

Supporting Information
for
Fullerene Size Controls the Selective Complexation of
[11]CPP with Pristine and Endohedral Fullerenes.

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Table S1. Results of fitting the carbon atoms in the nanoring to an ellipse for the different complexes studied. Radii in Å; f is the flattening $f=(R_1-R_2)/R_1$.

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Table S2. Second order perturbation analysis obtained as the energies of delocalization of electrons from filled NBOs into empty NBOs (E_2). Values greater than 0.5 kcal/mol for the π donation from [11]-CPP to the fullerenes are shown.

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Figure S2. Energy profiles obtained upon rotation of the different fullerenes along the Euler angles. The values in the X-axis correspond to Euler angles α - β - γ .

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Figure S3. Energy profiles obtained upon rotation of the C_{60} . Upper plots correspond to displacements inside the nanoring using two different orientations for C_{60} as explained in the top figures. Bottom plots show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when C_{60} is rotated along an axis perpendicular to the nanoring.

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Figure S4. Performance of different DFT methods to reproduce the interaction energy in corannulene dimer. Adapted from *J. Phys. Chem. A* 2012, 116, 11920-11926, adding values obtained at the TPSS-D/def2-TZVP level.

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Figure S5. Energy profiles obtained upon rotation of the C_{70} . Top figures correspond to displacements inside the nanoring using three different orientations for C_{70} . Bottom ones show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when C_{70} is rotated along an axis perpendicular to the nanoring.

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Figure S6. Energy profiles obtained upon rotation of the $Sc_3N@C_{80}$. Top figures correspond to displacements inside the nanoring using three different orientations for $Sc_3N@C_{80}$. Bottom ones show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when $Sc_3N@C_{80}$ is rotated along an axis perpendicular to the nanoring.

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Figure S7. Other structures obtained for C₆₀ ([11]CPP-C₆₀-6) and C₇₆ ([11]CPP-C₇₆-b) mentioned in the text.

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Figure S8. NCI two-dimensional plots for the complexes with endohedral fullerenes. In green the results obtained for C₇₀ are shown as reference, displaced by 0.05 a.u. for clarity.

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Figure S9. Correlation between dispersion and total complexation energy. It can be observed that the main outlier is C₇₆. The almost isoenergetic structure C₇₆-b follows the global trend.

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Cartesian coordinates (Å) for isolated molecules.

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Cartesian coordinates (Å) for the complexes studied.

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Table S1. Results of fitting the carbon atoms in the nanoring to an ellipse for the different complexes studied. Radii in Å; f is the flattening $f=(R_1-R_2)/R_1$.

	R_1	R_2	f	1/f
[11]CPP-C ₆₀	15.8	14.2	0.101	10
[11]CPP-C ₇₀	15.5	14.6	0.057	18
[11]CPP-C ₇₆	15.5	14.7	0.055	18
[11]CPP-C ₇₈	15.3	14.7	0.039	26
[11]CPP-Sc ₃ N@C ₈₀	15.1	15.1	0.001	1514
[11]CPP-Y@C ₈₂	15.4	14.9	0.028	36
[11]CPP-Tm@C ₈₂	15.3	15.0	0.024	41
[11]CPP-Y ₂ @C ₈₂	15.2	15.1	0.004	253
[11]CPP-Lu ₂ @C ₈₂	15.2	15.1	0.008	127

Table S2. Second order perturbation analysis obtained as the energies of delocalization of electrons from filled NBOs into empty NBOs (E_2). Values greater than 0.5 kcal/mol for the π donation from [11]-CPP to the fullerenes are shown.

Donor	Acceptor	E_2 (kcal/mol)
	[11]CPP-C₇₀	
BD(2)C85-C86	BD*(2)C45-C46	0.54
	[11]CPP-C₇₆	
BD(2)C91-C92	BD*(2)C3-C48	0.89
BD(2)C100-C101	BD*(2)C35-C40	0.87
CR(1)C185	RY*(7)C75	0.53
	[11]CPP-C₇₈	
BD(2)C81-C82	BD*(2)C13-C15	0.80
BD(2)C83-C188	BD*(2)C1-C3	0.82
BD(2)C114-C115	BD*(2)C63-C64	0.81
BD(2)C116-C117	BD*(2)C58-C61	0.81
BD(2)C123-C124	BD*(2)C59-C60	0.62
BD(2)C126-C127	BD*(2)C46-C49	0.60
BD(2)C135-C136	BD*(2)C8-C10	0.57
BD(2)C138-C139	BD*(2)C2-C4	0.57
	[11]CPP-Sc₃N@C₈₀	
BD(2)C96-C101	BD*(2)C45-C64	0.52
BD(2)C102-C107	BD*(2)C43-C63	0.67
BD(2)C108-C109	BD*(2)C58-C59	0.73
	[11]CPP-Y₂@C₈₂	
BD(2)C87-C88	BD*(2)C75-C76	0.62
BD(2)C89-C150	LP(1)C77	1.37
BD(2)C90-C91	LP(1)C21	1.64
BD(2)C114-C119	LP*(1)C47	0.60
BD(2)C122-C123	BD*(2)C41-C59	0.54
BD(2)C129-C130	BD*(2)C39-C40	0.51
BD(2)C132-C133	LP(1)C45	1.22
BD(2)C141-C142	BD*(2)C42-C69	0.55
	[11]CPP-Lu₂@C₈₂	
BD(2)C87-C88	BD*(2)C75-C76	0.61
BD(2)C89-C194	LP(1)C77	1.26
BD(2)C90-C91	LP(1)C21	1.62
BD(2)C99-C100	BD*(2)C4-C5	0.51
BD(2)C114-C119	LP*(1)C47	0.66
BD(2)C122-C123	BD*(2)C41-C59	0.52

Table S3. Highest occupied and lowest unoccupied orbitals for the molecules considered in this work.

	HOMO(eV)	LUMO(eV)
[11]CPP	-4.848	-2.554
C₆₀	-5.757	-4.039
C₇₀	-5.753	-3.980
C₇₆	-5.293	-4.184
C₇₈	-5.209	-4.408
Sc₃N@C₈₀	-5.208	-3.691
Y₂@C₈₂	-4.355	-3.923
Lu₂@C₈₂	-5.000	-3.863
Y@C₈₂-α	-4.767	-4.011
Y@C₈₂-β	-5.333	-4.643
Tm@C₈₂-α	-5.302	-4.620
Tm@C₈₂-β	-4.895	-4.594

