.997710
H	-5.735217	3.013018	2.161640
H	-7.424223	1.250852	-2.136933
H	-6.488381	0.701886	2.023262

C_{60}(5)···[10]CPP (B97-D2)

C	0.998729	0.725873	3.326085
C	0.998729	-0.725873	3.326085
C	1.961093	-1.425073	2.590599
C	2.960518	-0.699300	1.827581
C	2.960518	0.699300	1.827581
C	1.961093	1.425073	2.590599
C	-0.382035	1.174417	3.325750
C	-1.235336	0.000000	3.325550
C	-0.382035	-1.174417	3.325750
C	-0.749499	-2.305615	2.589939
C	1.579715	-2.599746	1.827311
C	3.195192	-1.425326	0.594093
C	3.422867	-0.725011	-0.592888
C	3.422868	0.725010	-0.592888
C	3.195192	1.425326	0.594093
C	2.342844	2.598425	0.593888
C	1.579715	2.599746	1.827311
C	0.249615	3.031882	1.827050
C	-0.749498	2.305615	2.589939
C	-2.424549	0.000000	2.589688
C	-2.806295	1.174354	1.826501
C	-1.984284	2.305874	1.826646
C	-1.747263	3.031199	0.593229
C	-0.368254	3.479304	0.593441
C	0.368254	3.479303	-0.593441
C	1.747264	3.031198	-0.593229
C	1.984285	2.305874	-1.826646
C	2.806295	1.174354	-1.826501
C	2.342844	-2.598426	0.593888
C	0.382035	-1.174417	-3.325750
C	0.749498	-2.305615	-2.589939
C	-0.249615	-3.031882	-1.827050
C	-1.579715	-2.599746	-1.827311
C	-1.961093	-1.425073	-2.590599
C	-0.998729	0.725873	-3.326085
C	0.382035	1.174417	-3.325750
C	1.235336	-0.000000	-3.325550
C	2.424549	-0.000000	-2.589688

C	2.806295	-1.174354	-1.826501
C	1.984284	-2.305874	-1.826646
C	0.368254	-3.479304	-0.593441
C	-0.368254	-3.479303	0.593441
C	-1.747264	-3.031198	0.593229
C	-2.342844	-2.598425	-0.593888
C	-3.195192	-1.425326	-0.594093
C	-2.960518	-0.699300	-1.827581
C	-2.960518	0.699300	-1.827581
C	-1.961093	1.425073	-2.590599
C	0.749499	2.305615	-2.589939
C	-0.249614	3.031882	-1.827050
C	-1.579715	2.599746	-1.827311
C	-2.342844	2.598426	-0.593888
C	-3.195192	1.425326	-0.594093
C	-3.422867	0.725011	0.592888
C	-3.422868	-0.725010	0.592888
C	-2.806295	-1.174354	1.826501
C	-1.984285	-2.305874	1.826646
C	1.747263	-3.031199	-0.593229
C	0.249614	-3.031882	1.827050
C	-0.998729	-0.725873	-3.326085
C	6.212012	3.653922	1.095076
C	5.394443	4.779069	1.095206
C	4.637136	5.129274	-0.040474
C	4.880112	4.404341	-1.222483
C	5.696389	3.280772	-1.222596
C	6.310863	2.825509	-0.040718
C	3.444897	5.995350	0.040793
C	2.877968	6.607273	-1.095002
C	2.680251	6.002296	1.222699
C	1.555195	7.036884	-1.095103
C	1.359438	6.431470	1.222671
C	0.736789	6.875055	0.040657
C	6.766024	1.423876	0.040288
C	6.537324	0.694435	1.222317
C	7.172136	0.695425	-1.095685
C	6.537324	-0.694454	1.222316
C	7.172135	-0.695445	-1.095685
C	6.766021	-1.423896	0.040289
C	6.310854	-2.825529	-0.040720
C	6.212007	-3.653934	1.095076
C	5.696383	-3.280782	-1.222598
C	5.394426	-4.779089	1.095206
C	4.880096	-4.404358	-1.222484
C	4.637123	-5.129283	-0.040476
C	-0.736771	6.875057	-0.040658
C	-1.555174	7.036890	1.095103
C	-1.359420	6.431472	-1.222672
C	-2.877953	6.607280	1.095003
C	-2.680236	6.002301	-1.222699
C	-3.444881	5.995358	-0.040794
C	-4.637123	5.129283	0.040476
C	-5.394426	4.779089	-1.095206
C	-4.880096	4.404358	1.222484
C	-6.212007	3.653934	-1.095076
C	-5.696383	3.280782	1.222598
C	-6.310854	2.825529	0.040720
C	3.444881	-5.995358	0.040794
C	2.877953	-6.607280	-1.095003
C	2.680236	-6.002301	1.222699
C	1.555174	-7.036890	-1.095103
C	1.359420	-6.431472	1.222672
C	0.736771	-6.875057	0.040658
C	-0.736789	-6.875055	-0.040657
C	-1.555195	-7.036884	1.095103
C	-1.359438	-6.431470	-1.222671
C	-2.877968	-6.607273	1.095002
C	-2.680251	-6.002296	-1.222699
C	-3.444897	-5.995350	-0.040793
C	-6.766021	1.423896	-0.040289
C	-7.172135	0.695445	1.095685
C	-6.537324	0.694454	-1.222316
C	-7.172136	-0.695425	1.095685
C	-6.537324	-0.694435	-1.222317
C	-6.766024	-1.423876	-0.040288
C	-6.310863	-2.825509	0.040718
C	-6.212012	-3.653922	-1.095076
C	-5.696389	-3.280772	1.222596
C	-5.394443	-4.779069	-1.095206
C	-4.880112	-4.404341	1.222483
C	-4.637136	-5.129274	0.040474
H	6.733293	3.375454	2.008081
H	5.290627	5.360789	2.008200
H	4.313101	4.638567	-2.119144
H	5.743981	2.669296	-2.119422
H	3.463333	6.688174	-2.007989
H	3.078372	5.535870	2.119545
H	1.129183	7.446219	-2.008164
H	0.763115	6.287974	2.119408
H	6.217384	1.217203	2.119387
H	7.429714	1.226970	-2.008818
H	6.217382	-1.217223	2.119387
H	7.429711	-1.226991	-2.008818
H	6.733284	-3.375474	2.008078
H	5.743971	-2.669310	-2.119422
H	5.290612	-5.360801	2.008197
H	4.313087	-4.638576	-2.119144
H	-1.129165	7.446222	2.008162
H	-0.763098	6.287972	-2.119408
H	-3.463313	6.688182	2.007988
H	-3.078357	5.535875	-2.119545
H	-5.290612	5.360801	-2.008197
H	-4.313087	4.638576	2.119144
H	-6.733284	3.375474	-2.008078
H	-5.743971	2.669310	2.119422
H	3.463313	-6.688182	-2.007988
H	3.078357	-5.535875	2.119545
H	1.129165	-7.446222	-2.008162
H	0.763098	-6.287972	2.119408
H	-1.129183	-7.446219	2.008164
H	-0.763115	-6.287974	-2.119408

H	-3.463333	-6.688174	2.007989
H	-3.078372	-5.535870	-2.119545
H	-7.429711	1.226991	2.008818
H	-6.217382	1.217223	-2.119387
H	-7.429714	-1.226970	2.008818
H	-6.217384	-1.217203	-2.119387
H	-6.733293	-3.375454	-2.008081
H	-5.743981	-2.669296	2.119422
H	-5.290627	-5.360789	-2.008200
H	-4.313101	-4.638567	2.119144

C_{60}(6)···[10]CPP (B97-D2)

C	1.807749	2.898658	0.943461
C	0.776741	3.459547	0.091758
C	-0.553733	3.466154	0.516680
C	-0.904381	2.914461	1.812689
C	0.090683	2.376102	2.635183
C	1.473532	2.370531	2.192842
C	2.768600	2.215787	0.098285
C	2.330617	2.353676	-1.277051
C	1.099441	3.122256	-1.281014
C	0.076739	2.802044	-2.179142
C	-1.613787	3.131501	-0.413995
C	-2.179464	2.235259	1.680053
C	-2.419227	1.047213	2.377566
C	-1.386081	0.488398	3.229744
C	-0.154405	1.140566	3.356522
C	1.076641	0.371526	3.360476
C	2.082952	1.131430	2.641618
C	3.007334	0.470975	1.825616
C	3.355900	1.024198	0.529614
C	2.495462	1.291344	-2.171272
C	3.105240	0.052777	-1.723120
C	3.524439	-0.078136	-0.396993
C	3.275182	-1.311272	0.323590
C	2.956749	-0.973084	1.697130
C	1.990757	-1.707466	2.392075
C	1.031302	-1.021678	3.237637
C	-0.246552	-1.697887	3.106394
C	-1.432875	-0.956909	3.102579
C	-2.616365	2.368890	0.303993
C	-2.768600	-2.215787	-0.098285
C	-3.355900	-1.024198	-0.529614
C	-3.007334	-0.470975	-1.825616
C	-2.082952	-1.131430	-2.641618
C	-1.473532	-2.370531	-2.192842
C	-0.776741	-3.459547	-0.091758
C	-1.099441	-3.122256	1.281014
C	-2.330617	-2.353676	1.277051
C	-2.495462	-1.291344	2.171272
C	-3.105240	-0.052777	1.723120
C	-3.524439	0.078136	0.396993
C	-2.956749	0.973084	-1.697130
C	-1.990757	1.707466	-2.392075
C	-1.031302	1.021678	-3.237637
C	-1.076641	-0.371526	-3.360476
C	0.154405	-1.140566	-3.356522
C	-0.090683	-2.376102	-2.635183
C	0.904381	-2.914461	-1.812689
C	0.553733	-3.466154	-0.516680
C	-0.076739	-2.802044	2.179142
C	1.305956	-2.808357	1.737675
C	1.613787	-3.131501	0.413995
C	2.616365	-2.368890	-0.303993
C	2.179464	-2.235259	-1.680053
C	2.419227	-1.047213	-2.377566
C	1.386081	-0.488398	-3.229744
C	1.432875	0.956909	-3.102579
C	0.246552	1.697887	-3.106394
C	-3.275182	1.311272	-0.323590
C	-1.305956	2.808357	-1.737675
C	-1.807749	-2.898658	-0.943461
C	-5.050393	5.018995	-1.160137
C	-3.973972	5.897488	-1.183292
C	-3.166245	6.094490	-0.044148
C	-3.608177	5.513820	1.158902
C	-4.683449	4.633865	1.181500
C	-5.374377	4.290521	0.003037
C	-1.795936	6.635864	-0.134935
C	-1.097614	7.118986	0.990449
C	-1.052490	6.437752	-1.314114
C	0.288647	7.228960	0.984874
C	0.331463	6.546229	-1.319093
C	1.044280	6.859138	-0.145592
C	-6.170648	3.048138	-0.041317
C	-6.185095	2.271452	-1.216204
C	-6.705438	2.455252	1.121112
C	-6.535123	0.926849	-1.189551
C	-7.053801	1.110369	1.148308
C	-6.886677	0.288862	0.014412
C	-6.803439	-1.181598	0.113266
C	-6.945768	-2.023876	-1.008079
C	-6.311499	-1.765798	1.296055
C	-6.458041	-3.326210	-0.996280
C	-5.823862	-3.065681	1.307641
C	-5.803059	-3.848200	0.136967
C	2.479441	6.523156	-0.065626
C	3.299364	6.454027	-1.210614
C	2.997994	5.983373	1.126461
C	4.474286	5.711265	-1.208468
C	4.172815	5.241024	1.128551
C	4.885657	5.002251	-0.061372
C	5.803059	3.848200	-0.136967
C	6.458041	3.326210	0.996280
C	5.823862	3.065681	-1.307641
C	6.945768	2.023876	1.008079
C	6.311499	1.765798	-1.296055
C	6.803439	1.181598	-0.113266
C	-4.885657	-5.002251	0.061372
C	-4.474286	-5.711265	1.208468
C	-4.172815	-5.241024	-1.128551

