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

Supporting information for

Assessment of Electronic Transitions Involving Intermolecular Charge Transfer in Complexes Formed by Fullerenes and Donor-Acceptor Nanohoops

Iván González-Veloso[1], Jesús Rodríguez-Otero[1*], and Enrique M. Cabaleiro-Lago [2]

[1] *Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Física, 15782, Universidade de Santiago de Compostela, Galicia (Spain).*

[2] *Departamento de Química Física, Facultad de Ciencias, Universidade de Santiago de Compostela, Campus de Lugo, Av. Alfonso X El Sabio, s/n 27002 Lugo, Galicia (Spain).*

[10]CPAq, [10]CPTcaq, [12]CPP

Table S1. Fitting the nanohoop into an ellipse, for the isolated nanohoops and in different complexes. Radii in Å; f is the flattening f=(R_1-R_2)/R_1

	R_1	R_2	f	$1/f$
[12]CPP	8.29	8.29	0.000	-16587.00
[10]CPAq	8.42	8.24	0.021	48.09
[10]CPTcaq	9.04	7.69	0.149	6.70
$(C_{60}(5)@[10]CPAq)_A$	9.22	7.21	0.218	4.59
$(C_{60}(6)@[10]CPAq)_A$	9.07	7.39	0.185	5.42
$(C_{60}(5)@[10]CPTcaq)_A$	9.47	7.16	0.244	4.10
$(C_{60}(6)@[10]CPTcaq)_A$	9.46	7.19	0.240	4.17
$C_{60}(5)@[12]CPP$	9.15	7.24	0.209	4.80
$C_{60}(6)@[12]CPP$	9.17	7.23	0.211	4.73
$C_{60}(5)@[10]CPAq$	9.24	7.21	0.220	4.54
$C_{60}(6)@[10]CPAq$	9.27	7.17	0.227	4.40
$C_{60}(5)@[10]CPTcaq$	9.77	6.87	0.297	3.37
$C_{60}(6)@[10]CPTcaq$	9.83	6.81	0.308	3.25
$(C_{70}(V)@[10]CPAq)_A$	9.18	7.26	0.209	4.78
$(C_{70}(H)@[10]CPAq)_A$	8.78	7.68	0.125	7.97
$(C_{70}(V)@[10]CPTcaq)_A$	9.56	7.06	0.261	3.83
$(C_{70}(H)@[10]CPTcaq)_A$	9.13	7.51	0.177	5.66
$C_{70}(V)@[12]CPP$	9.14	7.27	0.204	4.89
$C_{70}(H)@[12]CPP$	8.74	7.70	0.119	8.41
$C_{70}(V)@[10]CPAq$	9.25	7.20	0.222	4.51
$C_{70}(H)@[10]CPAq$	8.89	7.58	0.148	6.77
$C_{70}(V)@[10]CPTcaq$	9.74	6.91	0.290	3.45
$C_{70}(H)@[10]CPTcaq$	9.33	7.35	0.213	4.70

Table S2. Electron density for the bond critical points between the fullerene and the nanohoop for the most stable complexes

	N_{BCP}	density	N_{BCP}	density	N_{BCP}	density
C_{60}(5)@[10]CPAq	46	3.5488e-03	52	4.0001e-03	41	6.2832e-03
	58	6.0449e-03	71	5.9740e-03	126	5.3069e-03
	147	5.5101e-03	227	6.0365e-03	256	6.1260e-03
	260	5.7289e-03	262	4.1004e-03		
C_{60}(5)@[12]CPP	447	5.3130e-03	435	6.1156e-03	429	6.2170e-03
	396	5.6096e-03	378	5.2550e-03	316	5.2561e-03
	293	5.6104e-03	241	6.2164e-03	236	6.1170e-03
	225	5.3152e-03	317	1.4187e-06		
C_{60}(5)@[10]CPTcaq	234	5.6126e-03	229	6.1239e-03	231	6.3227e-03
	247	5.6299e-03	263	5.4047e-03	320	5.0822e-03
	340	5.3137e-03	429	6.1519e-03	460	6.1674e-03
	463	3.7299e-03				
$(C_{70}(H)$@[10]CPAq$)_A$	479	2.8962e-03	486	3.6466e-03	498	7.2906e-03
	475	8.9597e-03	471	5.0610e-03	440	5.6311e-03
	400	4.6650e-03	317	5.7298e-03	269	6.6851e-03
	245	7.2984e-03	229	5.3144e-03	240	2.3307e-03
	312	1.4615e-05				
$C_{70}(H)$@[12]CPP	509	5.1486e-04	456	5.2036e-03	463	3.0516e-03
	469	6.9759e-03	440	7.6802e-03	382	5.7325e-03
	294	6.3607e-03	242	6.9929e-03	232	7.1830e-03
	222	5.4532e-03	506	1.0358e-03	507	1.4853e-05
$C_{70}(H)$@[10]CPTcaq	536	4.9145e-04	242	3.9005e-03	241	8.3776e-03
	243	7.4993e-03	279	4.3445e-03	324	6.6088e-03
	369	7.0420e-03	416	6.1472e-03	451	5.5305e-03
	486	7.0265e-03	490	7.7682e-03		

Table S3. Amount of the charge transfer and the distance for the four most important transitions in monomers. N_{tr} is the number of the transition, q is the amount of charge that it transferred and R is the distance between positive and negative centre in the barycentre following ref. 85 and 86

	N_{tr}	q	R(Å)	N_{tr}	q	R(Å)
C_{60}	20	0.368	0.000	21	0.354	0.000
	22	0.375	0.000	24	0.405	0.000
C_{70}	5	0.325	0.584	6	0.348	0.633
	7	0.335	0.532	8	0.358	0.582
[10]CPAq	2	0.658	0.052	5	0.450	1.606
	6	0.465	1.517	7	0.665	0.317
[10]CPTcaq	6	0.869	15.001	7	0.423	2.036
	8	0.435	1.979	9	0.569	10.116
[12]CPP	2	0.401	0.000	3	0.362	0.001
	7	0.327	0.000	17	0.298	0.001

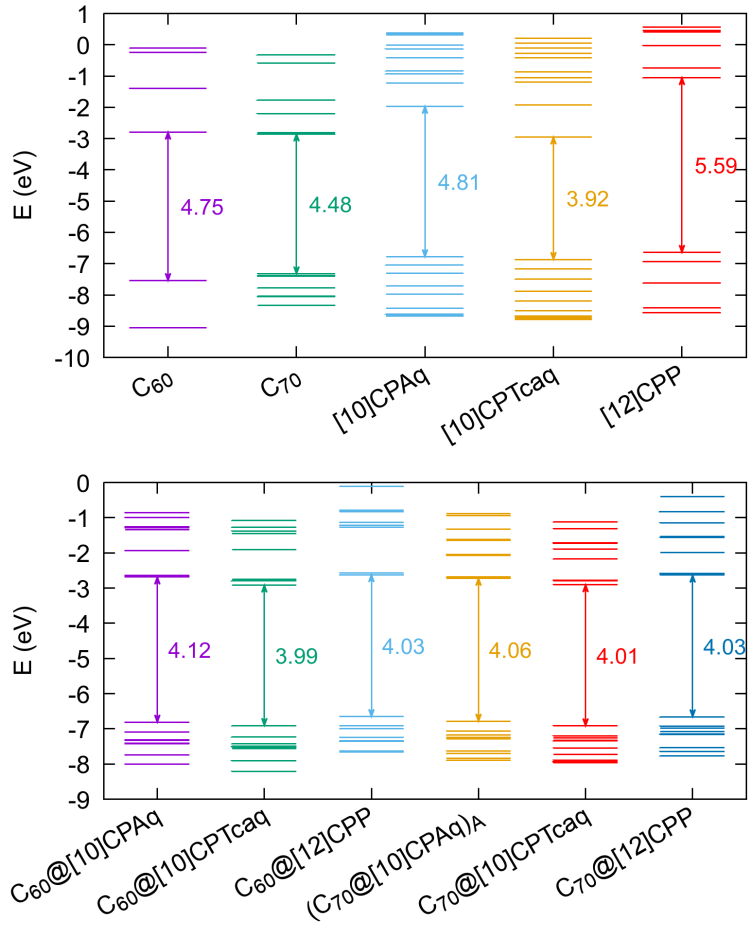

Figure S1. Schematic energy levels of the highest and lowest occupied molecular orbitals in monomers and complexes. CAM-B3LYP/def2-TZVP//B97-D/def2-TZVP.

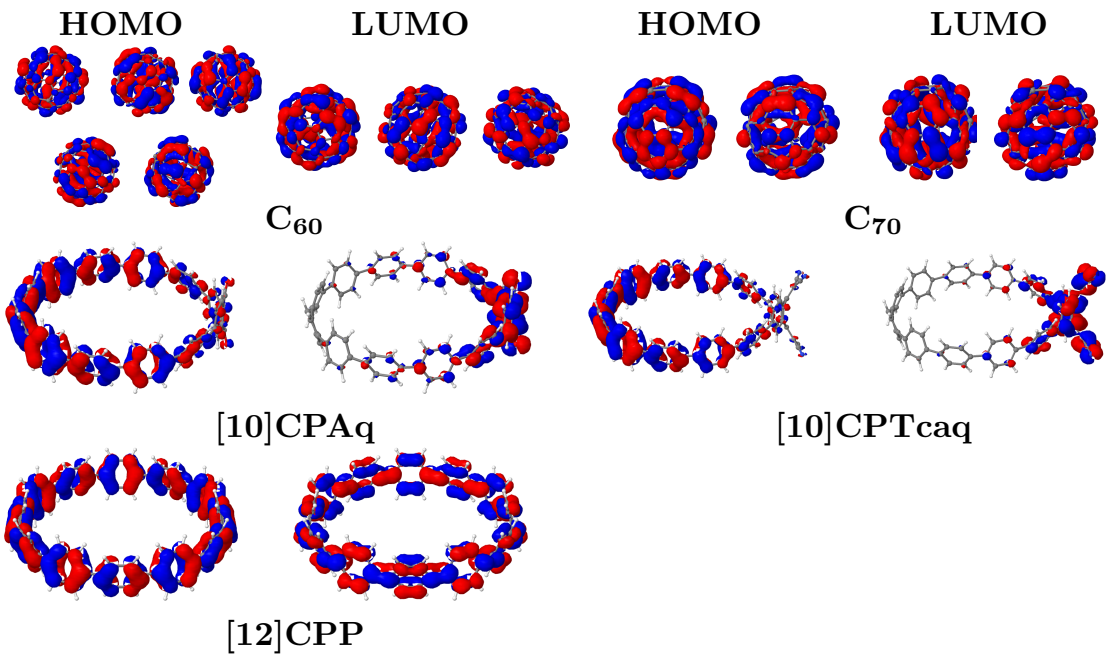

Figure S2. HOMO and LUMO orbitals in monomers at the CAM-B3LYP/def2-TZVP//B97-D2/def2-TZVP level.

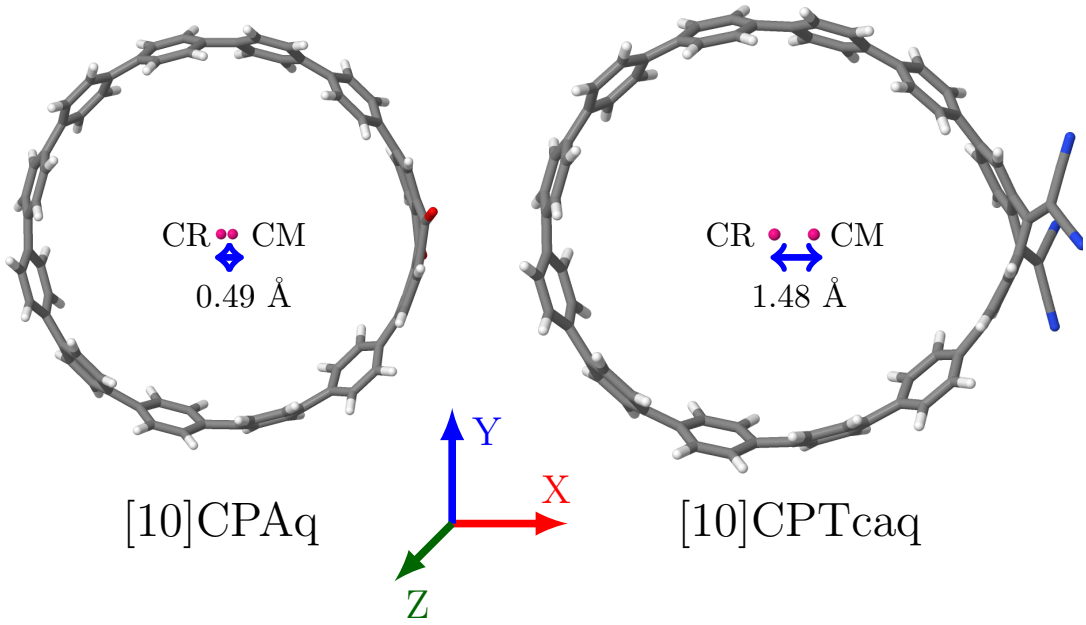

Figure S3. Distance between the center of mass (CM) and the center of the ring (CR) in [10]CPAq and [10]CPTcaq

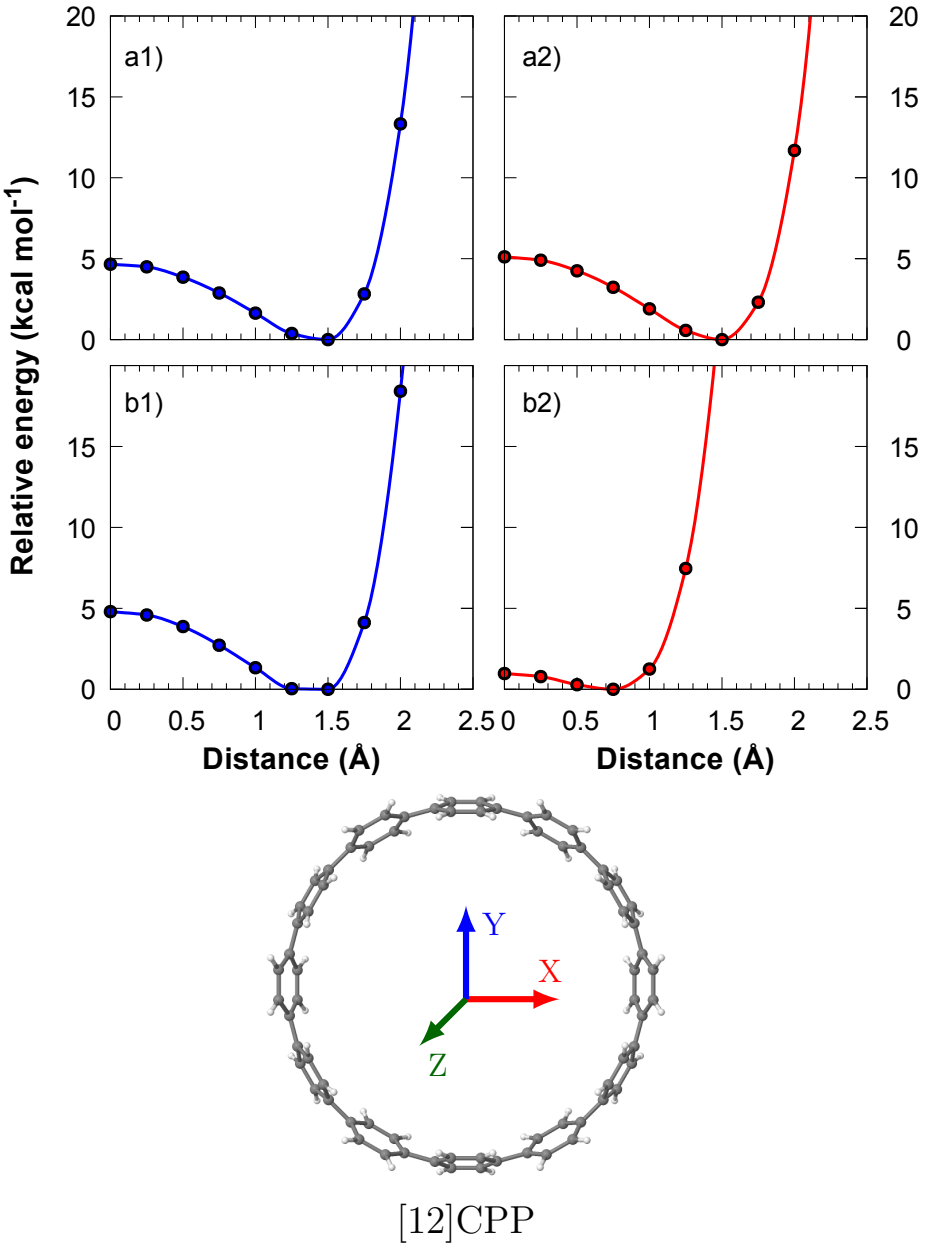

Figure S4. Energetic profile for the displacement inside the ring of the fullerene along the X axis in the [12]CPP. a1) C_{60}(5)@[12]CPP. a2) C_{60}(6)@[12]CPP. b1) C_{70}(V)@[12]CPP. b2) C_{70}(H)@[12]CPP.

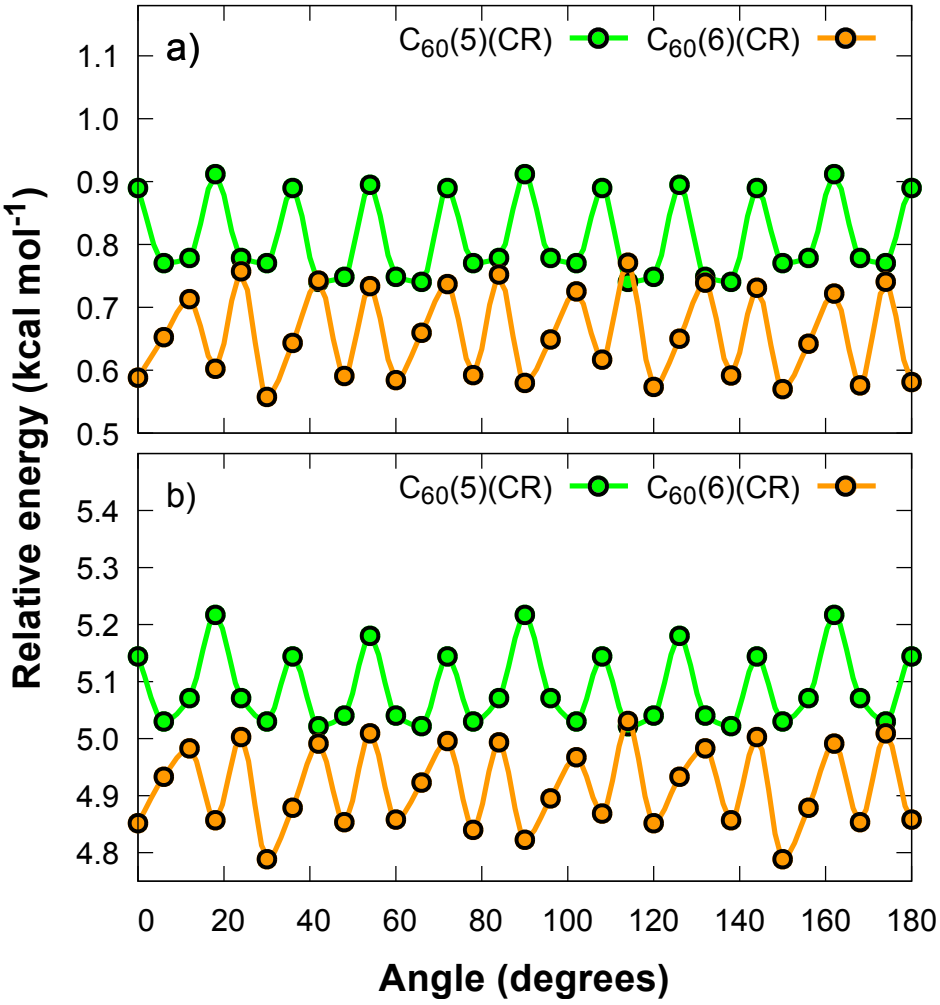

Figure S5. Energetic profile for C_{60} at the centre of different nanorings. The minimum energy is the one that was found in the center of mass. a) C_{60}@[10]CPAq. b) C_{60}@[10]CPTcaq.

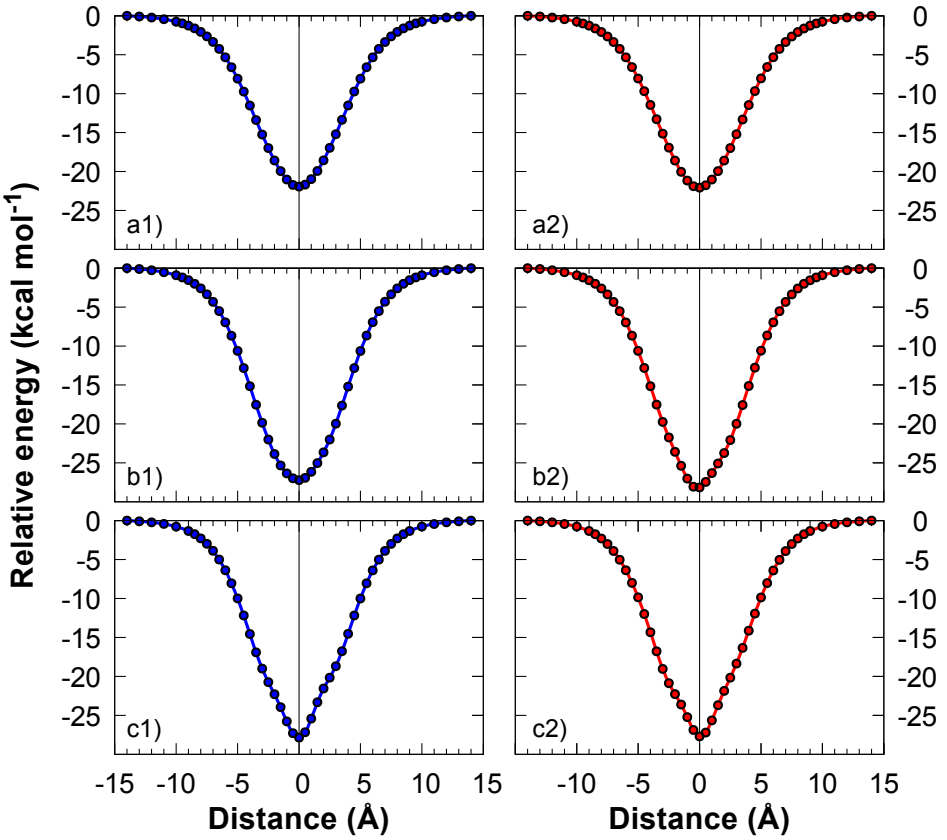

Figure S6. Energetic profile for the departure in Z axis of C_{60} inside different nanorings. a1) C_{60}(5)@[10]CPAq(CM). a2) C_{60}(6)@[10]CPAq(CM). b1) C_{60}(5)@[10]CPTcaq(CM). b2) C_{60}(6)@[10]CPTcaq(CM) c1) C_{60}(5)@[12]CPP c2) C_{60}(6)@[12]CPP. In all cases the zero position corresponds to the fullerene placed on the centre of mass, except for [12]CPP where it refers to an analogous off-centre location as commented in the text.

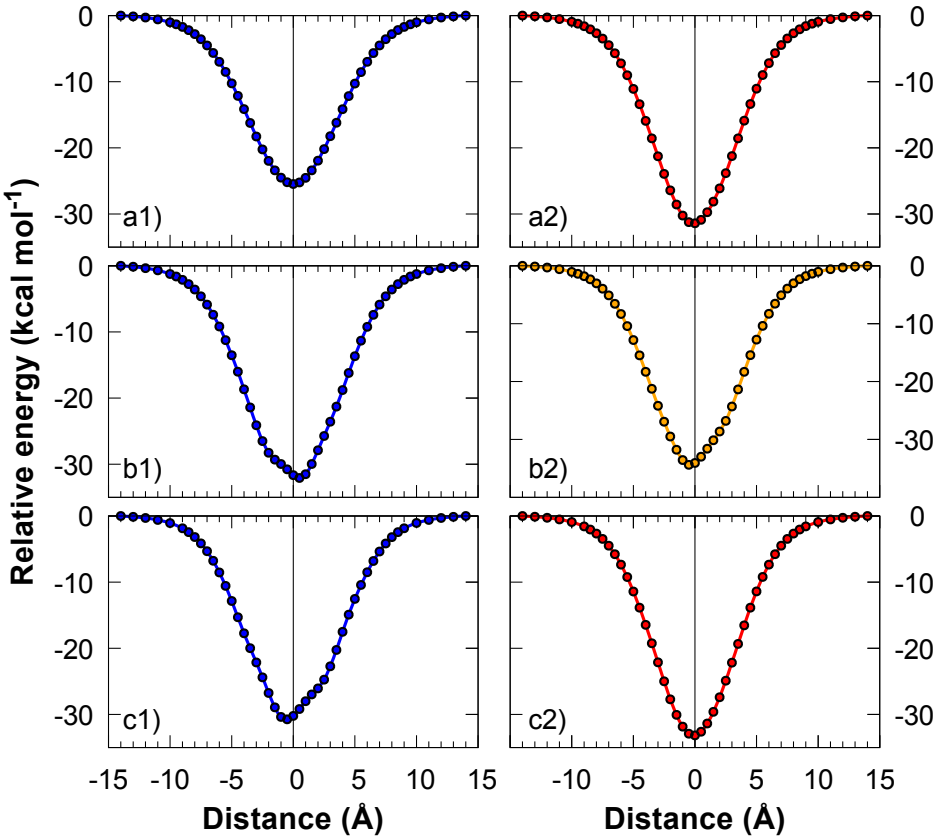

Figure S7. Energetic profile for the departure along the Z axis of C_{70} inside different nanorings. a1) C_{70}(V)@[10]CPAq. a2) C_{70}(H)@[10]CPAq. b1) C_{70}(V)@[10]CPTcaq. b2) C_{70}(H)@[10]CPTcaq. c1) C_{70}(V)@[12]CPP. c2) C_{70}(H)@[12]CPP. For the C_{70} location and orientation, see the colour code of Fig. 4.

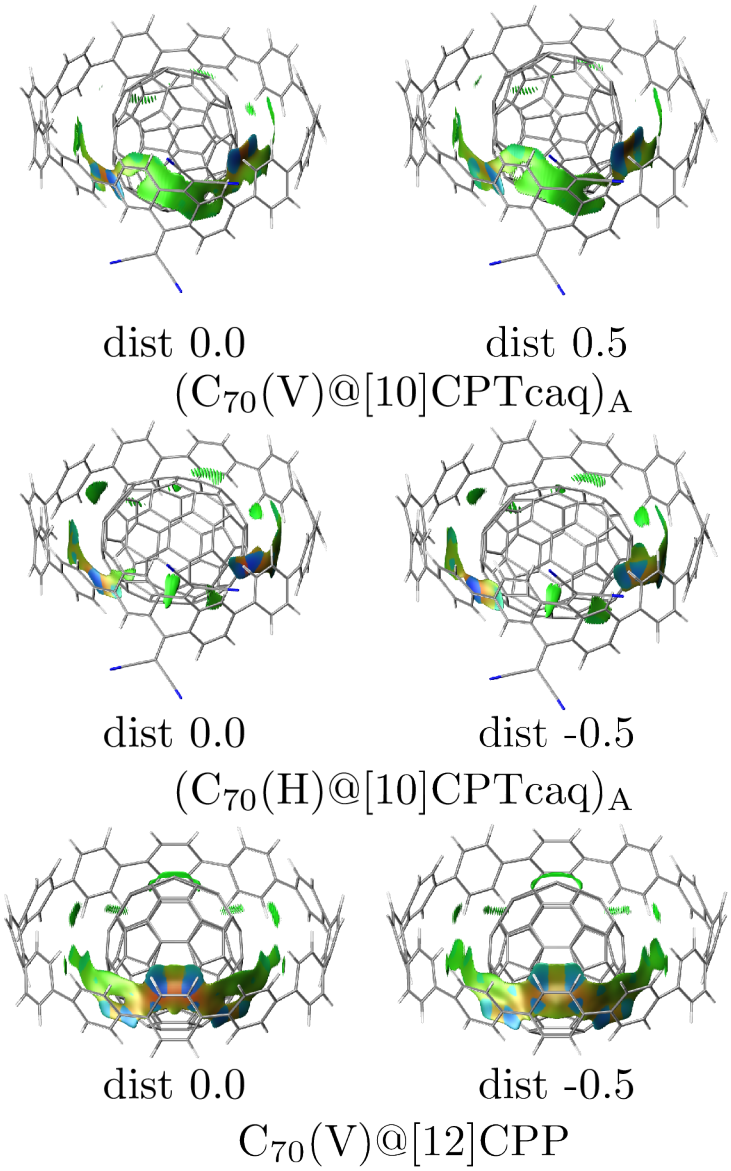

Figure S8. 3D NCI plot for some departures in Z axis. The gradient isosurface (0.3 a.u.) and the Blue-green-red scale over the range -0.020 and 0.020 are according to the sign of the second eigenvalue of the Hessian times the density.