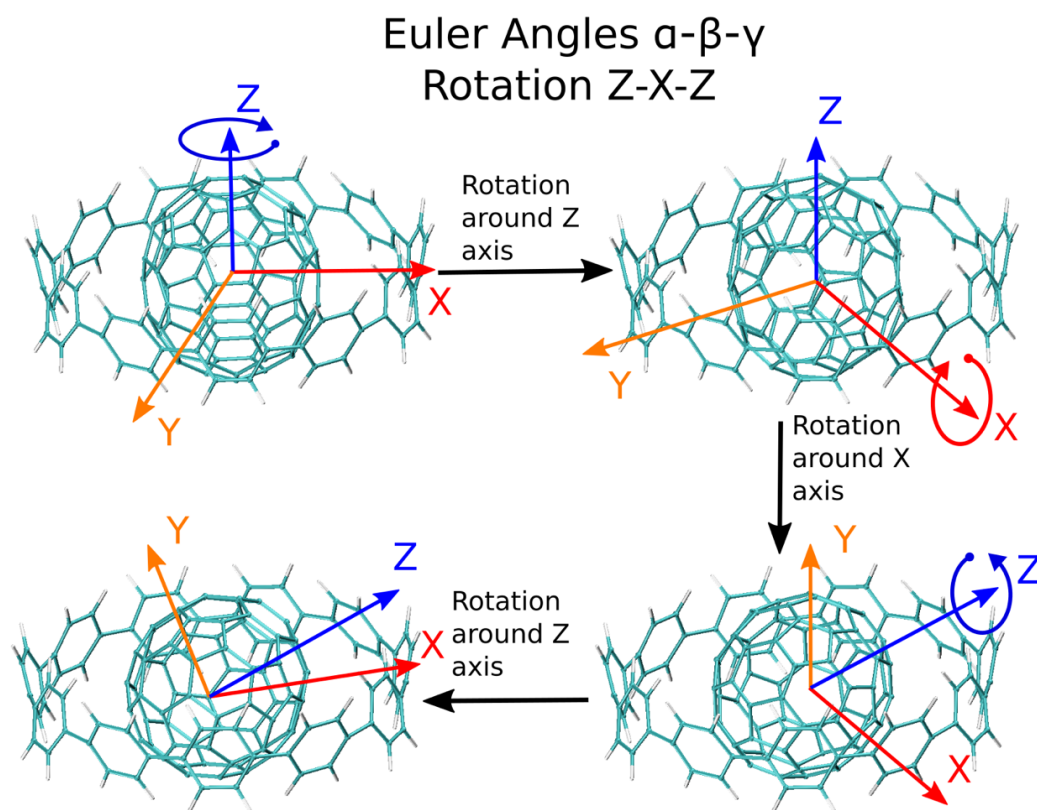


Figure S1. Diagram showing how the rotation along the Euler angles was performed.

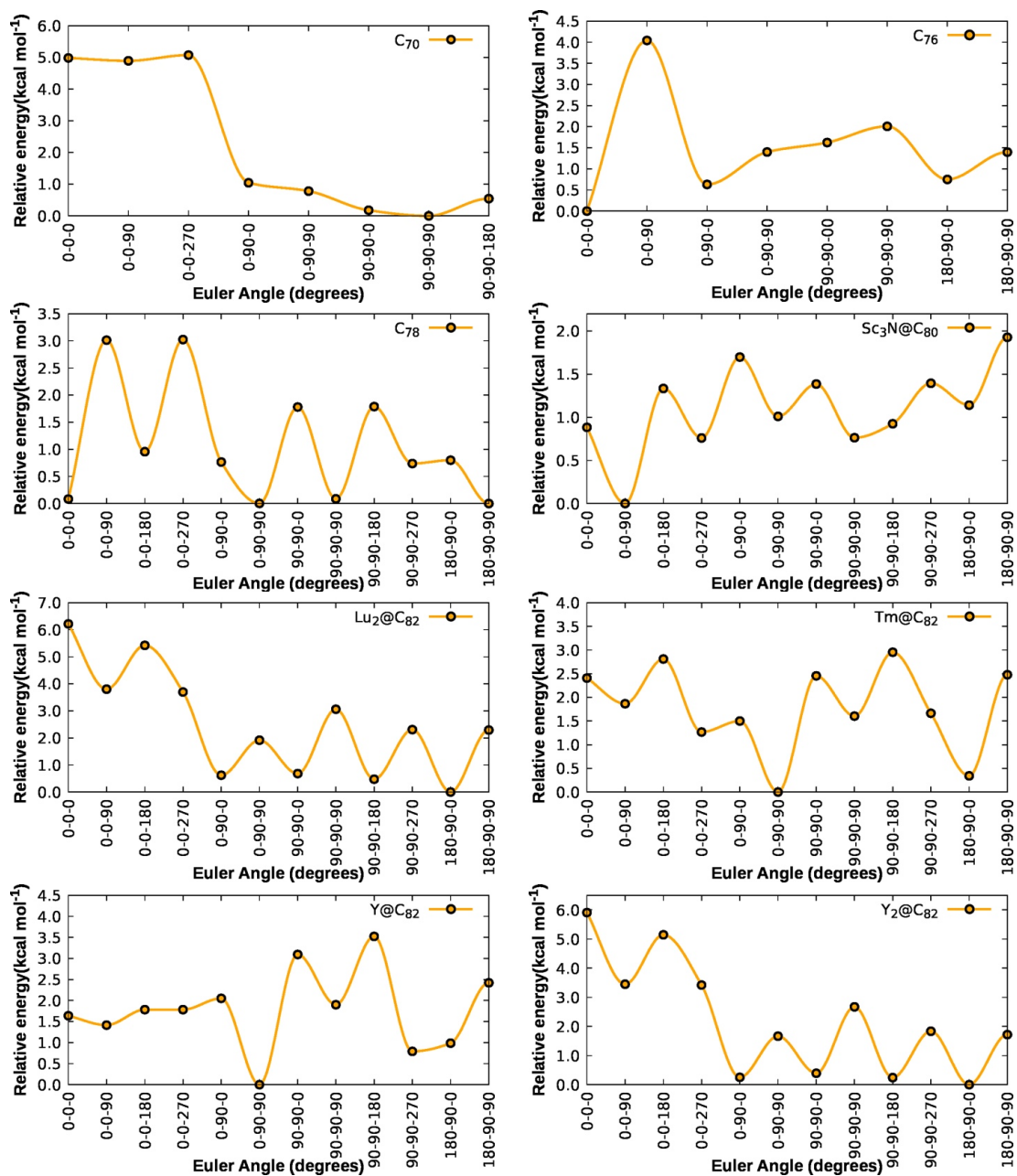


Figure S2. Energy profiles obtained upon rotation of the different fullerenes along the Euler angles. The values in the X-axis correspond to Euler angles α - β - γ .