C	-3.299364	-6.454027	1.210614
C	-2.997994	-5.983373	-1.126461
C	-2.479441	-6.523156	0.065626
C	-1.044280	-6.859138	0.145592
C	-0.288647	-7.228960	-0.984874
C	-0.331463	-6.546229	1.319093
C	1.097614	-7.118986	-0.990449
C	1.052490	-6.437752	1.314114
C	1.795936	-6.635864	0.134935
C	6.886677	-0.288862	-0.014412
C	7.053801	-1.110369	-1.148308
C	6.535123	-0.926849	1.189551
C	6.705438	-2.455252	-1.121112
C	6.185095	-2.271452	1.216204
C	6.170648	-3.048138	0.041317
C	5.374377	-4.290521	-0.003037
C	5.050393	-5.018995	1.160137
C	4.683449	-4.633865	-1.181500
C	3.973972	-5.897488	1.183292
C	3.608177	-5.513820	-1.158902
C	3.166245	-6.094490	0.044148
H	-5.611960	4.847542	-2.075175
H	-3.715578	6.394221	-2.115362
H	-3.018125	5.638473	2.062808
H	-4.897410	4.101583	2.103788
H	-1.644478	7.354858	1.900413
H	-1.548618	6.058722	-2.203041
H	0.800056	7.546708	1.890503
H	0.874656	6.248646	-2.211375
H	-5.783739	2.683799	-2.137429
H	-6.790470	3.041615	2.032773
H	-6.394417	0.333738	-2.089034
H	-7.403655	0.671992	2.079863
H	-7.389990	-1.631905	-1.920156
H	-6.178834	-1.151393	2.182054
H	-6.527619	-3.927948	-1.899523
H	-5.325395	-3.427741	2.202321
H	2.974393	6.932182	-2.131672
H	2.400384	6.016435	2.033417
H	5.047695	5.620870	-2.127958
H	4.456889	4.716772	2.036972
H	6.527619	3.927948	1.899523
H	5.325395	3.427741	-2.202321
H	7.389990	1.631905	1.920156
H	6.178834	1.151393	-2.182054
H	-5.047695	-5.620870	2.127958
H	-4.456889	-4.716772	-2.036972
H	-2.974393	-6.932182	2.131672
H	-2.400384	-6.016435	-2.033417
H	-0.800056	-7.546708	-1.890503
H	-0.874656	-6.248646	2.211375
H	1.644478	-7.354858	-1.900413
H	1.548618	-6.058722	2.203041
H	7.403655	-0.671992	-2.079863
H	6.394417	-0.333738	2.089034
H	6.790470	-3.041615	-2.032773
H	5.783739	-2.683799	2.137429
H	5.611960	-4.847542	2.075175
H	4.897410	-4.101583	-2.103788
H	3.715578	-6.394221	2.115362
H	3.018125	-5.638473	-2.062808

C_{60}(5)···[10]CPP (TPSS-D3(BJ))

C	0.999684	0.726663	3.328653
C	0.999683	-0.726662	3.328651
C	1.961168	-1.425172	2.594265
C	2.961964	-0.698543	1.830008
C	2.961966	0.698542	1.830008
C	1.961171	1.425171	2.594267
C	-0.382559	1.175713	3.328383
C	-1.236734	0.000001	3.328144
C	-0.382560	-1.175711	3.328380
C	-0.749596	-2.305857	2.593681
C	1.579467	-2.601489	1.829791
C	3.197069	-1.425448	0.593952
C	3.424409	-0.726015	-0.592790
C	3.424409	0.726013	-0.592790
C	3.197070	1.425446	0.593951
C	2.343532	2.600249	0.593797
C	1.579468	2.601489	1.829793
C	0.250782	3.033179	1.829557
C	-0.749595	2.305860	2.593684
C	-2.424888	0.000000	2.593407
C	-2.807189	1.175956	1.828980
C	-1.986086	2.306178	1.829105
C	-1.748762	3.032491	0.593101
C	-0.367787	3.481220	0.593360
C	0.367789	3.481218	-0.593364
C	1.748763	3.032488	-0.593104
C	1.986087	2.306176	-1.829106
C	2.807189	1.175953	-1.828982
C	2.343530	-2.600249	0.593797
C	0.382557	-1.175708	-3.328378
C	0.749595	-2.305856	-2.593677
C	-0.250781	-3.033178	-1.829559
C	-1.579468	-2.601489	-1.829794
C	-1.961170	-1.425172	-2.594265
C	-0.999683	0.726662	-3.328654
C	0.382558	1.175710	-3.328381
C	1.236730	-0.000000	-3.328142
C	2.424886	-0.000001	-2.593403
C	2.807189	-1.175955	-1.828981
C	1.986084	-2.306178	-1.829105
C	0.367788	-3.481218	-0.593365
C	-0.367791	-3.481220	0.593361
C	-1.748764	-3.032491	0.593102
C	-2.343529	-2.600245	-0.593800
C	-3.197067	-1.425443	-0.593955
C	-2.961964	-0.698541	-1.830011
C	-2.961965	0.698543	-1.830011
C	-1.961171	1.425174	-2.594267

C	0.749597	2.305857	-2.593682
C	-0.250780	3.033180	-1.829560
C	-1.579467	2.601490	-1.829796
C	-2.343527	2.600248	-0.593800
C	-3.197066	1.425445	-0.593954
C	-3.424412	0.726016	0.592787
C	-3.424413	-0.726013	0.592787
C	-2.807191	-1.175955	1.828979
C	-1.986087	-2.306177	1.829104
C	1.748761	-3.032490	-0.593104
C	0.250779	-3.033179	1.829555
C	-0.999683	-0.726660	-3.328652
C	6.197695	3.644633	1.099665
C	5.381239	4.768707	1.099725
C	4.633659	5.124614	-0.037647
C	4.883189	4.405847	-1.219405
C	5.698428	3.283377	-1.219474
C	6.304831	2.823624	-0.037761
C	3.441437	5.990705	0.038025
C	2.871944	6.591225	-1.099644
C	2.680793	6.006252	1.219831
C	1.550585	7.020223	-1.099734
C	1.361346	6.434745	1.219733
C	0.736816	6.868968	0.037834
C	6.759939	1.421980	0.037637
C	6.541029	0.693629	1.219615
C	7.154179	0.694607	-1.100249
C	6.541027	-0.693642	1.219615
C	7.154176	-0.694623	-1.100250
C	6.759936	-1.421994	0.037638
C	6.304827	-2.823639	-0.037759
C	6.197683	-3.644640	1.099666
C	5.698435	-3.283394	-1.219470
C	5.381217	-4.768717	1.099728
C	4.883187	-4.405866	-1.219404
C	4.633648	-5.124624	-0.037646
C	-0.736803	6.868970	-0.037837
C	-1.550572	7.020232	1.099736
C	-1.361335	6.434748	-1.219735
C	-2.871930	6.591239	1.099642
C	-2.680779	6.006261	-1.219833
C	-3.441423	5.990716	-0.038024
C	-4.633645	5.124624	0.037648
C	-5.381227	4.768722	-1.099723
C	-4.883163	4.405851	1.219407
C	-6.197687	3.644649	-1.099662
C	-5.698409	3.283380	1.219475
C	-6.304823	2.823640	0.037762
C	3.441425	-5.990716	0.038020
C	2.871930	-6.591218	-1.099646
C	2.680791	-6.006278	1.219828
C	1.550559	-7.020217	-1.099740
C	1.361333	-6.434769	1.219729
C	0.736800	-6.868972	0.037833
C	-0.736820	-6.868969	-0.037834
C	-1.550583	-7.020217	1.099741
C	-1.361356	-6.434765	-1.219731
C	-2.871948	-6.591217	1.099645
C	-2.680805	-6.006273	-1.219829
C	-3.441442	-5.990707	-0.038021
C	-6.759936	1.421997	-0.037638
C	-7.154187	0.694623	1.100246
C	-6.541021	0.693643	-1.219618
C	-7.154189	-0.694599	1.100250
C	-6.541022	-0.693619	-1.219618
C	-6.759939	-1.421973	-0.037642
C	-6.304834	-2.823618	0.037759
C	-6.197694	-3.644624	-1.099663
C	-5.698433	-3.283369	1.219470
C	-5.381233	-4.768701	-1.099727
C	-4.883188	-4.405843	1.219405
C	-4.633660	-5.124610	0.037647
H	6.716188	3.367695	2.013443
H	5.278092	5.347431	2.013462
H	4.323582	4.645109	-2.118328
H	5.752938	2.677381	-2.118517
H	3.454082	6.671494	-2.013485
H	3.081418	5.548384	2.118890
H	1.126717	7.427108	-2.013640
H	0.768037	6.299612	2.118709
H	6.230516	1.216015	2.119177
H	7.409921	1.223391	-2.014310
H	6.230515	-1.216029	2.119180
H	7.409920	-1.223408	-2.014312
H	6.716162	-3.367702	2.013444
H	5.752949	-2.677409	-2.118514
H	5.278065	-5.347430	2.013465
H	4.323594	-4.645130	-2.118330
H	-1.126702	7.427121	2.013642
H	-0.768025	6.299613	-2.118709
H	-3.454070	6.671510	2.013488
H	-3.081407	5.548392	-2.118886
H	-5.278081	5.347448	-2.013457
H	-4.323545	4.645106	2.118330
H	-6.716183	3.367715	-2.013437
H	-5.752909	2.677375	2.118517
H	3.454053	-6.671477	-2.013490
H	3.081414	-5.548432	2.118888
H	1.126695	-7.427084	-2.013644
H	0.768041	-6.299651	2.118710
H	-1.126718	-7.427092	2.013647
H	-0.768060	-6.299651	-2.118710
H	-3.454076	-6.671476	2.013491
H	-3.081430	-5.548425	-2.118886
H	-7.409938	1.223414	2.014312
H	-6.230499	1.216036	-2.119175
H	-7.409944	-1.223390	2.014311
H	-6.230501	-1.216011	-2.119178
H	-6.716179	-3.367686	-2.013440
H	-5.752940	-2.677374	2.118515
H	-5.278088	-5.347423	-2.013460
H	-4.323585	-4.645104	2.118333