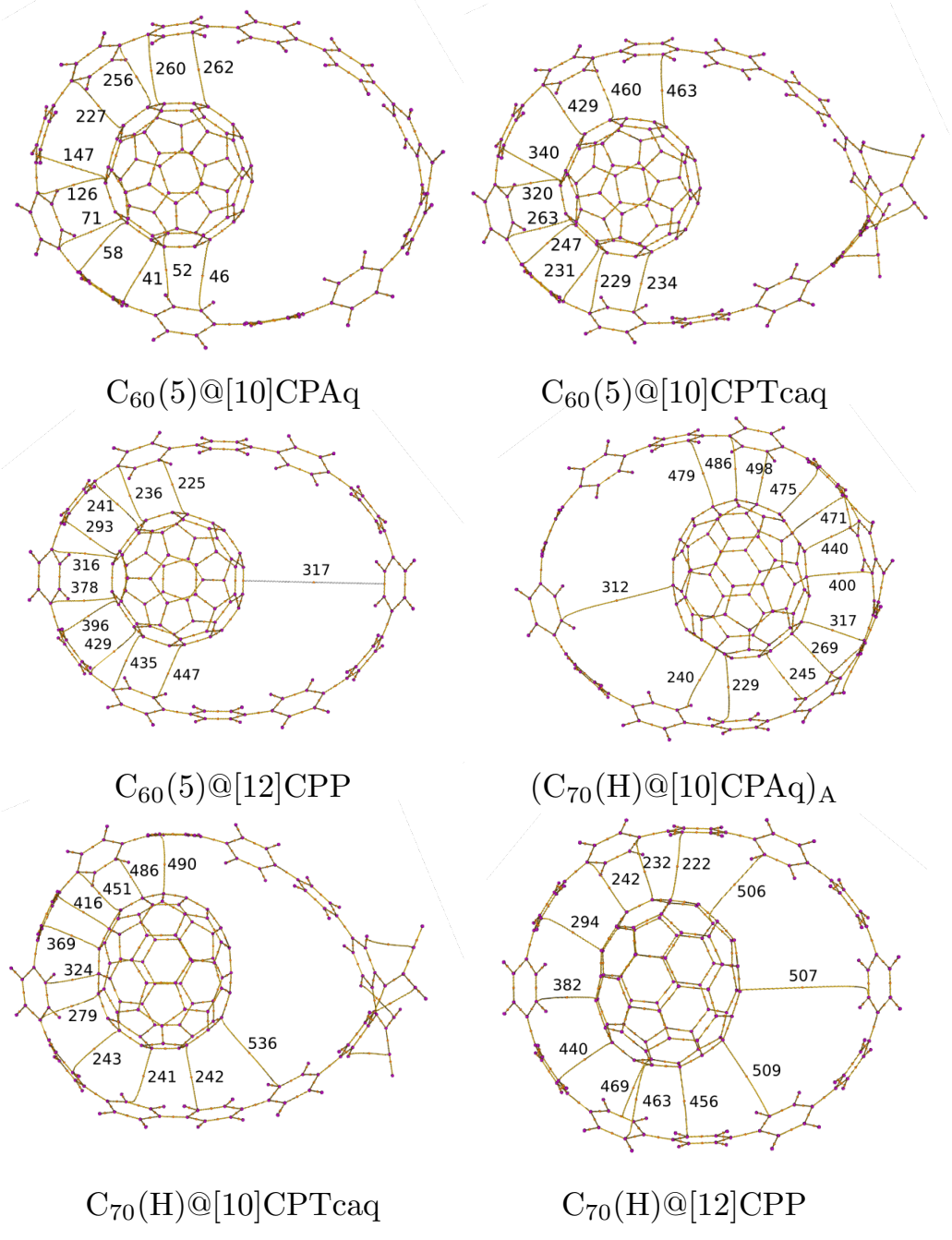

Figure S9. Bond critical points for the most stable complexes. The numbers refer to the values listed in Table S2.

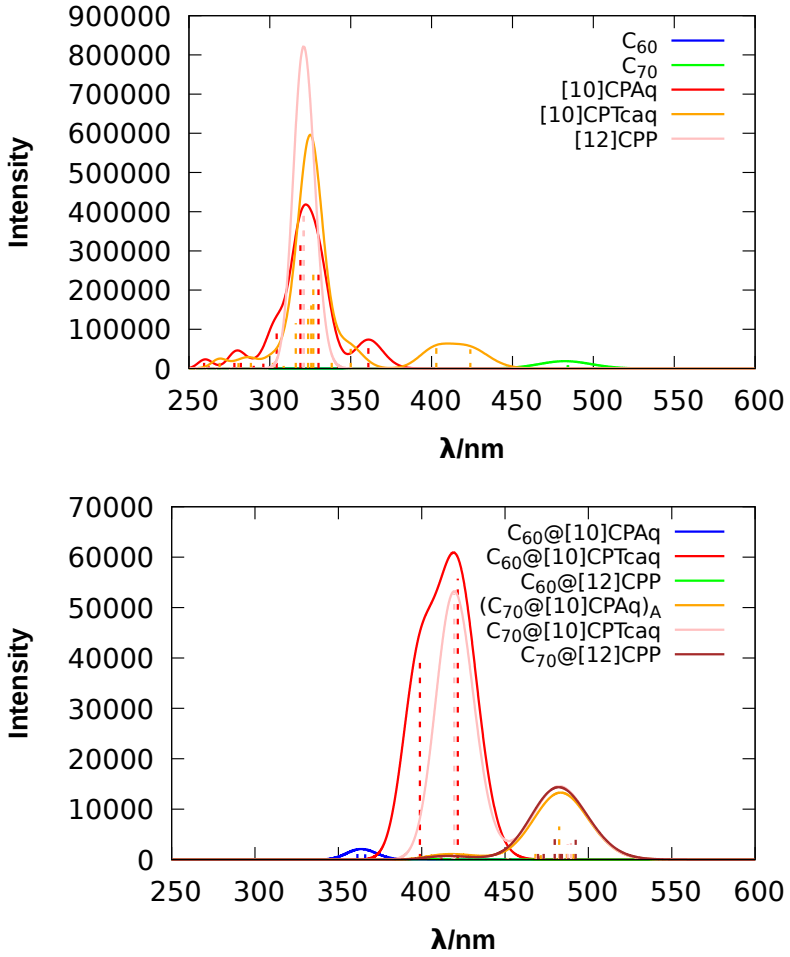

Figure S10. Absorption spectra for the monomers and complexes studied at CAM-B3LYP/TZVP level

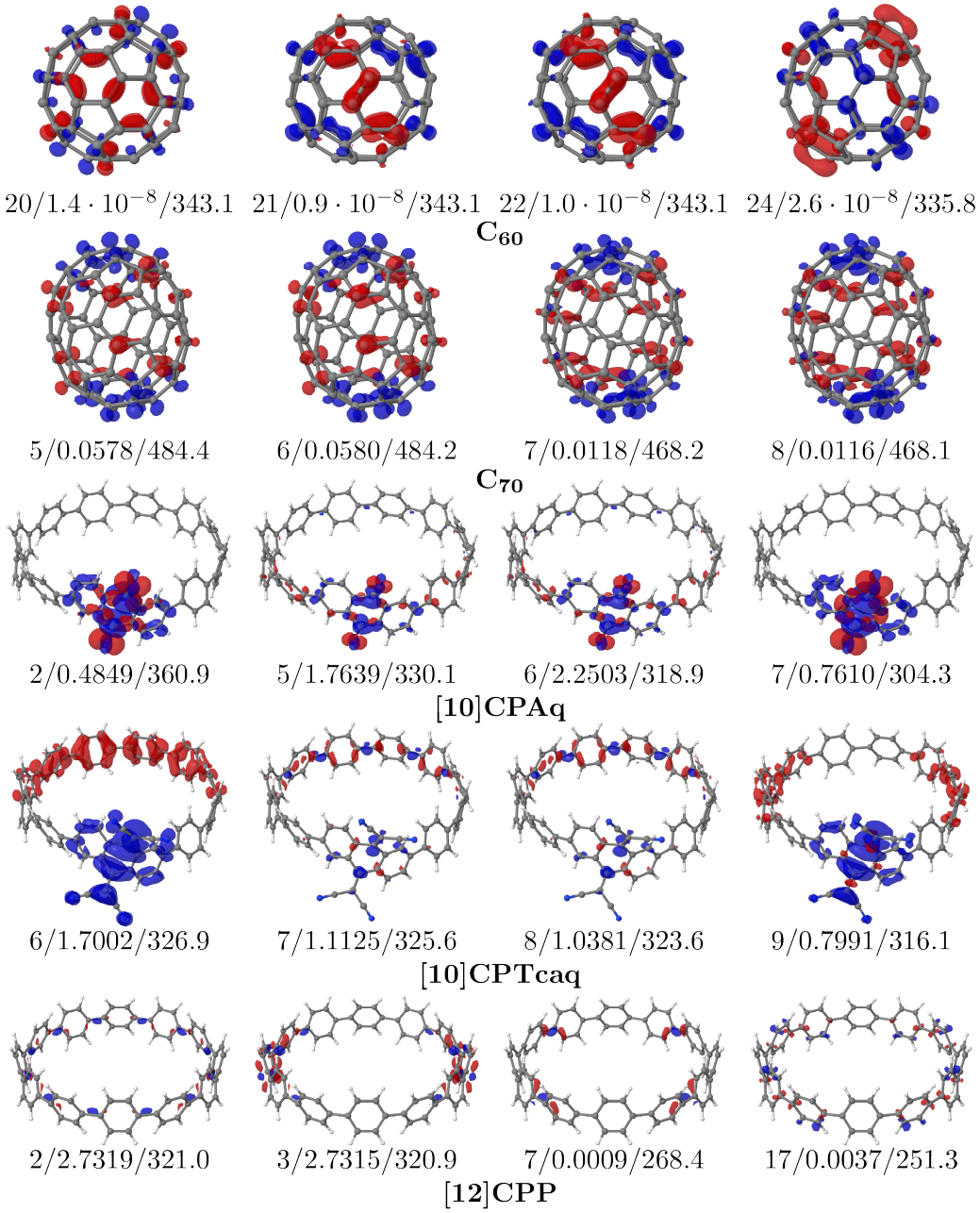

Figure S11. Difference density between the excited state and the ground state for the four most intense transitions in monomers. The numbers are the number of the transition/ oscillator strength/ wavelenght (nm). Surfaces correspond to -0.001 a.u. (red) and 0.001 a.u. (blue)

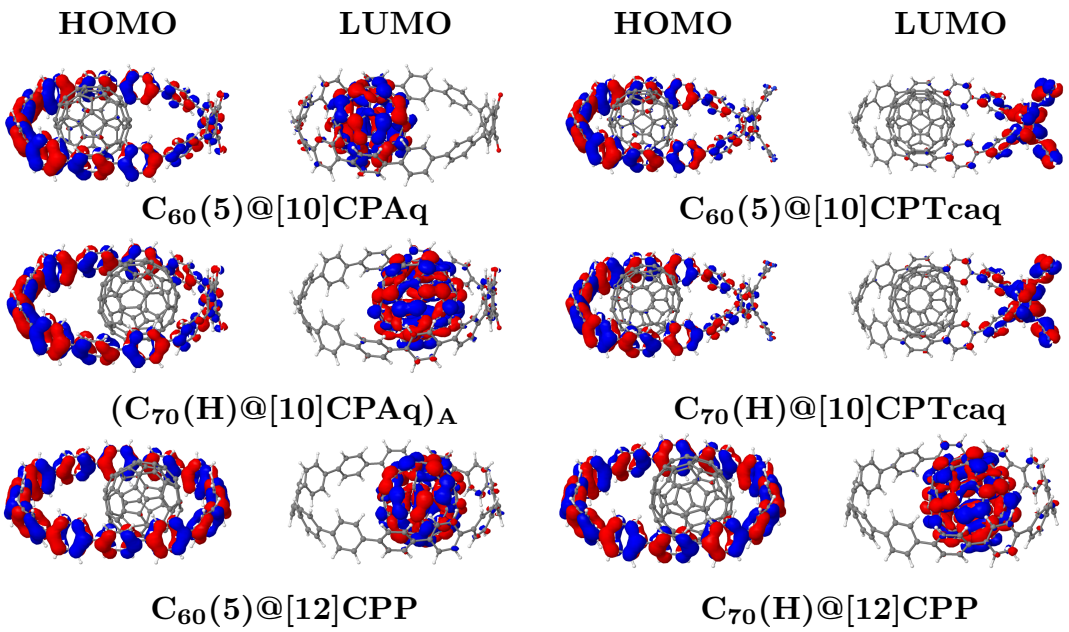

Figure S12. HOMO and LUMO orbitals in complexes at the CAM-B3LYP/def2-TZVP//B97-D2/def2-TZVP level

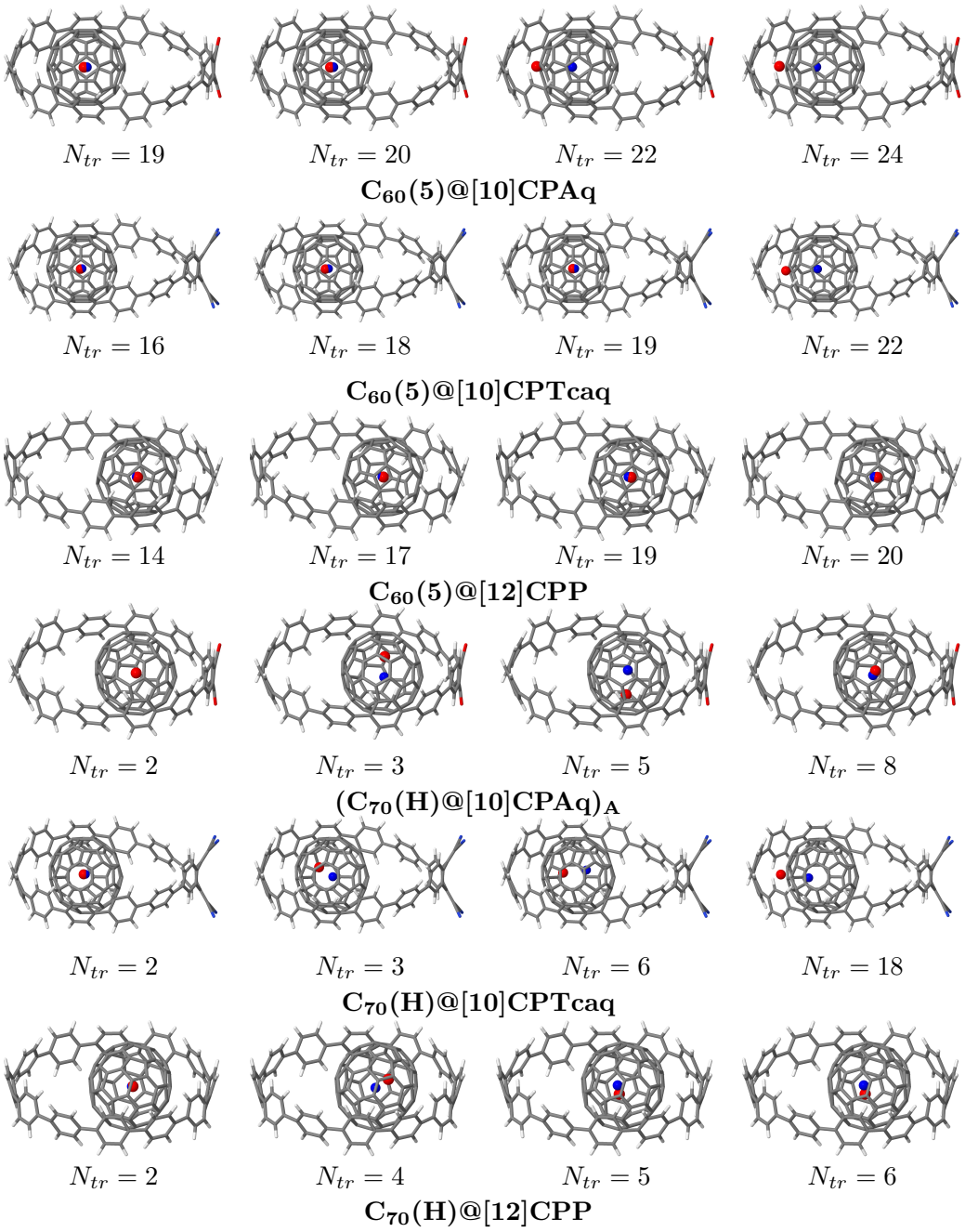

Figure S13. Position of the barycentres of charge in the most stable complexes. The blue sphere corresponds to the positive barycentre and the red sphere is the negative barycentre.

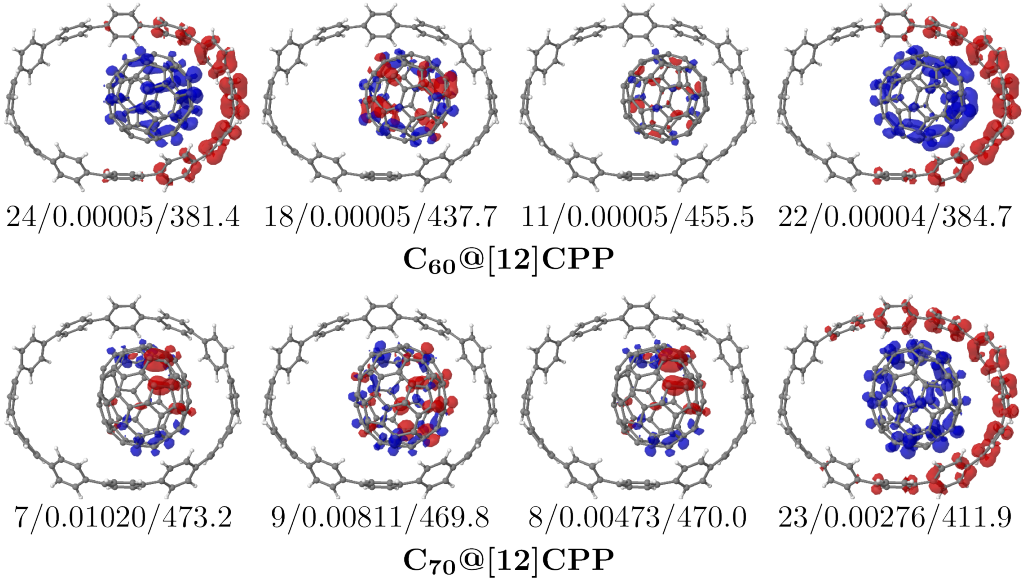

Figure S14. Difference density between the excited state and the ground state for the five to eight most intense transitions in C_{60}@[12]CPP and C_{70}@[12]CPP. The numbers are the number of the transition/oscillator strength/wavelength (nm). Surfaces correspond to −0.001 a.u.(red) and 0.001 a.u.(blue)

Table S4. Amount of the charge transfer and the distance for the five to eight most important transitions in the most stable complexes between fullerenes and [12]CPP. N_{tr} is the number of the transition, q is the amount of charge that it transferred and R is the distance between positive and negative centre in the barycentre following ref. 85 and 86.

	N_{tr}	q	R(Å)	N_{tr}	q	R(Å)
C_{60}@[12]CPP	11	0.257	0.145	18	0.431	0.083
	22	0.931	2.709	24	0.841	2.856
C_{70}@[12]CPP	07	0.329	1.401	08	0.357	1.371
	09	0.454	1.137	23	0.970	2.161

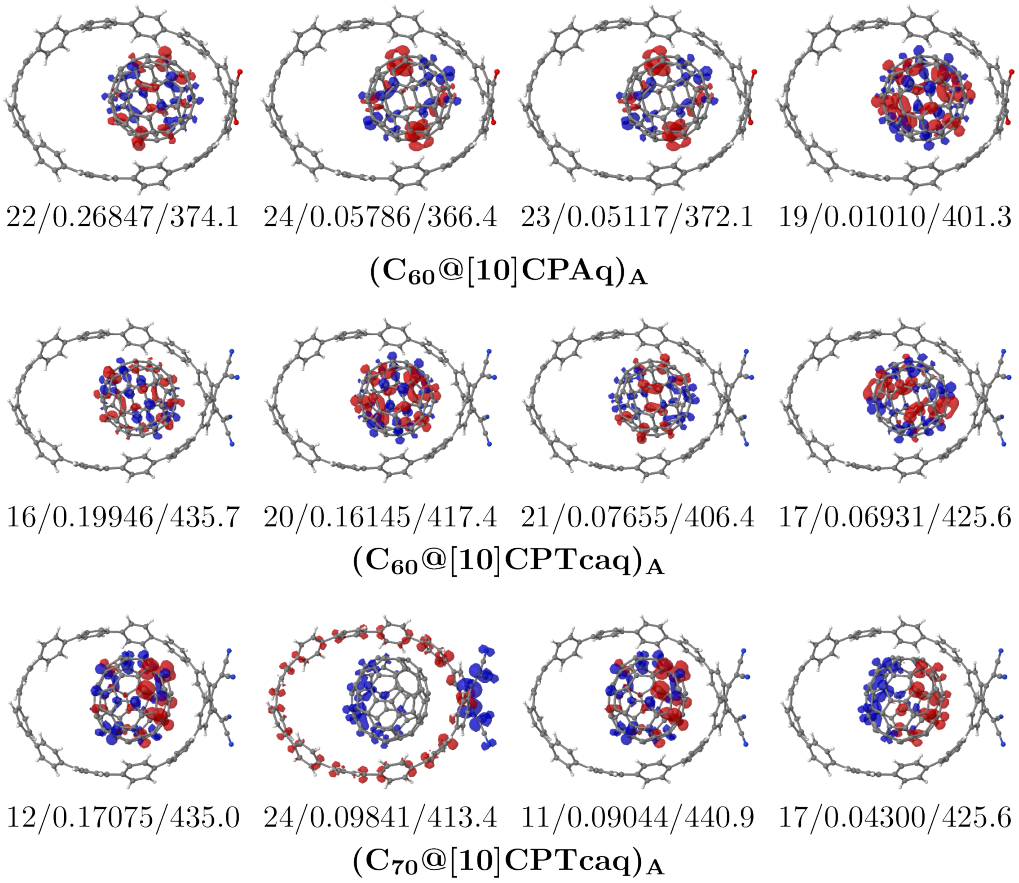

Figure S15. Difference density between the excited state and the ground state for the four most intense transitions with the fullerene near the anthracene unit. The numbers are the number of the transition/ oscillator strength/ wavelength (nm). Surfaces correspond to -0.001 a.u.(red) and 0.001 a.u.(blue)

Table S5. Amount of the charge transfer and the distance for the four most important transitions in complexes with the fullerene near the anthracene. N_{tr} is the number of the transition, q is the amount of charge that it transferred and R is the distance between positive and negative centre in the barycentre following ref. 85 and 86.

	N_{tr}	q	R (Å)	N_{tr}	q	R (Å)
$(C_{60}@[10]CPAq)_A$	19	0.476	0.038	22	0.375	0.122
	23	0.359	0.102	24	0.378	0.100
$(C_{60}@[10]CPTcaq)_A$	16	0.403	0.137	17	0.454	0.110
	20	0.471	0.116	21	0.381	0.234
$(C_{70}@[10]CPTcaq)_A$	11	0.511	1.463	12	0.526	1.459
	17	0.424	3.120	24	0.798	4.507

Table S6. Energies for the complexes with C_{60} (kcal mol^{-1}) obtained at the B3LYP-D3(BJ)/def2-TZVP level using the B97-D2/def2-TZVP geometries. ΔE_{comp} is the complexation energy, E_{def} the deformation energies of monomers, E_{disp} the contribution of dispersion to the total complexation energy.

Complex[a]	ΔE_{comp}	E_{def}		E_{disp}
		Full	Ring	
$(C_{60}(5)@[10]CPAq)_A$	−29.96	−0.10	3.31	−49.54
$(C_{60}(6)@[10]CPAq)_A$	−29.42	−0.09	2.77	−48.91
$(C_{60}(5)@[10]CPTcaq)_A$	−29.77	−0.02	2.78	−49.26
$(C_{60}(6)@[10]CPTcaq)_A$	−30.28	−0.09	2.65	−50.05
$C_{60}(5)@[12]CPP$	−30.67	−0.01	2.89	−49.91
$C_{60}(6)@[12]CPP$	−29.89	−0.12	3.26	−49.04
$C_{60}(5)@[10]CPAq$	−31.15	−0.04	2.37	−50.19
$C_{60}(6)@[10]CPAq$	−30.51	−0.09	2.99	−50.24
$C_{60}(5)@[10]CPTcaq$	−33.06	−0.06	2.04	−52.43
$C_{60}(6)@[10]CPTcaq$	−32.51	−0.12	2.67	−52.40

[a] The subscript A denotes when the fullerene is close to the anthracene unit.

Table S7. Energies for the complexes with C_{70} (kcal mol^{-1}) obtained at the B3LYP-D3(BJ)/def2-TZVP level using the B97-D2/def2-TZVP geometries. ΔE_{comp} is the complexation energy, E_{def} the deformation energies of monomers, E_{disp} the contribution of dispersion to the total complexation energy.

Complex[a]	ΔE_{comp}	E_{def}		E_{disp}
		Full	Ring	
$(C_{70}(V)@[10]CPAq)_A$	−33.73	0.04	3.58	−56.07
$(C_{70}(H)@[10]CPAq)_A$	−35.69	0.01	2.12	−55.76
$(C_{70}(V)@[10]CPTcaq)_A$	−34.91	−0.06	2.95	−57.24
$(C_{70}(H)@[10]CPTcaq)_A$	−35.42	0.10	2.35	−56.51
$C_{70}(V)@[12]CPP$	−34.12	−0.08	2.88	−55.51
$C_{70}(H)@[12]CPP$	−34.83	0.04	1.02	−53.17
$C_{70}(V)@[10]CPAq$	−34.40	−0.09	2.63	−55.62
$C_{70}(H)@[10]CPAq$	−35.18	0.13	1.77	−54.86
$C_{70}(V)@[10]CPTcaq$	−36.30	−0.06	1.94	−57.09
$C_{70}(H)@[10]CPTcaq$	−37.11	0.06	1.15	−56.74

[a] The subscript A denotes when the fullerene is close to the anthracene unit.

[10]CPA

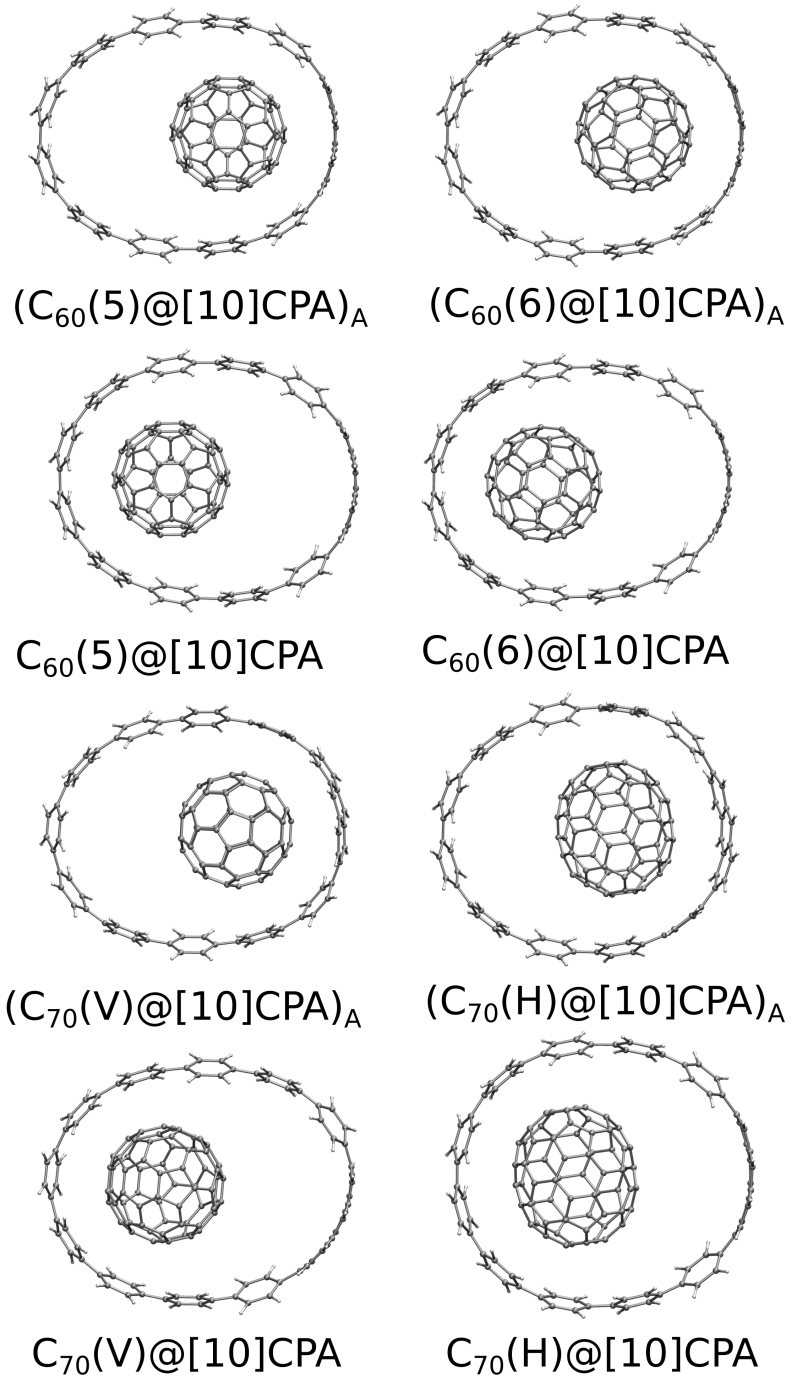

Figure S16. Most stable structures found for [10]CPA complexes.

Table S8. Energy for the complexes with [10]CPA (kcal mol^{-1}). ΔE_{comp} is the complexation energy, E_{def} the deformation energies of monomers, E_{disp} the contribution of dispersion to the total complexation energy, R_{centre} the distance between the center of host and guest.

Complex[a]	ΔE_{comp}	E_{def}		E_{disp}	R_{centre} (Å)
		Full	Ring		
$(C_{60}(5)@[10]CPA)_A$	−31.45	0.08	4.94	−59.01	2.288
$(C_{60}(6)@[10]CPA)_A$	−31.02	0.09	4.59	−57.68	2.270
$C_{60}(5)@[10]CPA$	−30.77	0.10	3.27	−55.74	2.389
$C_{60}(6)@[10]CPA$	−30.38	0.07	4.24	−56.90	2.422
$(C_{70}(V)@[10]CPA)_A$	−35.70	0.17	4.43	−65.24	2.206
$(C_{70}(H)@[10]CPA)_A$	−38.01	0.13	2.51	−64.66	1.670
$C_{70}(V)@[10]CPA$	−34.61	0.12	3.90	−63.15	2.290
$C_{70}(H)@[10]CPA$	−36.15	0.11	1.58	−60.11	1.779

[a] The subscript A denotes when the fullerene is close to the anthracene unit.