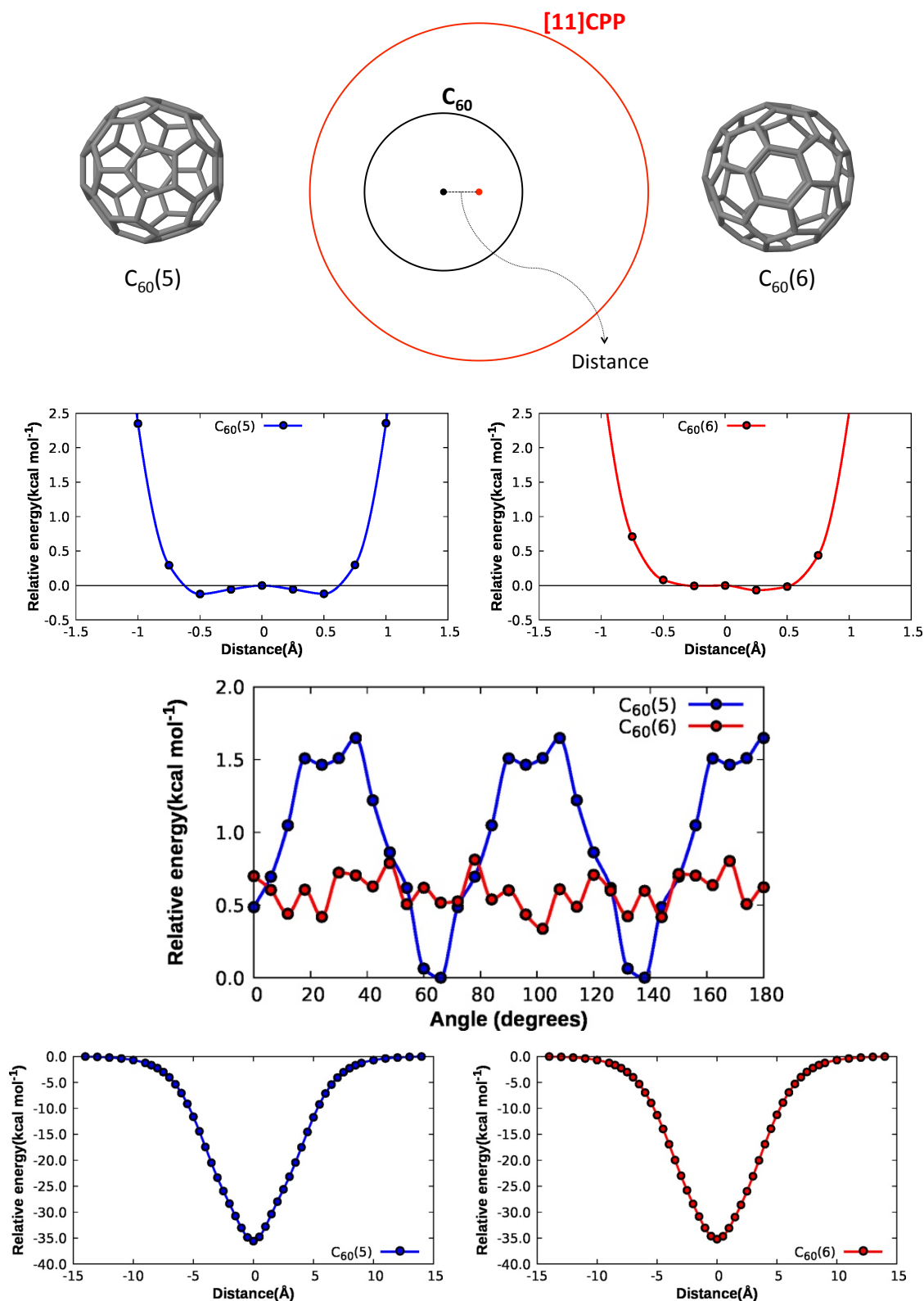


Figure S3. Energy profiles obtained upon rotation of the C_{60} . Upper plots correspond to displacements inside the nanoring using two different orientations for C_{60} as explained in the top figures. Bottom plots show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when C_{60} is rotated along an axis perpendicular to the nanoring.

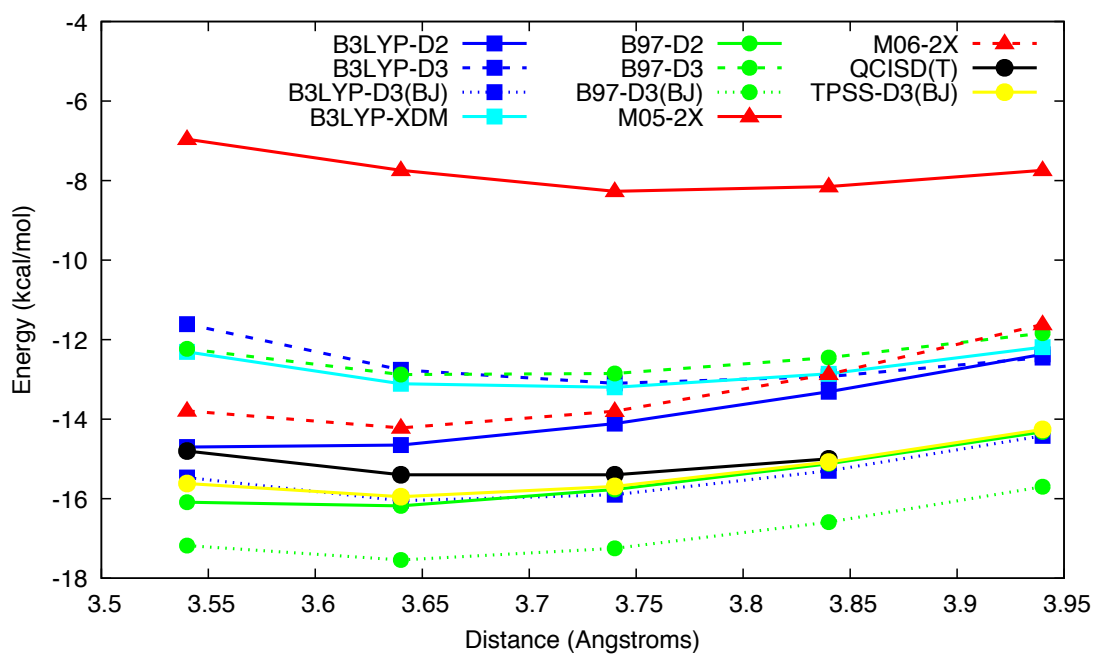


Figure S4. Performance of different DFT methods to reproduce the interaction energy in corannulene dimer. Adapted from *J. Phys. Chem. A* **2012**, *116*, 11920-11926, adding values obtained at the TPSS-D/def2-TZVP level.