C_{60}(6)···[10]CPP (TPSS-D3(BJ))

C	1.808428	2.898788	0.950251
C	0.776628	3.461563	0.096395
C	-0.552758	3.468120	0.520272
C	-0.904846	2.914377	1.817704
C	0.088518	2.375357	2.639528
C	1.473516	2.369955	2.197823
C	2.770996	2.215331	0.103277
C	2.333390	2.354818	-1.275213
C	1.100659	3.124899	-1.279405
C	0.079648	2.805826	-2.177959
C	-1.613708	3.133762	-0.413892
C	-2.181814	2.234475	1.683220
C	-2.421650	1.046992	2.378478
C	-1.387890	0.486426	3.231935
C	-0.157577	1.137529	3.360084
C	1.074727	0.367357	3.364323
C	2.083149	1.128689	2.646472
C	3.007168	0.469484	1.831430
C	3.357351	1.024603	0.533889
C	2.498379	1.294303	-2.169659
C	3.108245	0.053569	-1.721355
C	3.526168	-0.078475	-0.395925
C	3.276323	-1.314228	0.324899
C	2.956302	-0.976618	1.701218
C	1.990392	-1.710408	2.393905
C	1.029234	-1.024215	3.240326
C	-0.250152	-1.700930	3.107301
C	-1.435022	-0.960495	3.103265
C	-2.618692	2.369898	0.304322
C	-2.770996	-2.215330	-0.103278
C	-3.357350	-1.024604	-0.533888
C	-3.007168	-0.469484	-1.831430
C	-2.083148	-1.128689	-2.646471
C	-1.473516	-2.369954	-2.197822
C	-0.776627	-3.461563	-0.096396
C	-1.100660	-3.124898	1.279404
C	-2.333389	-2.354818	1.275212
C	-2.498379	-1.294303	2.169659
C	-3.108245	-0.053570	1.721354
C	-3.526168	0.078474	0.395925
C	-2.956302	0.976618	-1.701219
C	-1.990392	1.710408	-2.393905
C	-1.029234	1.024215	-3.240326
C	-1.074727	-0.367357	-3.364323
C	0.157577	-1.137529	-3.360084
C	-0.088518	-2.375356	-2.639527
C	0.904846	-2.914376	-1.817703
C	0.552757	-3.468120	-0.520271
C	-0.079648	-2.805826	2.177959
C	1.305213	-2.811966	1.736729
C	1.613708	-3.133761	0.413892
C	2.618692	-2.369898	-0.304322
C	2.181814	-2.234475	-1.683221
C	2.421650	-1.046992	-2.378478
C	1.387890	-0.486426	-3.231935
C	1.435022	0.960494	-3.103265
C	0.250151	1.700931	-3.107302
C	-3.276323	1.314228	-0.324898
C	-1.305213	2.811966	-1.736730
C	-1.808428	-2.898788	-0.950251
C	-5.038822	5.006096	-1.162835
C	-3.964283	5.884243	-1.186051
C	-3.164090	6.088383	-0.046031
C	-3.606589	5.511683	1.156175
C	-4.679493	4.631001	1.178546
C	-5.366138	4.285469	0.001148
C	-1.794899	6.631259	-0.133438
C	-1.097211	7.106045	0.992492
C	-1.054000	6.438739	-1.312345
C	0.287516	7.214942	0.986981
C	0.328639	6.546246	-1.317457
C	1.040675	6.852272	-0.144360
C	-6.162124	3.043841	-0.038848
C	-6.181356	2.270342	-1.212818
C	-6.688060	2.450984	1.124434
C	-6.533157	0.927613	-1.186399
C	-7.036103	1.107707	1.151943
C	-6.879058	0.290157	0.016804
C	-6.796300	-1.179982	0.111565
C	-6.931402	-2.018319	-1.010361
C	-6.309246	-1.764177	1.293627
C	-6.443287	-3.318751	-0.998723
C	-5.819862	-3.061807	1.304658
C	-5.794534	-3.841263	0.134783
C	2.474965	6.514170	-0.069132
C	3.287699	6.435161	-1.215571
C	2.996338	5.982383	1.122439
C	4.460841	5.693029	-1.213117
C	4.169455	5.240000	1.124801
C	4.876695	4.994419	-0.064231
C	5.794534	3.841263	-0.134783
C	6.443287	3.318751	0.998723
C	5.819863	3.061806	-1.304659
C	6.931401	2.018319	1.010361
C	6.309246	1.764177	-1.293627
C	6.796300	1.179982	-0.111565
C	-4.876694	-4.994419	0.064231
C	-4.460842	-5.693029	1.213117
C	-4.169456	-5.239998	-1.124801
C	-3.287698	-6.435162	1.215570
C	-2.996336	-5.982383	-1.122438
C	-2.474965	-6.514170	0.069132
C	-1.040675	-6.852271	0.144360
C	-0.287517	-7.214942	-0.986981
C	-0.328640	-6.546246	1.317457
C	1.097212	-7.106045	-0.992492
C	1.054001	-6.438739	1.312345
C	1.794898	-6.631259	0.133438
C	6.879058	-0.290157	-0.016804
C	7.036103	-1.107707	-1.151943

C	6.533157	-0.927613	1.186400
C	6.688060	-2.450984	-1.124434
C	6.181356	-2.270342	1.212818
C	6.162124	-3.043841	0.038848
C	5.366138	-4.285470	-0.001148
C	5.038823	-5.006096	1.162835
C	4.679494	-4.631001	-1.178546
C	3.964283	-5.884243	1.186051
C	3.606588	-5.511683	-1.156175
C	3.164090	-6.088383	0.046031
H	-5.598129	4.834255	-2.078018
H	-3.707054	6.378235	-2.118701
H	-3.018848	5.639866	2.059954
H	-4.896096	4.100128	2.100165
H	-1.641885	7.342617	1.902254
H	-1.551518	6.065547	-2.201887
H	0.795975	7.533059	1.892889
H	0.871446	6.253848	-2.210831
H	-5.783136	2.684571	-2.133616
H	-6.772416	3.035570	2.036065
H	-6.397896	0.335603	-2.086383
H	-7.383311	0.671714	2.084354
H	-7.375987	-1.629114	-1.922050
H	-6.182870	-1.151245	2.180405
H	-6.516077	-3.918631	-1.901669
H	-5.324460	-3.425267	2.199519
H	2.964614	6.910264	-2.137609
H	2.402864	6.022479	2.030749
H	5.031369	5.602701	-2.133235
H	4.456827	4.721891	2.034662
H	6.516077	3.918631	1.901669
H	5.324460	3.425267	-2.199519
H	7.375987	1.629113	1.922051
H	6.182870	1.151244	-2.180405
H	-5.031369	-5.602701	2.133234
H	-4.456827	-4.721891	-2.034662
H	-2.964614	-6.910264	2.137608
H	-2.402864	-6.022479	-2.030749
H	-0.795975	-7.533059	-1.892889
H	-0.871446	-6.253848	2.210831
H	1.641884	-7.342617	-1.902254
H	1.551518	-6.065547	2.201887
H	7.383311	-0.671714	-2.084354
H	6.397896	-0.335603	2.086383
H	6.772416	-3.035570	-2.036066
H	5.783136	-2.684571	2.133616
H	5.598129	-4.834255	2.078018
H	4.896096	-4.100128	-2.100165
H	3.707054	-6.378235	2.118701
H	3.018848	-5.639866	-2.059954

C_{60} (B97-D2)