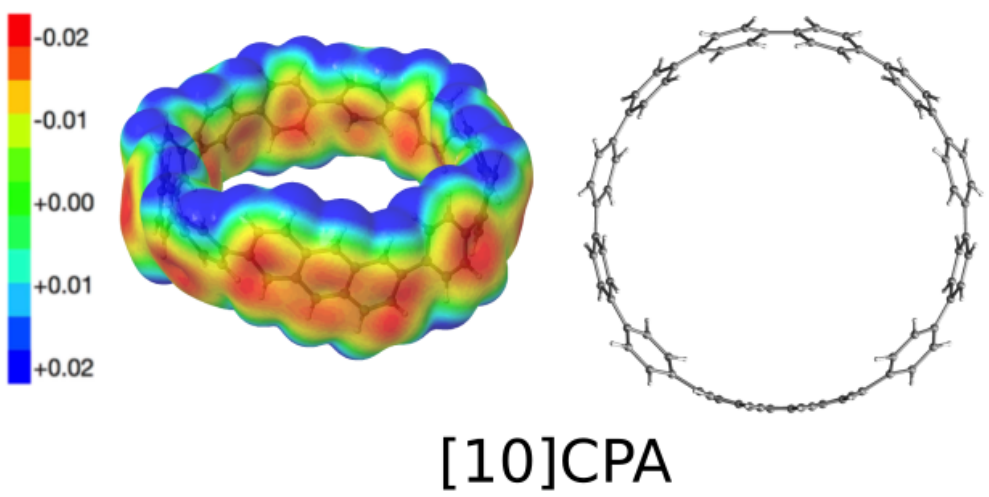

Figure S17. [10]CPA nanohoop studied together with its molecular electrostatic potential (MEPs) mapped on a 0.001 a.u. electron density isosurfaces at the B97-D2/def2-TZVP level.

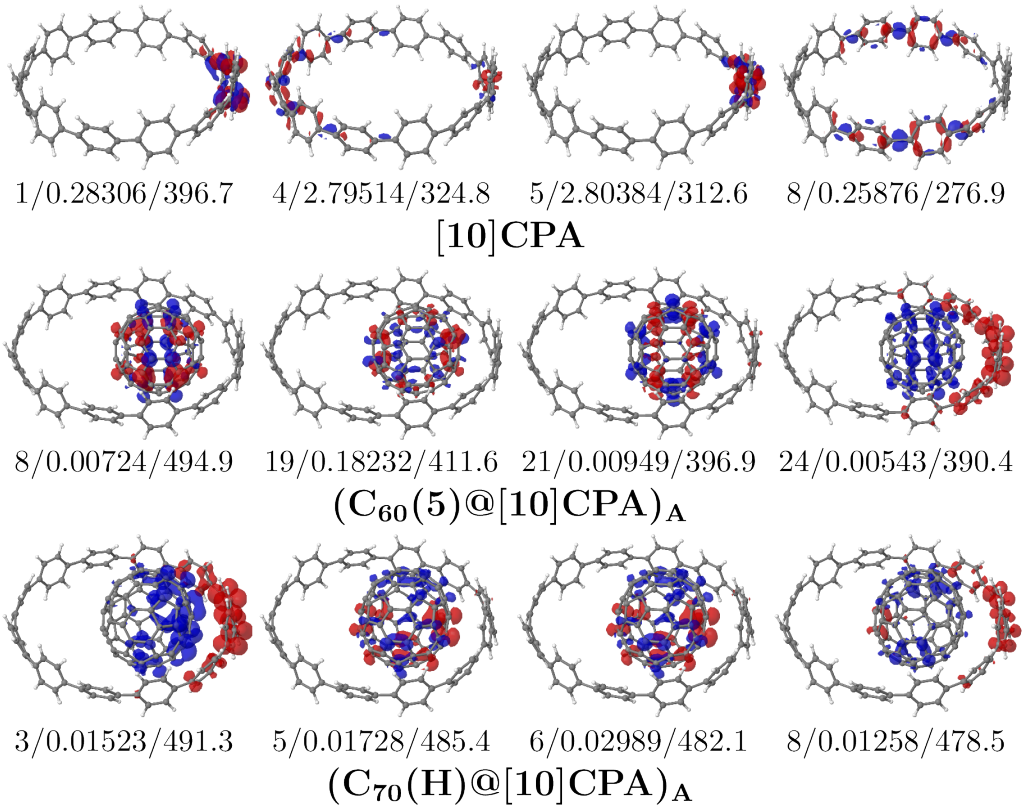

Figure S18. Difference density between the excited state and the ground state for the four most intense transitions in the most stable structures found in [10]CPA and their complexes. The numbers are the number of the transition/ oscillator strength/ wavelength (nm). Surfaces correspond to −0.001 a.u.(red) and 0.001 a.u.(blue)

Table S9. Amount of the charge transfer and the distance for the four most important transitions found in [10]CPA and the most stable [10]CPA complexes. N_{tr} is the number of the transition, q is the amount of charge that it transferred and R is the distance between positive and negative centre in the barycentre following ref. 85 and 86.

	N_{tr}	q	R (Å)	N_{tr}	q	R (Å)
[10]CPA	1	0.282	0.012	4	0.392	0.094
	5	0.216	0.132	8	0.414	0.219
$(C_{60}(5)@[10]CPA)_A$	8	0.570	0.433	19	0.387	0.388
	21	0.502	0.958	24	0.852	4.382
$(C_{70}(H)@[10]CPA)_A$	3	0.945	3.895	5	0.526	2.055
	6	0.548	2.006	8	0.555	3.599

[8]CPX

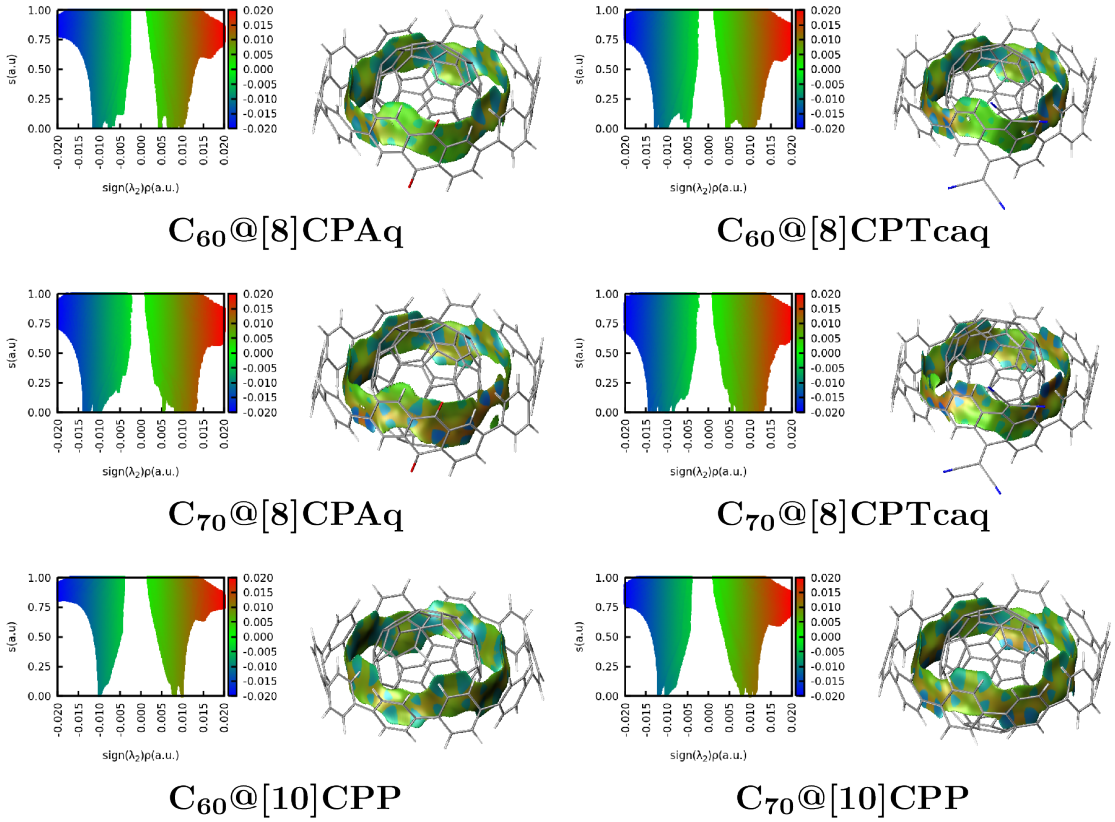

Figure S19. 2D and 3D NCI plots for the most stable structures found for anthracene-substituted [8]CPP complexes. The product of the density times the sign of the second eigenvalue of its Hessian is mapped onto an isosurface of reduced density gradient with value 0.3 a.u. The colour scale goes from −0.020 a.u. (blue) to +0.020 a.u. (red).

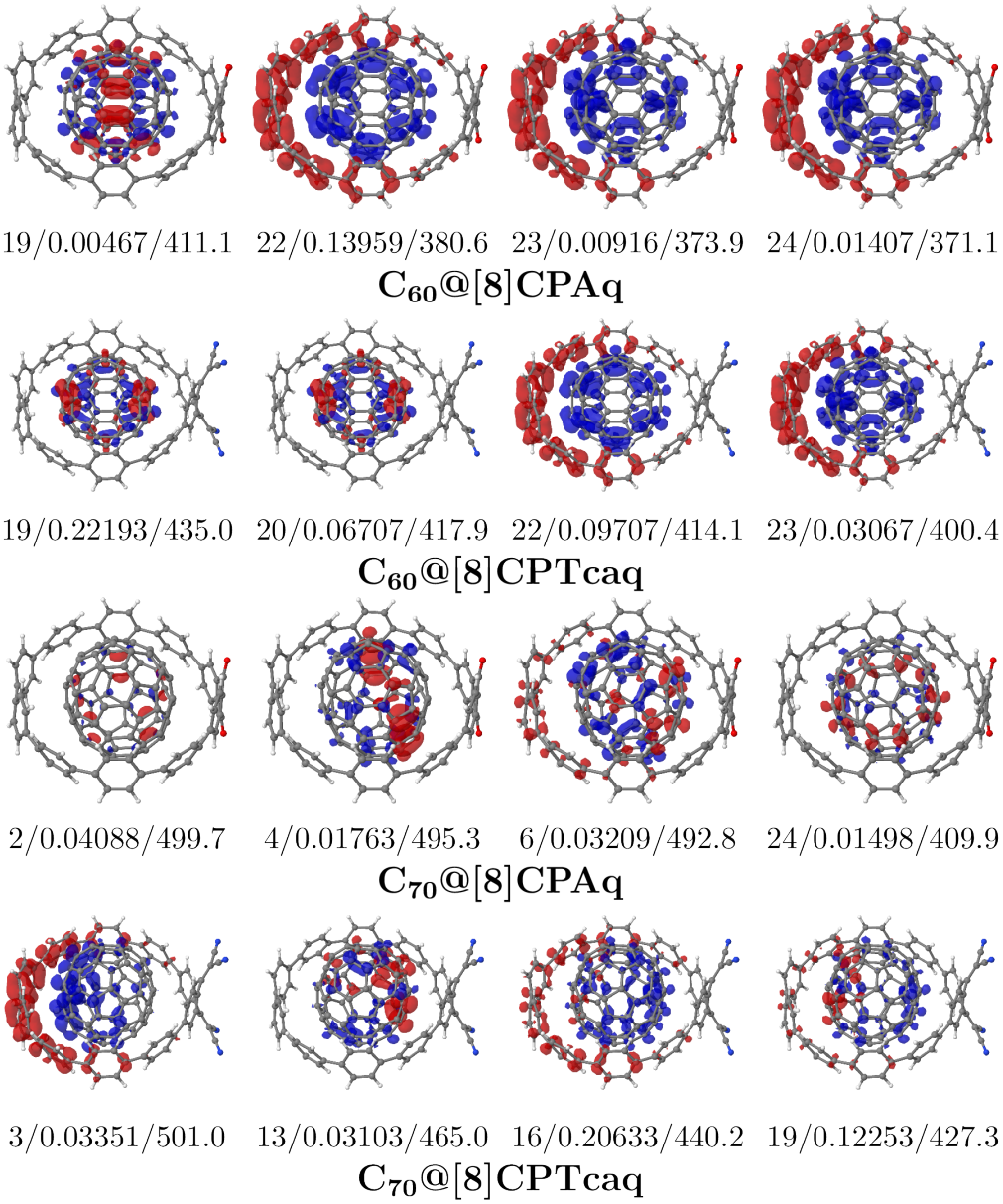

Figure S20. Difference density between the excited state and the ground state for the four most intense transitions in anthracene-substituted [8]CPX complexes. The numbers are the number of the transition/ oscillator strength/ wavelength (nm). Surfaces correspond to −0.001 a.u.(red) and 0.001 a.u.(blue).

C_{100}

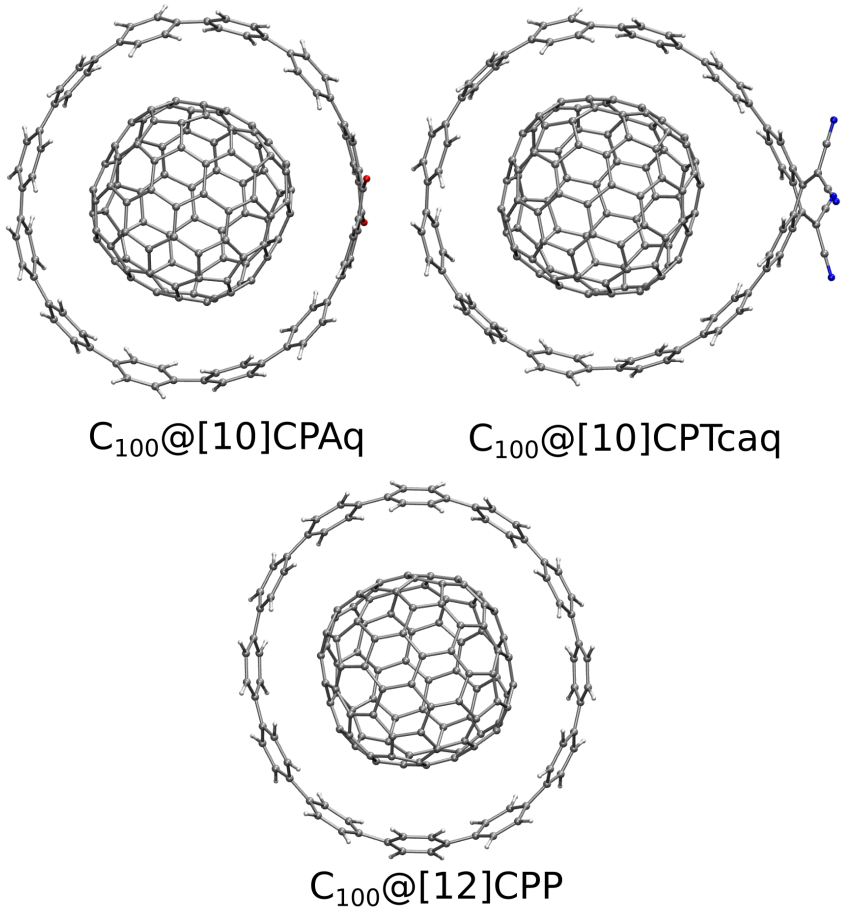

Figure S21. Most stable structures found for C_{100} complexes with the nanohoops.

Coordinates

Optimised coordinates in Å for the monomers

C_{60}

C	0.998874	0.725724	3.327532
C	0.998874	-0.725724	3.327532
C	1.961115	-1.424833	2.592445
C	2.959989	-0.699109	1.829374
C	2.959989	0.699109	1.829374
C	1.961115	1.424833	2.592445
C	-0.381536	1.174247	3.327532
C	-1.234676	0.000000	3.327532
C	-0.381536	-1.174247	3.327532
C	-0.749079	-2.305429	2.592445
C	1.579579	-2.599080	1.829374
C	3.195791	-1.424833	0.594698
C	3.422945	-0.725724	-0.594698
C	3.422945	0.725724	-0.594698
C	3.195791	1.424833	0.594698
C	2.342651	2.599080	0.594698
C	1.579579	2.599080	1.829374
C	0.249795	3.031153	1.829374
C	-0.749079	2.305429	2.592445
C	-2.424071	0.000000	2.592445
C	-2.805607	1.174247	1.829374
C	-1.983755	2.305429	1.829374
C	-1.747953	3.031153	0.594698
C	-0.367543	3.479675	0.594698
C	0.367543	3.479675	-0.594698
C	1.747953	3.031153	-0.594698
C	1.983755	2.305429	-1.829374
C	2.805607	1.174247	-1.829374
C	2.342651	-2.599080	0.594698
C	0.381536	-1.174247	-3.327532
C	0.749079	-2.305429	-2.592445
C	-0.249795	-3.031153	-1.829374
C	-1.579579	-2.599080	-1.829374
C	-1.961115	-1.424833	-2.592445
C	-0.998874	0.725724	-3.327532
C	0.381536	1.174247	-3.327532
C	1.234676	0.000000	-3.327532
C	2.424071	0.000000	-2.592445
C	2.805607	-1.174247	-1.829374
C	1.983755	-2.305429	-1.829374
C	0.367543	-3.479675	-0.594698
C	-0.367543	-3.479675	0.594698
C	-1.747953	-3.031153	0.594698
C	-2.342651	-2.599080	-0.594698
C	-3.195791	-1.424833	-0.594698
C	-2.959989	-0.699109	-1.829374
C	-2.959989	0.699109	-1.829374
C	-1.961115	1.424833	-2.592445
C	0.749079	2.305429	-2.592445
C	-0.249795	3.031153	-1.829374
C	-1.579579	2.599080	-1.829374
C	-2.342651	2.599080	-0.594698
C	-3.195791	1.424833	-0.594698
C	-3.422945	0.725724	0.594698
C	-3.422945	-0.725724	0.594698
C	-2.805607	-1.174247	1.829374
C	-1.983755	-2.305429	1.829374
C	1.747953	-3.031153	-0.594698
C	0.249795	-3.031153	1.829374
C	-0.998874	-0.725724	-3.327532

C_{70}

C	4.437515	-0.673982	-0.108239
C	4.259485	0.427886	-0.989443
C	3.634326	0.186370	-2.297440
C	3.234625	-1.138495	-2.624630
C	3.511017	-2.251165	-1.745299
C	4.103694	-2.022415	-0.505709
C	1.985222	-1.397310	-3.285833
C	1.488567	-2.669849	-2.815471
C	0.121877	-2.846995	-2.613143
C	-0.789406	-1.756898	-2.874943
C	-0.338165	-0.524917	-3.423088
C	-1.821818	-1.793855	-1.875955
C	-2.429369	-0.599613	-1.399651
C	-2.695775	-0.473609	0.040187
C	-2.334065	-1.551579	0.894213
C	-1.801574	-2.787599	0.368478
C	-1.549300	-2.906890	-0.996080
C	-1.722458	-1.315303	2.173037
C	-0.811803	-2.405229	2.438460
C	0.399167	-2.154264	3.079379
C	0.735951	-0.805924	3.474225
C	-0.179200	0.269500	3.306648
C	-1.457098	0.004760	2.630436
C	2.676557	0.639519	2.883625
C	3.732376	0.677192	1.862021
C	4.177193	-0.550803	1.299643
C	3.682391	-1.822867	1.773378
C	2.681695	-1.858507	2.741712
C	2.145963	-0.623193	3.265430
C	1.103896	-0.338046	-3.636828
C	1.636859	0.977797	-3.557883
C	-1.137640	0.618229	-3.146994
C	0.784918	2.128679	-3.365417
C	-0.581730	1.951592	-3.163002
C	-2.170068	0.581391	-2.147958
C	-2.252973	1.892182	-1.545784

C	-2.505293	2.011711	-0.181211
C	-2.682346	0.823905	0.622196
C	-2.070794	1.060054	1.901128
C	-1.515503	2.393876	1.888957
C	-0.304339	2.644546	2.529535
C	0.387733	1.569292	3.202008
C	1.797766	1.752010	2.993346
C	1.978065	2.940490	2.191936
C	2.978654	2.976283	1.223584
C	3.828843	1.824591	1.027649
C	4.088990	1.701520	-0.380335
C	3.399699	2.776994	-1.055489
C	2.807141	2.547942	-2.294966
C	2.886141	1.236760	-2.896534
C	-1.278333	2.752866	-2.180243
C	-1.792869	2.996664	0.603395
C	0.677390	3.508175	1.910702
C	2.718334	3.581282	-0.064603
C	1.509615	3.114101	-2.592983
C	2.437371	-3.213082	-1.868111
C	-0.350662	-3.574442	-1.455306
C	-0.865105	-3.330983	1.328065
C	1.605013	-2.819126	2.635722
C	3.646404	-2.746625	0.660373
C	0.562563	-4.094327	-0.531239
C	0.299985	-3.970095	0.889410
C	1.560660	-3.709087	1.556731
C	2.602507	-3.672036	0.548592
C	1.985527	-3.910035	-0.741939
C	1.459306	4.124129	-0.344669
C	0.417694	4.086876	0.663485
C	-0.842911	3.825666	-0.003681
C	-0.580394	3.701300	-1.424332
C	0.842460	3.885730	-1.635019

[10]CPAq

C	7.329889	-3.115048	1.903494
C	7.787502	-1.827823	2.159488
C	8.034440	-0.940406	1.102283
C	7.965268	-1.425496	-0.222399
C	7.560864	-2.739016	-0.466230
C	7.139564	-3.579293	0.581746
C	7.965223	1.425506	0.222263
C	7.560869	2.738970	0.466017
C	7.139535	3.579303	-0.581783
C	7.329841	3.115065	-1.903458
C	7.787474	1.827911	-2.159675
C	8.034364	0.940444	-1.102448
C	8.215722	0.511561	1.384328
C	8.215623	-0.511574	-1.384469
C	6.344850	-4.800960	0.323258
C	5.585363	-4.907301	-0.859322
C	6.145586	-5.794651	1.304466
C	4.591803	-5.868870	-0.996316
C	5.142745	-6.750526	1.172282
C	4.295978	-6.767105	0.046515
C	3.020225	-7.511349	0.016562
C	2.240437	-7.599798	1.185073
C	2.433557	-7.948427	-1.187375
C	0.895046	-7.949618	1.126787
C	1.091778	-8.310886	-1.242390
C	0.266674	-8.237685	-0.100746
C	-1.209360	-8.226469	-0.198111
C	-1.827110	-7.719936	-1.358425
C	-2.044148	-8.498756	0.905167
C	-3.171727	-7.367558	-1.366847
C	-3.389459	-8.141474	0.898563
C	-3.968992	-7.498373	-0.213716
C	-8.971643	-1.578779	1.057682
C	-8.769535	-0.737310	-0.055202
C	6.344849	4.801001	-0.323273
C	6.145593	5.794593	-1.304437
C	5.585425	4.907270	0.859353
C	5.142766	6.750519	-1.172274
C	4.591894	5.868898	0.996298
C	4.296025	6.767105	-0.046439
C	-8.026147	-3.491538	-0.128458
C	-7.030461	-5.528500	-1.252867
C	-7.284535	-4.770630	-0.091346
C	-5.255909	6.775379	0.134499
C	-6.039438	6.504860	1.274587
C	-5.621141	6.132148	-1.063570
C	-7.030465	5.528460	1.252811
C	-6.609479	5.153642	-1.084217
C	-7.284503	4.770628	0.091278
C	-8.026113	3.491548	0.128336
C	-8.609773	2.922262	-1.021784
C	-7.972324	2.687978	1.283888
C	-8.971551	1.578814	-1.057886
C	-8.335321	1.345971	1.248458
C	-8.769527	0.737340	0.055005
C	3.020262	7.511321	-0.016449
C	2.433556	7.948372	1.187510
C	2.240397	7.599824	-1.184953
C	1.091802	8.310866	1.242623
C	0.895056	7.949656	-1.126666
C	0.266688	8.237684	0.100883
C	-1.209327	8.226486	0.198291
C	-2.044125	8.498848	-0.904968
C	-1.827102	7.719921	1.358567
C	-3.389464	8.141554	-0.898395
C	-3.171738	7.367515	1.366977
C	-3.968987	7.498386	0.213838
C	-8.335261	-1.345960	-1.248617
C	-5.255912	-6.775379	-0.134424
C	-5.621204	-6.132103	1.063612
C	-6.039424	-6.504900	-1.274554
C	-7.972276	-2.687984	-1.284028
C	-8.609873	-2.922241	1.021624
C	-6.609549	-5.153595	1.084223
H	-5.834120	-7.035495	-2.201688

```
H  -3.993105  -8.321927   1.785260
H  -5.041953  -6.316119   1.965127
H  -6.778108  -4.596119   2.002077
H  -7.585008  -5.313868  -2.163630
H  -7.529763  -3.088512  -2.192538
H  -8.736899  -3.530961   1.914056
H   2.663409  -7.274481   2.132638
H  -3.993096   8.322073  -1.785088
H  -3.581606   6.874614   2.244919
H  -5.834155   7.035433   2.201748
H  -5.041859   6.316207  -1.965049
H  -7.585017   5.313821   2.163535
H  -6.777989   4.596224  -2.002083
H  -8.736738   3.530976  -1.914208
H  -7.529868   3.088484   2.192428
H  -9.374038   1.160733  -1.977881
H  -8.167865   0.731943   2.129814
H   7.028239  -3.739968   2.739452
H   7.873688  -1.459000   3.178229
H   7.511333  -3.067683  -1.500151
H   7.511313   3.067499   1.499815
H   7.028226   3.739946  -2.739421
H   7.873596   1.458811  -3.178428
H  -3.581592  -6.874703  -2.244797
H  -9.374185  -1.160706   1.977651
H   6.759357   5.797454  -2.201732
H   5.699265   4.164335   1.643415
H   4.984061   7.472661  -1.969950
H   3.958375   5.852742   1.879579
H   0.296793   7.886348  -2.032037
H   3.028797   7.960415   2.098051
H  -1.221130   7.491321   2.231336
H  -1.621671   8.955926  -1.796907
H  -1.221127  -7.491401  -2.231196
H  -1.621689  -8.955810   1.797150
H   2.663367   7.274531  -2.132510
H   0.661322   8.607204   2.196211
H   0.296858  -7.886273   2.032142
H   0.661340  -8.607282  -2.195939
H   5.699191  -4.164268  -1.643395
H   4.984207  -7.472690   1.970100
H   6.759500  -5.797333   2.201683
H  -8.167743  -0.731955  -2.129970
H   3.028760  -7.960508  -2.097896
H   3.958244  -5.852744  -1.879536
O   8.450720  -0.940351  -2.509039
O   8.450933   0.940190   2.508993
```

[10]CPTcaq

```
C   6.577059   2.845975  -2.011105
C   7.196161   1.621890  -2.227435
C   7.646708   0.844065  -1.148194
C   7.575253   1.399086   0.159297
C   6.977776   2.646071   0.354504
C   6.398966   3.361515  -0.710928
C   7.575380  -1.398931  -0.159337
C   6.977922  -2.645986  -0.354503
C   6.399182  -3.361434   0.710973
C   6.577315  -2.845902   2.011166
C   7.196380  -1.621770   2.227453
C   7.646844  -0.843925   1.148161
C   8.035637  -0.562828  -1.285339
C   8.035703   0.562997   1.285337
C   5.494763   4.505092  -0.474905
C   4.754001   4.588766   0.720745
C   5.205514   5.449389  -1.481475
C   3.703963   5.488580   0.857023
C   4.152507   6.347754  -1.345768
C   3.336118   6.347304  -0.196731
C   2.043748   7.059908  -0.143404
C   1.244778   7.147671  -1.299183
C   1.476483   7.495830   1.070361
C  -0.094624   7.514983  -1.221971
C   0.140523   7.875767   1.144359
C  -0.699695   7.822126   0.012725
C  -2.173571   7.870179   0.125209
C  -2.802081   7.391437   1.291269
C  -3.005341   8.186915  -0.968376
C  -4.162812   7.108183   1.314329
C  -4.367031   7.900014  -0.946645
C  -4.965689   7.284613   0.171090
C  -6.289611   6.630933   0.105090
C  -6.699725   6.009722  -1.089992
C  -7.072899   6.397790   1.253469
C  -7.732833   5.078785  -1.100124
C  -8.109547   5.469910   1.241981
C  -8.410103   4.724878   0.083199
C  -9.197148   3.473845   0.129430
C  -9.159776   2.671209   1.286245
C  -9.801315   2.918677  -1.017189
C  -9.549210   1.336943   1.251797
C -10.188759   1.582719  -1.052562
C  -9.993704   0.736678   0.057946
C   5.494992  -4.505066   0.474953
C   5.205726  -5.449353   1.481572
C   4.754234  -4.588795  -0.720703
C   4.152746  -6.347702   1.345836
C   3.704235  -5.488600  -0.856971
C   3.336354  -6.347312   0.196802
C   2.043988  -7.059878   0.143475
C   1.476721  -7.495822  -1.070286
C   1.245014  -7.147595   1.299265
C   0.140780  -7.875756  -1.144253
C  -0.094366  -7.514910   1.222047
C  -0.699440  -7.822103  -0.012629
C  -2.173328  -7.870188  -0.125117
C  -3.005096  -8.186907   0.968472
C  -2.801836  -7.391489  -1.291201
C  -4.366787  -7.900042   0.946716
C  -4.162565  -7.108268  -1.314274
C  -4.965454  -7.284683  -0.171044
```