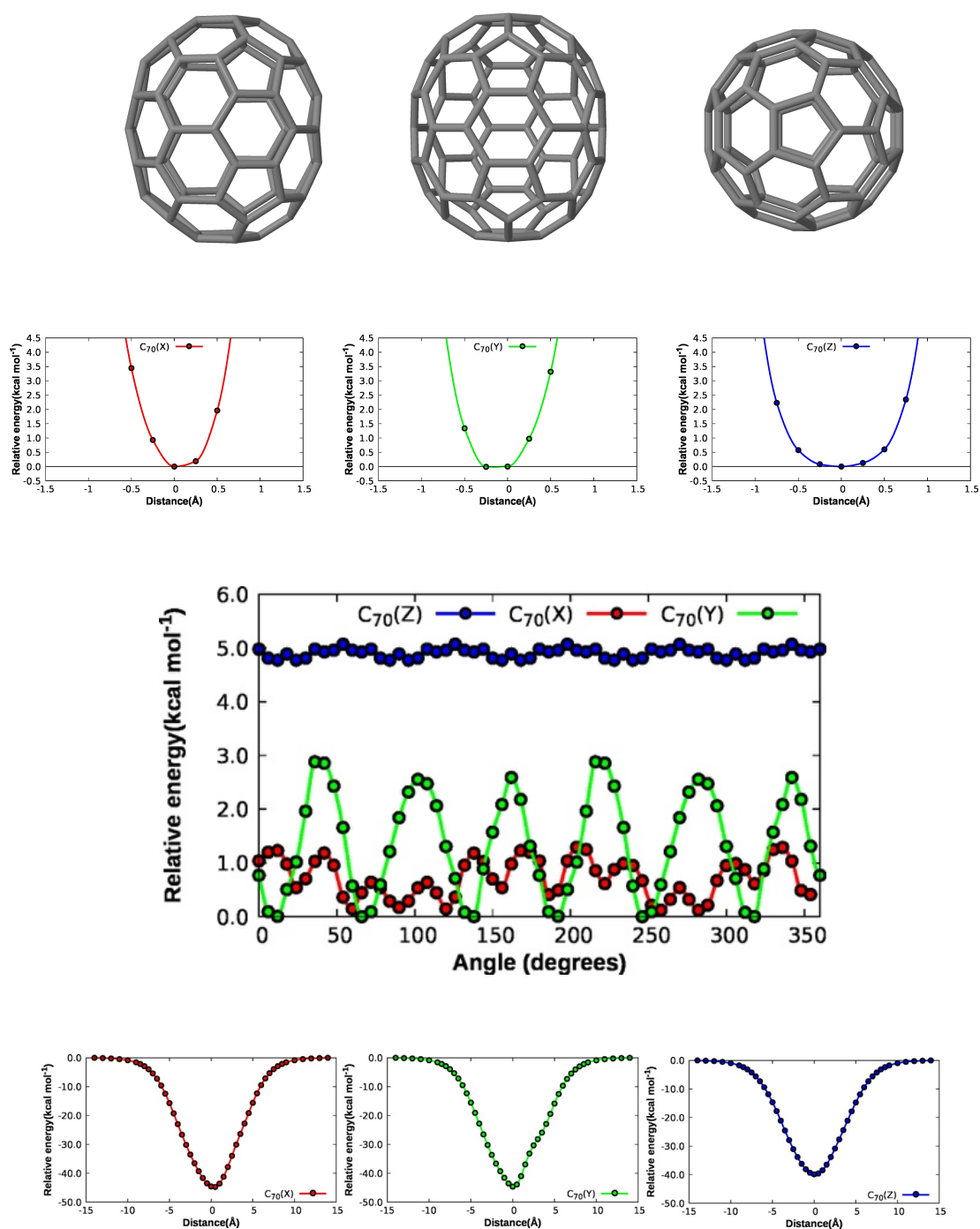


Figure S5. Energy profiles obtained upon rotation of the C₇₀. Top figures correspond to displacements inside the nanoring using three different orientations for C₇₀. Bottom ones show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when C₇₀ is rotated along an axis perpendicular to the nanoring.

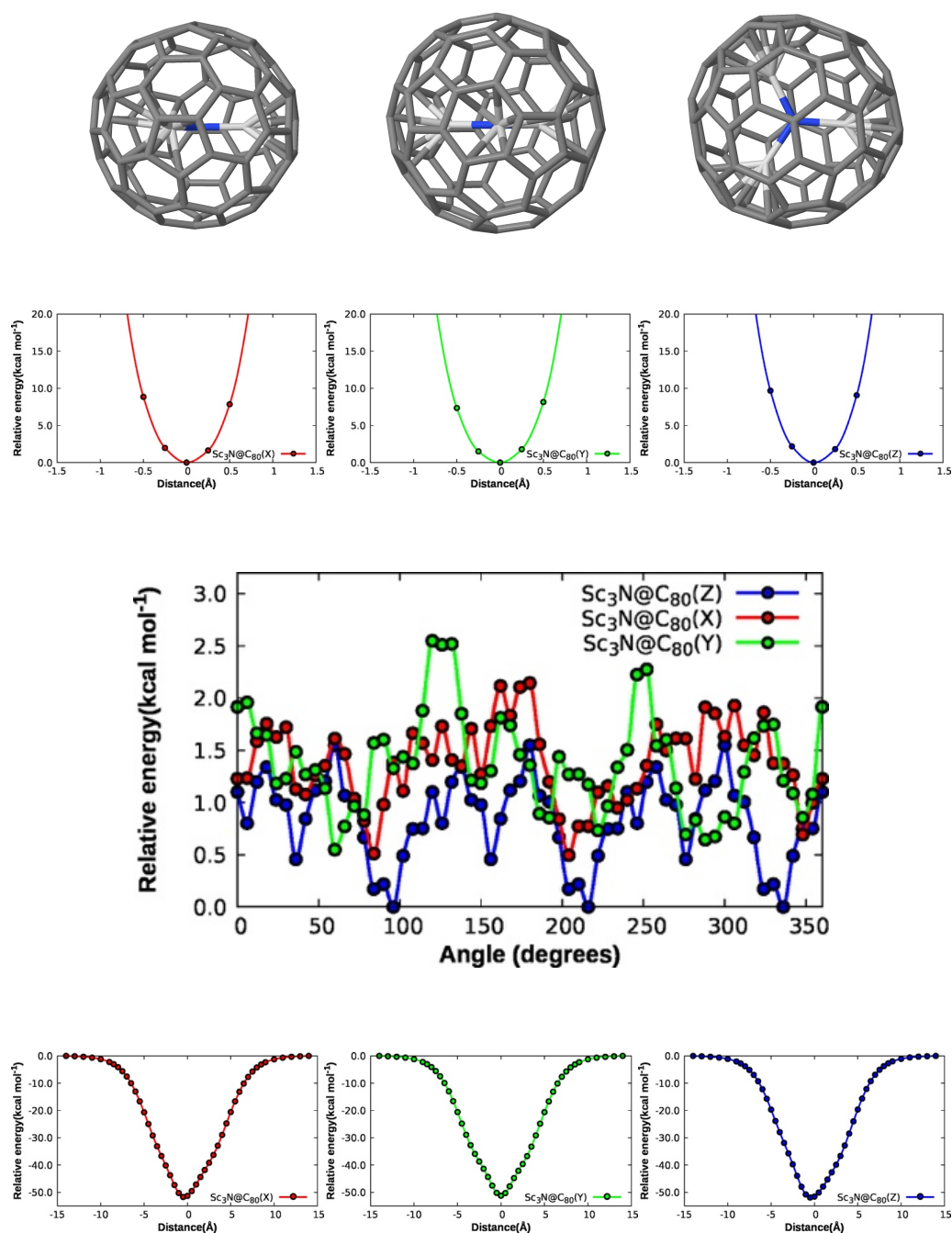
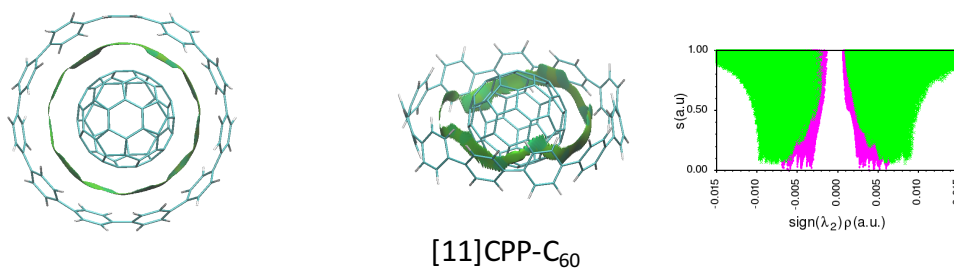
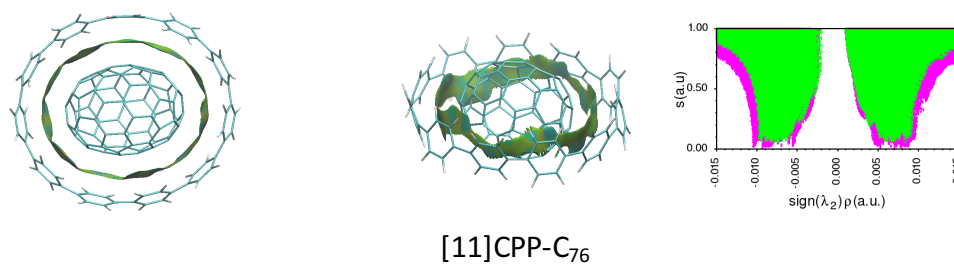


Figure S6. Energy profiles obtained upon rotation of the $\text{Sc}_3\text{N}@\text{C}_{80}$. Top figures correspond to displacements inside the nanoring using three different orientations for $\text{Sc}_3\text{N}@\text{C}_{80}$. Bottom ones show how energy changes as the fullerene is moved outside the nanoring. The plot in the centre shows energy changes when $\text{Sc}_3\text{N}@\text{C}_{80}$ is rotated along an axis perpendicular to the nanoring.