C	0.9988738	0.7257243	3.3275322
C	0.9988738	-0.7257243	3.3275322
C	1.9611150	-1.4248334	2.5924453
C	2.9599887	-0.6991091	1.8293737
C	2.9599887	0.6991091	1.8293737
C	1.9611150	1.4248334	2.5924453
C	-0.3815358	1.1742466	3.3275322
C	-1.2346759	0.0000000	3.3275322
C	-0.3815358	-1.1742466	3.3275322
C	-0.7490793	-2.3054289	2.5924453
C	1.5795791	-2.5990800	1.8293737
C	3.1957909	-1.4248334	0.5946977
C	3.4229452	-0.7257243	-0.5946977
C	3.4229452	0.7257243	-0.5946977
C	3.1957909	1.4248334	0.5946977
C	2.3426508	2.5990800	0.5946977
C	1.5795791	2.5990800	1.8293737
C	0.2497945	3.0311532	1.8293737
C	-0.7490793	2.3054289	2.5924453
C	-2.4240714	0.0000000	2.5924453
C	-2.8056072	1.1742466	1.8293737
C	-1.9837552	2.3054289	1.8293737
C	-1.7479531	3.0311532	0.5946977
C	-0.3675434	3.4796755	0.5946977
C	0.3675434	3.4796755	-0.5946977
C	1.7479531	3.0311532	-0.5946977
C	1.9837552	2.3054289	-1.8293737
C	2.8056072	1.1742466	-1.8293737
C	2.3426508	-2.5990800	0.5946977
C	0.3815358	-1.1742466	-3.3275322
C	0.7490793	-2.3054289	-2.5924453
C	-0.2497945	-3.0311532	-1.8293737
C	-1.5795791	-2.5990800	-1.8293737
C	-1.9611150	-1.4248334	-2.5924453
C	-0.9988738	0.7257243	-3.3275322
C	0.3815358	1.1742466	-3.3275322
C	1.2346759	0.0000000	-3.3275322
C	2.4240714	0.0000000	-2.5924453
C	2.8056072	-1.1742466	-1.8293737
C	1.9837552	-2.3054289	-1.8293737
C	0.3675434	-3.4796755	-0.5946977
C	-0.3675434	-3.4796755	0.5946977
C	-1.7479531	-3.0311532	0.5946977
C	-2.3426508	-2.5990800	-0.5946977
C	-3.1957909	-1.4248334	-0.5946977
C	-2.9599887	-0.6991091	-1.8293737
C	-2.9599887	0.6991091	-1.8293737
C	-1.9611150	1.4248334	-2.5924453
C	0.7490793	2.3054289	-2.5924453
C	-0.2497945	3.0311532	-1.8293737
C	-1.5795791	2.5990800	-1.8293737
C	-2.3426508	2.5990800	-0.5946977
C	-3.1957909	1.4248334	-0.5946977
C	-3.4229452	0.7257243	0.5946977
C	-3.4229452	-0.7257243	0.5946977
C	-2.8056072	-1.1742466	1.8293737
C	-1.9837552	-2.3054289	1.8293737
C	1.7479531	-3.0311532	-0.5946977
C	0.2497945	-3.0311532	1.8293737
C	-0.9988738	-0.7257243	-3.3275322

C_{60} (TPSS-D3(BJ))

C	0.3834385	0.7634533	3.3084320
C	0.5654300	-0.6778282	3.3277211
C	1.6028546	-1.2605220	2.5967670
C	2.5001962	-0.4254126	1.8168139
C	2.3252860	0.9599316	1.7982013
C	1.2459366	1.5661192	2.5588314
C	-1.0436781	1.0358487	3.3115356
C	-1.7437323	-0.2370796	3.3328365
C	-0.7492163	-1.2962665	3.3427950
C	-0.9755112	-2.4733770	2.6263400
C	1.3673050	-2.4850572	1.8511247
C	2.8192232	-1.1337986	0.5890547
C	2.9511237	-0.4294443	-0.6095288
C	2.7692265	1.0119217	-0.6289485
C	2.4624670	1.6927967	0.5511239
C	1.4678241	2.7518614	0.5411063
C	0.7159795	2.6735693	1.7819063
C	-0.6557103	2.9354371	1.7849497
C	-1.5530035	2.1003937	2.5649554
C	-2.9259278	-0.3961129	2.6067785
C	-3.4557429	0.7114716	1.8298510
C	-2.7829417	1.9350063	1.8094325
C	-2.6457589	2.6678639	0.5624575
C	-1.3310520	3.2861510	0.5473119
C	-0.6084840	3.3613763	-0.6453038
C	0.8186748	3.0889217	-0.6484805
C	1.1379095	2.3806510	-1.8762264
C	2.0939334	1.3626917	-1.8666773
C	2.1190174	-2.4066502	0.6103245
C	-0.0238773	-1.2940160	-3.3167626
C	0.4853548	-2.3586137	-2.5702681
C	-0.4118939	-3.1938363	-1.7903364
C	-1.7836101	-2.9320250	-1.7872241
C	-2.3133722	-1.8243032	-2.5639630
C	-1.6329973	0.4197025	-3.3328125
C	-0.3183406	1.0381102	-3.3481317
C	0.6761731	-0.0210752	-3.3381994
C	1.8584789	0.1379641	-2.6121936
C	2.3881793	-0.9696109	-1.8351964
C	1.7152454	-2.1930779	-1.8147048
C	0.2634238	-3.5443706	-0.5526298
C	-0.4591095	-3.6196562	0.6399686
C	-1.8863371	-3.3473646	0.6431869
C	-2.5354508	-3.0103376	-0.5464230
C	-3.5298811	-1.9510184	-0.5563747

C	-3.3925867	-1.2180188	-1.8032753
C	-3.5675471	0.1673233	-1.8219044
C	-2.6703696	1.0024519	-2.6019267
C	-0.0920962	2.2152757	-2.6317482
C	-1.1714293	2.8214606	-1.8710079
C	-2.4350032	2.2271572	-1.8564365
C	-3.1867580	2.1487942	-0.6156353
C	-3.8867637	0.8757939	-0.5943042
C	-4.0185781	0.1713543	0.6041808
C	-3.8366091	-1.2700259	0.6235599
C	-3.1613838	-1.6208033	1.8612446
C	-2.2055004	-2.6388880	1.8708375
C	1.5780120	-2.9258290	-0.5677000
C	0.1037784	-3.0795183	1.8656093
C	-1.4509931	-1.0215869	-3.3134849

$Li^{+}@C_{60}$(R6) (B97-D2)

C	-1.835945	-1.174501	2.799470
C	-2.609710	-1.714909	1.696763
C	-1.858564	-2.813422	1.117068
C	-0.619712	-2.952113	1.861804
C	-0.606103	-1.938827	2.901859
C	0.589250	-1.298276	3.239470
C	1.816085	-1.644694	2.544570
C	1.803218	-2.621317	1.544899
C	0.562457	-3.289228	1.197396
C	2.558294	-2.413912	0.322232
C	3.307124	-1.245758	0.145277
C	3.319147	-0.233343	1.184181
C	2.586278	-0.428513	2.359869
C	3.321842	-0.574189	-1.146142
C	3.332373	0.863370	-0.898544
C	3.326728	1.067293	0.542455
C	2.597593	2.122466	1.100607
C	1.836642	3.011942	0.243624
C	1.831649	2.815549	-1.141609
C	2.596551	1.725808	-1.729507
C	0.610852	3.363296	0.937399
C	-0.581071	3.494989	0.219752
C	-0.589746	3.284090	-1.216083
C	0.593848	2.952751	-1.884560
C	1.821010	1.183472	-2.840487
C	0.581169	1.942010	-2.925390
C	-0.617068	1.298394	-3.252935
C	-1.847666	1.646671	-2.565482
C	-1.833060	2.621078	-1.563806
C	1.810638	-0.202916	-3.080157
C	2.575583	-1.098273	-2.216825
C	-2.619994	0.431093	-2.385701
C	-1.867173	-0.667871	-2.962060
C	-0.629065	-0.131375	-3.497816
C	0.557317	-0.867773	-3.407843
C	-3.346207	0.235254	-1.207916
C	-3.332609	1.248503	-0.167837
C	-2.592425	2.421062	-0.342487
C	-1.818513	2.961251	0.759956
C	1.842672	1.923430	2.324518
C	0.614486	2.690035	2.223288
C	-0.575089	2.170700	2.740608
C	-1.813958	2.309176	1.995965
C	1.836231	0.669460	2.941503
C	0.549781	-2.167207	-2.762923
C	-0.641388	-2.682025	-2.239375
C	-1.872197	-1.920421	-2.342652
C	1.784899	-2.953508	-0.780177
C	1.788323	-2.307262	-2.021292
C	-3.352694	-1.066826	-0.565111
C	-2.631903	-2.126357	-1.122667
C	-2.585241	1.093178	2.178564
C	-3.330457	0.572653	1.116752
C	0.551229	-3.494870	-0.239441
C	-0.640724	-3.360114	-0.956366
C	-3.342901	-0.857814	0.871307
C	-1.870717	-3.016264	-0.265648
C	0.601765	0.132122	3.484747
C	-0.581618	0.868692	3.383427
C	-1.823943	0.203163	3.035819
Li	1.083837	0.120419	-0.886307

$Li^{+}@C_{60}$(R6) (TPSS-D3(BJ))

C	-1.834995	-1.173630	2.799002
C	-2.609542	-1.714483	1.695444
C	-1.857527	-2.813794	1.114990
C	-0.617793	-2.952837	1.860457
C	-0.603832	-1.938449	2.900996
C	0.590236	-1.298875	3.237923
C	1.818900	-1.646843	2.544380
C	1.805778	-2.624188	1.546476
C	0.562831	-3.291461	1.197683
C	2.564194	-2.419720	0.323392
C	3.314717	-1.251899	0.152073
C	3.330196	-0.234990	1.192090
C	2.592187	-0.429344	2.363048
C	3.308127	-0.574729	-1.137667
C	3.320211	0.861695	-0.891034
C	3.334891	1.070383	0.550423
C	2.603809	2.126882	1.103194
C	1.840254	3.019347	0.243637
C	1.831658	2.827542	-1.141819
C	2.584070	1.722472	-1.720075
C	0.611344	3.367370	0.937444
C	-0.579520	3.497931	0.219263
C	-0.590342	3.290527	-1.219438
C	0.592080	2.965587	-1.890151
C	1.807352	1.179918	-2.827670
C	0.575340	1.950254	-2.931783
C	-0.619702	1.301912	-3.260567
C	-1.850124	1.649054	-2.568835
C	-1.833735	2.622569	-1.567239
C	1.795751	-0.203636	-3.065484

C	2.560336	-1.097530	-2.204508
C	-2.622047	0.431187	-2.387475
C	-1.870115	-0.669533	-2.966204
C	-0.632084	-0.132668	-3.506393
C	0.550752	-0.873864	-3.416133
C	-3.345401	0.235513	-1.210054
C	-3.331235	1.249652	-0.169192
C	-2.591852	2.420587	-0.343973
C	-1.817177	2.961259	0.759405
C	1.845389	1.924999	2.326646
C	0.615089	2.691409	2.223792
C	-0.572966	2.171424	2.739268
C	-1.812720	2.309964	1.993898
C	1.839062	0.671055	2.941851
C	0.547113	-2.178322	-2.772441
C	-0.642593	-2.687907	-2.244742
C	-1.873312	-1.921253	-2.346452
C	1.788013	-2.961562	-0.782289
C	1.786856	-2.318867	-2.024691
C	-3.351297	-1.067533	-0.566664
C	-2.631537	-2.125687	-1.123784
C	-2.585027	1.093071	2.177081
C	-3.329328	0.573255	1.116658
C	0.551335	-3.499862	-0.240508
C	-0.639557	-3.363376	-0.957658
C	-3.341805	-0.858454	0.871057
C	-1.869533	-3.016415	-0.265984
C	0.602726	0.132794	3.483391
C	-0.579274	0.868278	3.382291
C	-1.822974	0.202288	3.035010
Li	1.109760	0.131025	-0.881351