C	-6.289391	-6.631041	-0.105076
C	-7.072655	-6.397932	-1.253484
C	-6.699553	-6.009831	1.089986
C	-8.109331	-5.470082	-1.242026
C	-7.732691	-5.078927	1.100083
C	-8.409941	-4.725053	-0.083262
C	-9.197027	-3.474046	-0.129518
C	-9.801246	-2.918897	1.017082
C	-9.159650	-2.671412	-1.286336
C	-10.188737	-1.582953	1.052440
C	-9.549130	-1.337158	-1.251900
C	-9.993678	-0.736906	-0.058062
C	8.746562	-1.072458	-2.354967
C	8.746582	1.072658	2.354890
C	9.244974	0.261003	3.420446
C	9.117262	2.449325	2.460762
C	9.117366	-2.449123	-2.460843
C	9.244851	-0.260768	-3.420528
H	5.801276	5.465832	-2.390834
H	3.094800	5.458893	1.756729
H	3.937049	7.044337	-2.152494
H	4.937024	3.877905	1.521869
H	6.901229	-3.042642	-1.360285
H	6.143352	-3.366295	2.859629
H	7.243715	-1.228959	3.237084
H	6.143017	3.366320	-2.859560
H	7.243467	1.229075	-3.237123
H	6.901093	3.042700	1.360245
H	1.649576	6.819322	-2.253560
H	2.085653	7.505621	1.971475
H	-0.706753	7.461129	-2.118579
H	-0.272191	8.180570	2.103091
H	-2.198849	7.131966	2.157366
H	-2.569832	8.626116	-1.863003
H	-4.587828	6.635162	2.195911
H	-4.971542	8.115071	-1.824931
H	-6.123293	6.167386	-1.998214
H	-6.831638	6.916395	2.178696
H	-7.936382	4.530630	-2.016454
H	-8.662867	5.279498	2.158757
H	-8.705282	3.061317	2.193372
H	-9.918812	3.530074	-1.909048
H	-9.389181	0.719475	2.132073
H	-10.600497	1.171479	-1.971528
H	5.801509	-5.465729	2.390931
H	4.937307	-3.877911	-1.521845
H	3.937300	-7.044252	2.152589
H	3.095099	-5.458921	-1.756679
H	2.085893	-7.505631	-1.971396
H	1.649812	-6.819212	2.253624
H	-0.271936	-8.180574	-2.102970
H	-0.706509	-7.461018	2.118636
H	-2.569577	-8.626078	1.863121
H	-2.198587	-7.132030	-2.157299
H	-4.971293	-8.115087	1.824997
H	-4.587573	-6.635283	-2.195871
H	-6.831356	-6.916539	-2.178697
H	-6.123139	-6.167470	1.998225
H	-8.662632	-5.279696	-2.158817
H	-7.936281	-4.530775	2.016401
H	-9.918748	-3.530297	1.908939
H	-8.705119	-3.061508	-2.193449
H	-10.600515	-1.171725	1.971395
H	-9.389098	-0.719688	-2.132173
N	9.433437	-3.562318	-2.580573
N	9.662491	0.374128	-4.301373
N	9.662636	-0.373895	4.301241
N	9.433177	3.562579	2.580496

[12]CPP

C	-0.695335	7.923823	1.222780
C	0.695480	7.923776	1.222547
C	1.426429	8.177969	0.045904
C	0.695572	8.585911	-1.088361
C	-0.696115	8.585960	-1.088153
C	2.852934	7.795384	-0.026341
C	3.688389	7.775650	1.108924
C	4.893756	7.080025	1.105471
C	5.324094	6.368935	-0.033223
C	4.564427	6.521477	-1.209340
C	3.359927	7.216633	-1.205882
C	6.368748	5.324281	0.032617
C	6.521378	4.564736	1.208785
C	7.216557	3.360243	1.205436
C	7.795263	2.853159	0.025891
C	7.775445	3.688497	-1.109433
C	7.079786	4.893840	-1.106091
C	8.177896	1.426663	-0.046229
C	8.585819	0.695926	1.088112
C	8.585899	-0.695750	1.088037
C	8.178073	-1.426459	-0.046410
C	7.923909	-0.695204	-1.222934
C	7.923778	0.695610	-1.222822
C	7.795430	-2.853019	0.025511
C	7.216612	-3.360290	1.205009
C	6.521314	-4.564721	1.208115
C	6.368781	-5.324071	0.031856
C	7.079811	-4.893544	-1.106797
C	7.775542	-3.688236	-1.109965
C	5.324229	-6.368760	-0.034179
C	4.893952	-7.080018	1.104387
C	3.688624	-7.775692	1.107705
C	2.853189	-7.795354	-0.027566
C	3.360267	-7.216456	-1.207038
C	4.564695	-6.521203	-1.210297
C	1.426683	-8.177950	0.044547
C	0.695651	-7.923950	1.221247
C	-0.695164	-7.924049	1.221411
C	-1.426439	-8.178107	0.044894
C	-0.695846	-8.585755	-1.089695
C	0.695846	-8.585676	-1.089864

C	-2.853029	-7.795501	-0.026914
C	-3.688100	-7.775713	1.108632
C	-4.893329	-7.079866	1.105681
C	-5.323960	-6.368725	-0.032825
C	-4.564781	-6.521268	-1.209210
C	-3.360377	-7.216597	-1.206252
C	-6.368545	-5.324166	0.033374
C	-6.520949	-4.564798	1.209642
C	-7.216296	-3.360410	1.206570
C	-7.795271	-2.853232	0.027191
C	-7.775562	-3.688438	-1.108229
C	-7.079813	-4.893716	-1.105129
C	-8.177927	-1.426674	-0.044700
C	-8.585683	-0.696101	1.089851
C	-8.585665	0.695585	1.090016
C	-8.177967	1.426428	-0.044405
C	-7.923809	0.695398	-1.221080
C	-7.923784	-0.695425	-1.221219
C	-7.795495	2.852976	0.027688
C	-7.216615	3.360099	1.207162
C	-6.521342	4.564514	1.210365
C	-6.368911	5.324021	0.034247
C	-7.080147	4.893694	-1.104325
C	-7.775830	3.688377	-1.107591
C	-5.324310	6.368642	-0.031783
C	-4.893748	7.079610	1.106882
C	-3.688454	7.775387	1.110042
C	-3.360680	7.216697	-1.204998
C	-4.565076	6.521357	-1.208095
H	-1.221559	7.606902	2.119713
H	1.221889	7.606844	2.119348
H	1.227650	8.860599	-1.996414
H	-1.228559	8.860682	-1.995998
H	3.363932	8.273573	2.019958
H	5.491143	7.046023	2.013844
H	4.862250	5.989356	-2.109359
H	2.746205	7.210345	-2.103231
H	5.989324	4.862644	2.108819
H	7.210350	2.746637	2.102847
H	8.273371	3.363954	-2.020458
H	7.045732	5.491131	-2.014520
H	8.860445	1.228121	1.996116
H	8.860555	-1.228091	1.995966
H	7.607075	-1.221522	-2.119826
H	7.606822	1.221908	-2.119672
H	7.210485	-2.746747	2.102498
H	5.989222	-4.862652	2.108126
H	7.045740	-5.490609	-2.015360
H	8.273507	-3.363497	-2.020932
H	5.491250	-7.046176	2.012774
H	3.364067	-8.273741	2.018646
H	2.746551	-7.210125	-2.104372
H	4.862475	-5.989014	-2.110260
H	1.222056	-7.607119	2.118117
H	-1.221413	-7.607351	2.118419
H	-1.228240	-8.860290	-1.997634
H	1.228013	-8.860147	-1.997965
H	-3.363299	-8.273786	2.019471
H	-5.490252	-7.045798	2.014337
H	-4.862790	-5.989139	-2.109141
H	-2.746948	-7.210396	-2.103793
H	-5.988717	-4.862643	2.109564
H	-7.210059	-2.746856	2.104008
H	-8.273607	-3.363698	-2.019110
H	-7.045875	-5.490814	-2.013671
H	-8.860221	-1.228513	1.997787
H	-8.860119	1.227760	1.998124
H	-7.606935	1.221828	-2.117926
H	-7.606954	-1.221666	-2.118181
H	-7.210339	2.746418	2.104506
H	-5.989120	4.862266	2.110323
H	-7.046272	5.490913	-2.012752
H	-8.273908	3.363783	-2.018512
H	-5.490774	7.045514	2.015470
H	-3.363703	8.273322	2.021000
H	-2.747201	7.210688	-2.102544
H	-4.863056	5.989369	-2.108148
C	-2.853297	7.795383	-0.025501
C	-1.426719	8.178035	0.046346

[8]CPAq

C	5.883160	-3.074133	1.858561
C	6.441537	-1.831422	2.136238
C	6.749658	-0.948204	1.092097
C	6.666625	-1.415334	-0.237944
C	6.171102	-2.692174	-0.503212
C	5.655063	-3.500461	0.529656
C	6.666705	1.414927	0.237963
C	6.171257	2.691798	0.503218
C	5.655361	3.500117	-0.529601
C	5.883452	3.073881	-1.858599
C	6.441795	1.831098	-2.136147
C	6.749816	0.947802	-1.092136
C	6.967795	0.496456	1.385668
C	6.967828	-0.496884	-1.385625
C	4.706848	-4.603897	0.250404
C	3.969800	-4.605169	-0.951589
C	4.317387	-5.536526	1.235759
C	2.818965	-5.370224	-1.094476
C	3.158150	-6.294131	1.097609
C	2.334669	-6.166397	-0.039131
C	0.925314	-6.610184	-0.063214
C	0.150705	-6.510573	1.108102
C	0.243124	-6.890343	-1.264371
C	-1.239262	-6.509645	1.053297
C	-1.147058	-6.899978	-1.316640
C	-1.923869	-6.615790	-0.173710
C	-3.335850	-6.182738	-0.265333
C	-3.779478	-5.501327	-1.415908
C	-4.205285	-6.192106	0.845505
C	-4.933263	-4.726050	-1.396336

C	-5.358129	-5.412510	0.866880
C	-5.701747	-4.587510	-0.223885
C	4.707189	4.603648	-0.250411
C	4.317734	5.536297	-1.235777
C	3.970116	4.605008	0.951572
C	3.158597	6.293899	-1.097701
C	2.819318	5.370063	1.094485
C	2.335024	6.166277	0.039010
C	-7.694427	-1.516627	-1.156320
C	-7.552309	-0.739683	0.012571
C	-6.613886	3.430966	0.095372
C	-7.233969	2.829082	1.209849
C	-6.662295	2.723465	-1.121646
C	-7.694297	1.517050	1.156412
C	-7.118903	1.410746	-1.173518
C	-7.552260	0.740092	-0.012475
C	0.925710	6.610100	0.063139
C	0.243545	6.890341	1.264305
C	0.151056	6.510510	-1.108227
C	-1.146634	6.900089	1.316628
C	-1.238886	6.509692	-1.053390
C	-1.923490	6.615912	0.173648
C	-3.335476	6.182965	0.265292
C	-4.204941	6.192314	-0.845508
C	-3.779132	5.501595	1.415917
C	-5.357797	5.412757	-0.866868
C	-4.932949	4.726353	1.396337
C	-5.701436	4.587813	0.223929
C	-6.614127	-3.430621	-0.095288
C	-6.662451	-2.723108	1.121722
C	-7.234212	-2.828674	-1.209787
C	-7.118943	-1.410374	1.173632
H	-7.293542	-3.375461	-2.148354
H	-5.971264	-5.394286	1.765279
H	-6.208905	-3.156305	2.009799
H	-7.007198	-0.855739	2.101535
H	-8.106803	-1.062912	-2.054575
H	0.641576	-6.300996	2.055341
H	-5.970911	5.394503	-1.765277
H	-5.167887	4.114062	2.263250
H	-7.293263	3.375862	2.148424
H	-6.208747	3.156611	-2.009723
H	-8.106679	1.063379	2.054658
H	-7.007215	0.856114	-2.101431
H	5.521979	-3.678248	2.685866
H	6.545004	-1.483578	3.160891
H	6.108612	-3.001133	-1.542462
H	6.108680	3.000734	1.542465
H	5.522396	3.678006	-2.685903
H	6.545315	1.483246	-3.160864
H	-5.168201	-4.113728	-2.263222
H	4.901307	5.635423	-2.147626
H	4.228846	3.912758	1.747271
H	2.856895	6.957675	-1.904987
H	2.218316	5.252594	1.992440
H	-1.798079	6.296794	-1.960689
H	0.812656	7.048445	2.177665
H	-3.146424	5.472065	2.299254
H	-3.941449	6.772673	-1.726950
H	-3.146757	-5.471775	-2.299273
H	-3.941820	-6.772499	1.726916
H	0.641918	6.300869	-2.055457
H	-1.639853	7.070540	2.270681
H	-1.798383	-6.296731	1.960580
H	-1.640294	-7.070342	-2.270684
H	4.228549	-3.912917	-1.747268
H	2.856475	-6.957826	1.904860
H	4.900858	-5.635634	2.147608
H	0.812187	-7.048479	-2.177740
H	2.217983	-5.252685	-1.992472
O	7.245207	-0.915941	-2.503322
O	7.245144	0.915491	2.503329

[8]CPTcaq

C	-4.975592	2.853675	1.951431
C	-5.637406	1.657383	2.195439
C	-6.099763	0.864208	1.132366
C	-6.017493	1.391425	-0.185652
C	-5.383003	2.614774	-0.408897
C	-4.766875	3.326649	0.639067
C	-6.016856	-1.392939	0.185880
C	-5.381819	-2.616021	0.408995
C	-4.765584	-3.327634	-0.639092
C	-4.974693	-2.854716	-1.951400
C	-5.637057	-1.658700	-2.195296
C	-6.099585	-0.865746	-1.132106
C	-6.488111	-0.539825	1.295291
C	-6.488583	0.538116	-1.294990
C	-3.773182	4.388165	0.376823
C	-3.038496	4.384556	-0.826037
C	-3.367107	5.299389	1.374685
C	-1.880376	5.138876	-0.966559
C	-2.205044	6.050492	1.235642
C	-1.390900	5.930192	0.090804
C	0.009091	6.399067	0.056101
C	0.793637	6.320059	1.222515
C	0.673833	6.701491	-1.149277
C	2.182261	6.362842	1.158999
C	2.062223	6.758490	-1.209309
C	2.855360	6.495721	-0.072007
C	4.279976	6.110221	-0.175215
C	4.740261	5.462200	-1.338500
C	5.152059	6.125730	0.933703
C	5.913016	4.716085	-1.333599
C	6.324149	5.375565	0.940232
C	6.684054	4.574617	-0.163331
C	7.611134	3.428139	-0.049750
C	7.660518	2.704653	1.157668
C	8.237183	2.845073	-1.170980
C	8.121305	1.393189	1.192738
C	8.702031	1.534089	-1.134562

C	8.558733	0.740497	0.023120
C	-3.771484	-4.388817	-0.377045
C	-3.365186	-5.299798	-1.375014
C	-3.036687	-4.385093	0.825773
C	-2.202892	-6.050573	-1.236160
C	-1.878353	-5.139101	0.966121
C	-1.388723	-5.930175	-0.091317
C	0.011367	-6.398769	-0.056709
C	0.676095	-6.701452	1.148602
C	0.795932	-6.319276	-1.223072
C	2.064494	-6.758280	1.208672
C	2.184576	-6.361876	-1.159511
C	2.857635	-6.495049	0.071483
C	4.282188	-6.109364	0.174867
C	5.154349	-6.124430	-0.933997
C	4.742295	-5.461547	1.338344
C	6.326267	-5.374029	-0.940280
C	5.914871	-4.715165	1.333675
C	6.685930	-4.573216	0.163470
C	7.612641	-3.426416	0.050136
C	8.238128	-2.843085	1.171541
C	7.662101	-2.702910	-1.157273
C	8.702399	-1.531891	1.135275
C	8.122335	-1.391244	-1.192201
C	8.559090	-0.738358	-0.022444
C	-7.192720	-1.036448	2.374531
C	-7.193584	1.034436	-2.374086
C	-7.695857	0.207061	-3.425530
C	-7.546604	2.413693	-2.504009
C	-7.545117	-2.415845	2.504513
C	-7.695195	-0.209283	3.426026
H	-3.950031	5.394883	2.287410
H	-1.283268	5.025563	-1.867603
H	-1.896221	6.709948	2.043309
H	-3.311045	3.702596	-1.626614
H	-5.293840	-2.984688	1.424570
H	-4.522890	-3.375882	-2.789874
H	-5.700393	-1.292045	-3.214009
H	-4.523868	3.375061	2.789802
H	-5.700431	1.290729	3.214183
H	-5.295344	2.983462	-1.424512
H	0.315486	6.096191	2.173029
H	0.093868	6.845725	-2.058202
H	2.752841	6.167024	2.062865
H	2.542976	6.951198	-2.165250
H	4.107964	5.431242	-2.221863
H	4.876808	6.684616	1.825205
H	6.161628	4.124581	-2.210975
H	6.939207	5.358016	1.837253
H	7.202213	3.123424	2.050051
H	8.296903	3.404723	-2.101866
H	8.008162	0.824871	2.112219
H	9.118322	1.093876	-2.037819
H	-3.948153	-5.395395	-2.287723
H	-3.309381	-3.703296	1.626417
H	-1.893913	-6.709846	-2.043904
H	-1.281203	-5.025717	1.867151
H	0.096107	-6.846052	2.057454
H	0.317790	-6.095191	-2.173530
H	2.545238	-6.951228	2.164570
H	2.755165	-6.165692	-2.063287
H	4.879251	-6.683154	-1.825662
H	4.109951	-5.430951	2.221682
H	6.941375	-5.356143	-1.837274
H	6.163289	-4.123814	2.211207
H	8.297824	-3.402702	2.102451
H	7.204256	-3.121858	-2.049803
H	9.118212	-1.091499	2.038662
H	8.009233	-0.822991	-2.111722
N	-7.843592	-3.531883	2.641679
N	-8.114201	0.440843	4.295004
N	-8.114683	-0.443215	-4.294487
N	-7.845566	3.529607	-2.641158

[10]CPA

C	7.357198	-3.159713	1.862381
C	7.724214	-1.868343	2.135870
C	7.882770	-0.911405	1.086889
C	7.835350	-1.393742	-0.277647
C	7.512688	-2.758887	-0.514724
C	7.159977	-3.620045	0.513254
C	7.835478	1.393591	0.277180
C	7.512710	2.758698	0.514360
C	7.159779	3.619991	-0.513415
C	7.356651	3.159770	-1.862589
C	7.723622	1.868399	-2.136150
C	7.882498	0.911296	-1.087352
C	7.928513	0.465960	1.329366
C	7.928075	-0.466083	-1.329833
C	6.390747	-4.862921	0.267195
C	5.630838	-5.001599	-0.913453
C	6.195866	-5.845834	1.261509
C	4.643397	-5.970219	-1.034487
C	5.192310	-6.805657	1.149353
C	4.343614	-6.845700	0.027108
C	3.056470	-7.571053	0.016484
C	2.276159	-7.621178	1.187146
C	2.459035	-8.021604	-1.177448
C	0.924779	-7.949181	1.137635
C	1.110304	-8.358931	-1.224405
C	0.289477	-8.251123	-0.082870
C	-1.186374	-8.221804	-0.176678
C	-1.802002	-7.717575	-1.339063
C	-2.021227	-8.480363	0.929696
C	-3.144887	-7.358080	-1.348604
C	-3.364908	-8.116759	0.921648
C	-3.942911	-7.479921	-0.194883
C	-8.976929	-1.579183	1.057223
C	-8.776113	-0.737140	-0.055362
C	6.390740	4.862952	-0.267144
C	6.195949	5.846020	-1.261294

C	5.630777	5.001499	0.913488
C	5.192325	6.805793	-1.149181
C	4.643335	5.970100	1.034582
C	4.343621	6.845666	-0.026928
C	-8.017622	-3.486804	-0.126039
C	-7.004586	-5.516446	-1.246988
C	-7.268377	-4.761163	-0.086104
C	-5.230446	6.757398	0.120789
C	-6.009655	6.488884	1.264295
C	-5.603998	6.115862	-1.075709
C	-7.004590	5.516456	1.246895
C	-6.596737	5.141678	-1.092272
C	-7.268377	4.761230	0.085963
C	-8.017680	3.486897	0.125838
C	-8.607842	2.920742	-1.022544
C	-7.966343	2.683670	1.281703
C	-8.976877	1.579288	-1.057527
C	-8.337008	1.343901	1.247596
C	-8.776119	0.737220	0.055064
C	3.056503	7.571009	-0.016210
C	2.459031	8.021280	1.177778
C	2.276208	7.621325	-1.186827
C	1.110271	8.358528	1.224771
C	0.924803	7.949242	-1.137236
C	0.289450	8.250959	0.083256
C	-1.186401	8.221767	0.177018
C	-2.021176	8.480503	-0.929346
C	-1.802105	7.717489	1.339369
C	-3.364861	8.116938	-0.921454
C	-3.144982	7.358015	1.348757
C	-3.942897	7.479940	0.194994
C	-8.336933	-1.343837	-1.247865
C	-5.230510	-6.757418	-0.120810
C	-5.604121	-6.115853	1.075647
C	-6.009702	-6.488920	-1.264346
C	-7.966245	-2.683612	-1.281912
C	-8.607847	-2.920636	1.022312
C	-6.596805	-5.141629	1.092176
H	-5.798261	-7.018226	-2.190785
H	-3.968763	-8.289027	1.809863
H	-5.029238	-6.298196	1.980243
H	-6.772046	-4.585668	2.009709
H	-7.555026	-5.302857	-2.160411
H	-7.518783	-3.081328	-2.189207
H	-8.733088	-3.529850	1.914619
H	2.705582	-7.281891	2.126901
H	-3.968677	8.289320	-1.809657
H	-3.552978	6.868288	2.229363
H	-5.798153	7.018136	2.190750
H	-5.029058	6.298174	-1.980270
H	-7.555053	5.302901	2.160310
H	-6.771988	4.585731	-2.009828
H	-8.733061	3.529988	-1.914846
H	-7.518913	3.081367	2.189022
H	-9.382815	1.162565	-1.976644
H	-8.170288	0.728882	2.128365
H	7.135025	-3.827635	2.689325
H	7.809618	-1.531365	3.167673
H	7.432799	-3.079865	-1.550758
H	7.432700	3.079615	1.550381
H	7.134308	3.827959	-2.689292
H	7.809053	1.531574	-3.167944
H	-3.552813	-6.868436	-2.229276
H	-9.382968	-1.162458	1.976300
H	6.806684	5.834576	-2.160318
H	5.731217	4.269920	1.709759
H	5.033421	7.508698	-1.964308
H	4.010116	5.969856	1.918436
H	0.328460	7.857339	-2.041458
H	3.052392	8.060912	2.088688
H	-1.195188	7.498189	2.213962
H	-1.599077	8.933252	-1.823683
H	-1.195003	-7.498304	-2.213623
H	-1.599210	-8.932988	1.824114
H	2.705650	7.282323	-2.126639
H	0.671827	8.663737	2.172009
H	0.328405	-7.857118	2.041871
H	0.671904	-8.664355	-2.171652
H	5.731240	-4.270187	-1.709904
H	5.033447	-7.508491	1.964542
H	6.806413	-5.834267	2.160661
H	-8.170200	-0.728849	-2.128647
H	3.052456	-8.061316	-2.088359
H	4.010222	-5.970112	-1.918342
H	7.904903	-0.825323	-2.358290
H	7.905674	0.825245	2.357847

$\mathbf{C}_{100}$

C	-0.490536	4.467293	-0.545798
C	-1.851535	4.351060	-0.173705
C	-2.839040	3.814437	-1.070848
C	-0.092865	4.050849	-1.901169
C	-1.086975	3.528981	-2.759876
C	-2.454721	3.406173	-2.344705
C	3.470315	3.225920	-1.086910
C	2.245103	3.967559	-1.191624
C	1.281575	3.666325	-2.184368
C	3.758929	2.229751	-2.014326
C	2.828727	1.944546	-3.069108
C	1.573182	2.586248	-3.150152
C	4.281403	1.772799	0.772833
C	3.794875	3.025607	0.300163
C	4.363070	0.996226	-1.586817
C	4.578280	0.707898	-0.213963
C	-3.957594	0.018908	-2.505422
C	-3.917050	1.392475	-2.150028
C	-3.015154	2.202217	-2.903017
C	-1.995226	1.604848	-3.730168
C	-0.604787	-0.426148	-4.074644
C	-1.904179	0.199316	-3.908293
C	-2.995441	-0.561009	-3.394501

C	0.791417	-2.423694	-3.644585
C	-0.490258	-1.860589	-3.769622
C	0.471278	1.847181	-3.777553
C	-0.809661	2.410630	-3.646635
C	2.978621	0.548600	-3.413361
C	1.884390	-0.213130	-3.918710
C	0.584052	0.411890	-4.079261
C	1.976473	-1.618165	-3.737221
C	-4.279213	1.769014	-0.777944
C	-3.793152	3.023305	-0.308719
C	-3.468655	3.227556	1.077792
C	-4.575679	0.706721	0.211786
C	-4.360560	0.998919	1.583838
C	-3.756882	2.233840	2.007945
C	-3.767639	-2.238291	-1.986350
C	-4.369298	-1.003603	-1.558759
C	-4.576571	-0.711488	-0.185483
C	-3.473669	-3.231918	-1.057879
C	-3.790207	-3.027789	0.330486
C	-4.273989	-1.773670	0.802509
C	-1.588497	-2.597918	-3.133808
C	-2.843558	-1.955999	-3.047268
C	-2.249068	-3.973834	-1.167634
C	-1.291300	-3.675333	-2.166755
C	-1.280083	3.671805	2.174015
C	-1.571273	2.594284	3.142761
C	-2.243729	3.969933	1.180457
C	-2.826574	1.951896	3.063493
C	-2.975934	0.556856	3.411594
C	-1.972978	-1.608618	3.741451
C	-1.881422	-0.203056	3.919047
C	-0.581329	0.422900	4.077872
C	-0.469101	1.857378	3.772195
C	0.811609	2.420967	3.639732
C	-3.904013	-1.396983	2.172469
C	-3.943001	-0.023428	2.528089
C	-2.997457	-2.206377	2.920224
C	1.088495	3.536976	2.749909
C	0.094199	4.056086	1.889763
C	0.491711	4.468964	0.533257
C	2.456282	3.413561	2.335085
C	2.840462	3.818471	1.060114
C	1.852758	4.352244	0.161488
C	3.017164	2.211363	2.896703
C	3.919375	1.399904	2.145952
C	3.960442	0.027338	2.505144
C	-0.787618	-2.413950	3.651051
C	0.493835	-1.850014	3.774544
C	0.607823	-0.414685	4.075589
C	1.906959	0.210816	3.907502
C	1.997471	1.615882	3.725491
C	2.998510	-0.550499	3.395818
C	1.295580	-3.668887	2.176698
C	1.592361	-2.588680	3.140777
C	2.847170	-1.946501	3.052446
C	2.253470	-3.969763	1.178390
C	-1.848893	-4.354806	0.184231
C	-2.831381	-3.818551	1.087084
C	-2.439820	-3.410118	2.358682
C	-0.485704	-4.470517	0.548425
C	-0.080345	-4.053922	1.901471
C	-1.069645	-3.532412	2.765919
C	2.444003	-3.415678	-2.349479
C	1.073866	-3.539604	-2.756369
C	0.084763	-4.059086	-1.890474
C	2.835719	-3.820454	-1.076758
C	1.853432	-4.354591	-0.172421
C	0.490287	-4.471813	-0.536296
C	3.945911	-0.028881	-2.528255
C	3.907435	-1.401469	-2.168836
C	3.001180	-2.213272	-2.914346
C	3.771365	-2.231355	1.992305
C	4.372546	-0.997614	1.561301
C	4.579709	-0.709207	0.187221
C	3.477782	-3.227657	1.066577
C	3.794239	-3.027230	-0.322352
C	4.277539	-1.774233	-0.797840

Optimised coordinates in Å for the complexes

$C_{60}(5)$@[10]CPAq

C	-1.450044	1.010193	3.347224
C	-0.997383	-0.368926	3.323650
C	0.135320	-0.720489	2.583274
C	0.858369	0.294140	1.838276
C	0.422846	1.623144	1.860951
C	-0.753529	1.987596	2.629297
C	-2.901494	1.005555	3.346875
C	-3.345656	-0.376436	3.322787
C	-2.168850	-1.225942	3.308420
C	-2.164450	-2.402615	2.552658
C	0.140461	-1.942940	1.799655
C	1.310081	-0.301116	0.594080
C	1.308623	0.455659	-0.581565
C	0.857127	1.835659	-0.558320
C	0.421799	2.409297	0.640345
C	-0.754855	3.259459	0.654521
C	-1.481354	2.998061	1.883074
C	-2.879773	2.992252	1.881641
C	-3.602934	1.978096	2.627558
C	-4.474852	-0.734672	2.579761
C	-5.203106	0.274952	1.833095
C	-4.775200	1.605794	1.856394
C	-4.774365	2.388458	0.635784
C	-3.604423	3.243248	0.650943
C	-2.904984	3.495660	-0.531180
C	-1.455027	3.503349	-0.530312
C	-1.003062	2.909072	-1.775182