Another structure for C₆₀ complex (radii of [11]CPP are 15.2 Å, 15.0 Å)

	ΔE_{comp}	ΔE_{disp}	N _{contacts}	R _{average} (Å)
C ₆₀ -6	-34.74	-39.01	34	3.85



Another structure for C₇₆ complex (radii of [11]CPP are 15.2 Å, 15.0 Å)

	ΔE_{comp}	ΔE_{disp}	N _{contacts}	R _{average} (Å)
C ₇₆ -b	-48.15	-63.5	124	3.98

Figure S7. Other structures obtained for C₆₀ ([11]CPP-C₆₀-6) and C₇₆ ([11]CPP-C₇₆-b) mentioned in the text.

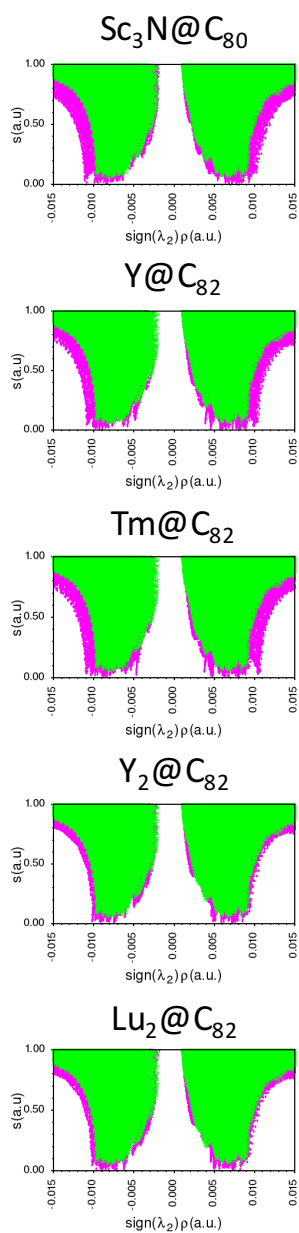


Figure S8. NCI two-dimensional plots for the complexes with endohedral fullerenes. In green the results obtained for C_{70} are shown as reference, displaced by 0.05 a.u. for clarity.

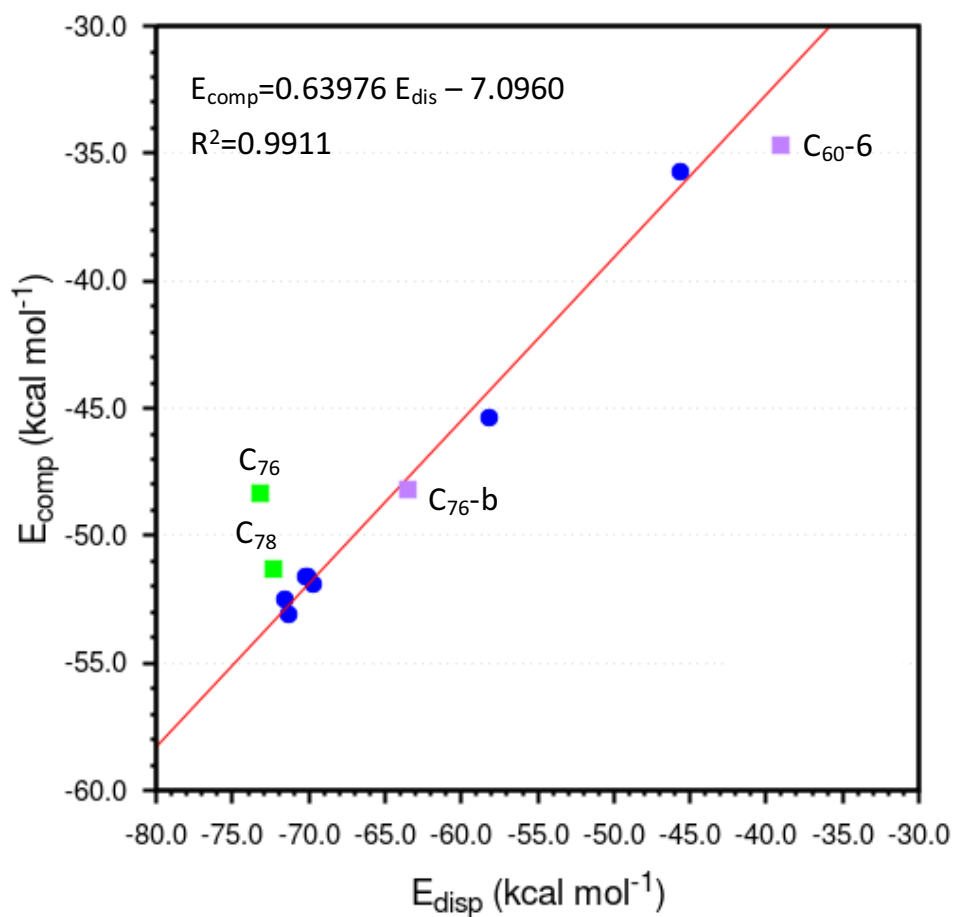


Figure S9. Correlation between dispersion and total complexation energy. It can be observed that the main outlier is C_{76} . The almost isoenergetic C_{76-b} follows the global trend.

Cartesian coordinates (Å) for the isolated molecules**C₆₀**

C 0.3834385 0.7634533 3.3084320
C 0.5654300 -0.6778282 3.3277211
C 1.6028546 -1.2605220 2.5967670
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C₇₀

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C₇₆

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C₇₈

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 C -1.7326211 -2.0304621 3.1573166
 C -1.2720380 -3.1401590 2.3488798
 C 0.1269416 -3.4057114 2.3720626
 C -1.9877433 -3.4702214 1.1639585
 C -2.7830301 -1.2017558 2.6367697
 C -4.0302791 -0.4087048 0.7190636
 C -3.4914497 -1.5071072 1.4290610
 C -3.1037946 -2.6763777 0.7148320
 C 0.0763569 3.4124579 2.5819654
 C -0.9369934 2.5073572 3.0250440
 C -2.2036020 2.4850929 2.2841750
 C -3.0023339 1.2639015 2.2808972
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 C -3.8236662 0.9489952 1.1688373
 C -1.2998464 -3.9672563 -0.0001634
 C 0.1094963 -4.1516836 -0.0002028
 C 0.8125446 -3.9046101 1.2175828
 C 0.8124981 -3.9040189 -1.2179113
 C -1.9876178 -3.4698444 -1.1643335
 C -1.7331234 -2.0307185 -3.1582351
 C -1.2721034 -3.1400939 -2.3495743
 C 0.1270849 -3.4053677 -2.3725679
 C -4.0303217 -0.4086223 -0.7194855