$Na^+@C_{60}$(R6) (B97-D2)

C	-1.830607	-1.174107	2.795007
C	-2.604257	-1.714568	1.691956
C	-1.852346	-2.812683	1.111982
C	-0.613603	-2.950858	1.856507
C	-0.600412	-1.938191	2.896914
C	0.595255	-1.297297	3.233398
C	1.822193	-1.643292	2.538662
C	1.809623	-2.618615	1.538324
C	0.568967	-3.286254	1.191278
C	2.565898	-2.412012	0.316145
C	3.313640	-1.243829	0.138429
C	3.324565	-0.231956	1.177777
C	2.592494	-0.427369	2.353703
C	3.323197	-0.570794	-1.150467
C	3.334220	0.862856	-0.903764
C	3.332929	1.068461	0.535514
C	2.604576	2.122930	1.094560
C	1.844248	3.012370	0.237935
C	1.839957	2.814735	-1.146487
C	2.600214	1.722481	-1.731946
C	0.617744	3.362614	0.931467
C	-0.574151	3.495212	0.214611
C	-0.581854	3.284023	-1.221044
C	0.601659	2.951882	-1.888836
C	1.826473	1.181336	-2.839182
C	0.590033	1.941446	-2.929991
C	-0.607873	1.299178	-3.258192
C	-1.838007	1.646657	-2.569678
C	-1.824979	2.621195	-1.568614
C	1.815947	-0.200482	-3.077787
C	2.578542	-1.093077	-2.217068
C	-2.610613	0.431660	-2.389566
C	-1.857705	-0.666498	-2.966558
C	-0.619925	-0.130180	-3.503265
C	0.566368	-0.865518	-3.412354
C	-3.338942	0.235886	-1.212752
C	-3.326151	1.248983	-0.172886
C	-2.584821	2.420924	-0.347806
C	-1.811384	2.961246	0.754752
C	1.848712	1.923110	2.317799
C	0.620444	2.689134	2.216960
C	-0.569438	2.170904	2.735599
C	-1.808094	2.309600	1.991173
C	1.842259	0.670087	2.935864
C	0.558015	-2.164915	-2.767260
C	-0.632973	-2.680245	-2.244606
C	-1.863833	-1.918960	-2.347682
C	1.792997	-2.951638	-0.786026
C	1.796879	-2.304381	-2.025902
C	-3.346255	-1.066083	-0.570268
C	-2.624048	-2.124748	-1.128007
C	-2.580018	1.093775	2.174007
C	-3.325095	0.573273	1.111993
C	0.558715	-3.491879	-0.245210
C	-0.633167	-3.358351	-0.961766
C	-3.337457	-0.857398	0.866392
C	-1.863095	-3.014702	-0.271039
C	0.607676	0.132958	3.478904
C	-0.576096	0.869285	3.378757
C	-1.818698	0.203624	3.031455
Na	0.682865	0.068550	-0.591804

$Na^+@C_{60}$(C) (TPSS-D3(BJ))

C	-1.8197596	-1.1735054	2.7876699
C	-2.5950909	-1.7152484	1.6821539
C	-1.8418416	-2.8164027	1.1016329
C	-0.6008536	-2.9551694	1.8483975
C	-0.5872565	-1.9398445	2.8903708
C	0.6084318	-1.2985615	3.2256513
C	1.8394329	-1.6463883	2.5327151
C	1.8264921	-2.6220120	1.5317092
C	0.5817693	-3.2894429	1.1827029
C	2.5862188	-2.4184224	0.3074998
C	3.3287750	-1.2471647	0.1324742
C	3.3423584	-0.2317084	1.1744834
C	2.6127842	-0.4273480	2.3506336
C	3.3265848	-0.5698780	-1.1551505

C	3.3387121	0.8640312	-0.9089366
C	3.3486463	1.0730753	0.5308751
C	2.6251535	2.1308918	1.0884838
C	1.8620118	3.0230669	0.2291499
C	1.8523838	2.8222633	-1.1539901
C	2.6056227	1.7211407	-1.7345153
C	0.6308244	3.3707334	0.9220414
C	-0.5613008	3.5039818	0.2047375
C	-0.5711618	3.2952832	-1.2350932
C	0.6114395	2.9610336	-1.9007966
C	1.8303050	1.1794693	-2.8401097
C	0.5977848	1.9457859	-2.9428383
C	-0.5979491	1.3045412	-3.2782390
C	-1.8289521	1.6523592	-2.5852724
C	-1.8159223	2.6278857	-1.5841560
C	1.8186837	-0.1980477	-3.0766534
C	2.5818323	-1.0902292	-2.2172514
C	-2.6023393	0.4332813	-2.4031979
C	-1.8489710	-0.6678595	-2.9836181
C	-0.6102162	-0.1293934	-3.5243154
C	0.5738219	-0.8654940	-3.4255595
C	-3.3318632	0.2376389	-1.2269424
C	-3.3182487	1.2530624	-0.1848399
C	-2.5756139	2.4242815	-0.3598769
C	-1.8000613	2.9657654	0.7456252
C	1.8656206	1.9271024	2.3125525
C	0.6330535	2.6933067	2.2096100
C	-0.5569930	2.1760220	2.7292254
C	-1.7980424	2.3150330	1.9825181
C	1.8594487	0.6738040	2.9310175
C	0.5675893	-2.1701420	-2.7816739
C	-0.6224739	-2.6874797	-2.2620867
C	-1.8550924	-1.9212357	-2.3650667
C	1.8107064	-2.9599393	-0.7979656
C	1.8086586	-2.3091709	-2.0349144
C	-3.3381460	-1.0671810	-0.5832697
C	-2.6146221	-2.1250038	-1.1409148
C	-2.5712215	1.0961256	2.1648471
C	-3.3160403	0.5757823	1.1028166
C	0.5719557	-3.4981694	-0.2571229
C	-0.6202155	-3.3649221	-0.9744610
C	-3.3282164	-0.8581243	0.8565937
C	-1.8514256	-3.0172348	-0.2815361
C	0.6206942	0.1353454	3.4717033
C	-0.5632877	0.8714236	3.3730400
C	-1.8080880	0.2039648	3.0241663
Na	0.0048790	0.0027340	-0.0267292

$K^+@C_{60}$(C) (B97-D2)

C	0.5950718	2.9533917	-1.8721968
C	1.8329786	2.8149773	-1.1270770
C	2.5844790	1.7163996	-1.7062165
C	-0.6142866	1.2990780	-3.2472503
C	-1.8423418	1.6460835	-2.5559394
C	-1.8294299	2.6218615	-1.5546957
C	-0.5876824	3.2878707	-1.2064550
C	1.8425750	3.0158510	0.2563432
C	0.6142417	3.3628839	0.9476803
C	-0.5780423	3.4959047	0.2301463
C	3.3176419	0.8591871	-0.8805087
C	3.3276578	1.0677926	0.5560151
C	-0.6265872	-0.1315518	-3.4927258
C	2.5607641	-1.0918562	-2.1883925
C	3.3056301	-0.5714022	-1.1261720
C	-2.6141717	0.4298961	-2.3745028
C	-1.8624817	-0.6687281	-2.9535172
C	-1.8138551	2.9589049	0.7696137
C	-2.5875788	2.4187476	-0.3333900
C	1.7894335	-2.3079153	-2.0065581
C	0.5513393	-2.1693191	-2.7517578
C	3.3211712	-0.2340381	1.1980864
C	3.3076364	-1.2470179	0.1585074
C	-3.3301863	1.2471884	-0.1583801
C	-3.3437215	0.2341959	-1.1979757
C	-0.6389848	-2.6867149	-2.2321732
C	-1.8686451	-1.9221487	-2.3347568
C	2.5650045	-2.4185780	0.3335167
C	1.7912767	-2.9587314	-0.7694811
C	1.8399018	0.6688796	2.9536262
C	2.5915913	-0.4297370	2.3746195
C	-0.5739207	2.1694796	2.7518936
C	-1.8120120	2.3080830	2.0067003
C	-3.3502113	-1.0676475	-0.5558911
C	-2.6263648	-2.1254973	-1.1135645
C	-0.5801825	0.8679061	3.3942546
C	0.6040053	0.1317066	3.4928425
C	1.8197608	-1.6459176	2.5560477
C	1.8068496	-2.6216853	1.5548184
C	0.5554627	-3.4957399	-0.2300156
C	-0.6368204	-3.3627389	-0.9475531
C	0.5651028	-3.2877070	1.2065787
C	0.5917076	-1.2989160	3.2473694
C	0.5576028	-0.8677489	-3.3941165
C	1.7994701	-0.2018154	-3.0458209
C	1.8110301	1.1759164	-2.8092623
C	0.5814989	1.9404606	-2.9117464
C	2.6037896	2.1256402	1.1136866
C	1.8460628	1.9222933	2.3348719
C	0.6164067	2.6868625	2.2322935
C	-1.8651555	-3.0157140	-0.2562132
C	-0.6176524	-2.9532435	1.8723309
C	-1.8555571	-2.8148395	1.1272121
C	-3.3401938	-0.8590441	0.8806474
C	-3.3281806	0.5715637	1.1263130
C	-2.6070553	-1.7162513	1.7063539
C	-2.5833369	1.0920168	2.1885330
C	-1.8220499	0.2019753	3.0459678
C	-0.6040790	-1.9403092	2.9118821
C	-1.8336077	-1.1757691	2.8094069
K	-0.0111167	0.0002854	0.0000322

$K^+@C_{60}$(R5) (TPSS-D3(BJ))