C	0.130700	2.090246	-1.788781
C	0.866816	-1.683737	0.570142
C	-1.439465	-0.873028	-3.338582
C	-0.737926	-1.846290	-2.619833
C	-1.460452	-2.861730	-1.874859
C	-2.858970	-2.864932	-1.875349
C	-3.587301	-1.854603	-2.621842
C	-3.343722	0.501772	-3.316611
C	-2.172191	1.358681	-3.300732
C	-0.995387	0.508924	-3.314322
C	0.134119	0.867685	-2.572343
C	0.862243	-0.142476	-1.826333
C	0.434858	-1.474194	-1.849663
C	-0.734130	-3.118361	-0.645009
C	-1.434389	-3.366490	0.539122
C	-2.884440	-3.367933	0.537841
C	-3.583657	-3.120533	-0.645515
C	-4.758401	-2.272186	-0.631521
C	-4.762585	-1.489452	-1.852093
C	-5.199333	-0.161371	-1.829638
C	-4.476210	0.852910	-2.575120
C	-2.176113	2.535432	-2.545029
C	-3.351665	2.899440	-1.775440
C	-4.480488	2.074046	-1.790393
C	-5.204905	1.812800	-0.561532
C	-5.649082	0.433522	-0.585808
C	-5.647081	-0.322742	0.588459
C	-5.194267	-1.699134	0.565043
C	-4.470391	-1.955850	1.795046
C	-3.336452	-2.774090	1.781486
C	0.436964	-2.260309	-0.629090
C	-0.988018	-2.768870	1.784480
C	-2.890985	-0.877485	-3.340106
C	8.642600	-3.024328	1.953436
C	9.205425	-1.776758	2.200365
C	9.524627	-0.926244	1.132709
C	9.459537	-1.433121	-0.183453
C	8.963191	-2.714931	-0.416179
C	8.425040	-3.483318	0.634593
C	9.376618	1.399653	0.204330
C	8.812315	2.654442	0.430184
C	8.253175	3.397154	-0.627866
C	8.504210	2.946612	-1.943569
C	9.130866	1.728441	-2.182812
C	9.484291	0.897358	-1.110790
C	9.713367	0.530738	1.380572
C	9.759844	-0.546288	-1.355957
C	7.459525	-4.573863	0.373524
C	6.702240	-4.557382	-0.815567
C	7.082927	-5.507269	1.361415
C	5.555801	-5.329019	-0.953202
C	5.928208	-6.272432	1.227671
C	5.099914	-6.149868	0.094652
C	3.725072	-6.686081	0.052222
C	2.932231	-6.677788	1.215263
C	3.100590	-7.042044	-1.158754
C	1.561691	-6.907434	1.153106
C	1.731881	-7.280258	-1.218596
C	0.919425	-7.165560	-0.072993
C	-0.554631	-7.168777	-0.160734
C	-1.197951	-6.672397	-1.310180
C	-1.368313	-7.529579	0.931037
C	-2.571266	-6.462699	-1.334585
C	-2.742608	-7.315638	0.908341
C	-3.371716	-6.733541	-0.208974
C	-9.133363	-1.657143	1.033724
C	-9.000556	-0.784509	-0.064752
C	7.249876	4.455786	-0.379081
C	6.863726	5.381392	-1.370278
C	6.481722	4.421108	0.802507
C	5.696859	6.128914	-1.243456
C	5.323518	5.176475	0.934138
C	4.866509	5.996670	-0.113466
C	-8.017882	-3.455461	-0.179833
C	-6.682637	-5.277896	-1.313061
C	-7.101297	-4.612259	-0.143477
C	-4.980811	6.255375	0.147467
C	-5.761406	6.084278	1.307439
C	-5.477854	5.706649	-1.048978
C	-6.888914	5.269976	1.302182
C	-6.600435	4.889313	-1.053126
C	-7.285170	4.581305	0.138307
C	-8.158184	3.391837	0.183907
C	-8.782239	2.870506	-0.967545
C	-8.161353	2.581822	1.335307
C	-9.208061	1.547683	-1.018280
C	-8.588911	1.261619	1.285631
C	-9.032197	0.683689	0.081056
C	3.493924	6.537589	-0.070503
C	2.882381	6.922228	1.137866
C	2.695367	6.521060	-1.229206
C	1.519990	7.194119	1.198775
C	1.330664	6.781858	-1.165245
C	0.701077	7.083407	0.057565
C	-0.771439	7.136782	0.147476
C	-1.574994	7.491608	-0.953570
C	-1.428654	6.691514	1.309606
C	-2.953537	7.308283	-0.929541
C	-2.805740	6.512079	1.335043
C	-3.596830	6.762697	0.198034
C	-8.540517	-1.341381	-1.272962
C	-4.758186	-6.232850	-0.160409
C	-5.268809	-5.703186	1.038601
C	-5.535726	-6.064584	-1.322330
C	-8.060707	-2.643043	-1.328751
C	-8.654978	-2.961823	0.976770
C	-6.409151	-4.910474	1.046292
H	-5.208055	-6.518942	-2.254484
H	-3.338690	-7.583073	1.777794
H	-4.694465	-5.806963	1.955257
H	-6.690702	-4.411422	1.969169
H	-7.232123	-5.131494	-2.239797

H	-7.582084	-2.980982	-2.243372
H	-8.716381	-3.587649	1.863927
H	3.381749	-6.392959	2.163574
H	-3.540475	7.564277	-1.808550
H	-3.262605	6.067668	2.214604
H	-5.448200	6.554348	2.236751
H	-4.903061	5.812670	-1.964930
H	-7.436873	5.117096	2.228827
H	-6.867670	4.375961	-1.972423
H	-8.872976	3.491170	-1.855821
H	-7.690855	2.942156	2.245638
H	-9.621099	1.157352	-1.945569
H	-8.438845	0.631155	2.157540
H	8.263609	-3.602779	2.791458
H	9.295727	-1.396977	3.214849
H	8.907599	-3.057845	-1.445131
H	8.727572	2.994817	1.458005
H	8.106914	3.505531	-2.786339
H	9.251168	1.352844	-3.195755
H	-3.017674	-5.988195	-2.204040
H	-9.556159	-1.286186	1.964554
H	7.464961	5.491514	-2.269465
H	6.733930	3.717707	1.590758
H	5.403939	6.804740	-2.043794
H	4.706280	5.050434	1.820127
H	0.727883	6.668272	-2.062655
H	3.484003	6.991309	2.041410
H	-0.842714	6.389301	2.173488
H	-1.107521	7.895569	-1.848379
H	-0.602030	-6.361656	-2.164326
H	-0.912245	-7.967509	1.815750
H	3.135326	6.210406	-2.173936
H	1.076040	7.479567	2.149400
H	0.965692	-6.798408	2.055682
H	1.277150	-7.538380	-2.172000
H	6.948385	-3.852076	-1.603955
H	5.640047	-6.950328	2.027959
H	7.678496	-5.606267	2.265724
H	-8.421260	-0.703685	-2.144360
H	3.696123	-7.109501	-2.066430
H	4.942947	-5.210881	-1.843185
O	10.068602	-0.992605	-2.454056
O	9.982660	0.993964	2.482142

$\mathbf{C_{60}(5)@[10]CPTcaq}$

C	-2.467478	0.530873	3.383823
C	-2.055948	-0.861098	3.358454
C	-0.924155	-1.242786	2.631346
C	-0.161390	-0.246244	1.901696
C	-0.557643	1.095091	1.926148
C	-1.732501	1.490955	2.681116
C	-3.918318	0.569947	3.364211
C	-4.403439	-0.797794	3.326466
C	-3.252440	-1.682305	3.323090
C	-3.273251	-2.854370	2.560665
C	-0.944704	-2.460712	1.840863
C	0.289242	-0.848240	0.660199
C	0.325781	-0.085199	-0.511144
C	-0.085083	1.307440	-0.485883
C	-0.518950	1.887483	0.710240
C	-1.669374	2.773112	0.713827
C	-2.419624	2.527232	1.931341
C	-3.817488	2.563505	1.911178
C	-4.580528	1.567061	2.641273
C	-5.532900	-1.117706	2.566395
C	-6.220470	-0.082696	1.816046
C	-5.752724	1.234332	1.852509
C	-5.712231	2.023233	0.636742
C	-4.517787	2.842883	0.672378
C	-3.795541	3.080679	-0.498987
C	-2.346033	3.044389	-0.478869
C	-1.895583	2.443424	-1.721045
C	-0.786895	1.590733	-1.724369
C	-0.194121	-2.217112	0.622683
C	-2.424432	-1.314767	-3.311783
C	-1.761828	-2.312132	-2.589159
C	-2.524656	-3.307709	-1.858994
C	-3.922317	-3.269108	-1.878218
C	-4.610289	-2.234753	-2.629081
C	-4.286763	0.116487	-3.307309
C	-3.090308	0.937592	-3.270921
C	-1.939382	0.052931	-3.273721
C	-0.809386	0.373166	-2.515099
C	-0.121445	-0.662565	-1.765416
C	-0.588044	-1.980576	-1.801890
C	-1.822942	-3.592123	-0.621619
C	-2.545989	-3.825648	0.550802
C	-3.994738	-3.784317	0.530416
C	-4.670903	-3.510096	-0.660154
C	-5.820980	-2.628587	-0.657184
C	-5.785287	-1.839379	-1.873417
C	-6.181783	-0.498847	-1.848913
C	-5.418062	0.497270	-2.578794
C	-3.069040	2.109704	-2.508442
C	-4.243285	2.504756	-1.752455
C	-5.395895	1.713488	-1.786949
C	-6.144043	1.467373	-0.569265
C	-6.629815	0.102414	-0.607381
C	-6.666702	-0.659958	0.562572
C	-6.255618	-2.049641	0.537205
C	-5.554978	-2.334246	1.774884
C	-4.445713	-3.185784	1.771719
C	-0.625944	-2.772783	-0.585662
C	-2.098018	-3.251247	1.805662
C	-3.875232	-1.275540	-3.332676
C	7.730405	2.731892	-2.089257
C	8.386882	1.525877	-2.300046
C	8.856969	0.770977	-1.212762
C	8.814896	1.356200	0.081503
C	8.195805	2.591789	0.268973
C	7.543583	3.250384	-0.791289

C	8.671666	-1.425443	-0.161116
C	7.938666	-2.601052	-0.325757
C	7.267283	-3.203491	0.755751
C	7.523137	-2.692832	2.044810
C	8.288507	-1.548917	2.232217
C	8.803861	-0.847241	1.130344
C	9.180015	-0.654965	-1.314446
C	9.274465	0.537612	1.221049
C	6.523421	4.287882	-0.541112
C	5.805080	4.281798	0.671741
C	6.074842	5.161036	-1.553319
C	4.631313	5.009348	0.818330
C	4.897165	5.885767	-1.407428
C	4.112054	5.775325	-0.241974
C	2.728669	6.283592	-0.171616
C	1.908608	6.246093	-1.315127
C	2.131346	6.657758	1.047657
C	0.540729	6.478364	-1.226442
C	0.764312	6.897776	1.133948
C	-0.072156	6.767535	0.007714
C	-1.543395	6.795581	0.120274
C	-2.177893	6.317067	1.281774
C	-2.364906	7.165904	-0.961971
C	-3.553692	6.126515	1.324091
C	-3.741402	6.974043	-0.920070
C	-4.363676	6.401700	0.206154
C	-5.753730	5.910599	0.168213
C	-6.277300	5.394248	-1.031233
C	-6.522898	5.736956	1.334896
C	-7.423601	4.611047	-1.037051
C	-7.675743	4.958580	1.327558
C	-8.108644	4.307224	0.155269
C	-9.031606	3.155516	0.186094
C	-9.073239	2.331975	1.326980
C	-9.677471	2.677879	-0.972582
C	-9.561225	1.033732	1.259895
C	-10.161861	1.376212	-1.041516
C	-10.028464	0.492314	0.047548
C	6.192529	-4.192645	0.539749
C	5.743801	-5.046254	1.568094
C	5.455075	-4.182791	-0.661491
C	4.563869	-5.770345	1.438515
C	4.279970	-4.912094	-0.792886
C	3.777900	-5.681978	0.272531
C	2.422419	-6.259328	0.196851
C	1.877020	-6.721431	-1.016058
C	1.584667	-6.246753	1.327459
C	0.540702	-7.095965	-1.106474
C	0.245833	-6.609201	1.233281
C	-0.317682	-7.013862	0.007673
C	-1.776289	-7.201015	-0.112533
C	-2.571103	-7.580362	0.986445
C	-2.443387	-6.848639	-1.299950
C	-3.957495	-7.486338	0.939565
C	-3.828237	-6.752703	-1.346372
C	-4.617387	-7.003393	-0.207637
C	-6.015618	-6.533527	-0.170528
C	-6.787618	-6.367398	-1.337423
C	-6.531624	-5.992502	1.021941
C	-7.919396	-5.558691	-1.342620
C	-7.659085	-5.182625	1.016228
C	-8.330793	-4.873257	-0.181984
C	-9.203318	-3.683754	-0.231491
C	-9.842405	-3.172121	0.916090
C	-9.186289	-2.862867	-1.375022
C	-10.261736	-1.847694	0.975019
C	-9.608384	-1.540974	-1.317652
C	-10.065470	-0.973993	-0.112946
C	9.835159	-1.240011	-2.378893
C	10.015853	1.052005	2.264748
C	10.487633	0.252439	3.351132
C	10.428937	2.419658	2.318535
C	10.104986	-2.642254	-2.446156
C	10.356070	-0.490143	-3.478238
H	6.639397	5.249646	-2.478285
H	4.052849	4.902316	1.732228
H	4.558875	6.524879	-2.219466
H	6.108156	3.619965	1.478114
H	7.815783	-3.010293	-1.322084
H	7.031485	-3.134841	2.906168
H	8.391653	-1.141080	3.231968
H	7.257570	3.219727	-2.936304
H	8.428769	1.117707	-3.304015
H	8.134428	3.003271	1.270139
H	2.335880	5.942904	-2.267905
H	2.747574	6.746528	1.939481
H	-0.076608	6.352784	-2.112211
H	0.330515	7.175631	2.091509
H	-1.574527	6.003130	2.129557
H	-1.913041	7.593528	-1.853839
H	-3.995325	5.661205	2.200800
H	-4.344535	7.248456	-1.782288
H	-5.710159	5.501031	-1.951907
H	-6.184960	6.180220	2.268692
H	-7.716062	4.122687	-1.962192
H	-8.218192	4.806544	2.257502
H	-8.588976	2.658123	2.242910
H	-9.741315	3.314195	-1.852055
H	-9.443056	0.385688	2.123848
H	-10.590303	1.016246	-1.974132
H	6.318296	-5.131800	2.487087
H	5.754425	-3.528524	-1.475557
H	4.232498	-6.405390	2.256585
H	3.694551	-4.818044	-1.703981
H	2.512058	-6.783957	-1.896885
H	1.970271	-5.871324	2.272377
H	0.149696	-7.449341	-2.057522
H	-0.393593	-6.504509	2.105813
H	-2.091670	-7.924278	1.899812
H	-1.865837	-6.538971	-2.166720
H	-4.537948	-7.752529	1.819584
H	-4.296562	-6.362735	-2.245368

H	-6.462951	-6.832137	-2.265422
H	-5.967104	-6.093350	1.944533
H	-8.457744	-5.405572	-2.274920
H	-7.939177	-4.673616	1.934113
H	-9.949655	-3.802280	1.795784
H	-8.704614	-3.217162	-2.282042
H	-10.686098	-1.464011	1.900002
H	-9.444465	-0.901449	-2.180582
N	10.333490	-3.779843	-2.529852
N	10.785606	0.099707	-4.384222
N	10.879292	-0.379010	4.246141
N	10.774022	3.528281	2.390162

$C_{60}(5)$@[12]CPP

C	2.366997	1.174233	3.340229
C	3.220047	-0.000292	3.344708
C	4.413041	-0.000201	2.615195
C	4.798467	1.173999	1.853861
C	3.976012	2.305081	1.849395
C	2.738008	2.305808	2.607074
C	0.986514	0.725539	3.332590
C	0.986491	-0.726201	3.332548
C	2.366988	-1.174838	3.340161
C	2.738076	-2.306385	2.606828
C	4.798592	-1.174275	1.853700
C	5.421411	0.724807	0.623542
C	5.199349	1.424499	-0.564678
C	4.346444	2.595900	-0.568758
C	3.744834	3.028929	0.614625
C	2.367244	3.479468	0.607784
C	1.743047	3.033509	1.839303
C	0.412827	2.601693	1.832733
C	0.028310	1.425489	2.592923
C	0.028224	-1.426040	2.592752
C	-0.966306	-0.699669	1.824641
C	-0.966291	0.699283	1.824749
C	-1.196419	1.426540	0.589901
C	-0.344736	2.602706	0.594742
C	0.257501	3.034625	-0.590871
C	1.637772	3.481564	-0.583643
C	2.261992	3.031781	-1.813534
C	3.591521	2.598874	-1.806684
C	5.421515	-0.724766	0.623426
C	3.019416	-0.725582	-3.309932
C	3.977589	-1.424638	-2.569116
C	3.591654	-2.598581	-1.807355
C	2.261991	-3.031537	-1.814290
C	1.267483	-2.305707	-2.582817
C	0.786022	0.000343	-3.320351
C	1.638962	1.174900	-3.316036
C	3.019398	0.726297	-3.309687
C	3.977529	1.425212	-2.568666
C	4.972513	0.699347	-1.799966
C	4.972580	-0.698867	-1.800168
C	4.346648	-2.595884	-0.569307
C	3.744987	-3.029224	0.614070
C	2.367289	-3.479832	0.607136
C	1.637723	-3.481595	-0.584430
C	0.257421	-3.034580	-0.591502
C	0.028071	-2.306962	-1.826861
C	-0.792827	-1.174660	-1.830942
C	-0.406904	0.000260	-2.591409
C	1.267512	2.306149	-2.582181
C	0.028143	2.307274	-1.826309
C	-0.792769	1.175015	-1.830650
C	-1.417158	0.726128	-0.599797
C	-1.417172	-0.726008	-0.599952
C	-1.196419	-1.426645	0.589609
C	-0.344811	-2.602868	0.594262
C	0.412730	-2.602160	1.832333
C	1.743016	-3.034032	1.838836
C	5.199542	-1.424289	-0.564946
C	3.976151	-2.305508	1.849085
C	1.638950	-1.174208	-3.316400
C	-0.926660	6.744967	1.157396
C	0.463273	6.761176	1.156869
C	1.188987	7.106637	0.001275
C	0.454216	7.505420	-1.132061
C	-0.937063	7.488820	-1.131746
C	2.648867	6.898691	-0.041950
C	3.448993	6.984371	1.113673
C	4.756677	6.511298	1.121660
C	5.325949	5.921866	-0.024163
C	4.568214	5.959418	-1.210452
C	3.263987	6.437229	-1.219739
C	6.531520	5.073351	0.043281
C	6.810668	4.356228	1.221880
C	7.658079	3.256298	1.211901
C	8.269318	2.816879	0.022261
C	8.134556	3.643070	-1.111331
C	7.285518	4.744526	-1.100961
C	8.747939	1.423569	-0.067367
C	9.172674	0.695489	1.062346
C	9.172709	-0.695461	1.062221
C	8.747973	-1.423292	-0.067705
C	8.511881	-0.693995	-1.248357
C	8.511839	0.694528	-1.248145
C	8.269450	-2.816582	0.021709
C	7.658328	-3.256188	1.211387
C	6.811037	-4.356278	1.221361
C	6.531893	-5.073311	0.042632
C	7.285856	-4.744341	-1.101644
C	8.134753	-3.642729	-1.112005
C	5.326311	-5.921836	-0.024904
C	4.756932	-6.511298	1.120924
C	3.449173	-6.984337	1.112776
C	2.649084	-6.898536	-0.042906
C	3.264250	-6.436921	-1.220670
C	4.568584	-5.959161	-1.211281
C	1.189265	-7.106595	0.000228
C	0.463533	-6.761358	1.155952

C	-0.926399	-6.745148	1.156427
C	-1.660917	-7.072046	0.000837
C	-0.936793	-7.488711	-1.132855
C	0.454519	-7.505288	-1.133155
C	-3.117402	-6.833919	-0.040855
C	-3.923805	-6.941696	1.109223
C	-5.229746	-6.462565	1.121014
C	-5.790597	-5.845753	-0.015078
C	-5.025450	-5.854156	-1.197683
C	-3.721411	-6.337178	-1.210740
C	-7.010709	-5.015382	0.059199
C	-7.287306	-4.292484	1.235168
C	-8.165587	-3.215259	1.227734
C	-8.810362	-2.806961	0.043607
C	-8.676205	-3.645504	-1.081963
C	-7.796042	-4.723117	-1.074474
C	-9.322234	-1.423439	-0.051633
C	-9.749095	-0.695701	1.078375
C	-9.749222	0.695301	1.078484
C	-9.322443	1.423256	-0.051429
C	-9.108506	0.695058	-1.237837
C	-9.108394	-0.695038	-1.237953
C	-8.810558	2.806782	0.044017
C	-8.165719	3.214844	1.228179
C	-7.287372	4.292032	1.235772
C	-7.010765	5.015094	0.059913
C	-7.796072	4.723000	-1.073820
C	-8.676342	3.645453	-1.081435
C	-5.790754	5.845601	-0.014243
C	-5.229996	6.462352	1.121916
C	-3.924104	6.941625	1.110189
C	-3.721651	6.337446	-1.209818
C	-5.025621	5.854299	-1.196853
H	-1.453546	6.392924	2.040804
H	0.997829	6.419523	2.039475
H	0.984346	7.820154	-2.028036
H	-1.476154	7.791196	-2.026774
H	3.025101	7.395630	2.026729
H	5.332636	6.558353	2.042797
H	4.962784	5.498259	-2.111330
H	2.675600	6.345881	-2.128834
H	6.250887	4.573891	2.126848
H	7.732844	2.646869	2.108203
H	8.651960	3.379643	-2.030975
H	7.156952	5.324209	-2.011919
H	9.440630	1.226881	1.972737
H	9.440665	-1.227144	1.972452
H	8.180639	-1.215786	-2.141835
H	8.180598	1.216465	-2.141493
H	7.732996	-2.646736	2.107753
H	6.251258	-4.574050	2.126420
H	7.157431	-5.324146	-2.012619
H	8.652127	-3.379267	-2.031681
H	5.332832	-6.558494	2.042108
H	3.025284	-7.395779	2.025819
H	2.675799	-6.345195	-2.129806
H	4.963189	-5.497721	-2.112107
H	0.998127	-6.419815	2.038652
H	-1.453278	-6.393232	2.039921
H	-1.475845	-7.791124	-2.027848
H	0.984672	-7.820029	-2.029164
H	-3.506894	-7.381305	2.012587
H	-5.814343	-6.530663	2.035598
H	-5.421253	-5.378280	-2.091305
H	-3.127110	-6.235658	-2.115636
H	-6.709671	-4.492664	2.133963
H	-8.247297	-2.599705	2.119859
H	-9.219382	-3.408748	-1.994254
H	-7.669377	-5.314082	-1.978835
H	-10.009644	-1.227620	1.990668
H	-10.009899	1.227033	1.990851
H	-8.793141	1.218556	-2.136683
H	-8.792978	-1.218370	-2.136861
H	-8.247456	2.599149	2.120205
H	-6.709761	4.492024	2.134589
H	-7.669342	5.314031	-1.978089
H	-9.219526	3.408885	-1.993777
H	-5.814631	6.530279	2.036471
H	-3.507254	7.381236	2.013554
H	-3.127393	6.236168	-2.114726
H	-5.421401	5.378623	-2.090549
C	-3.117697	6.834012	-0.039868
C	-1.661162	7.072101	0.001861

$(C_{70}(H)@[10]CPAq)_A$

C	4.437917	-0.673274	-0.107917
C	4.262883	0.428449	-0.989527
C	3.638006	0.186890	-2.297796
C	3.236336	-1.137968	-2.623884
C	3.511404	-2.250500	-1.743987
C	4.101491	-2.020137	-0.504869
C	1.986238	-1.397012	-3.284137
C	1.488937	-2.669614	-2.813754
C	0.121472	-2.848517	-2.612385
C	-0.789274	-1.757426	-2.873364
C	-0.337389	-0.524778	-3.420621
C	-1.822686	-1.795206	-1.875262
C	-2.429504	-0.599851	-1.399009
C	-2.695677	-0.473435	0.040161
C	-2.334103	-1.552675	0.893283
C	-1.803107	-2.790133	0.368045
C	-1.551257	-2.909949	-0.996541
C	-1.721430	-1.315650	2.171390
C	-0.811181	-2.406084	2.437477
C	0.399877	-2.154434	3.079002
C	0.736843	-0.805891	3.472968
C	-0.178573	0.269791	3.304783
C	-1.456190	0.005184	2.628514
C	2.678010	0.639531	2.883020
C	3.735194	0.676597	1.861871
C	4.181011	-0.551164	1.299735

C	3.684454	-1.823503	1.772776
C	2.683931	-1.859028	2.741553
C	2.147387	-0.623289	3.264664
C	1.104652	-0.337681	-3.634562
C	1.638394	0.978005	-3.556850
C	-1.136809	0.618559	-3.144805
C	0.786122	2.128831	-3.363911
C	-0.581016	1.952192	-3.161183
C	-2.169910	0.581803	-2.146616
C	-2.253244	1.893214	-1.545004
C	-2.505348	2.013568	-0.180612
C	-2.682127	0.824760	0.621854
C	-2.070326	1.061151	1.900012
C	-1.516811	2.396610	1.888553
C	-0.304814	2.646582	2.529245
C	0.387586	1.570014	3.200879
C	1.797703	1.751897	2.992193
C	1.976828	2.940260	2.191011
C	2.971838	2.968694	1.219251
C	3.828069	1.822608	1.025736
C	4.089214	1.700684	-0.380913
C	3.398804	2.774925	-1.055126
C	2.809649	2.548824	-2.296062
C	2.889569	1.237413	-2.897512
C	-1.278231	2.754106	-2.179277
C	-1.794117	2.999833	0.603905
C	0.676174	3.510705	1.910582
C	2.710459	3.571229	-0.066344
C	1.510928	3.115066	-2.592804
C	2.436745	-3.211883	-1.866342
C	-0.351858	-3.576976	-1.455526
C	-0.865776	-3.333650	1.327663
C	1.606246	-2.819526	2.635283
C	3.643777	-2.744648	0.659388
C	0.562266	-4.095061	-0.531025
C	0.299774	-3.970891	0.888510
C	1.560480	-3.707577	1.555059
C	2.600428	-3.667686	0.547570
C	1.982698	-3.905946	-0.740365
C	1.457365	4.119699	-0.344219
C	0.416154	4.089223	0.663567
C	-0.843835	3.829405	-0.002677
C	-0.580832	3.703693	-1.423181
C	0.842291	3.883767	-1.633304
C	7.238122	-3.102950	1.856922
C	7.701543	-1.807683	2.046823
C	7.894055	-0.955386	0.951165
C	7.760138	-1.485620	-0.349127
C	7.367939	-2.811053	-0.527121
C	6.996167	-3.620669	0.562658
C	7.765718	1.376104	0.000913
C	7.405030	2.702260	0.233306
C	6.890252	3.512264	-0.795378
C	6.926857	2.991737	-2.109690
C	7.349962	1.694098	-2.362899
C	7.707567	0.846167	-1.305879
C	8.089536	0.501685	1.173869
C	7.884937	-0.608954	-1.556871
C	6.175594	-4.836647	0.366977
C	5.553904	-5.088083	-0.873401
C	5.782184	-5.658587	1.444876
C	4.485145	-5.964053	-0.984000
C	4.705945	-6.530714	1.336052
C	3.968514	-6.635312	0.139847
C	2.609887	-7.207266	0.093598
C	1.791644	-7.160692	1.238477
C	2.004353	-7.600755	-1.116928
C	0.420737	-7.372393	1.154532
C	0.632396	-7.806007	-1.202050
C	-0.201105	-7.635803	-0.079549
C	-1.668855	-7.556129	-0.200272
C	-2.247927	-6.976613	-1.344736
C	-2.526881	-7.895872	0.863525
C	-3.601608	-6.662035	-1.384664
C	-3.881367	-7.582855	0.822432
C	-4.441064	-6.911469	-0.282339
C	-10.057549	-1.644868	1.063251
C	-9.859532	-0.721247	0.017248
C	6.137895	4.748849	-0.497690
C	5.732732	5.642586	-1.512069
C	5.595097	4.959706	0.784350
C	4.704764	6.552327	-1.303502
C	4.567880	5.870245	0.992786
C	4.025617	6.616779	-0.069253
C	-8.942949	-3.406169	-0.203818
C	-7.661922	-5.246167	-1.378888
C	-8.058644	-4.590485	-0.195768
C	-5.704671	6.296994	0.551815
C	-6.456958	6.043608	1.715300
C	-6.199502	5.787144	-0.662858
C	-7.571010	5.210854	1.684073
C	-7.306794	4.947419	-0.692263
C	-7.977882	4.580302	0.490587
C	-8.874589	3.405384	0.483196
C	-9.544205	2.975080	-0.680911
C	-8.877887	2.529468	1.585619
C	-10.014360	1.671136	-0.800233
C	-9.352440	1.228476	1.468886
C	-9.841689	0.738895	0.242454
C	2.680512	7.208162	0.057577
C	2.111247	7.524207	1.307716
C	1.828688	7.243582	-1.063896
C	0.743444	7.728865	1.444744
C	0.462818	7.455245	-0.927621
C	-0.123580	7.635927	0.337897
C	-1.588382	7.553736	0.491253
C	-2.466820	7.929174	-0.543786
C	-2.146589	6.934862	1.625458
C	-3.818536	7.608020	-0.491792
C	-3.498811	6.615374	1.678407
C	-4.356612	6.896617	0.598254
C	-9.377706	-1.227178	-1.205430

```
C  -5.791104  -6.315469  -0.236622
C  -6.278901  -5.782441   0.970903
C  -6.551657  -6.084417  -1.399809
C  -8.928135  -2.538330  -1.312733
C  -9.610949  -2.957697   0.954277
C  -7.383985  -4.939544   0.990602
H  -6.241297  -6.537528  -2.338791
H  -4.515190  -7.837941   1.668640
H  -5.717389  -5.939132   1.888547
H  -7.655922  -4.451783   1.923060
H  -8.202060  -5.055680  -2.303432
H  -8.433601  -2.849550  -2.229399
H  -9.719400  -3.628789   1.803300
H   2.214695  -6.842494   2.187289
H  -4.467665   7.887936  -1.318248
H  -3.879164   6.051997   2.526917
H  -6.138931   6.476750   2.661068
H  -5.642428   5.960585  -1.580229
H  -8.107013   5.005555   2.607741
H  -7.584752   4.477926  -1.632207
H  -9.638106   3.653461  -1.525850
H  -8.380413   2.824277   2.505907
H -10.462102   1.348173  -1.737620
H  -9.212067   0.540917   2.299034
H   6.980999  -3.688071   2.733983
H   7.832049  -1.405497   3.047934
H   7.272192  -3.158079  -1.549988
H   7.462574   3.060307   1.256047
H   6.534908   3.578873  -2.934532
H   7.325251   1.286689  -3.370024
H  -3.997537  -6.127897  -2.244830
H -10.503508  -1.307603   1.996373
H   6.190823   5.591319  -2.495991
H   5.876235   4.315128   1.610280
H   4.381186   7.181706  -2.128493
H   4.088939   5.893102   1.967095
H  -0.173701   7.367152  -1.804022
H   2.743774   7.569356   2.190779
H  -1.494071   6.614001   2.433509
H  -2.076602   8.459114  -1.409600
H  -1.609425  -6.682923  -2.174122
H  -2.118726  -8.393050   1.740683
H   2.220672   6.987366  -2.044082
H   0.330596   7.931160   2.430070
H  -0.192930  -7.223423   2.039264
H   0.189789  -8.071077  -2.159291
H   5.820460  -4.509767  -1.750691
H   4.397388  -7.100286   2.209174
H   6.285508  -5.580906   2.404129
H  -9.221701  -0.546994  -2.039032
H   2.612841  -7.710091  -2.011198
H   3.961958  -6.023108  -1.933322
O   8.016083  -1.070647  -2.685999
O   8.392577   0.966606   2.267857
```