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 C 2.1417526 -3.3505034 -1.2199257
 C 2.8157718 -3.0236697 -0.0002660
 C 2.1419878 -3.3511698 1.2195279
 C 3.6852974 -1.8965682 -0.0002849
 C 2.2790592 -2.5234404 -2.3766088
 C 2.6768321 -0.2543300 -3.1571538
 C 3.0909035 -1.3496737 -2.3498123
 C 3.8139996 -1.0577736 -1.1613011
 C -0.8506642 -1.2044144 -3.9694114
 C 0.5871563 -1.4528126 -3.9267172
 C 1.0348217 -2.5529366 -3.1172783
 C 1.4335035 -0.2953183 -3.9108307
 C 3.8143644 -1.0579146 1.1609435
 C 3.0912106 -1.3499286 2.3497333
 C 2.2793337 -2.5240487 2.3765063
 C 2.6766161 -0.2543128 3.1575882
 C 3.9915496 0.3019427 0.7161082
 C 3.4790126 1.3984312 1.4495261
 C 2.9135876 1.0941176 2.7294959
 C 1.4715155 3.0587914 2.6328841
 C 1.8617792 1.8980682 3.2684831
 C 2.1195301 3.4619697 -1.4057939
 C 3.0250173 2.5916029 -0.7321814
 C 3.0249776 2.5917708 0.7319318
 C 2.1195146 3.4621799 1.4056894
 C 3.9914434 0.3018490 -0.7165516
 C 2.9137422 1.0939380 -2.7295642
 C 3.4790797 1.3983610 -1.4498044
 C -0.0939277 4.2354166 -1.4172517
 C 1.1684126 4.2645937 -0.6912976
 C 1.1683361 4.2646829 0.6911893
 C -1.2910094 4.2150791 -0.7275770
 C 1.8621285 1.8977513 -3.2682972
 C 0.0765410 3.4121206 -2.5818944
 C 1.4716445 3.0584801 -2.6329081
 C -1.3630291 0.1708638 -3.8671964
 C -2.3604798 3.3691279 -1.1789413
 C -2.2034649 2.4848013 -2.2840975
 C -0.9367900 2.5070404 -3.0247659
 C -0.5017045 1.3229083 -3.7794319
 C 0.8934359 1.0567972 -3.9099226
 C -3.0846788 2.9558033 -0.0000247
 C -3.7996340 1.7783628 -0.0000852
 C -3.8236608 0.9489704 -1.1689723
 C -3.0021845 1.2637086 -2.2808280
 C -2.5437286 0.1472823 -3.0534176
 C -0.0940127 4.2355654 1.4171262
 C -1.2910766 4.2151451 0.7274269
 C -2.3605307 3.3692201 1.1788182
 Y -0.1552174 -0.5199064 -1.7998407
 Y -0.1513818 -0.5146715 1.8016895

[11]CPP

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 C 7.9027052 -0.4051843 -1.1450321
 C 7.6208746 0.3456789 0.0113018
 C 7.2867067 -0.3697676 1.1742210
 C 7.0854072 -1.7426317 1.1428478
 C 7.4182741 1.8090235 -0.0161387
 C 6.9047941 2.4184088 -1.1741169
 C 6.3261806 3.6805278 -1.1271230
 C 6.2281244 4.3888070 0.0824864
 C 6.8947052 3.8535359 1.1994128
 C 7.4806782 2.5951097 1.1495915
 C 5.2437237 5.4830756 0.2023600
 C 4.9121559 6.3396511 -0.8621156
 C 3.7394392 7.0868079 -0.8451380
 C 2.8326727 7.0008266 0.2287696
 C 3.2455528 6.2613766 1.3516017
 C 4.4225525 5.5271659 1.3416941

C 1.4239335 7.4364593 0.1218423
C 0.7958694 7.5280424 -1.1336675
C -0.5874487 7.5403456 -1.2521702
C -1.4191022 7.4373648 -0.1220136
C -0.7909831 7.5286373 1.1335036
C 0.5923539 7.5400531 1.2519958
C -2.8281198 7.0026137 -0.2289056
C -3.2414409 6.2632798 -1.3516628
C -4.4189167 5.5298204 -1.3416766
C -5.2401344 5.4864044 -0.2023651
C -4.9080436 6.3428944 0.8620274
C -3.7348430 7.0893034 0.8449693
C -6.2252690 4.3927980 -0.0823968
C -6.8923014 3.8579758 -1.1992862
C -7.4791045 2.5999409 -1.1494045
C -7.4171214 1.8138042 0.0162965
C -6.9031565 2.4228560 1.1742551
C -6.3237182 3.6845959 1.1272108
C -7.6206520 0.3505899 -0.0111314
C -7.2869974 -0.3650560 -1.1740833
C -7.0865806 -1.7380468 -1.1427370
C -7.2072506 -2.4645708 0.0542929
C -7.6994812 -1.7750328 1.1774755
C -7.9028891 -0.4001112 1.1452038
C -6.5903759 -3.8038253 0.1463073
C -6.4560382 -4.6495905 -0.9702507
C -5.5401808 -5.6945806 -0.9738149
C -4.7167663 -5.9432722 0.1393243
C -4.9753141 -5.2063595 1.3076816
C -5.8902018 -4.1616705 1.3111806
C -3.4727040 -6.7338359 0.0430658
C -2.7331861 -6.7045190 -1.1515231
C -1.3998564 -7.0901874 -1.1819851
C -0.7408464 -7.5254493 -0.0191056
C -1.5266288 -7.7109739 1.1334226
C -2.8608937 -7.3231590 1.1643197
C 0.7359632 -7.5259209 0.0189882
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C 2.8561433 -7.3249535 -1.1644229
C 3.4683140 -6.7360283 -0.0431594
C 2.7288149 -6.7062631 1.1514304
C 1.3952387 -7.0910944 1.1818797
C 4.7128806 -5.9462466 -0.1393901
C 4.9718850 -5.2094377 -1.3077017
C 5.8874640 -4.1653530 -1.3111599
C 6.4530101 -4.6537688 0.9702427
C 5.5364631 -5.6981615 0.9737632
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H 8.2405987 0.1013180 -2.0449784
H 7.0599967 0.1724884 2.0872604
H 6.7072407 -2.2391501 2.0315883
H 6.8440477 1.8469825 -2.0956216
H 5.8278427 4.0668733 -2.0117226
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H 3.5016699 7.7091281 -1.7031886
H 2.5807244 6.1615896 2.2035803
H 4.6457962 4.8773328 2.1827503
H 1.3949749 7.4903044 -2.0386079
H -1.0253720 7.5538572 -2.2457517
H -1.3901040 7.4913429 2.0384427
H 1.0302814 7.5533590 2.2455796
H -2.5766581 6.1629608 -2.2035978
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H -6.8427161 1.8513894 2.0957558
H -5.8250566 4.0706254 2.0117871
H -7.0599916 0.1770746 -2.0871082
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H -7.8809735 -2.3165027 2.1021932

H -8.2404034 0.1065938 2.0451898
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H -4.3613248 -5.3713578 2.1882218
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H -3.1718087 -6.2565737 -2.0383841
H -0.8281785 -6.9343301 -2.0920902
H -1.0727602 -8.1209969 2.0317224
H -3.4254061 -7.4356481 2.0859921
H 1.0675074 -8.1216639 -2.0318385
H 3.4205968 -7.4377862 -2.0860863
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H 5.9675794 -3.5382368 -2.1943222
H 7.0393895 -4.4591544 1.8643853
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C 6.5878968 -3.8080441 -0.1462750
C 7.2056646 -2.4692078 -0.0542116

Cartesian coordinates (Å) for the complexes studied.