C	0.586766	2.959153	-1.875827
C	1.824800	2.816614	-1.127311
C	2.577153	1.716182	-1.705855
C	-0.622447	1.302249	-3.253030
C	-1.853407	1.649947	-2.559479
C	-1.840339	2.625577	-1.558253
C	-0.595784	3.293782	-1.209286
C	1.834074	3.017289	0.256088
C	0.605766	3.368901	0.949634
C	-0.586075	3.502741	0.231192
C	3.314658	0.860230	-0.881488
C	3.324521	1.069017	0.556594
C	-0.634678	-0.132283	-3.499245
C	2.553067	-1.091637	-2.187969
C	3.302538	-0.571951	-1.127397
C	-2.625810	0.430547	-2.377257
C	-1.873397	-0.670860	-2.958027
C	-1.824809	2.963880	0.772165
C	-2.599128	2.421728	-0.333711
C	1.780772	-2.309319	-2.007418
C	0.542774	-2.173212	-2.756772
C	3.318075	-0.234306	1.199545
C	3.304584	-1.248470	0.158825
C	-3.339400	1.249759	-0.158675
C	-3.352950	0.234706	-1.200403
C	-0.646979	-2.691514	-2.236822
C	-1.879484	-1.924719	-2.339554
C	2.557127	-2.417736	0.333474
C	1.782753	-2.960089	-0.770235
C	1.831286	0.669560	2.954703
C	2.583675	-0.429557	2.373754
C	-0.581897	2.174323	2.756866
C	-1.822878	2.313132	2.009624
C	-3.359201	-1.069609	-0.556958
C	-2.638189	-2.128277	-1.114929
C	-0.588338	0.868983	3.400814
C	0.595428	0.131775	3.499353
C	1.811656	-1.646642	2.556753
C	1.798646	-2.622287	1.555573
C	0.546845	-3.502368	-0.230165
C	-0.645041	-3.369276	-0.948649
C	0.556638	-3.293601	1.208603
C	0.583257	-1.301060	3.253403
C	0.549052	-0.869439	-3.400038
C	1.791000	-0.201435	-3.047098
C	1.802834	1.176268	-2.810631
C	0.573174	1.944370	-2.917132
C	2.596093	2.125389	1.113465
C	1.837332	1.923211	2.336274
C	0.607844	2.691984	2.236305
C	-1.876158	-3.021166	-0.255385
C	-0.625887	-2.959375	1.875362
C	-1.866754	-2.820321	1.128146
C	-3.349588	-0.860711	0.882383
C	-3.337303	0.572721	1.128529
C	-2.619142	-1.718535	1.708667
C	-2.595142	1.093561	2.191522
C	-1.833034	0.201148	3.051473
C	-0.612339	-1.943449	2.917951
C	-1.844783	-1.176702	2.814892
K	0.507825	-0.003862	-0.003053

[10]CPP (B97-D2)

C	6.6281934	-2.8852949	1.0908711
C	7.0582548	-1.5617017	1.0908711
C	6.8887644	-0.7384879	-0.0416254
C	6.4440005	-1.3627011	-1.2235450
C	6.0142815	-2.6852401	-1.2235450
C	6.0071998	-3.4516649	-0.0416254
C	6.8887644	0.7384879	0.0416254
C	7.0582548	1.5617017	-1.0908711
C	6.4440005	1.3627011	1.2235450
C	6.6281934	2.8852949	-1.0908711
C	6.0142815	2.6852401	1.2235450
C	6.0071998	3.4516649	0.0416254
C	5.1390552	-4.6465634	0.0416254
C	4.4123303	-4.8901368	1.2235450
C	4.7923029	-5.4121813	-1.0908711
C	3.2873115	-5.7075108	1.2235450
C	3.6663873	-6.2302069	-1.0908711
C	2.8310890	-6.3233990	0.0416254
C	1.4264016	-6.7798096	-0.0416254
C	0.6958541	-7.1953916	1.0908711
C	0.6952999	-6.5497065	-1.2235450
C	-0.6958541	-7.1953916	1.0908711
C	-0.6952999	-6.5497065	-1.2235450
C	-1.4264016	-6.7798096	-0.0416254
C	5.1390552	4.6465634	-0.0416254
C	4.7923029	5.4121813	1.0908711
C	4.4123303	4.8901368	-1.2235450
C	3.6663873	6.2302069	1.0908711
C	3.2873115	5.7075108	-1.2235450
C	2.8310890	6.3233990	-0.0416254
C	1.4264016	6.7798096	0.0416254
C	0.6958541	7.1953916	-1.0908711
C	0.6952999	6.5497065	1.2235450
C	-0.6958541	7.1953916	-1.0908711
C	-0.6952999	6.5497065	1.2235450
C	-1.4264016	6.7798096	0.0416254
C	-2.8310890	-6.3233990	0.0416254
C	-3.6663873	-6.2302069	-1.0908711
C	-3.2873115	-5.7075108	1.2235450
C	-4.7923029	-5.4121813	-1.0908711
C	-4.4123303	-4.8901368	1.2235450
C	-5.1390552	-4.6465634	0.0416254
C	-6.0071998	-3.4516649	-0.0416254
C	-6.6281934	-2.8852949	1.0908711

C	-6.0142815	-2.6852401	-1.2235450
C	-7.0582548	-1.5617017	1.0908711
C	-6.4440005	-1.3627011	-1.2235450
C	-6.8887644	-0.7384879	-0.0416254
C	-2.8310890	6.3233990	-0.0416254
C	-3.6663873	6.2302069	1.0908711
C	-3.2873115	5.7075108	-1.2235450
C	-4.7923029	5.4121813	1.0908711
C	-4.4123303	4.8901368	-1.2235450
C	-5.1390552	4.6465634	-0.0416254
C	-6.0071998	3.4516649	0.0416254
C	-6.6281934	2.8852949	-1.0908711
C	-6.0142815	2.6852401	1.2235450
C	-7.0582548	1.5617017	-1.0908711
C	-6.4440005	1.3627011	1.2235450
C	-6.8887644	0.7384879	0.0416254
H	6.7162844	-3.4723135	2.0023928
H	7.4745629	-1.1385722	2.0023928
H	6.3065814	-0.7671546	-2.1224607
H	5.5530537	-3.0862745	-2.1224607
H	7.4745629	1.1385722	-2.0023928
H	6.3065814	0.7671546	2.1224607
H	6.7162844	3.4723135	-2.0023928
H	5.5530537	3.0862745	2.1224607
H	4.6512094	-4.3275566	2.1224607
H	5.3778124	-5.3145621	-2.0023928
H	2.6784482	-5.7608516	2.1224607
H	3.3926135	-6.7568936	-2.0023928
H	1.2269204	-7.4605699	2.0023928
H	1.2192335	-6.2349792	-2.1224607
H	-1.2269204	-7.4605699	2.0023928
H	-1.2192335	-6.2349792	-2.1224607
H	5.3778124	5.3145621	2.0023928
H	4.6512094	4.3275566	-2.1224607
H	3.3926135	6.7568936	2.0023928
H	2.6784482	5.7608516	-2.1224607
H	1.2269204	7.4605699	-2.0023928
H	1.2192335	6.2349792	2.1224607
H	-1.2269204	7.4605699	-2.0023928
H	-1.2192335	6.2349792	2.1224607
H	-3.3926135	-6.7568936	-2.0023928
H	-2.6784482	-5.7608516	2.1224607
H	-5.3778124	-5.3145621	-2.0023928
H	-4.6512094	-4.3275566	2.1224607
H	-6.7162844	-3.4723135	2.0023928
H	-5.5530537	-3.0862745	-2.1224607
H	-7.4745629	-1.1385722	2.0023928
H	-6.3065814	-0.7671546	-2.1224607
H	-3.3926135	6.7568936	2.0023928
H	-2.6784482	5.7608516	-2.1224607
H	-5.3778124	5.3145621	2.0023928
H	-4.6512094	4.3275566	-2.1224607
H	-6.7162844	3.4723135	-2.0023928
H	-5.5530537	3.0862745	2.1224607
H	-7.4745629	1.1385722	-2.0023928
H	-6.3065814	0.7671546	2.1224607

[10]CPP (TPSS-D3(BJ))

C	6.6126392	-2.8791881	1.0913864
C	7.0418152	-1.5575146	1.0913734
C	6.8736402	-0.7376548	-0.0401598
C	6.4293453	-1.3592868	-1.2201367
C	6.0004398	-2.6796824	-1.2201030
C	5.9947592	-3.4436846	-0.0401345
C	6.8736402	0.7376548	0.0401598
C	7.0418152	1.5575146	-1.0913734
C	6.4293453	1.3592868	1.2201367
C	6.6126392	2.8791881	-1.0913864
C	6.0004398	2.6796825	1.2201030
C	5.9947592	3.4436846	0.0401345
C	5.1276331	-4.6372211	0.0402586
C	4.4026948	-4.8788218	1.2201122
C	4.7817355	-5.3992587	-1.0912438
C	3.2794647	-5.6947781	1.2200263
C	3.6574952	-6.2160435	-1.0913438
C	2.8256941	-6.3095064	0.0401040
C	1.4226274	-6.7653498	-0.0402757
C	0.6947954	-7.1783755	1.0913102
C	0.6941575	-6.5350765	-1.2202705
C	-0.6947954	-7.1783755	1.0913103
C	-0.6941575	-6.5350765	-1.2202705
C	-1.4226274	-6.7653498	-0.0402757
C	5.1276331	4.6372211	-0.0402585
C	4.7817355	5.3992587	1.0912438
C	4.4026948	4.8788218	-1.2201122
C	3.6574952	6.2160435	1.0913438
C	3.2794648	5.6947781	-1.2200263
C	2.8256941	6.3095064	-0.0401040
C	1.4226274	6.7653498	0.0402757
C	0.6947954	7.1783755	-1.0913103
C	0.6941575	6.5350765	1.2202705
C	-0.6947954	7.1783755	-1.0913103
C	-0.6941575	6.5350765	1.2202705
C	-1.4226274	6.7653498	0.0402757
C	-2.8256941	-6.3095064	0.0401040
C	-3.6574952	-6.2160435	-1.0913438
C	-3.2794648	-5.6947781	1.2200263
C	-4.7817355	-5.3992587	-1.0912438
C	-4.4026948	-4.8788218	1.2201122
C	-5.1276331	-4.6372211	0.0402585
C	-5.9947592	-3.4436846	-0.0401345
C	-6.6126392	-2.8791881	1.0913864
C	-6.0004398	-2.6796825	-1.2201030
C	-7.0418152	-1.5575146	1.0913734
C	-6.4293453	-1.3592868	-1.2201367
C	-6.8736402	-0.7376548	-0.0401598
C	-2.8256941	6.3095064	-0.0401040
C	-3.6574952	6.2160435	1.0913438
C	-3.2794647	5.6947781	-1.2200263
C	-4.7817355	5.3992587	1.0912438
C	-4.4026948	4.8788218	-1.2201122