C_{70}(H)@[10]CPTcaq

```
C   1.094690  -0.687770  -0.205406
C   0.961523   0.497573  -0.980945
C   0.421664   0.386152  -2.343088
C   0.056633  -0.901179  -2.825637
C   0.289049  -2.096338  -2.047431
C   0.800396  -1.991603  -0.755806
C  -1.146805  -1.096945  -3.586708
C  -1.658423  -2.412783  -3.280399
C  -3.034134  -2.612911  -3.181735
C  -3.938652  -1.506061  -3.391747
C  -3.465765  -0.223581  -3.783987
C  -5.032377  -1.647431  -2.469496
C  -5.679254  -0.509162  -1.915004
C  -6.036006  -0.529988  -0.490870
C  -5.719298  -1.687324   0.271296
C  -5.140722  -2.859327  -0.340191
C  -4.804061  -2.842131  -1.689664
C  -5.193578  -1.579417   1.604095
C  -4.288152  -2.685747   1.815404
C  -3.122004  -2.497145   2.554895
C  -2.824423  -1.193207   3.101681
C  -3.738788  -0.109866   2.984449
C  -4.970019  -0.310238   2.206914
C  -0.864994   0.312079   2.783201
C   0.252804   0.456732   1.840356
C   0.744395  -0.707780   1.187961
C   0.234328  -2.023866   1.499625
C  -0.825422  -2.160003   2.393963
C  -1.405712  -0.984992   3.002324
C  -2.015006  -0.010818  -3.884721
C  -1.500911   1.292766  -3.641417
C  -4.292630   0.882877  -3.446653
C  -2.374366   2.415704  -3.390516
C  -3.749681   2.212829  -3.293323
C  -5.386396   0.741863  -2.524297
C  -5.519970   1.985129  -1.800596
C  -5.856201   1.963798  -0.450686
C  -6.070427   0.701374   0.215349
C  -5.545470   0.810639   1.548021
C  -5.005663   2.141204   1.705312
C  -3.839182   2.331288   2.444309
C  -3.179356   1.196393   3.046886
C  -1.760250   1.404732   2.947682
C  -1.541580   2.668513   2.283060
C  -0.481268   2.807408   1.389392
C   0.390715   1.683849   1.133454
C   0.741152   1.704488  -0.260390
C   0.085217   2.840968  -0.866617
C  -0.426509   2.734591  -2.158203
C  -0.297472   1.489416  -2.880440
C  -4.514814   2.908112  -2.281906
C  -5.205489   2.867405   0.470694
C  -2.828598   3.255957   1.978412
C  -0.666297   3.538056   0.154112
```

C	-1.708906	3.322714	-2.480408
C	-0.765650	-3.045033	-2.333951
C	-3.570969	-3.453503	-2.135179
C	-4.258963	-3.491476	0.615233
C	-1.883436	-3.110266	2.125406
C	0.277920	-2.831655	0.300245
C	-2.711670	-4.056516	-1.211708
C	-3.064334	-4.080357	0.192482
C	-1.851246	-3.885665	0.960666
C	-0.748252	-3.744156	0.030292
C	-1.281227	-3.851443	-1.312809
C	-1.911862	4.096482	-0.149677
C	-3.014219	3.949802	0.778908
C	-4.226835	3.753072	0.012053
C	-3.873785	3.775281	-1.391806
C	-2.443773	3.989090	-1.492702
C	7.351620	2.712636	-2.485359
C	8.030814	1.521096	-2.704985
C	8.538342	0.779681	-1.625766
C	8.486464	1.354804	-0.327120
C	7.836536	2.573339	-0.129999
C	7.174486	3.228876	-1.185464
C	8.478536	-1.433696	-0.591697
C	7.818227	-2.651221	-0.758838
C	7.199621	-3.302673	0.325137
C	7.432708	-2.784793	1.615411
C	8.125610	-1.596011	1.804193
C	8.588682	-0.858127	0.702986
C	8.932980	-0.627106	-1.741859
C	8.990885	0.547567	0.801224
C	6.178825	4.287992	-0.929564
C	5.469419	4.309137	0.288062
C	5.768909	5.186259	-1.935521
C	4.346960	5.110798	0.454738
C	4.641428	5.982417	-1.771076
C	3.873710	5.923813	-0.591288
C	2.548804	6.563406	-0.491024
C	1.694893	6.578499	-1.608855
C	2.038220	7.043706	0.729826
C	0.367983	6.973036	-1.492320
C	0.713858	7.453474	0.841884
C	-0.166273	7.385275	-0.256169
C	-1.623555	7.561587	-0.109280
C	-2.265406	7.211153	1.092127
C	-2.445438	7.898357	-1.203679
C	-3.644292	7.044328	1.149088
C	-3.823545	7.732984	-1.146411
C	-4.448978	7.218333	0.007302
C	-5.802409	6.631394	-0.032448
C	-6.268730	6.056105	-1.229945
C	-6.557976	6.388225	1.131856
C	-7.321067	5.151568	-1.233677
C	-7.613519	5.483364	1.127908
C	-7.965296	4.775611	-0.039965
C	-8.761136	3.532921	-0.004433
C	-8.740051	2.720935	1.144972
C	-9.347512	2.987312	-1.165056
C	-9.120854	1.385725	1.090682
C	-9.722331	1.650658	-1.221604
C	-9.538524	0.795292	-0.116969
C	6.188898	-4.357471	0.114744
C	5.819689	-5.252555	1.139116
C	5.425167	-4.374712	-1.069502
C	4.680589	-6.041556	1.027109
C	4.291145	-5.168791	-1.183712
C	3.860712	-5.978375	-0.116661
C	2.529049	-6.609849	-0.160333
C	1.967636	-7.086489	-1.360007
C	1.718649	-6.618894	0.989238
C	0.636532	-7.483192	-1.421691
C	0.383645	-6.998499	0.922413
C	-0.203258	-7.403031	-0.292627
C	-1.667829	-7.557154	-0.390625
C	-2.465189	-7.844053	0.736014
C	-2.340154	-7.236774	-1.583947
C	-3.841436	-7.656184	0.711818
C	-3.716718	-7.046132	-1.607280
C	-4.492299	-7.164787	-0.438712
C	-5.834640	-6.553554	-0.379083
C	-6.599830	-6.295298	-1.535106
C	-6.282742	-5.975655	0.824009
C	-7.641534	-5.375111	-1.519227
C	-7.323368	-5.056410	0.839963
C	-7.970782	-4.665465	-0.346638
C	-8.745244	-3.409621	-0.373613
C	-9.337669	-2.869064	0.786255
C	-8.704991	-2.589179	-1.516218
C	-9.716440	-1.533289	0.845832
C	-9.088246	-1.254949	-1.458129
C	-9.528131	-0.673119	-0.253983
C	9.616142	-1.164671	-2.813605
C	9.722982	1.083033	1.841237
C	10.246994	0.293091	2.910705
C	10.080315	2.465610	1.906261
C	9.968440	-2.547858	-2.893468
C	10.091728	-0.376810	-3.906936
H	6.329379	5.247298	-2.865082
H	3.773459	5.040018	1.375557
H	4.332924	6.648085	-2.573576
H	5.742156	3.623204	1.085270
H	7.709295	-3.060220	-1.756976
H	6.976682	-3.263321	2.476864
H	8.210701	-1.188300	2.805602
H	6.863474	3.195464	-3.326577
H	8.071568	1.115197	-3.709913
H	7.771531	2.980782	0.872569
H	2.054183	6.190669	-2.558910
H	2.688460	7.086200	1.600800
H	-0.287683	6.877695	-2.353483
H	0.347536	7.814396	1.799960
H	-1.669249	6.942757	1.960301
H	-1.991098	8.252653	-2.125587

H	-4.084902	6.646193	2.058684
H	-4.421477	7.957357	-2.026191
H	-5.715175	6.212121	-2.151075
H	-6.276916	6.871252	2.064770
H	-7.554338	4.630930	-2.157855
H	-8.138603	5.279029	2.057714
H	-8.293065	3.098378	2.060587
H	-9.456986	3.605286	-2.052798
H	-8.965793	0.760645	1.965889
H	-10.115057	1.246681	-2.151734
H	6.422312	-5.316491	2.041835
H	5.665962	-3.691085	-1.878885
H	4.405258	-6.705502	1.843044
H	3.676270	-5.094264	-2.076992
H	2.583807	-7.134745	-2.255002
H	2.117272	-6.234411	1.924960
H	0.233686	-7.840783	-2.365913
H	-0.236383	-6.894663	1.808509
H	-1.993164	-8.178969	1.656231
H	-1.767881	-7.011176	-2.479456
H	-4.415700	-7.845381	1.615245
H	-4.172694	-6.670111	-2.518303
H	-6.338792	-6.780679	-2.472333
H	-5.725106	-6.141511	1.740963
H	-8.171393	-5.159192	-2.443830
H	-7.541202	-4.534146	1.767375
H	-9.456069	-3.493593	1.668475
H	-8.249121	-2.962532	-2.429078
H	-10.120354	-1.135215	1.773751
H	-8.923550	-0.624275	-2.327283
N	10.265900	-3.668470	-2.988397
N	10.487600	0.243594	-4.807769
N	10.682945	-0.329082	3.791596
N	10.382776	3.585910	1.988073

C_{70}(H)@[12]CPP

C	4.515939	-1.731374	-0.347260
C	4.573852	-0.542092	-1.121749
C	3.793924	-0.477175	-2.364632
C	3.014014	-1.607629	-2.736553
C	3.048425	-2.834565	-1.974937
C	3.787896	-2.893455	-0.796700
C	1.686842	-1.454241	-3.267626
C	0.900865	-2.586714	-2.834658
C	-0.438431	-2.409502	-2.492013
C	-1.029962	-1.093422	-2.570984
C	-0.305233	0.020283	-3.078267
C	-1.939303	-0.949823	-1.467467
C	-2.145656	0.311794	-0.843585
C	-2.235883	0.362281	0.621901
C	-2.112266	-0.852905	1.351033
C	-1.994441	-2.129474	0.683798
C	-1.909669	-2.177521	-0.705490
C	-1.346099	-0.916601	2.564920
C	-0.754380	-2.232379	2.649096
C	0.531064	-2.380091	3.165628
C	1.262898	-1.217148	3.612656
C	0.671216	0.076178	3.624642
C	-0.684784	0.232493	3.080163
C	3.467718	-0.295513	2.908577
C	4.396521	-0.442918	1.778552
C	4.427170	-1.681953	1.084586
C	3.643520	-2.813898	1.520306
C	2.766300	-2.676922	2.592953
C	2.643978	-1.400594	3.259330
C	1.106793	-0.167437	-3.440311
C	1.989382	0.942641	-3.331634
C	-0.727916	1.303970	-2.634978
C	1.511185	2.255522	-2.963613
C	0.172122	2.434413	-2.621259
C	-1.637338	1.448535	-1.531444
C	-1.299478	2.668694	-0.834483
C	-1.384054	2.716303	0.554952
C	-1.810729	1.545453	1.287397
C	-1.044425	1.480929	2.501295
C	-0.144636	2.611856	2.520026
C	1.141271	2.463290	3.036541
C	1.564750	1.180108	3.548487
C	2.945633	0.996259	3.194802
C	3.376208	2.165684	2.463379
C	4.252077	2.023309	1.390873
C	4.732992	0.712908	1.020839
C	4.820473	0.664070	-0.410888
C	4.400479	1.945997	-0.926532
C	3.659447	2.008735	-2.104419
C	3.316598	0.790085	-2.801199
C	-0.184051	3.293620	-1.513057
C	-0.358173	3.391002	1.320446
C	2.264451	3.088570	2.372864
C	4.054486	2.798666	0.187907
C	2.547604	2.929206	-2.212507
C	1.742626	-3.455623	-2.041969
C	-0.989115	-3.094509	-1.343216
C	-1.162798	-2.996873	1.490393
C	1.460264	-3.297915	2.542398
C	3.252193	-3.577951	0.358134
C	-0.175576	-3.928385	-0.567165
C	-0.264246	-3.877537	0.878289
C	1.073950	-4.029529	1.414256
C	1.989449	-4.172712	0.300895
C	1.217013	-4.110159	-0.922912
C	2.978685	3.683734	0.091922
C	2.064254	3.834554	1.205704
C	0.726447	3.989458	0.669394
C	0.815339	3.939638	-0.776200
C	2.207531	3.749551	-1.131698
C	-0.991074	7.284956	1.168896
C	0.398375	7.315512	1.163550
C	1.117536	7.638007	-0.002897
C	0.374564	8.032456	-1.133177
C	-1.015675	7.998506	-1.129055

C	2.568200	7.377298	-0.068589
C	3.385421	7.393258	1.079452
C	4.658693	6.836216	1.065592
C	5.177093	6.226949	-0.095217
C	4.418179	6.348274	-1.274866
C	3.147530	6.910696	-1.262480
C	6.314777	5.287627	-0.049944
C	6.568321	4.554598	1.124704
C	7.333957	3.395462	1.100947
C	7.881724	2.908702	-0.100033
C	7.777356	3.737596	-1.235684
C	7.014938	4.899143	-1.210501
C	8.297921	1.496183	-0.191128
C	8.722118	0.762220	0.934956
C	8.722857	-0.627767	0.928659
C	8.301376	-1.352137	-0.204940
C	8.042346	-0.616955	-1.376903
C	8.039992	0.771969	-1.370133
C	7.892496	-2.767838	-0.130080
C	7.337853	-3.269090	1.062299
C	6.583631	-4.435720	1.071128
C	6.344354	-5.158621	-0.112133
C	7.044354	-4.751149	-1.266026
C	7.799780	-3.584529	-1.274895
C	5.222322	-6.115700	-0.171172
C	4.724244	-6.766785	0.975025
C	3.462581	-7.350814	0.980280
C	2.636771	-7.315440	-0.160774
C	3.200353	-6.803068	-1.344960
C	4.459021	-6.218758	-1.349990
C	1.188624	-7.591248	-0.095173
C	0.475333	-7.341135	1.092243
C	-0.913891	-7.293905	1.103981
C	-1.660323	-7.493550	-0.071800
C	-0.952200	-7.863591	-1.231923
C	0.436868	-7.912917	-1.242769
C	-3.094327	-7.147433	-0.108927
C	-3.918998	-7.235288	1.029826
C	-5.182588	-6.653378	1.050211
C	-5.681058	-5.955286	-0.067137
C	-4.903430	-5.970455	-1.240853
C	-3.640726	-6.550746	-1.260690
C	-6.846726	-5.052857	0.019066
C	-7.075382	-4.323996	1.201114
C	-7.904156	-3.207745	1.207402
C	-8.545839	-2.768934	0.032756
C	-8.454044	-3.601301	-1.101158
C	-7.620996	-4.715291	-1.108872
C	-9.031004	-1.375333	-0.046674
C	-9.450956	-0.654537	1.089791
C	-9.466385	0.736514	1.092922
C	-9.061655	1.471887	-0.039943
C	-8.834679	0.748303	-1.226650
C	-8.819754	-0.641542	-1.229920
C	-8.602528	2.873980	0.047768
C	-7.974045	3.317677	1.227635
C	-7.158628	4.443347	1.229548
C	-6.930914	5.179937	0.051624
C	-7.697859	4.838433	-1.080424
C	-8.516656	3.713601	-1.081488
C	-5.770047	6.090288	-0.024194
C	-5.261438	6.755025	1.109317
C	-3.991983	7.323212	1.100857
C	-3.732845	6.711331	-1.212169
C	-5.000672	6.140393	-1.202764
H	-1.509783	6.934261	2.057535
H	0.935922	6.986426	2.048837
H	0.897161	8.344275	-2.034471
H	-1.560353	8.282108	-2.026737
H	2.998418	7.812347	2.005242
H	5.242978	6.828872	1.982509
H	4.771633	5.882344	-2.190524
H	2.549640	6.875593	-2.169243
H	6.048248	4.814421	2.042392
H	7.389550	2.788096	2.000095
H	8.254745	3.435413	-2.164868
H	6.911132	5.484098	-2.121075
H	9.002810	1.289724	1.843508
H	9.004177	-1.163243	1.832389
H	7.708446	-1.136017	-2.271168
H	7.704141	1.298939	-2.259143
H	7.382940	-2.668741	1.966835
H	6.061171	-4.712098	1.982435
H	6.948547	-5.327765	-2.182803
H	8.279841	-3.269239	-2.198339
H	5.314495	-6.771294	1.888204
H	3.090517	-7.802779	1.896576
H	2.596110	-6.747968	-2.245840
H	4.799947	-5.722612	-2.254112
H	1.016567	-7.073073	1.995300
H	-1.424787	-6.994177	2.015354
H	-1.500681	-8.085362	-2.144319
H	0.951085	-8.173130	-2.164687
H	-3.549670	-7.741926	1.918577
H	-5.782523	-6.708386	1.955871
H	-5.250596	-5.427727	-2.116492
H	-3.026829	-6.451243	-2.152280
H	-6.499372	-4.559707	2.092600
H	-7.952497	-2.593713	2.103078
H	-8.997080	-3.335263	-2.005295
H	-7.525539	-5.305623	-2.017515
H	-9.702496	-1.192133	2.001317
H	-9.730072	1.263702	2.007072
H	-8.529241	1.277815	-2.125441
H	-8.503246	-1.160450	-2.131097
H	-8.019566	2.700858	2.121507
H	-6.590678	4.680281	2.125673
H	-7.606699	5.433196	-1.986631
H	-9.051688	3.445221	-1.989734
H	-5.855600	6.789378	2.019649
H	-3.611346	7.796224	2.003333
H	-3.124813	6.638018	-2.110643

H	-5.356375	5.628609	-2.093545
C	-3.172594	7.258945	-0.043087
C	-1.731098	7.572090	0.007066

$C_{60}(5)$@[10]CPA

C	1.366874	1.418108	3.292782
C	2.523845	0.541639	3.317543
C	3.658401	0.861241	2.564735
C	3.678368	2.069513	1.759933
C	2.563620	2.914287	1.737383
C	1.386496	2.582883	2.518726
C	0.176127	0.588625	3.325399
C	0.597362	-0.800114	3.370022
C	2.048619	-0.829331	3.366004
C	2.725897	-1.829486	2.660679
C	4.360752	-0.176656	1.832483
C	4.392275	1.777160	0.532657
C	3.967105	2.342027	-0.671638
C	2.811676	3.215934	-0.695249
C	2.121297	3.497193	0.485955
C	0.672210	3.529865	0.492016
C	0.216166	2.963949	1.748259
C	-0.931060	2.164769	1.780115
C	-0.950852	0.954740	2.583033
C	-0.124092	-1.772669	2.670233
C	-1.293682	-1.392752	1.899159
C	-1.699214	-0.054638	1.856400
C	-2.141316	0.531088	0.604213
C	-1.667009	1.902739	0.556922
C	-1.227462	2.449727	-0.652672
C	-0.036945	3.279421	-0.685642
C	0.679470	2.987071	-1.913632
C	2.077659	2.957872	-1.918824
C	4.814959	0.390878	0.578367
C	2.480136	-0.440985	-3.306973
C	3.606400	-0.805707	-2.562514
C	3.584213	-2.013976	-1.757746
C	2.437177	-2.814075	-1.727068
C	1.268381	-2.435414	-2.499540
C	0.132549	-0.394118	-3.297275
C	0.608345	0.976683	-3.345043
C	2.059498	0.947885	-3.351939
C	2.781102	1.919987	-2.651686
C	3.951607	1.541393	-1.880836
C	4.354639	0.203376	-1.835457
C	4.317608	-1.750025	-0.535677
C	3.879214	-2.297995	0.671757
C	2.690619	-3.126015	0.704070
C	1.981270	-3.379923	-0.472367
C	0.531660	-3.354159	-0.467497
C	0.089509	-2.769514	-1.720407
C	-1.024807	-1.924619	-1.743614
C	-1.002564	-0.714786	-2.546540
C	-0.068691	1.976956	-2.639985
C	-1.247102	1.644435	-1.860547
C	-1.705005	0.323592	-1.814663
C	-2.160780	-0.244054	-0.559170
C	-1.740652	-1.633368	-0.515146
C	-1.314711	-2.197889	0.691220
C	-0.158403	-3.075351	0.715595
C	0.577916	-2.812114	1.938572
C	1.976330	-2.838890	1.933295
C	4.794584	-0.381725	-0.584528
C	3.904826	-1.497671	1.881007
C	1.289397	-1.270591	-3.273543
C	7.306169	-3.103994	1.933168
C	7.758882	-1.833738	2.170882
C	7.960448	-0.915983	1.096874
C	7.889382	-1.435420	-0.250315
C	7.488297	-2.783392	-0.449593
C	7.062332	-3.585631	0.598701
C	7.954592	1.363141	0.222145
C	7.616913	2.727158	0.429534
C	7.199891	3.545420	-0.609727
C	7.390806	3.054765	-1.949098
C	7.784763	1.766890	-2.196209
C	7.972945	0.841752	-1.126200
C	8.042469	0.465085	1.299819
C	7.990964	-0.541523	-1.330048
C	6.143740	-4.727440	0.381904
C	5.490579	-4.896936	-0.858146
C	5.668249	-5.521385	1.447834
C	4.340083	-5.660238	-0.979197
C	4.505662	-6.276984	1.330807
C	3.762820	-6.295204	0.136408
C	2.362020	-6.751515	0.083935
C	1.539662	-6.620600	1.219551
C	1.746954	-7.149278	-1.119243
C	0.164266	-6.802311	1.139297
C	0.369822	-7.326346	-1.200617
C	-0.459447	-7.120010	-0.081621
C	-1.930945	-7.104623	-0.190888
C	-2.553883	-6.604088	-1.349179
C	-2.759448	-7.465810	0.889159
C	-3.927304	-6.388419	-1.391290
C	-4.133315	-7.252503	0.846034
C	-4.744784	-6.662662	-0.277662
C	-10.582010	-1.673277	0.948718
C	-10.400225	-0.768856	-0.117549
C	6.328042	4.719260	-0.374838
C	5.883888	5.548853	-1.426956
C	5.676763	4.886145	0.866139
C	4.740250	6.331612	-1.301970
C	4.545978	5.676757	0.995370
C	3.988048	6.341141	-0.112934
C	-9.445980	-3.445522	-0.284910
C	-8.070842	-5.248494	-1.413579
C	-8.511163	-4.590421	-0.246922
C	-5.899168	5.979423	0.231205
C	-6.669487	5.822565	1.400445
C	-6.432214	5.466965	-0.966045

C	-7.841359	5.072372	1.396252
C	-7.598973	4.711066	-0.968824
C	-8.294604	4.432776	0.224470
C	-9.268078	3.320377	0.253807
C	-9.958507	2.892144	-0.899262
C	-9.327601	2.480288	1.382504
C	-10.489855	1.609400	-0.985053
C	-9.861261	1.199543	1.298330
C	-10.357947	0.695439	0.080276
C	2.586838	6.797563	-0.065868
C	1.953464	7.154164	1.140767
C	1.777172	6.684376	-1.212469
C	0.571839	7.294255	1.215347
C	0.397357	6.829703	-1.138886
C	-0.243818	7.091545	0.085861
C	-1.713807	7.016369	0.187491
C	-2.552516	7.371419	-0.886542
C	-2.319794	6.464432	1.331462
C	-3.919162	7.114548	-0.848945
C	-3.686083	6.207129	1.368782
C	-4.512755	6.487443	0.263797
C	-9.934102	-1.301165	-1.335610
C	-6.136103	-6.167690	-0.245171
C	-6.665533	-5.646149	0.949970
C	-6.909064	-6.014356	-1.413460
C	-9.466591	-2.607736	-1.416855
C	-10.117159	-2.981713	0.865888
C	-7.822647	-4.875980	0.948786
H	-6.567386	-6.466253	-2.342042
H	-4.743325	-7.525394	1.704129
H	-6.099639	-5.746137	1.872866
H	-8.126813	-4.386696	1.870366
H	-8.616439	-5.111411	-2.344401
H	-8.977628	-2.931010	-2.332196
H	-10.205894	-3.632507	1.732800
H	1.973754	-6.280458	2.155979
H	-4.538264	7.387873	-1.700395
H	-4.108303	5.701681	2.233864
H	-6.321361	6.265050	2.331174
H	-5.865662	5.568373	-1.888456
H	-8.389226	4.937924	2.326093
H	-7.911261	4.232090	-1.893105
H	-10.014921	3.549047	-1.764235
H	-8.823428	2.776414	2.298793
H	-10.946068	1.282994	-1.917119
H	-9.755672	0.531004	2.148977
H	7.052887	-3.726673	2.784702
H	7.867479	-1.476065	3.193249
H	7.378613	-3.112062	-1.479145
H	7.545810	3.062703	1.460517
H	7.138371	3.687304	-2.793625
H	7.852562	1.404447	-3.220284
H	-4.363309	-5.914638	-2.267276
H	-11.020756	-1.321775	1.880067
H	6.397249	5.540862	-2.383984
H	5.968889	4.287985	1.722162
H	4.391805	6.899576	-2.161297
H	4.009108	5.664012	1.939400
H	-0.203531	6.645681	-2.025800
H	2.551466	7.297395	2.037556
H	-1.697149	6.157591	2.168396
H	-2.120433	7.845053	-1.765151
H	-1.940970	-6.299477	-2.194139
H	-2.313152	-7.905778	1.778161
H	2.225660	6.379077	-2.153928
H	0.110470	7.547631	2.167034
H	-0.449084	-6.610681	2.016276
H	-0.077123	-7.618104	-2.148224
H	5.804141	-4.325825	-1.724920
H	4.138930	-6.820480	2.198315
H	6.174331	-5.509647	2.408520
H	-9.794880	-0.641025	-2.187947
H	2.356457	-7.303243	-2.006472
H	3.808956	-5.654010	-1.926671
H	7.934135	-0.928405	-2.346815
H	8.026219	0.853702	2.317533

C_{70}(V)@[10]CPA

C	1.084728	2.128957	3.013383
C	2.226163	2.563263	2.236889
C	1.139767	0.932169	3.737669
C	3.386047	1.791157	2.214416
C	4.100324	1.607090	0.974142
C	3.703247	2.269955	-0.217362
C	4.090084	1.653900	-1.436954
C	-1.139879	0.360625	2.993873
C	-1.188471	1.594416	2.239867
C	0.004790	0.029958	3.727682
C	-0.098136	2.462264	2.249272
C	0.312352	3.113398	1.026463
C	-0.425577	2.961512	-0.179279
C	0.298537	3.151970	-1.387152
C	2.482076	3.081206	-0.194726
C	1.747971	3.173603	1.018336
C	1.733546	3.212375	-1.394304
C	-0.148089	-2.302703	2.940179
C	-1.326637	-1.953349	2.176507
C	0.511058	-1.329115	3.699967
C	-1.812026	-0.647615	2.202688
C	-2.287232	-0.033584	0.984503
C	-2.357047	-0.760278	-0.235792
C	-2.302410	0.010444	-1.429693
C	-1.575763	2.046451	-0.189322
C	-1.901926	1.351216	1.007485
C	-1.916938	1.395515	-1.406769
C	2.690951	-2.182106	2.925982
C	2.004120	-3.180786	2.134176
C	1.959525	-1.267598	3.693318
C	0.611945	-3.239789	2.141193
C	-0.103769	-3.479177	0.909167
C	0.581209	-3.744707	-0.307162