[11]CPP-C₆₀

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C 2.1501480 0.9608716 1.7965793
C 1.0697194 1.5673518 2.5566842
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C -1.9205497 -0.2367283 3.3306914
C -0.9257785 -1.2960960 3.3404650
C -1.1520116 -2.4739771 2.6247719
C 1.1927686 -2.4875893 1.8497878
C 2.6468312 -1.1360082 0.5885251
C 2.7789329 -0.4296671 -0.6091921
C 2.5962754 1.0129061 -0.6283596
C 2.2887594 1.6959273 0.5506162
C 1.2943556 2.7569273 0.5409416
C 0.5406310 2.6774891 1.7812215
C -0.8322137 2.9391832 1.7842042
C -1.7297999 2.1019327 2.5635556
C -3.1036012 -0.3958335 2.6053649
C -3.6351078 0.7126352 1.8287764
C -2.9613959 1.9369979 1.8083328
C -2.8237401 2.6710070 0.5619255
C -1.5090430 3.2905629 0.5468309
C -0.7845836 3.3659182 -0.6443463
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C 1.9188085 1.3637144 -1.8651893
C 1.9470618 -2.4104987 0.6098840
C -0.2001698 -1.2942209 -3.3147736
C 0.3096681 -2.3594144 -2.5687649
C -0.5880635 -3.1954337 -1.7889285
C -1.9606810 -2.9330088 -1.7857617
C -2.4907146 -1.8246029 -2.5626684
C -1.8096645 0.4198877 -3.3310511
C -0.4947941 1.0383807 -3.3456979
C 0.4998164 -0.0209870 -3.3356929
C 1.6824976 0.1380360 -2.6100078
C 2.2140575 -0.9705232 -1.8341604
C 1.5415671 -2.1953538 -1.8139802
C 0.0885833 -3.5473809 -0.5521711
C -0.6360808 -3.6218812 0.6388555
C -2.0632728 -3.3492683 0.6423442
C -2.7142432 -3.0114400 -0.5456420
C -3.7097698 -1.9530026 -0.5557952
C -3.5723676 -1.2186947 -1.8025446
C -3.7475291 0.1674439 -1.8210825
C -2.8477936 1.0026733 -2.6005231
C -0.2683181 2.2159925 -2.6293659
C 1.3480990 2.8231564 -1.8689385
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C 1.4811855 -7.1795238 -1.1590883
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C 3.4330454 -6.2058938 -0.0843669
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C 4.9822128 -4.7113159 -1.3259104
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C 5.5821956 -5.3474487 0.9143322
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H 8.7509507 0.2286666 -2.0431224
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H 7.0866345 -2.0422668 2.0229023
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H 7.3428264 4.5051786 2.1699287
H 8.4902396 2.3386814 2.0619252
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H -4.4926600 -5.2196969 2.2327392
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H 1.0181997 -7.5895697 -2.0521940
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H 3.1564693 -5.7204312 1.9976577
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H 6.0992471 -3.1000171 -2.1821178
H 7.2306354 -4.2932202 1.7884748
H 5.4386388 -5.9753570 1.7895724
C 6.7752998 -3.5334779 -0.1812886
C 7.5341502 -2.2735809 -0.0734290

[11]CPP-C₇₀

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C 7.3867519 1.7013887 0.0118296
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 H 1.0150014 -7.9717290 -2.0230940
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 H 0.8382829 -6.7809233 2.1029858
 H 4.4291652 -5.4291432 -2.1895363
 H 6.0775956 -3.6331355 -2.2002120
 H 7.1050125 -4.5446985 1.8728365
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[11]CPP-C₇₆

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 C 3.0403253 0.1215634 2.5842577
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[11]CPP-C₇₈

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 C 0.4675771 3.7371384 -1.3494141
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 C -6.9280129 2.4370543 1.3842773
 C -6.3249289 3.6863971 1.3421523
 C -7.7023542 0.4004785 0.1832528
 C -7.4372805 -0.2967589 -1.0080877
 C -7.2346586 -1.6690893 -1.0080101
 C -7.2827384 -2.4116886 0.1842176
 C -7.7163074 -1.7401953 1.3421402
 C -7.9216472 -0.3669937 1.3416884
 C -6.6493186 -3.7423783 0.2358174
 C -6.4953588 -4.5466983 -0.9082658
 C -5.5731692 -5.5838860 -0.9370763
 C -4.7595258 -5.8660513 0.1754954
 C -5.0355411 -5.1710786 1.3652798
 C -5.9569162 -4.1339393 1.3942833
 C -3.5160972 -6.6505952 0.0612312
 C -2.8127604 -6.6567924 -1.1546394
 C -1.4809539 -7.0414254 -1.2126518
 C -0.7875495 -7.4381349 -0.0573627
 C -1.5384195 -7.5908248 1.1229514
 C -2.8702848 -7.2049897 1.1816433
 C 0.6872377 -7.4403512 -0.0565126
 C 1.4394180 -7.6023625 -1.2348188
 C 2.7762948 -7.2334170 -1.2900124
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 C 2.7170453 -6.6728928 1.0432560
 C 1.3806181 -7.0416807 1.0983454
 C 4.6818949 -5.9191820 -0.2823653
 C 4.9708532 -5.2315819 -1.4732855
 C 5.8996597 -4.2006120 -1.5002002
 C 6.4232909 -4.6130925 0.8059143
 C 5.4937286 -5.6431330 0.8330916
 C 6.5834641 -3.8087570 -0.3373183
 C 7.2101304 -2.4753544 -0.2761753
 H 7.7930897 -2.3488842 -2.3539370
 H 8.1742274 0.0675907 -2.3341416
 H 7.1791317 0.1817662 1.8465974
 H 6.7984530 -2.2209700 1.8266909
 H 6.8461718 1.8188588 -2.3570587
 H 5.8441434 4.0384545 -2.2728463
 H 7.0148656 4.4159509 1.8456718
 H 8.0267787 2.1888845 1.7602800
 H 5.4630662 6.2570397 -2.0659481
 H 3.3820881 7.5297268 -1.9653855
 H 2.8028606 6.2357966 2.0977104
 H 4.8804663 4.9944768 1.9999640
 H 1.3104047 7.3714056 -2.1363103
 H -1.1102172 7.4403341 -2.2145036
 H -1.2466378 7.3793501 2.0850707
 H 1.1743262 7.4411600 2.1630017
 H -2.7407740 6.2392994 -2.1461000
 H -4.8249519 5.0055985 -2.0467316
 H -5.4038041 6.2809982 2.0163569
 H -3.3190470 7.5492908 1.9115454
 H -6.9926624 4.4872221 -1.8845675
 H -8.0619835 2.2845570 -1.8083840
 H -6.8502294 1.8482043 2.2930752
 H -5.7918684 4.0451040 2.2176948
 H -7.2606048 0.2576955 -1.9247149
 H -6.9055964 -2.1493444 -1.9244889
 H -7.8472595 -2.2940064 2.2674979
 H -8.2086040 0.1253644 2.2665931
 H -7.0726569 -4.3272688 -1.8020743
 H -5.4472958 -6.1545072 -1.8527527
 H -4.4305306 -5.3590188 2.2467182