C	-5.1276331	4.6372211	-0.0402586
C	-5.9947592	3.4436847	0.0401345
C	-6.6126392	2.8791881	-1.0913864
C	-6.0004398	2.6796824	1.2201030
C	-7.0418152	1.5575146	-1.0913734
C	-6.4293453	1.3592868	1.2201367
C	-6.8736402	0.7376548	0.0401598
H	6.7064167	-3.4662125	2.0010474
H	7.4625561	-1.1375319	2.0010377
H	6.2918309	-0.7636252	-2.1177122
H	5.5391647	-3.0809129	-2.1176520
H	7.4625561	1.1375319	-2.0010377
H	6.2918309	0.7636252	2.1177122
H	6.7064167	3.4662125	-2.0010474
H	5.5391647	3.0809129	2.1176520
H	4.6415077	-4.3161315	2.1177140
H	5.3690339	-5.3068947	-2.0008667
H	2.6703731	-5.7480247	2.1174967
H	3.3883232	-6.7459455	-2.0010563
H	1.2241307	-7.4487222	2.0010368
H	1.2181452	-6.2205487	-2.1179701
H	-1.2241307	-7.4487222	2.0010367
H	-1.2181452	-6.2205487	-2.1179701
H	5.3690339	5.3068947	2.0008667
H	4.6415077	4.3161315	-2.1177140
H	3.3883233	6.7459455	2.0010563
H	2.6703731	5.7480246	-2.1174967
H	1.2241307	7.4487222	-2.0010367
H	1.2181452	6.2205487	2.1179701
H	-1.2241307	7.4487222	-2.0010368
H	-1.2181452	6.2205487	2.1179701
H	-3.3883233	-6.7459455	-2.0010563
H	-2.6703731	-5.7480246	2.1174967
H	-5.3690339	-5.3068947	-2.0008667
H	-4.6415077	-4.3161315	2.1177140
H	-6.7064167	-3.4662125	2.0010474
H	-5.5391647	-3.0809129	-2.1176520
H	-7.4625561	-1.1375319	2.0010377
H	-6.2918309	-0.7636252	-2.1177122
H	-3.3883232	6.7459455	2.0010563
H	-2.6703731	5.7480247	-2.1174967
H	-5.3690338	5.3068947	2.0008667
H	-4.6415077	4.3161315	-2.1177140
H	-6.7064167	3.4662125	-2.0010474
H	-5.5391647	3.0809129	2.1176520
H	-7.4625561	1.1375319	-2.0010377
H	-6.2918309	0.7636252	2.1177122

$Li^+@C_{60}$(6)···[10]CPP···BF_4^- (B97-D2)

C	-1.457048	-3.180543	-0.165838
C	-0.718357	-3.129973	-1.414281
C	-1.426194	-2.240545	-2.317820
C	-2.602868	-1.742249	-1.627430
C	-2.621394	-2.324417	-0.296605
C	-3.051505	-1.562823	0.795090
C	-3.482396	-0.192082	0.599768
C	-3.462782	0.367462	-0.679939
C	-3.015898	-0.420392	-1.814214
C	-2.994136	1.727313	-0.867572
C	-2.557307	2.472343	0.231456
C	-2.584736	1.893665	1.562890
C	-3.036506	0.584321	1.742415
C	-1.370523	3.297046	0.123033
C	-0.661896	3.230904	1.384255
C	-1.409360	2.360315	2.275207
C	-0.730764	1.502740	3.145315
C	0.719850	1.485095	3.157455
C	1.438118	2.328030	2.301151
C	0.736346	3.224350	1.398587
C	1.150860	0.114401	3.353691
C	2.283697	-0.365263	2.691076
C	3.026042	0.507599	1.801417
C	2.613531	1.830505	1.614034
C	1.481975	3.300705	0.151979
C	2.634362	2.422892	0.284003
C	3.061810	1.652566	-0.806349
C	3.490053	0.278709	-0.609890
C	3.474140	-0.281402	0.668645
C	0.796857	3.379108	-1.073980
C	-0.657804	3.363754	-1.077745
C	3.048104	-0.496811	-1.752607
C	2.341477	0.393481	-2.652170
C	2.354963	1.727647	-2.071095
C	1.243900	2.576109	-2.206078
C	2.600883	-1.809109	-1.575409
C	2.579749	-2.391385	-0.244874
C	3.008951	-1.642396	0.856118
C	2.273129	-1.694596	2.106002
C	-1.200231	0.142980	3.332119
C	-0.036622	-0.715086	3.459894
C	-0.046648	-1.995054	2.900435
C	1.129416	-2.493391	2.208245
C	-2.330707	-0.306475	2.644883
C	0.063489	2.085126	-2.906821
C	0.050815	0.803161	-3.463965
C	1.212835	-0.057791	-3.339374
C	-2.254531	1.781010	-2.113162
C	-1.109252	2.581356	-2.212248
C	1.426472	-2.277808	-2.289308
C	0.744646	-1.418742	-3.157756
C	0.681064	-3.267787	1.065089
C	1.393492	-3.220302	-0.137976
C	-2.268156	0.452561	-2.700272

C	-1.136616	-0.026666	-3.364652
C	0.680484	-3.150687	-1.400828
C	-0.707038	-1.399056	-3.173179
C	-2.341011	-1.634441	2.058845
C	-1.220407	-2.462570	2.184373
C	-0.770111	-3.248773	1.051019
Li	0.591324	1.273510	-0.388561
C	6.517985	1.310437	2.795195
C	6.954972	1.191778	1.481439
C	6.815760	-0.019725	0.772875
C	6.396732	-1.145719	1.509220
C	5.961971	-1.027488	2.824232
C	5.921226	0.223545	3.467872
C	6.822029	-0.074102	-0.701833
C	6.941734	-1.288383	-1.409097
C	6.435896	1.060995	-1.442224
C	6.515733	-1.397438	-2.727275
C	6.012025	0.952365	-2.761676
C	5.949620	-0.297747	-3.405693
C	5.054086	0.409242	4.647490
C	4.332491	1.610290	4.787320
C	4.712009	-0.651607	5.511058
C	3.219219	1.687783	5.613077
C	3.597260	-0.573407	6.339606
C	2.771252	0.568806	6.342155
C	1.376978	0.540700	6.825570
C	0.658546	1.720638	7.108845
C	0.638002	-0.654672	6.740437
C	-0.731193	1.734090	7.099432
C	-0.752146	-0.641119	6.730688
C	-1.468517	0.568485	6.805666
C	5.090099	-0.465117	-4.593778
C	4.775670	0.603389	-5.458617
C	4.346415	-1.651800	-4.741676
C	3.667537	0.547453	-6.297857
C	3.239561	-1.706816	-5.577805
C	2.820219	-0.578793	-6.310097
C	1.432076	-0.524117	-6.808573
C	0.695622	-1.690214	-7.103007
C	0.715313	0.685251	-6.732091
C	-0.694230	-1.677141	-7.113600
C	-0.674854	0.698234	-6.742578
C	-1.412878	-0.497492	-6.829479
C	-2.855197	0.623943	6.303324
C	-3.703742	-0.501409	6.290691
C	-3.270343	1.750785	5.567092
C	-4.809409	-0.557417	5.448093
C	-4.374496	1.695575	4.727508
C	-5.119157	0.509758	4.579951
C	-5.977939	0.342005	3.391572
C	-6.549830	1.440453	2.716573
C	-6.032617	-0.906659	2.744309
C	-6.977829	1.331914	1.398997
C	-6.457880	-1.014621	1.425408
C	-6.853228	0.119790	0.689256
C	-2.808101	-0.526309	-6.349217
C	-3.636384	0.614049	-6.353041
C	-3.253195	-1.642880	-5.614741
C	-4.752709	0.693164	-5.526754
C	-4.368498	-1.564576	-4.791660
C	-5.093684	-0.364727	-4.659443
C	-5.961478	-0.176430	-3.480755
C	-6.563407	-1.261507	-2.809961
C	-5.995406	1.074136	-2.835963
C	-6.997932	-1.142435	-1.495295
C	-6.427223	1.192542	-1.520120
C	-6.850237	0.067355	-0.785502
H	6.585699	2.275805	3.290699
H	7.356932	2.067055	0.977270
H	6.284034	-2.103275	1.008249
H	5.520778	-1.894041	3.309566
H	7.321417	-2.171652	-0.901087
H	6.341692	2.021888	-0.944086
H	6.568810	-2.363540	-3.223579
H	5.601029	1.830598	-3.252111
H	4.563281	2.453763	4.142756
H	5.295708	-1.569244	5.491390
H	2.613708	2.589246	5.588359
H	3.329274	-1.431696	6.951576
H	1.197272	2.651346	7.269866
H	1.151790	-1.590001	6.534602
H	-1.253885	2.675089	7.253287
H	-1.281504	-1.565960	6.517191
H	5.374056	1.510983	-5.431105
H	4.554387	-2.499962	-4.095118
H	3.421879	1.412413	-6.909253
H	2.614659	-2.595375	-5.559732
H	1.219414	-2.630441	-7.260129
H	1.243422	1.611421	-6.522598
H	-1.233691	-2.607178	-7.278185
H	-1.188861	1.633863	-6.539996
H	-3.461980	-1.364292	6.907273
H	-2.645318	2.638924	5.549396
H	-5.411897	-1.462771	5.421552
H	-4.580000	2.542828	4.079447
H	-6.605063	2.405410	3.214323
H	-5.610274	-1.781534	3.231746
H	-7.361006	2.214381	0.892819
H	-6.355403	-1.972014	0.921607
H	-3.368472	1.470949	-6.966469
H	-2.642626	-2.541097	-5.583080
H	-5.336993	1.610147	-5.510572
H	-4.598335	-2.404292	-4.141405
H	-6.637541	-2.225166	-3.308734
H	-5.552479	1.939614	-3.321100
H	-7.405500	-2.015436	-0.990776
H	-6.309409	2.148765	-1.018354
B	0.556043	6.786347	-1.268252
F	0.681667	7.238800	-2.592341
F	1.682089	5.945790	-0.946760
F	0.482039	7.843021	-0.349419
F	-0.642571	5.981041	-1.156598

$Li^+@C_{60}$(6)···[10]CPP···$TFPB^-$ (B97-D2)