C	-0.118429	-3.434806	-1.505042
C	-1.845677	-2.138445	-0.263885
C	-1.301315	-2.685765	0.930862
C	-1.316383	-2.640675	-1.483884
C	3.451193	0.557135	2.969340
C	4.194293	-0.390458	2.168294
C	2.347884	0.130093	3.716174
C	3.826180	-1.733491	2.149167
C	3.846474	-2.462910	0.903094
C	4.325384	-1.868214	-0.294763
C	3.828998	-2.413881	-1.507767
C	2.046679	-3.678219	-0.314367
C	2.722170	-3.355723	0.893483
C	2.703433	-3.306583	-1.517390
C	4.717722	-0.455319	-0.272486
C	4.598234	0.260909	0.947031
C	4.589137	0.307163	-1.463053
C	2.651457	-2.062378	-3.506012
C	3.795931	-1.641066	-2.726701
C	4.171519	-0.298907	-2.705001
C	1.911771	-1.121673	-4.231113
C	-0.187988	-2.185049	-3.492094
C	0.580935	-3.150620	-2.736694
C	1.973190	-3.088447	-2.742653
C	0.463018	-1.184082	-4.223400
C	-1.179497	0.477885	-3.437362
C	-1.842534	-0.558327	-2.674985
C	-1.356977	-1.864314	-2.701859
C	-0.042942	0.174609	-4.195676
C	1.046735	2.245205	-3.418161
C	-0.127096	2.549393	-2.628096
C	-1.218773	1.683081	-2.638091
C	1.092616	1.076734	-4.186779
C	3.415509	0.676341	-3.461569
C	3.359696	1.881082	-2.660788
C	2.197856	2.650405	-2.640175
C	2.301490	0.275694	-4.208073
C	7.173419	-3.152294	2.282454
C	7.477981	-1.846265	2.553352
C	7.745282	-0.926459	1.497134
C	7.914574	-1.457805	0.162407
C	7.646055	-2.835200	-0.065233
C	7.149156	-3.657633	0.935688
C	7.671599	1.334430	0.587327
C	7.161200	2.653545	0.703835
C	6.938096	3.457987	-0.401899
C	7.467225	3.004412	-1.661773
C	7.972120	1.740481	-1.816121
C	7.984934	0.817313	-0.725419
C	7.660568	0.455835	1.681605
C	8.132146	-0.562839	-0.901261
C	6.342055	-4.861294	0.637393
C	5.740661	-5.010584	-0.629150
C	5.894008	-5.737234	1.650336
C	4.629489	-5.819627	-0.814139
C	4.770171	-6.535334	1.469935
C	4.045006	-6.512262	0.262184
C	2.637699	-6.945853	0.178291
C	1.817636	-6.858236	1.320297
C	2.006207	-7.232526	-1.048335
C	0.435242	-6.952581	1.226409
C	0.621330	-7.321078	-1.142875
C	-0.201048	-7.135347	-0.015095
C	-1.664649	-6.988973	-0.126527
C	-2.236063	-6.381484	-1.260174
C	-2.526522	-7.325254	0.935581
C	-3.587443	-6.054225	-1.297197
C	-3.877489	-6.997756	0.898745
C	-4.432629	-6.317186	-0.202328
C	-10.355681	-1.339567	1.110767
C	-10.233754	-0.412868	0.055718
C	5.977629	4.580453	-0.335608
C	5.334877	5.048176	-1.499882
C	5.475259	5.067234	0.890369
C	4.187409	5.829439	-1.437830
C	4.312568	5.822286	0.952751
C	3.592089	6.170459	-0.208760
C	-9.115531	-3.024072	-0.146414
C	-7.712008	-4.775114	-1.317005
C	-8.151380	-4.144831	-0.135075
C	-6.234963	6.573580	0.395430
C	-6.996604	6.397639	1.568297
C	-6.764757	6.047803	-0.798346
C	-8.137507	5.600568	1.574019
C	-7.902094	5.249586	-0.792262
C	-8.569112	4.935349	0.408093
C	-9.460827	3.756566	0.446619
C	-10.128079	3.278548	-0.700678
C	-9.432653	2.907422	1.569846
C	-10.543205	1.953867	-0.790905
C	-9.852267	1.584946	1.481859
C	-10.315670	1.048022	0.265055
C	2.218097	6.707608	-0.130880
C	1.693855	7.278105	1.048220
C	1.323583	6.531966	-1.205634
C	0.339184	7.570831	1.173937
C	-0.024710	6.840738	-1.087375
C	-0.559432	7.327804	0.118489
C	-2.023049	7.426813	0.276224
C	-2.856493	7.792472	-0.798303
C	-2.642398	6.999731	1.464758
C	-4.235201	7.628027	-0.727139
C	-4.021534	6.824667	1.531635
C	-4.845556	7.076465	0.417095
C	-9.720223	-0.893562	-1.164655
C	-5.796196	-5.751717	-0.165259
C	-6.312901	-5.238588	1.038919
C	-6.559285	-5.554414	-1.332824
C	-9.172299	-2.167338	-1.262538
C	-9.811005	-2.615926	1.010799
C	-7.459989	-4.453094	1.053123
H	-6.223087	-5.993533	-2.269531

H	-4.514486	-7.258508	1.740895
H	-5.749130	-5.369237	1.959451
H	-7.761751	-3.980428	1.984205
H	-8.258243	-4.615285	-2.243721
H	-8.660568	-2.447461	-2.179711
H	-9.866533	-3.285812	1.865897
H	2.262673	-6.607210	2.279214
H	-4.848467	7.895214	-1.584488
H	-4.456315	6.389098	2.427780
H	-6.659456	6.851673	2.497470
H	-6.210375	6.163054	-1.726153
H	-8.670219	5.442331	2.509005
H	-8.201640	4.758699	-1.714464
H	-10.253013	3.934022	-1.559611
H	-8.942395	3.240776	2.480901
H	-10.980667	1.593786	-1.719602
H	-9.678066	0.921556	2.325261
H	6.849420	-3.789816	3.098673
H	7.407827	-1.468314	3.571543
H	7.698988	-3.189693	-1.091706
H	6.789100	2.943126	1.681795
H	7.426277	3.660517	-2.526091
H	8.301404	1.399537	-2.796055
H	-3.979141	-5.508869	-2.152440
H	-10.820885	-1.029188	2.043933
H	5.680478	4.732957	-2.479064
H	5.958522	4.795755	1.824202
H	3.717210	6.127526	-2.370265
H	3.916924	6.077389	1.931611
H	-0.694696	6.617574	-1.913922
H	2.351903	7.482228	1.888615
H	-2.024785	6.705783	2.310435
H	-2.408364	8.184729	-1.708511
H	-1.594877	-6.085938	-2.086523
H	-2.124716	-7.840426	1.805090
H	1.665081	6.067900	-2.125008
H	-0.034791	7.986031	2.107296
H	-0.167572	-6.783299	2.114847
H	0.163257	-7.513918	-2.110167
H	6.046551	-4.376039	-1.454228
H	4.409090	-7.136394	2.301039
H	6.385179	-5.745992	2.619416
H	-9.618837	-0.211923	-2.005431
H	2.607924	-7.354838	-1.945723
H	4.120727	-5.789541	-1.772907
H	8.284627	-0.957119	-1.905323
H	7.439516	0.845778	2.674263

$C_{60}(5)$@[8]CPAq

C	1.088103	0.438913	3.326797
C	0.687549	-0.956523	3.334168
C	1.416857	-1.897030	2.600017
C	2.574385	-1.477841	1.830909
C	2.960489	-0.134052	1.824098
C	2.203293	0.842195	2.585771
C	-0.115044	1.251019	3.327933
C	-1.259219	0.357750	3.335797
C	-0.763259	-1.006575	3.339482
C	-1.432052	-1.995431	2.610773
C	0.722898	-2.923899	1.843441
C	2.593664	-2.244311	0.599695
C	3.000510	-1.638679	-0.591353
C	3.403099	-0.245197	-0.599408
C	3.382144	0.494148	0.585986
C	2.884497	1.856594	0.581732
C	2.157042	2.073185	1.817340
C	0.998097	2.856363	1.818782
C	-0.159249	2.437077	2.588299
C	-2.405263	0.682896	2.603331
C	-2.450557	1.913516	1.835305
C	-1.348563	2.774175	1.827994
C	-0.926300	3.402101	0.590572
C	0.522814	3.452038	0.584443
C	1.226046	3.244973	-0.604914
C	2.427354	2.432764	-0.606222
C	2.451344	1.666322	-1.837541
C	2.928970	0.352203	-1.833619
C	1.451292	-3.137397	0.607624
C	-0.055300	-1.241952	-3.313849
C	-0.011626	-2.428060	-2.574265
C	-1.168795	-2.846594	-1.804908
C	-2.327621	-2.064060	-1.803556
C	-2.373586	-0.833413	-2.571601
C	-0.858013	0.965367	-3.320129
C	0.592822	1.015557	-3.325999
C	1.088819	-0.348760	-3.321686
C	2.234640	-0.673880	-2.589186
C	2.279432	-1.904619	-1.820893
C	1.177831	-2.766038	-1.813777
C	-0.694381	-3.444081	-0.571228
C	-1.397648	-3.236898	0.618097
C	-2.599883	-2.425193	0.619373
C	-3.056773	-1.848440	-0.568439
C	-3.553007	-0.486016	-0.571721
C	-3.131936	0.142531	-1.809550
C	-2.745818	1.486838	-1.816175
C	-1.587691	1.905696	-2.585709
C	1.261356	2.004497	-2.597587
C	0.504132	2.981251	-1.835220
C	-0.894036	2.932829	-1.829174
C	-1.622982	3.146572	-0.592915
C	-2.765948	2.253872	-0.584966
C	-3.172638	1.647710	0.606093
C	-3.573461	0.254331	0.612848
C	-3.100517	-0.343315	1.847080
C	-2.622482	-1.657841	1.850505
C	0.754694	-3.393083	-0.576049
C	-0.675211	-2.972628	1.848631
C	-1.258490	-0.430027	-3.313024
C	6.130446	-2.917773	1.889503
C	6.586649	-1.635124	2.164161

C	6.871954	-0.748000	1.117802
C	6.852130	-1.232806	-0.207572
C	6.463613	-2.546076	-0.466830
C	5.989883	-3.381618	0.561390
C	6.758823	1.608391	0.240179
C	6.286450	2.896648	0.486119
C	5.792403	3.703913	-0.555829
C	5.995695	3.247033	-1.878571
C	6.535977	1.994244	-2.138259
C	6.846293	1.126170	-1.083180
C	7.023679	0.704021	1.404926
C	7.098071	-0.312981	-1.363992
C	5.152046	-4.562965	0.267884
C	4.475724	-4.655055	-0.965220
C	4.786441	-5.490208	1.265869
C	3.380411	-5.491107	-1.126302
C	3.683120	-6.320621	1.108408
C	2.896571	-6.270240	-0.059421
C	1.504166	-6.753233	-0.097463
C	0.718958	-6.657292	1.066788
C	0.839344	-7.049116	-1.303575
C	-0.667777	-6.682899	1.000901
C	-0.549418	-7.081995	-1.367675
C	-1.337862	-6.810791	-0.230980
C	-2.750015	-6.394063	-0.329951
C	-3.186873	-5.703187	-1.475810
C	-3.618522	-6.412161	0.780412
C	-4.335542	-4.923040	-1.450497
C	-4.765907	-5.627348	0.807767
C	-5.100896	-4.792188	-0.276638
C	4.883370	4.838266	-0.286275
C	4.463609	5.721533	-1.303456
C	4.201308	4.918344	0.944810
C	3.312662	6.488156	-1.163820
C	3.058981	5.692663	1.088861
C	2.530238	6.418655	0.005772
C	-7.072024	-1.697335	-1.158165
C	-6.929889	-0.943118	0.024105
C	-6.186798	3.267156	0.160403
C	-6.744205	2.614492	1.277693
C	-6.199445	2.570334	-1.062803
C	-7.129065	1.279602	1.211924
C	-6.580481	1.236595	-1.127465
C	-6.970954	0.532293	0.027376
C	1.113263	6.824179	0.036533
C	0.435322	7.110714	1.237655
C	0.332192	6.657590	-1.122556
C	-0.952805	7.066487	1.305939
C	-1.053774	6.606272	-1.052230
C	-1.727135	6.724011	0.178972
C	-3.112122	6.227398	0.293615
C	-3.984885	6.171691	-0.811679
C	-3.502436	5.534272	1.454825
C	-5.083640	5.319952	-0.816874
C	-4.601080	4.684590	1.450426
C	-5.362532	4.484795	0.283596
C	-5.994662	-3.627476	-0.131270
C	-6.020428	-2.934742	1.093930
C	-6.612886	-3.007769	-1.235082
C	-6.474864	-1.624515	1.169098
H	-6.676270	-3.540463	-2.181223
H	-5.378699	-5.609841	1.706326
H	-5.549516	-3.377764	1.967441
H	-6.345635	-1.080323	2.100416
H	-7.490320	-1.228835	-2.045855
H	1.195621	-6.422963	2.014821
H	-5.698982	5.251194	-1.710921
H	-4.782958	4.060873	2.321083
H	-6.818572	3.143567	2.224991
H	-5.774629	3.036309	-1.947572
H	-7.500671	0.789709	2.108738
H	-6.442259	0.699839	-2.061737
H	5.782917	-3.531785	2.714799
H	6.628934	-1.266010	3.185324
H	6.449548	-2.867683	-1.503299
H	6.226574	3.214555	1.522067
H	5.635951	3.837885	-2.715339
H	6.629875	1.628863	-3.157299
H	-4.560043	-4.293714	-2.307228
H	5.010569	5.769926	-2.241256
H	4.482745	4.270718	1.768144
H	2.979312	7.104648	-1.995424
H	2.490930	5.619548	2.011751
H	-1.612127	6.336529	-1.944373
H	1.007671	7.312110	2.140292
H	-2.858060	5.548647	2.329189
H	-3.761300	6.755391	-1.701556
H	-2.546909	-5.660090	-2.352521
H	-3.355589	-6.999211	1.657326
H	0.819515	6.427835	-2.066493
H	-1.443137	7.237300	2.261298
H	-1.237318	-6.465786	1.900304
H	-1.032912	-7.258213	-2.325544
H	4.718235	-3.972262	-1.772366
H	3.387137	-6.974043	1.925732
H	5.336520	-5.523107	2.202503
H	1.419249	-7.196840	-2.211774
H	2.806834	-5.429557	-2.046463
O	7.369834	-0.731389	-2.484149
O	7.230242	1.137369	2.533393

$C_{60}(5)$@[8]CPTcaq

C	1.308563	0.919595	3.334305
C	1.718077	-0.472804	3.310537
C	2.831858	-0.860914	2.559137
C	3.580280	0.127724	1.803749
C	3.185477	1.468983	1.826499
C	2.028255	1.871919	2.605760
C	-0.142624	0.960218	3.347686
C	-0.629836	-0.407200	3.331550
C	0.520184	-1.292650	3.308773

C	0.480734	-2.470834	2.556660
C	2.790044	-2.083312	1.778245
C	3.999259	-0.485125	0.557510
C	4.009590	0.267371	-0.619346
C	3.599597	1.657770	-0.595909
C	3.194609	2.248726	0.603352
C	2.045601	3.132908	0.625994
C	1.324042	2.901582	1.863211
C	-0.073939	2.940859	1.876762
C	-0.821211	1.952172	2.633142
C	-1.778100	-0.732398	2.602255
C	-2.483614	0.297164	1.860708
C	-2.012701	1.613855	1.875110
C	-1.997831	2.390864	0.650997
C	-0.802725	3.210711	0.652554
C	-0.106978	3.434684	-0.537526
C	1.341897	3.395722	-0.551359
C	1.762376	2.784565	-1.797300
C	2.869797	1.931434	-1.818861
C	3.511773	-1.850337	0.542159
C	1.194719	-0.983626	-3.345896
C	1.873233	-1.975019	-2.630208
C	1.126324	-2.964438	-1.874700
C	-0.271715	-2.925543	-1.862849
C	-0.976267	-1.896204	-2.606082
C	-0.666258	0.449261	-3.308988
C	0.531577	1.269090	-3.307261
C	1.681618	0.383689	-3.330147
C	2.828908	0.708743	-2.599620
C	3.534558	-0.320500	-1.857438
C	3.065037	-1.637678	-1.872321
C	1.856162	-3.236230	-0.650562
C	1.160398	-3.459847	0.539525
C	-0.288407	-3.418061	0.552025
C	-0.992050	-3.154799	-0.625429
C	-2.139157	-2.269330	-0.602581
C	-2.132805	-1.492042	-1.826516
C	-2.529163	-0.151173	-1.804221
C	-1.781101	0.837727	-2.559089
C	0.571607	2.447218	-2.555220
C	-0.584467	2.850091	-1.775597
C	-1.738614	2.060041	-1.777391
C	-2.458258	1.825600	-0.540701
C	-2.950078	0.461414	-0.557308
C	-2.960509	-0.290330	0.621817
C	-2.545895	-1.679882	0.596940
C	-1.818064	-1.954881	1.820521
C	-0.710052	-2.808331	1.798343
C	3.052888	-2.417333	-0.649221
C	1.636726	-2.873359	1.777222
C	-0.256466	-0.943209	-3.333216
C	-5.509915	2.997454	1.970946
C	-6.143109	1.782942	2.192041
C	-6.628172	1.019083	1.119630
C	-6.552700	1.569477	-0.188729
C	-5.954314	2.815021	-0.385395
C	-5.361325	3.528759	0.672694
C	-6.638174	-1.233975	0.156196
C	-6.116631	-2.510310	0.373484
C	-5.532610	-3.257712	-0.665447
C	-5.611659	-2.724090	-1.968550
C	-6.165312	-1.475278	-2.210345
C	-6.639064	-0.682222	-1.154054
C	-7.071506	-0.369196	1.268192
C	-6.995636	0.729674	-1.316562
C	-4.446939	4.660336	0.426295
C	-3.809847	4.809887	-0.821766
C	-4.003638	5.496795	1.472165
C	-2.682056	5.604962	-0.964743
C	-2.872612	6.290262	1.330138
C	-2.127088	6.288058	0.133876
C	-0.720144	6.724575	0.082160
C	0.083817	6.570127	1.227564
C	-0.066373	7.033112	-1.127460
C	1.468537	6.549930	1.135774
C	1.321260	7.018673	-1.217665
C	2.120672	6.686354	-0.104895
C	3.512472	6.214715	-0.240506
C	3.899461	5.533884	-1.410185
C	4.398164	6.163853	0.855182
C	5.006265	4.694678	-1.420551
C	5.505051	5.322851	0.845366
C	5.778826	4.494013	-0.261281
C	6.607797	3.278412	-0.149982
C	6.627287	2.574635	1.069123
C	7.160275	2.632972	-1.273888
C	7.010637	1.241207	1.124262
C	7.547964	1.298435	-1.217563
C	7.397340	0.544116	-0.036314
C	-4.685278	-4.433594	-0.392533
C	-4.288132	-5.314365	-1.419932
C	-4.057369	-4.587903	0.859338
C	-3.200603	-6.162740	-1.259303
C	-2.970880	-5.436039	1.019903
C	-2.453171	-6.170180	-0.064002
C	-1.069103	-6.674350	-0.008291
C	-0.422065	-6.986778	1.203848
C	-0.267257	-6.589075	-1.162526
C	0.965331	-7.044368	1.283338
C	1.117085	-6.640143	-1.081539
C	1.772078	-6.782265	0.157018
C	3.188765	-6.384111	0.270251
C	4.062201	-6.396401	-0.836651
C	3.626407	-5.708508	1.424950
C	5.211706	-5.614936	-0.853118
C	4.777278	-4.930920	1.410131
C	5.544090	-4.788222	0.238666
C	6.434736	-3.620024	0.101735
C	7.049413	-3.003223	1.209075
C	6.460220	-2.921509	-1.120295
C	7.505134	-1.691194	1.138132
C	6.909925	-1.609451	-1.189260

C	7.361039	-0.931537	-0.040629
C	-7.808573	-0.831742	2.342253
C	-7.665737	1.232606	-2.416307
C	-8.136476	0.411571	-3.487274
C	-8.020840	2.610202	-2.554956
C	-8.246763	-2.186672	2.465232
C	-8.269781	0.016381	3.396066
H	-4.523489	5.493909	2.426400
H	-2.146766	5.585741	-1.909350
H	-2.526330	6.877456	2.176981
H	-4.114271	4.204265	-1.668875
H	-6.097575	-2.901930	1.383150
H	-5.149709	-3.250602	-2.797289
H	-6.139894	-1.077141	-3.218543
H	-5.046228	3.494375	2.816661
H	-6.175440	1.384163	3.199876
H	-5.883693	3.204080	-1.393400
H	-0.379981	6.325326	2.179096
H	-0.655154	7.230167	-2.020271
H	2.045488	6.288860	2.018408
H	1.792496	7.205549	-2.179569
H	3.247409	5.547147	-2.278861
H	4.178366	6.741514	1.749872
H	5.186908	4.078087	-2.296467
H	6.130725	5.256021	1.732355
H	6.206583	3.035347	1.958640
H	7.229367	3.167685	-2.218364
H	6.878198	0.699056	2.056238
H	7.916661	0.814888	-2.119019
H	-4.808488	-5.302800	-2.373976
H	-4.330389	-3.946023	1.690603
H	-2.886519	-6.787190	-2.091805
H	-2.432767	-5.421785	1.963033
H	-1.012471	-7.130645	2.105737
H	-0.725060	-6.343280	-2.116640
H	1.433676	-7.233562	2.246193
H	1.698664	-6.431495	-1.974905
H	3.800950	-6.974150	-1.720050
H	2.985315	-5.673181	2.301132
H	5.827824	-5.591482	-1.749055
H	5.002228	-4.312025	2.274224
H	7.114243	-3.539861	2.152865
H	5.993558	-3.362584	-1.996840
H	7.923597	-1.226324	2.027599
H	6.781268	-1.062536	-2.119006
N	-8.615543	-3.282069	2.598386
N	-8.658746	0.681131	4.267987
N	-8.530995	-0.229961	-4.373969
N	-8.321279	3.724574	-2.701890

C_{70}(V)@[8]CPAq

C	-1.105646	1.842771	3.582126
C	-0.470033	2.851544	2.762467
C	-0.332144	0.866044	4.219678
C	0.915337	2.855997	2.613782
C	1.492475	3.120597	1.319011
C	0.691808	3.480091	0.203228
C	1.242642	3.205325	-1.077524
C	-1.974420	-0.862842	3.591445
C	-2.765186	0.149083	2.924563
C	-0.775496	-0.514553	4.224174
C	-2.338692	1.475824	2.919731
C	-2.466036	2.263992	1.717159
C	-3.103666	1.752104	0.555814
C	-2.723112	2.341095	-0.679848
C	-0.766611	3.475429	0.359536
C	-1.312449	3.114776	1.620437
C	-1.570895	3.192174	-0.777059
C	0.314967	-2.521717	3.296370
C	-0.924686	-2.871825	2.635175
C	0.393064	-1.361075	4.074369
C	-2.047527	-2.059017	2.780056
C	-2.890199	-1.789878	1.638418
C	-2.656157	-2.406892	0.380125
C	-3.145819	-1.714063	-0.759647
C	-3.553067	0.355631	0.560827
C	-3.333077	-0.425196	1.727572
C	-3.587967	-0.351791	-0.670437
C	2.600772	-0.841713	3.104311
C	2.508933	-2.036367	2.293887
C	1.558689	-0.503894	3.976501
C	1.389254	-2.860285	2.388371
C	0.815451	-3.428751	1.191871
C	1.417557	-3.244762	-0.079488
C	0.558492	-3.356852	-1.205037
C	-1.474238	-3.262442	0.227780
C	-0.612562	-3.435413	1.343849
C	-0.868879	-3.363563	-1.053225
C	1.721188	1.855457	3.280356
C	2.789531	1.498503	2.371800
C	1.110336	0.872757	4.066625
C	3.221809	0.177331	2.285826
C	3.526469	-0.391945	0.995117
C	3.489299	0.389041	-0.191109
C	3.273421	-0.318226	-1.403714
C	2.595066	-2.376169	-0.178999
C	3.085151	-1.757910	1.000272
C	2.832120	-1.685436	-1.397219
C	3.034824	1.780442	-0.099850
C	2.648599	2.283309	1.169731
C	2.399120	2.366562	-1.227198
C	1.915619	-0.643303	-3.289520
C	2.703538	0.328538	-2.562476
C	2.273524	1.651564	-2.475819
C	0.716177	-0.260143	-3.900256
C	-0.368861	-2.323934	-3.096969
C	0.871108	-2.711772	-2.459245
C	1.991129	-1.887648	-2.553936
C	-0.449454	-1.117598	-3.802034
C	-2.656687	-0.664922	-2.800811
C	-2.564128	-1.907953	-2.066749

C	-1.442111	-2.720215	-2.211263
C	-1.617048	-0.271218	-3.651355
C	-1.787352	2.040463	-2.810505
C	-2.854090	1.624848	-1.926292
C	-3.280481	0.299187	-1.921716
C	-1.173363	1.109348	-3.656165
C	1.038324	2.054765	-3.113070
C	0.398825	3.010300	-2.233163
C	-0.986963	3.003891	-2.084986
C	0.268727	1.116426	-3.810344
C	5.969065	-3.082391	1.968768
C	6.437119	-1.799970	2.222711
C	6.700952	-0.918953	1.164903
C	6.647024	-1.416289	-0.155051
C	6.242474	-2.727595	-0.394663
C	5.789577	-3.558400	0.647439
C	6.657634	1.437769	0.260328
C	6.270424	2.758503	0.489156
C	5.836966	3.588372	-0.562991
C	5.999064	3.096376	-1.879640
C	6.448454	1.806302	-2.122964
C	6.710823	0.934837	-1.057718
C	6.881366	0.533788	1.435509
C	6.888451	-0.516229	-1.326543
C	4.952365	-4.746231	0.370393
C	4.363472	-4.927998	-0.898437
C	4.499725	-5.600172	1.399713
C	3.262593	-5.755123	-1.075800
C	3.397666	-6.426750	1.223059
C	2.685085	-6.445458	0.006285
C	1.285582	-6.902796	-0.080888
C	0.458759	-6.800024	1.053737
C	0.653284	-7.178763	-1.311150
C	-0.924581	-6.778355	0.937169
C	-0.731576	-7.160854	-1.426894
C	-1.552814	-6.859656	-0.319938
C	-2.935518	-6.364853	-0.471359
C	-3.295574	-5.663149	-1.637816
C	-3.842290	-6.320872	0.607849
C	-4.402016	-4.823880	-1.661716
C	-4.946806	-5.476985	0.585886
C	-5.202209	-4.639514	-0.518898
C	5.017109	4.794415	-0.315748
C	4.630666	5.663447	-1.360591
C	4.364587	4.969102	0.920328
C	3.510859	6.475862	-1.244665
C	3.249121	5.787797	1.038993
C	2.723132	6.466948	-0.074427
C	-7.025348	-1.481323	-1.501621
C	-6.924294	-0.728972	-0.313081
C	-6.091054	3.468181	-0.159776
C	-6.695290	2.828732	0.941701
C	-6.084907	2.768225	-1.380972
C	-7.106278	1.502208	0.866698
C	-6.492532	1.442989	-1.454744
C	-6.930241	0.747714	-0.311762
C	1.305558	6.874655	-0.075501
C	0.595370	7.163628	1.107160
C	0.550913	6.710382	-1.253264
C	-0.794709	7.132286	1.137811
C	-0.836639	6.675108	-1.221297
C	-1.544526	6.804606	-0.010747
C	-2.946639	6.347862	0.059164
C	-3.778995	6.301996	-1.078592
C	-3.407590	5.690316	1.214870
C	-4.900701	5.482686	-1.115918
C	-4.529342	4.871783	1.178001
C	-5.245016	4.669194	-0.016766
C	-6.056670	-3.440304	-0.421248
C	-6.129311	-2.745718	0.800733
C	-6.598598	-2.803243	-1.555507
C	-6.549999	-1.423423	0.853110
H	-6.630144	-3.334242	-2.504053
H	-5.590269	-5.420207	1.460734
H	-5.719740	-3.199976	1.698470
H	-6.454534	-0.884417	1.791082
H	-7.385604	-1.004198	-2.409782
H	0.901346	-6.588456	2.022979
H	-5.482417	5.419491	-2.032562
H	-4.764864	4.269834	2.050972
H	-6.788157	3.360786	1.885673
H	-5.624039	3.221238	-2.254135
H	-7.514788	1.023805	1.753619
H	-6.337076	0.903385	-2.384280
H	5.649735	-3.687308	2.811349
H	6.506281	-1.425762	3.240569
H	6.207426	-3.048552	-1.430208
H	6.231330	3.091074	1.521380
H	5.680535	3.697645	-2.725166
H	6.512723	1.421622	-3.137284
H	-4.563598	-4.196128	-2.533285
H	5.171511	5.657328	-2.302821
H	4.634484	4.354897	1.772643
H	3.196934	7.071622	-2.098307
H	2.691863	5.773914	1.971097
H	-1.372022	6.413741	-2.129666
H	1.141913	7.361773	2.026161
H	-2.802597	5.703279	2.116815
H	-3.505591	6.866780	-1.966649
H	-2.625414	-5.664446	-2.492566
H	-3.644071	-6.910071	1.499963
H	1.057807	6.474542	-2.184868
H	-1.307017	7.309195	2.080281
H	-1.516091	-6.550699	1.819411
H	-1.182995	-7.314047	-2.404127
H	4.678298	-4.323414	-1.741748
H	3.042334	-7.018546	2.062922
H	4.977231	-5.580586	2.375175
H	1.257160	-7.345426	-2.199874
H	2.761417	-5.751029	-2.039589
O	7.111479	-0.956416	-2.449893
O	7.091807	0.972226	2.561450