H -6.0479279 -3.5396064 2.2983215
 H -3.2719930 -6.2304381 -2.0410088
 H -0.9379219 -6.9058825 -2.1427458
 H -1.0583464 -7.9724700 2.0194879
 H -3.4052138 -7.2919944 2.1232307
 H 0.9583984 -7.9820372 -2.1318738
 H 3.3135335 -7.3300524 -2.2293621
 H 3.1781513 -6.2462403 1.9284238
 H 0.8358431 -6.8952356 2.0256988
 H 4.3666272 -5.4136393 -2.3566507
 H 5.9923038 -3.6037626 -2.4025050
 H 6.9969796 -4.3939441 1.7020028
 H 5.3587283 -6.2100397 1.7499068

[11]CPP-Tm@C₈₂

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 C 2.6092079 -1.1550872 3.1813111
 C 1.8361200 -2.3760810 3.0499929
 C 2.2088865 -3.0459539 1.8238200
 C 3.3291046 -2.3155055 1.2966280
 C 2.0193699 0.0282620 3.7143535
 C 0.6332234 -0.0207283 4.1903420
 C -0.0737950 -1.2554008 4.1052724
 C 0.5353038 -2.4200097 3.4984055
 C -0.1570699 1.1639788 4.1156345
 C -1.5498152 1.1208579 3.8008256
 C -2.2180778 -0.1151618 3.5947273
 C -1.4668184 -1.3050601 3.7903447
 C -3.2826568 -0.1465000 2.6289557
 C -3.6580636 1.0054886 1.8616938
 C -2.8849644 2.2202271 1.9924949
 C -1.8758031 2.2823503 2.9820294
 C -0.6653525 3.0302626 2.7662245
 C 0.3704609 2.3712241 3.5165111
 C -1.7111351 -2.4803714 2.9638802
 C -2.7170914 -2.4771737 1.9707589
 C -3.5623591 -1.3129832 1.8477001
 C -4.2328007 0.5622043 0.6085887
 C -4.1602599 -0.8995786 0.6005216
 C -0.4533050 -3.1429056 2.7437979
 C 2.5260794 1.2529633 3.1907131
 C 1.6711245 2.4194116 3.0685597
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 C -1.1881224 -3.8256192 0.5451489
 C -2.4626333 -3.2201741 0.7855388
 C -3.0125430 -2.8008226 -0.4839479
 C -3.8158915 -1.6308784 -0.6058084
 C -2.0750481 -3.1932483 -1.5109672
 C -0.9490056 -3.8078363 -0.8751528
 C 1.2422692 -3.6459552 0.9765710
 C 1.4867998 -3.6315434 -0.4727502
 C 0.3608068 -3.6997569 -1.4066584
 C 3.9209401 0.1019976 1.4696472
 C 3.4516452 1.2855228 2.1002747
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 C 1.9964221 3.1219014 1.8475426
 C -1.9223420 -2.4284527 -2.7019641
 C -2.7506744 -1.2682927 -2.8478710
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 C -3.7208053 0.5805025 -1.8066508
 C -3.9450945 1.3240467 -0.5973407
 C -2.8333078 1.0494577 -2.8417787
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 C 0.4686406 -3.0885138 -2.6924320
 C -0.6438740 -2.4208651 -3.3069887
 C -0.9288504 -0.0397612 -4.0324681
 C -0.1460644 -1.2277414 -3.9829829
 C 1.2701845 -1.1753496 -3.8147793
 C 1.6493729 -2.3526836 -3.0609787
 C 3.5538359 -2.2979019 -0.0578521
 C 2.6732103 -3.0150231 -0.9387999
 C 2.7279274 -2.3219690 -2.2083918
 C -2.0820296 2.2592382 -2.6847992

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 C -1.4458593 3.6763181 0.5745389
 C -1.2051921 3.6839462 -0.8435665
 C -0.2279939 1.1978462 -3.9742275
 C -0.8057370 2.3463955 -3.2881224
 C 0.1107456 3.6752167 -1.3765521
 C 0.2596184 3.0843886 -2.6663660
 C 1.4879139 2.4356656 -3.0416381
 C 1.1894307 1.2412915 -3.8046392
 C 1.9645559 0.0573251 -3.6371221
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 C 0.9926978 3.6668312 1.0052972
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 C 2.4687645 3.1539017 -0.9156408
 C 2.5679343 2.4736869 -2.1897656
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 C 3.9255729 1.3123240 -0.7059956
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 C 3.1143940 0.0925977 -2.7283836
 C 3.4991345 -1.1031122 -2.0527559
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 C 7.3378185 -0.3658794 0.9590997
 C 7.1197372 -1.7354895 0.9438410
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 C 6.2976733 4.3890477 -0.1556542
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 C 7.5349028 2.5864583 0.9112185
 C 5.3201060 5.4842778 -0.0270848
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 C 3.7205011 6.9915728 -1.0710001
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 C 3.3884540 6.3020798 1.2013861
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 C 6.4155767 -4.6123415 0.8242188
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 H 7.8002397 -2.3425570 -2.3222815
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 H 6.8697210 1.8358541 -2.3284889
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 H 3.4149547 7.5509165 -1.9500612
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 H 4.8625140 4.9986616 2.0235046
 H 1.3435122 7.3940289 -2.1452580
 H -1.0771876 7.4652421 -2.2514412
 H -1.2635259 7.3766859 2.0453907
 H 1.1567972 7.4399782 2.1523529
 H -2.7096204 6.2485424 -2.1970782
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 H -5.4231724 6.3210913 1.9322232
 H -3.3329643 7.5820130 1.8459363
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 H -8.0084556 2.2752044 -1.8950372
 H -6.8566974 1.8889549 2.2283178
 H -5.8141360 4.0931135 2.1464224
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 H -7.8674757 -2.2665434 2.2146855
 H -8.2236647 0.1557351 2.1915860
 H -7.0671015 -4.3375219 -1.8151453
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 H -4.4281932 -5.3370382 2.2438912
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 H 4.3596212 -5.4100255 -2.3396416
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[11]CPP-Y₂@C₈₂

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 C 1.4160647 3.8853352 -0.1062467
 C 0.7947226 3.7954013 1.1904100
 C -0.6249186 3.9290059 1.2027078
 C 1.3456927 3.1815006 -2.3387948
 C 0.6710635 2.3738492 -3.3347885
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 C 2.5370351 2.6540497 -1.7322593

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 C 3.1650158 1.4412356 -2.1719446
 C 2.5526867 0.7306028 -3.2451428
 C 0.6307138 2.5950899 3.3506443
 C 1.4507293 3.0376732 2.2658049
 C 2.6861723 2.2918585 1.9951910
 C 3.2306559 2.2887500 0.6413746
 C 2.5676556 3.0693209 -0.3617289
 C 3.9647422 1.1715428 0.1705862
 C 0.5251240 0.0255913 -4.1548511
 C -0.8933265 0.0317958 -4.0607973
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 C -1.5392566 -1.1844554 -3.6834360
 C 1.2920627 -1.1431177 -3.8043834
 C 1.3191523 -3.1480848 -2.3539672
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 C 3.9005185 -0.7161130 -1.2057756
 C 3.1529730 -1.4213990 -2.1781517
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 C 2.5113377 -2.6279636 -1.7428621
 C -2.7361472 -1.1841287 -2.8827146
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 C -3.9540439 0.0397735 -1.1507561
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 C -1.4513057 -3.8779174 -0.0298546
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 C -2.7254389 -6.8378077 -1.2633465
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 C -2.9499542 -7.2775187 1.0847065
 C 0.6904185 -7.5321418 0.1250748
 C 1.5293777 -7.7005155 -0.9923891
 C 2.8582452 -7.3001562 -0.9605201
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