C	-1.375938	-6.132060	-0.279072
C	-0.666274	-6.054587	-1.542955
C	-1.406770	-5.164266	-2.419392
C	-2.574884	-4.692130	-1.695238
C	-2.554200	-5.290706	-0.372231
C	-2.970726	-4.550358	0.739945
C	-3.423459	-3.183221	0.573041
C	-3.441261	-2.608047	-0.699618
C	-3.009184	-3.373415	-1.853607
C	-2.990731	-1.242097	-0.877155
C	-2.542080	-0.508562	0.221039
C	-2.531256	-1.100752	1.543841
C	-2.963157	-2.416110	1.716584
C	-1.370820	0.335344	0.097628
C	-0.632134	0.259724	1.340936
C	-1.349045	-0.626540	2.236615
C	-0.638198	-1.483998	3.079455
C	0.811524	-1.482398	3.057664
C	1.501078	-0.620173	2.198439
C	0.766347	0.273372	1.324003
C	1.265491	-2.848719	3.226263
C	2.389792	-3.303630	2.532118
C	3.100939	-2.409300	1.638900
C	2.665737	-1.090628	1.478308
C	1.485506	0.385121	0.063617
C	2.653927	-0.480682	0.158105
C	3.060889	-1.230634	-0.952249
C	3.513472	-2.599747	-0.785290
C	3.534451	-3.176929	0.486194
C	0.766151	0.465148	-1.145957
C	-0.688659	0.426893	-1.118400
C	3.055021	-3.365169	-1.927810
C	2.315289	-2.473519	-2.799560
C	2.322436	-1.150551	-2.200110
C	1.194863	-0.323749	-2.296815
C	2.630729	-4.686157	-1.759282
C	2.647476	-5.286697	-0.436720
C	3.093278	-4.547590	0.665329
C	2.384857	-4.626000	1.929854
C	-1.085051	-2.852091	3.258284
C	0.092288	-3.696159	3.348114
C	0.087099	-4.968472	2.771411
C	1.254180	-5.441462	2.046467
C	-2.224719	-3.308376	2.590762
C	0.009505	-0.814272	-2.980362
C	0.002156	-2.087168	-3.559794
C	1.178665	-2.931304	-3.469854
C	-2.282436	-1.161660	-2.139324
C	-1.151661	-0.347733	-2.253926
C	1.446867	-5.161709	-2.453630
C	0.734097	-4.301458	-3.296068
C	0.790557	-6.206944	0.903119
C	1.474895	-6.133235	-0.315098
C	-2.292160	-2.478693	-2.744308
C	-1.170604	-2.933092	-3.443046
C	0.732804	-6.056150	-1.560765
C	-0.718098	-4.301838	-3.278493
C	-2.230076	-4.628809	1.986061
C	-1.095992	-5.442709	2.074843
C	-0.660686	-6.207209	0.921113
Li	0.677750	-1.669525	-0.430881
C	6.648940	-1.164127	2.637501
C	7.075254	-1.304932	1.324225
C	6.915231	-2.523826	0.633832
C	6.506389	-3.640917	1.388667
C	6.083375	-3.500695	2.706460
C	6.046338	-2.236963	3.325796
C	6.880053	-2.580841	-0.839550
C	7.009739	-3.785898	-1.559119
C	6.444496	-1.448612	-1.556862
C	6.567852	-3.888690	-2.873823
C	6.003996	-1.551024	-2.869900
C	5.974240	-2.792492	-3.533439
C	5.165660	-2.017618	4.488171
C	4.426233	-0.821014	4.558786
C	4.825358	-3.043704	5.392000
C	3.301014	-0.719012	5.364876
C	3.699332	-2.939839	6.202563
C	2.860322	-1.808462	6.141203
C	1.463892	-1.827259	6.616559
C	0.730638	-0.640732	6.824486
C	0.741012	-3.035438	6.606144
C	-0.658310	-0.646564	6.824112
C	-0.649128	-3.041147	6.605900
C	-1.381949	-1.839071	6.615868
C	5.123996	-2.952019	-4.728296
C	4.781900	-1.860518	-5.552885
C	4.415051	-4.152857	-4.923567
C	3.670474	-1.910157	-6.385427
C	3.305133	-4.203043	-5.756773
C	2.850414	-3.054855	-6.434947
C	1.454893	-3.001389	-6.909039
C	0.728942	-4.162792	-7.242625
C	0.726012	-1.804855	-6.767978
C	-0.661189	-4.164843	-7.240499
C	-0.663529	-1.807024	-6.765268
C	-1.389664	-3.005794	-6.903736
C	-2.779594	-1.831127	6.144266
C	-3.609429	-2.969061	6.207892
C	-3.232107	-0.744137	5.371436
C	-4.740199	-3.079244	5.404846
C	-4.362590	-0.852250	4.573558
C	-5.094489	-2.053641	4.505905
C	-5.980122	-2.277427	3.347870
C	-6.592385	-1.207651	2.663362
C	-6.009179	-3.540312	2.726109
C	-7.018501	-1.348639	1.349972
C	-6.431801	-3.680458	1.408237
C	-6.848481	-2.564350	0.656659
C	-2.783474	-3.063782	-6.424314

C	-3.604827	-1.920396	-6.366441
C	-3.233342	-4.214998	-5.747812
C	-4.712364	-1.875508	-5.528673
C	-4.338707	-4.169228	-4.908242
C	-5.048602	-2.970289	-4.705914
C	-5.896932	-2.816325	-3.509098
C	-6.492413	-3.915392	-2.855953
C	-5.923411	-1.578601	-2.838901
C	-6.936519	-3.818412	-1.541492
C	-6.367452	-1.481664	-1.526794
C	-6.807907	-2.616430	-0.816703
H	6.715608	-0.190171	3.115269
H	7.469651	-0.438061	0.801956
H	6.388068	-4.604630	0.900429
H	5.644137	-4.356402	3.212849
H	7.413658	-4.666173	-1.064514
H	6.329549	-0.500417	-1.040521
H	6.637223	-4.846960	-3.383157
H	5.558305	-0.679421	-3.340173
H	4.654551	-0.005946	3.878209
H	5.419990	-3.954270	5.419340
H	2.686602	0.172630	5.288822
H	3.433625	-3.771407	6.851213
H	1.253096	0.307679	6.915988
H	1.267952	-3.974491	6.458563
H	-1.188567	0.297460	6.915496
H	-1.168314	-3.984491	6.458449
H	5.353574	-0.938227	-5.491004
H	4.650030	-5.020554	-4.313291
H	3.397075	-1.026061	-6.956035
H	2.703673	-5.107813	-5.773300
H	1.261766	-5.089485	-7.443352
H	1.244026	-0.884083	-6.513692
H	-1.191667	-5.093184	-7.439522
H	-1.183225	-0.888078	-6.508366
H	-3.333419	-3.800124	6.852919
H	-2.624576	0.151951	5.292148
H	-5.327866	-3.994259	5.433965
H	-4.600199	-0.037953	3.895562
H	-6.665200	-0.235019	3.142969
H	-5.561619	-4.393706	3.229213
H	-7.417993	-0.483275	0.828830
H	-6.303182	-4.641078	0.916378
H	-3.335733	-1.033689	-6.935034
H	-2.630830	-5.118914	-5.770272
H	-5.285347	-0.954544	-5.460452
H	-4.569045	-5.038906	-4.298994
H	-6.561559	-4.871080	-3.370189
H	-5.470233	-0.707021	-3.301854
H	-7.341342	-4.700710	-1.051163
H	-6.249729	-0.537182	-1.004207
B	0.032100	4.582736	-0.296963
C	0.038863	4.888946	1.320571
C	0.025472	6.174034	1.883552
H	0.011072	7.042428	1.229388
C	0.020581	6.377843	3.270914
C	0.035080	5.297365	4.154566
H	0.030142	5.454889	5.227039
C	0.051549	4.007723	3.618143
C	0.053644	3.818964	2.233698
H	0.064166	2.801949	1.852314
C	0.039992	7.798814	3.789858
F	1.257862	8.380850	3.588798
F	-0.219663	7.880297	5.121862
F	-0.874572	8.580180	3.156427
C	-0.036013	5.983554	-1.158186
C	-1.250603	6.684799	-1.267716
H	-2.146017	6.271265	-0.808996
C	-1.349943	7.895095	-1.958686
C	-0.225573	8.457305	-2.569721
H	-0.299254	9.392429	-3.113273
C	0.991757	7.784834	-2.465860
C	1.081164	6.572895	-1.768092
H	2.049927	6.083336	-1.705297
C	-2.682048	8.608300	-1.990419
F	-2.936065	9.237584	-0.805943
F	-3.715968	7.745209	-2.198410
F	-2.755210	9.555225	-2.962122
C	2.233255	8.313753	-3.144805
F	2.093866	9.584348	-3.601683
F	3.311518	8.305210	-2.311821
F	2.574096	7.541734	-4.221125
C	1.410596	3.744194	-0.709831
C	1.668838	3.361008	-2.040372
H	0.975028	3.637094	-2.825565
C	2.808253	2.640260	-2.415641
C	3.776565	2.299480	-1.471485
H	4.660859	1.741826	-1.755378
C	3.568298	2.698484	-0.152430
C	2.418245	3.410962	0.211540
H	2.314751	3.701193	1.251992
C	2.990986	2.269836	-3.868743
F	3.396110	3.327473	-4.616166
F	3.915845	1.280057	-4.046643
F	1.830756	1.817355	-4.430033
C	4.584639	2.381551	0.917255
F	3.995240	1.878942	2.044556
F	5.280269	3.481002	1.304074
F	5.501128	1.453643	0.516528
C	-1.338684	3.712343	-0.685763
C	-2.328129	3.361469	0.248076
H	-2.209546	3.637778	1.290742
C	-3.483066	2.652727	-0.108177
C	-3.706403	2.264591	-1.427359
H	-4.591731	1.705260	-1.704456
C	-2.753501	2.620607	-2.382275
C	-1.616624	3.348986	-2.017117
H	-0.939872	3.646224	-2.809701
C	-4.491397	2.336338	0.969020
F	-5.178818	3.440073	1.362060
F	-3.895734	1.831573	2.091532
F	-5.415544	1.414159	0.575397

C	-2.954893	2.264158	-3.836190
F	-3.875221	1.270891	-4.012544
F	-1.799700	1.827541	-4.420031
F	-3.378358	3.327798	-4.566646
C	0.051794	2.784362	4.496595
F	1.112484	1.960199	4.219829
F	0.107189	3.058232	5.822700
F	-1.068668	2.018450	4.299437