C_{70}(V)@[8]CPTcaq

C	-0.750296	2.241349	3.003399
C	-0.096531	3.187024	2.124276
C	0.008396	1.312157	3.724790
C	1.291010	3.181345	2.000917
C	1.897941	3.356829	0.702136
C	1.113819	3.625585	-0.451463
C	1.682819	3.254491	-1.698924
C	-1.626828	-0.455815	3.194155
C	-2.403509	0.506690	2.442684
C	-0.438445	-0.063880	3.821583
C	-1.973087	1.829035	2.348675
C	-2.076009	2.528236	1.089302
C	-2.691277	1.929371	-0.042533
C	-2.284460	2.420404	-1.310476
C	-0.346214	3.628312	-0.321784
C	-0.919050	3.366384	0.951346
C	-1.127054	3.258779	-1.448160
C	0.664072	-2.133984	3.059587
C	-0.563705	-2.530054	2.403637
C	0.730063	-0.920391	3.753318
C	-1.686983	-1.707611	2.470333
C	-2.507891	-1.519068	1.296713
C	-2.246595	-2.220935	0.089499
C	-2.716866	-1.617047	-1.104964
C	-3.149851	0.540127	0.056091
C	-2.953642	-0.153442	1.281396
C	-3.163170	-0.252977	-1.122751
C	2.953931	-0.474425	2.786506
C	2.876764	-1.725554	2.064041
C	1.899048	-0.073634	3.614375
C	1.753674	-2.538215	2.197465
C	1.201906	-3.193631	1.035825
C	1.829894	-3.105047	-0.235196
C	0.988768	-3.290877	-1.364306
C	-1.066204	-3.087863	0.020231
C	-0.227749	-3.187325	1.162131
C	-0.441392	-3.284201	-1.237822
C	2.080325	2.228705	2.751535
C	3.163683	1.806053	1.891271
C	1.452972	1.306112	3.596489
C	3.591950	0.481413	1.908265
C	3.922500	-0.182485	0.669426
C	3.908232	0.511557	-0.569874
C	3.710069	-0.281958	-1.731821
C	3.012890	-2.249897	-0.375634
C	3.481167	-1.544322	0.765258
C	3.268164	-1.646251	-1.636028
C	3.456838	1.906872	-0.587796
C	3.053240	2.508285	0.634687
C	2.840016	2.405493	-1.766116
C	2.386579	-0.742032	-3.615403
C	3.163694	0.278339	-2.945221
C	2.735347	1.604385	-2.962620
C	1.198796	-0.402740	-4.273172
C	0.094940	-2.401289	-3.342944
C	1.323189	-2.742412	-2.656232
C	2.447015	-1.929375	-2.789647
C	0.028849	-1.249511	-4.134597
C	-2.197535	-0.724092	-3.210442
C	-2.118008	-1.909087	-2.385285
C	-0.994565	-2.730917	-2.450234
C	-1.139677	-0.393591	-4.066753
C	-1.318807	1.972918	-3.400119
C	-2.402872	1.623583	-2.506982
C	-2.836582	0.302442	-2.414709
C	-0.691967	0.982502	-4.163867
C	1.513480	1.961736	-3.650675
C	0.861360	2.977840	-2.853018
C	-0.526671	2.981714	-2.729727
C	0.753142	0.976954	-4.291568
C	-5.586545	2.976241	2.040057
C	-6.137409	1.720945	2.241075
C	-6.590978	0.949907	1.160152
C	-6.545758	1.518493	-0.142650
C	-6.019383	2.800916	-0.319110
C	-5.483634	3.542168	0.751730
C	-6.559495	-1.294946	0.173920
C	-6.026337	-2.568542	0.372181
C	-5.477415	-3.320249	-0.682510
C	-5.611955	-2.786630	-1.982703
C	-6.167097	-1.534660	-2.203508
C	-6.598569	-0.734937	-1.132652
C	-6.987954	-0.450884	1.301688
C	-6.970494	0.675677	-1.277610
C	-4.658608	4.746419	0.535480
C	-4.054483	4.994980	-0.711854
C	-4.251772	5.567783	1.610385
C	-2.958789	5.839704	-0.825763
C	-3.156980	6.412111	1.496384
C	-2.408641	6.477219	0.301332
C	-1.003849	6.925447	0.277770
C	-0.220859	6.771981	1.438388
C	-0.323453	7.242987	-0.915869
C	1.165198	6.768196	1.378304
C	1.066228	7.242259	-0.975002
C	1.846370	6.919438	0.154923
C	3.253557	6.484575	0.056182
C	3.707991	5.849973	-1.115106
C	4.100561	6.430048	1.183003
C	4.835163	5.037799	-1.101953
C	5.227070	5.617269	1.196501
C	5.562780	4.819694	0.083000
C	6.413134	3.619355	0.203277
C	6.422148	2.907358	1.417603
C	7.006662	2.991745	-0.910690
C	6.833354	1.582666	1.474161
C	7.423078	1.665972	-0.852438
C	7.261348	0.898986	0.320349
C	-4.620055	-4.493877	-0.425192
C	-4.159054	-5.319813	-1.472967

C	-4.047050	-4.709247	0.845140
C	-3.067558	-6.160190	-1.304219
C	-2.952997	-5.546850	1.012986
C	-2.369308	-6.216440	-0.079609
C	-0.978136	-6.697281	0.009638
C	-0.352807	-6.988653	1.240386
C	-0.145924	-6.603233	-1.122095
C	1.031643	-6.987942	1.360597
C	1.236734	-6.598283	-1.000878
C	1.860132	-6.688345	0.258028
C	3.245203	-6.202110	0.415248
C	4.150808	-6.148443	-0.664753
C	3.609328	-5.514096	1.588829
C	5.257032	-5.307120	-0.635750
C	4.717747	-4.677466	1.619769
C	5.516760	-4.482186	0.477567
C	6.377887	-3.286914	0.391984
C	6.918209	-2.660787	1.533277
C	6.462404	-2.584297	-0.824701
C	7.351674	-1.340736	1.491070
C	6.888646	-1.263367	-0.864951
C	7.257282	-0.577839	0.308266
C	-7.696875	-0.942357	2.383622
C	-7.661392	1.176958	-2.367277
C	-8.136340	0.360274	-3.439433
C	-8.046183	2.547540	-2.493858
C	-8.100082	-2.308270	2.504002
C	-8.169008	-0.118110	3.451441
H	-4.764949	5.506383	2.566045
H	-2.437687	5.886530	-1.777115
H	-2.833203	6.978548	2.365679
H	-4.348034	4.426334	-1.587662
H	-5.975636	-2.952810	1.382483
H	-5.190360	-3.311654	-2.833014
H	-6.173290	-1.139822	-3.212967
H	-5.151552	3.484719	2.893480
H	-6.134395	1.302768	3.241208
H	-5.964133	3.205243	-1.321658
H	-0.699861	6.518117	2.379551
H	-0.891305	7.438493	-1.822355
H	1.722293	6.512111	2.274700
H	1.554957	7.437756	-1.926340
H	3.094154	5.873034	-2.010869
H	3.834884	6.981618	2.081500
H	5.065702	4.451215	-1.986576
H	5.819637	5.545920	2.105405
H	5.971117	3.350395	2.300901
H	7.087437	3.532464	-1.850830
H	6.689169	1.034935	2.400717
H	7.824831	1.198958	-1.748364
H	-4.630708	-5.273396	-2.450417
H	-4.370137	-4.127573	1.701691
H	-2.711170	-6.736863	-2.153627
H	-2.464757	-5.572398	1.982827
H	-0.960746	-7.154631	2.126435
H	-0.579938	-6.383632	-2.093173
H	1.477840	-7.153223	2.338171
H	1.832604	-6.374514	-1.880926
H	3.951093	-6.728464	-1.562463
H	2.942283	-5.524965	2.445962
H	5.898894	-5.242962	-1.511243
H	4.883282	-4.061496	2.498938
H	6.942870	-3.198721	2.478097
H	6.057604	-3.030056	-1.728866
H	7.711161	-0.873588	2.404601
H	6.801786	-0.718344	-1.800204
N	-8.441534	-3.412334	2.639181
N	-8.567979	0.523786	4.335962
N	-8.539214	-0.274527	-4.327330
N	-8.373659	3.655150	-2.634604

C_{100}@[10]CPAq

C	-4.159628	1.798078	-0.611587
C	-4.737363	0.560088	-0.239816
C	-4.741103	-0.573208	-1.122926
C	-3.571159	1.921857	-1.955831
C	-3.592136	0.788501	-2.802334
C	-4.173723	-0.455969	-2.387192
C	-1.095041	4.614551	-1.120472
C	-2.346363	3.916986	-1.241853
C	-2.545819	2.920032	-2.227643
C	-0.066515	4.358575	-2.023907
C	-0.261268	3.395044	-3.070066
C	-1.441704	2.623705	-3.165765
C	0.534145	4.615266	0.769677
C	-0.786859	4.809625	0.270287
C	1.297325	4.275402	-1.569936
C	1.627377	4.332720	-0.190990
C	-1.979956	-3.450762	-2.473225
C	-3.159522	-2.728173	-2.149663
C	-3.396787	-1.548550	-2.918456
C	-2.353228	-0.967998	-3.727454
C	0.107303	-0.775390	-4.022550
C	-1.084769	-1.590279	-3.873276
C	-0.978622	-2.911039	-3.346210
C	2.526246	-0.552839	-3.547878
C	1.402331	-1.386323	-3.686150
C	-1.335250	1.292764	-3.775475
C	-2.463974	0.462662	-3.659393
C	1.030940	2.826495	-3.381698
C	1.157444	1.492035	-3.869049
C	-0.028357	0.673216	-4.044003
C	2.418907	0.875136	-3.657700
C	-3.695308	-2.842078	-0.787472
C	-4.547471	-1.788775	-0.346820
C	-4.594517	-1.391722	1.033241
C	-2.940413	-3.619542	0.222921
C	-3.113459	-3.270960	1.587334
C	-3.892578	-2.127641	1.983874
C	0.063177	-4.404492	-1.904327
C	-1.316908	-4.309301	-1.506227

C	-1.702010	-4.330464	-0.140917
C	1.055104	-4.636214	-0.955070
C	0.692227	-4.795510	0.427104
C	-0.647398	-4.586708	0.868699
C	1.483387	-2.700527	-3.037760
C	0.299746	-3.469841	-2.968001
C	2.308986	-3.939723	-1.045110
C	2.548257	-2.969735	-2.048467
C	-3.910913	0.742017	2.119578
C	-3.138708	-0.037875	3.109574
C	-4.627504	0.042249	1.119516
C	-3.204543	-1.448154	3.044574
C	-2.075072	-2.266802	3.421777
C	0.296184	-2.469909	3.799470
C	-0.880974	-1.689615	3.945121
C	-0.780204	-0.249025	4.090471
C	-1.962791	0.558304	3.754217
C	-1.811950	1.948726	3.610686
C	-0.817286	-4.060274	2.228887
C	-2.035934	-3.405955	2.552109
C	0.321559	-3.666771	2.994573
C	-2.627433	2.737283	2.701424
C	-3.557993	2.124963	1.829755
C	-3.693407	2.664072	0.466814
C	-1.831180	3.858974	2.292086
C	-1.965354	4.380570	1.009308
C	-2.903952	3.781382	0.100451
C	-0.518757	3.752987	2.879518
C	0.650018	4.126615	2.149212
C	1.854264	3.480524	2.537178
C	1.586272	-1.843390	3.728699
C	1.732591	-0.449733	3.840510
C	0.538191	0.365854	4.108390
C	0.644962	1.802097	3.928973
C	-0.525388	2.577893	3.716349
C	1.859033	2.365347	3.437700
C	3.745265	-0.676386	2.290411
C	2.933842	0.128991	3.227169
C	3.001714	1.536843	3.126305
C	4.504453	-0.003829	1.301696
C	2.812783	-3.767560	0.313599
C	1.841009	-4.345865	1.201039
C	1.655864	-3.788175	2.462702
C	3.587251	-2.640086	0.680931
C	3.400817	-2.065828	2.023362
C	2.435719	-2.655029	2.872873
C	4.186121	0.401145	-2.234345
C	3.619392	-0.854023	-2.638292
C	3.562598	-1.963862	-1.763117
C	4.708275	0.553020	-0.953424
C	4.664580	-0.556733	-0.039569
C	4.096609	-1.803198	-0.400552
C	1.997648	3.390545	-2.486153
C	3.163727	2.677525	-2.097445
C	3.431320	1.477704	-2.824115
C	3.731264	2.187413	2.075714
C	2.967805	3.318787	1.618226
C	2.848689	3.629749	0.239701
C	4.470195	1.426928	1.173978
C	4.480769	1.787804	-0.217715
C	3.644499	2.827335	-0.719227
C	7.260525	-2.994940	1.946600
C	7.677694	-1.678644	2.148801
C	7.936811	-0.838221	1.048151
C	7.886817	-1.382040	-0.261409
C	7.536997	-2.724752	-0.446487
C	7.135426	-3.534975	0.638050
C	7.954536	1.490021	0.063411
C	7.658333	2.843262	0.260999
C	7.254725	3.669841	-0.810182
C	7.339584	3.134024	-2.123797
C	7.704675	1.804169	-2.339503
C	7.950008	0.947788	-1.247492
C	8.135096	0.621553	1.274466
C	8.069070	-0.520618	-1.478395
C	6.431166	-4.816999	0.411868
C	5.774958	-5.056692	-0.819802
C	6.221234	-5.753021	1.455146
C	4.851049	-6.092025	-0.955334
C	5.288714	-6.784241	1.323157
C	4.530320	-6.931371	0.137239
C	3.292556	-7.735791	0.084204
C	2.460780	-7.797244	1.226850
C	2.780267	-8.242216	-1.134677
C	1.125403	-8.190405	1.119180
C	1.446138	-8.641397	-1.240355
C	0.568641	-8.541805	-0.133517
C	-0.901057	-8.533226	-0.298264
C	-1.458726	-7.974924	-1.473078
C	-1.779286	-8.829933	0.772036
C	-2.798752	-7.585309	-1.516935
C	-3.119419	-8.437814	0.729122
C	-3.635868	-7.735506	-0.386759
C	-8.420048	-1.675500	1.011739
C	-8.200829	-0.815350	-0.091574
C	6.575590	4.960161	-0.556248
C	6.356338	5.913318	-1.582064
C	5.939924	5.185935	0.689099
C	5.432329	6.948551	-1.419315
C	5.024177	6.223639	0.854679
C	4.690788	7.080364	-0.220030
C	-7.568689	-3.593729	-0.247699
C	-6.617548	-5.628308	-1.423713
C	-6.855394	-4.889361	-0.238980
C	-4.670525	6.796184	0.338222
C	-5.393170	6.415127	1.493871
C	-5.011411	6.172249	-0.885864
C	-6.324884	5.375857	1.448590
C	-5.941873	5.132889	-0.930249
C	-6.573946	4.669124	0.246943
C	-7.297826	3.380422	0.234571
C	-7.900864	2.871170	-0.941412

C	-7.241176	2.530076	1.363121
C	-8.304565	1.536803	-1.024870
C	-7.647117	1.197474	1.280822
C	-8.125854	0.652168	0.065354
C	3.446331	7.873870	-0.139226
C	2.941910	8.358026	1.092405
C	2.595490	7.929305	-1.268203
C	1.599996	8.724125	1.223247
C	1.253388	8.289811	-1.135705
C	0.706698	8.614106	0.129385
C	-0.760319	8.560945	0.311784
C	-1.656092	8.811616	-0.756312
C	-1.291838	7.994685	1.494778
C	-2.974262	8.353290	-0.709153
C	-2.612073	7.542359	1.544490
C	-3.454296	7.632325	0.411298
C	-7.821675	-1.408303	-1.318649
C	-4.892862	-6.960745	-0.310281
C	-5.231996	-6.319929	0.904416
C	-5.654133	-6.639762	-1.459836
C	-7.509291	-2.767353	-1.394069
C	-8.115660	-3.035713	0.933704
C	-6.189465	-5.305372	0.938504
H	-5.452337	-7.163145	-2.402503
H	-3.768612	-8.628968	1.592307
H	-4.651019	-6.535991	1.808404
H	-6.336088	-4.747022	1.869661
H	-7.164616	-5.372008	-2.338954
H	-7.088862	-3.162834	-2.325610
H	-8.249176	-3.669024	1.818701
H	2.828423	-7.408586	2.183456
H	-3.631949	8.507154	-1.573311
H	-2.953383	6.994109	2.429453
H	-5.191625	6.919263	2.446722
H	-4.458562	6.431325	-1.795915
H	-6.846396	5.080329	2.366729
H	-6.098006	4.599420	-1.874644
H	-8.020211	3.525430	-1.813210
H	-6.769848	2.885270	2.286236
H	-8.731127	1.159063	-1.961863
H	-7.485542	0.538926	2.140945
H	6.952966	-3.590658	2.812656
H	7.733680	-1.247968	3.155104
H	7.511167	-3.095387	-1.475864
H	7.670135	3.210077	1.291846
H	7.035089	3.744933	-2.980748
H	7.720805	1.375773	-3.348308
H	-3.168424	-7.040564	-2.393427
H	-8.788392	-1.257815	1.956351
H	6.885572	5.817873	-2.537308
H	6.067383	4.474666	1.510876
H	5.241974	7.639405	-2.249723
H	4.463743	6.291710	1.793770
H	0.589729	8.191467	-2.002431
H	3.600582	8.390828	1.969079
H	-0.627107	7.785600	2.340892
H	-1.292204	9.319209	-1.657947
H	-0.804132	-7.725093	-2.315827
H	-1.388043	-9.325758	1.668795
H	2.956083	7.558272	-2.234830
H	1.219318	9.042400	2.201465
H	0.471442	-8.100195	1.994131
H	1.056883	-8.979612	-2.208329
H	5.898059	-4.360045	-1.654907
H	5.110016	-7.463294	2.165580
H	6.768002	-5.649906	2.399356
H	-7.643101	-0.773485	-2.193216
H	3.426775	-8.270917	-2.020275
H	4.280327	-6.176547	-1.886470
O	8.197476	-1.001252	-2.601989
O	8.325504	1.094653	2.392367

C_{100}@[10]CPTcaq

C	-4.553585	0.776588	-0.390055
C	-4.818614	-0.555515	0.007130
C	-4.561999	-1.673755	-0.860963
C	-4.026008	1.013521	-1.745236
C	-3.787562	-0.105387	-2.575607
C	-4.052053	-1.446016	-2.134309
C	-2.251756	4.226341	-0.980819
C	-3.302353	3.251225	-1.075324
C	-3.270295	2.221439	-2.045742
C	-1.202525	4.208861	-1.895647
C	-1.174180	3.212913	-2.928174
C	-2.138373	2.181859	-2.996673
C	-0.650814	4.642487	0.883407
C	-1.984250	4.510746	0.400784
C	0.145126	4.457636	-1.458357
C	0.466380	4.613971	-0.085850
C	-1.210719	-3.830026	-2.209852
C	-2.525702	-3.406573	-1.879638
C	-3.043329	-2.329712	-2.660888
C	-2.176445	-1.531294	-3.493592
C	0.164389	-0.764171	-3.828771
C	-0.798411	-1.836169	-3.650554
C	-0.376395	-3.084639	-3.106899
C	2.466501	0.034766	-3.391074
C	1.571029	-1.043703	-3.502159
C	-1.725604	0.905076	-3.589477
C	-2.623340	-0.167576	-3.444200
C	0.212629	2.963320	-3.250038
C	0.647554	1.689708	-3.720861
C	-0.311640	0.609825	-3.867840
C	2.021597	1.393943	-3.517739
C	-3.005858	-3.622877	-0.509425
C	-4.079373	-2.794954	-0.071208
C	-4.201544	-2.393677	1.304160
C	-2.076580	-4.179407	0.501703
C	-2.313710	-3.860318	1.863763
C	-3.337260	-2.926248	2.254942
C	1.004696	-4.258702	-1.656172

C	-0.352337	-4.484018	-1.238808
C	-0.707086	-4.572664	0.131102
C	2.031226	-4.229733	-0.717106
C	1.730891	-4.444345	0.670316
C	0.385914	-4.553447	1.127218
C	1.968538	-2.289490	-2.836286
C	1.002059	-3.315648	-2.738190
C	3.084361	-3.260929	-0.836075
C	3.076591	-2.280841	-1.857192
C	-4.037390	-0.141551	2.353181
C	-3.090992	-0.698921	3.342441
C	-4.578768	-1.009047	1.372548
C	-2.819469	-2.085286	3.296347
C	-1.524325	-2.606869	3.669513
C	0.831629	-2.235722	4.018900
C	-0.496121	-1.754175	4.168859
C	-0.739489	-0.328342	4.292633
C	-2.083765	0.169901	3.962100
C	-2.269208	1.553922	3.797441
C	0.110961	-4.068238	2.483622
C	-1.225096	-3.718728	2.815572
C	1.132522	-3.405589	3.229542
C	-3.257485	2.111109	2.888425
C	-4.023417	1.279799	2.037956
C	-4.295928	1.746701	0.669203
C	-2.754686	3.382672	2.451413
C	-3.021889	3.834291	1.162949
C	-3.800628	3.013340	0.276052
C	-1.448398	3.600284	3.021324
C	-0.409042	4.225009	2.268028
C	0.918018	3.893992	2.650174
C	1.935454	-1.322042	3.921688
C	1.746547	0.068339	4.010992
C	0.395215	0.582072	4.283728
C	0.155693	1.999719	4.082552
C	-1.167515	2.472091	3.875864
C	1.195902	2.827201	3.566223
C	3.738614	0.299559	2.435263
C	2.768948	0.905017	3.372189
C	2.498728	2.286840	3.249304
C	4.305040	1.116374	1.425235
C	3.548205	-2.953514	0.513331
C	2.749891	-3.730557	1.422201
C	2.451700	-3.215251	2.680374
C	4.037572	-1.670000	0.854627
C	3.733049	-1.135920	2.193061
C	2.944879	-1.923278	3.065148
C	3.866092	1.378199	-2.113463
C	3.608942	0.016968	-2.491905
C	3.826814	-1.059081	-1.600475
C	4.351313	1.670199	-0.841414
C	4.584764	0.596707	0.088606
C	4.323992	-0.754755	-0.247422
C	1.026758	3.754936	-2.374305
C	2.332682	3.347004	-1.992274
C	2.870475	2.234001	-2.707258
C	3.041767	3.073859	2.179884
C	2.029295	3.986930	1.718050
C	1.825706	4.235659	0.337138
C	3.926573	2.492663	1.277267
C	3.840601	2.824448	-0.118665
C	2.778569	3.629113	-0.622480
C	7.829910	2.633655	-1.839925
C	8.449299	1.392560	-1.998693
C	8.972608	0.700983	-0.884895
C	8.958890	1.348877	0.389459
C	8.379435	2.619114	0.518206
C	7.741868	3.257733	-0.570414
C	8.940823	-1.471573	0.254064
C	8.340580	-2.733426	0.141429
C	7.721665	-3.362664	1.246375
C	7.856048	-2.742462	2.513663
C	8.497557	-1.509992	2.655335
C	8.998377	-0.824397	1.527454
C	9.380240	-0.711288	-0.937578
C	9.423728	0.583289	1.567915
C	6.880425	4.441517	-0.360306
C	6.302124	4.692276	0.907933
C	6.478567	5.273933	-1.434268
C	5.297418	5.645114	1.070998
C	5.470083	6.225121	-1.271660
C	4.812665	6.392006	-0.027178
C	3.556867	7.160120	0.101444
C	2.674667	7.258945	-0.999764
C	3.100887	7.645403	1.351959
C	1.358658	7.689903	-0.830054
C	1.783615	8.076391	1.521761
C	0.860465	8.041968	0.447907
C	-0.600657	8.126891	0.658436
C	-1.170511	7.660585	1.867420
C	-1.486600	8.435161	-0.403335
C	-2.527125	7.336760	1.946076
C	-2.841576	8.114307	-0.323491
C	-3.373128	7.465645	0.819415
C	-4.654733	6.728749	0.762789
C	-5.083695	6.181488	-0.469783
C	-5.365456	6.348283	1.927673
C	-6.072149	5.198594	-0.518482
C	-6.358094	5.366597	1.878415
C	-6.684438	4.716735	0.662744
C	-7.447645	3.450990	0.624043
C	-7.363783	2.548823	1.710918
C	-8.092624	2.999923	-0.554112
C	-7.781629	1.223265	1.580112
C	-8.505319	1.671636	-0.687797
C	-8.297273	0.737407	0.354840
C	6.835903	-4.532198	1.055541
C	6.453861	-5.368623	2.134051
C	6.221269	-4.765989	-0.198225
C	5.435567	-6.313329	1.990252
C	5.211036	-5.715427	-0.343615
C	4.751419	-6.472102	0.759768

C	3.492881	-7.237458	0.646147
C	3.020552	-7.708180	-0.604249
C	2.620820	-7.342725	1.755320
C	1.696414	-8.115785	-0.767366
C	1.294640	-7.745781	1.590815
C	0.778890	-8.065393	0.311165
C	-0.683783	-8.102780	0.095633
C	-1.588515	-8.379843	1.149714
C	-1.226951	-7.621343	-1.119974
C	-2.936675	-8.032769	1.048936
C	-2.575372	-7.272373	-1.220426
C	-3.441499	-7.390537	-0.109008
C	-4.728593	-6.663351	-0.093203
C	-5.442786	-6.351391	-1.275682
C	-5.170034	-6.070857	1.113082
C	-6.467496	-5.400482	-1.270476
C	-6.187784	-5.118543	1.116886
C	-6.820238	-4.712824	-0.083612
C	-7.617367	-3.466446	-0.089666
C	-8.226413	-2.970613	1.090384
C	-7.575984	-2.606182	-1.212189
C	-8.587880	-1.627170	1.202459
C	-7.943547	-1.262506	-1.102489
C	-8.363328	-0.723435	0.135587
C	10.063961	-1.286983	-2.003456
C	10.145986	1.150474	2.612645
C	10.611381	0.392545	3.740765
C	10.553437	2.528208	2.625301
C	10.453352	-2.669798	-2.027938
C	10.504829	-0.535151	-3.145547
H	6.949812	5.161778	-2.417398
H	4.807273	5.731785	2.046267
H	5.165316	6.834856	-2.129980
H	6.564939	4.068214	1.767711
H	8.289563	-3.207275	-0.841108
H	7.380299	-3.189001	3.392901
H	8.525460	-1.035256	3.640455
H	7.334265	3.084705	-2.705498
H	8.440996	0.916573	-2.983476
H	8.361258	3.093514	1.501701
H	2.985418	6.883876	-1.981333
H	3.780827	7.647955	2.211994
H	0.673364	7.638490	-1.682855
H	1.449233	8.407561	2.512177
H	-0.519720	7.418946	2.715181
H	-1.093357	8.882149	-1.324163
H	-2.901266	6.846658	2.852034
H	-3.492033	8.315494	-1.182662
H	-4.552479	6.438114	-1.392394
H	-5.102790	6.798746	2.892265
H	-6.289852	4.714973	-1.477104
H	-6.860764	5.063244	2.804518
H	-6.860177	2.857896	2.633756
H	-8.233033	3.693825	-1.391495
H	-7.594829	0.522547	2.401767
H	-8.958134	1.336794	-1.629091
H	6.949765	-5.265306	3.106049
H	6.463031	-4.134573	-1.059202
H	5.146494	-6.925832	2.852168
H	4.699525	-5.796110	-1.307806
H	3.693732	-7.714836	-1.469425
H	2.947685	-6.985226	2.738381
H	1.350547	-8.433123	-1.758032
H	0.616657	-7.691905	2.449730
H	-1.217040	-8.828779	2.078661
H	-0.560840	-7.395809	-1.959522
H	-3.604402	-8.214579	1.899369
H	-2.930350	-6.782415	-2.134221
H	-5.162910	-6.836558	-2.218574
H	-4.631168	-6.272400	2.045310
H	-6.976073	-5.153682	-2.210157
H	-6.416154	-4.597573	2.052490
H	-8.359226	-3.636689	1.951044
H	-7.121127	-2.954988	-2.145711
H	-8.993625	-1.252452	2.150010
H	-7.764942	-0.591228	-1.950511
N	10.779702	-3.794163	-2.081208
N	10.873694	0.050866	-4.091036
N	11.000622	-0.199055	4.674534
N	10.895756	3.648257	2.668824

C_{100}@[12]CPP

C	-4.217385	-1.584351	-0.554222
C	-3.762175	-2.872891	-0.183464
C	-2.995515	-3.695616	-1.078172
C	-3.910707	-1.094435	-1.908457
C	-3.156083	-1.928402	-2.766648
C	-2.697320	-3.223861	-2.352292
C	-3.991006	2.567813	-1.096049
C	-4.403683	1.195076	-1.198691
C	-3.875430	0.334216	-2.190801
C	-3.095132	3.094526	-2.022878
C	-2.587588	2.260885	-3.075918
C	-2.899006	0.884370	-3.155038
C	-2.780527	3.715787	0.760105
C	-3.873210	2.931156	0.289573
C	-2.048815	3.986721	-1.596907
C	-1.821525	4.268807	-0.224849
C	0.959884	-3.843929	-2.513809
C	-0.382123	-4.145101	-2.158553
C	-1.390766	-3.469566	-2.910164
C	-1.064302	-2.331476	-3.734411
C	0.559976	-0.481700	-4.078637
C	0.275496	-1.895411	-3.912856
C	1.283082	-2.765537	-3.401748
C	2.150598	1.365628	-3.650565
C	1.921859	-0.016153	-3.775085
C	-1.909578	-0.000847	-3.780743
C	-2.138690	-1.381955	-3.649694
C	-1.271958	2.750545	-3.419945
C	-0.262794	1.877711	-3.923483

C	-0.546738	0.463082	-4.082717
C	1.076505	2.314776	-3.743445
C	-0.657091	-4.591471	-0.787165
C	-1.992724	-4.427120	-0.318472
C	-2.272286	-4.165162	1.066529
C	0.448066	-4.617276	0.199387
C	0.111192	-4.478892	1.570802
C	-1.235167	-4.197859	1.994709
C	3.101969	-3.102093	-1.997582
C	2.054542	-3.992083	-1.570114
C	1.823262	-4.267035	-0.197409
C	3.995081	-2.570585	-1.071001
C	3.873225	-2.926687	0.316052
C	2.779222	-3.708797	0.787397
C	2.909362	-0.898061	-3.141893
C	2.597639	-2.274105	-3.056429
C	4.408030	-1.198498	-1.179572
C	3.882820	-0.342877	-2.177701
C	-3.244072	-2.150683	2.160768
C	-2.124934	-2.165437	3.126450
C	-3.293316	-3.159088	1.168375
C	-1.191323	-3.223570	3.047961
C	0.197216	-3.022262	3.394042
C	2.048192	-1.513996	3.720926
C	0.663323	-1.772861	3.898830
C	-0.264358	-0.667924	4.056930
C	-1.682159	-0.914319	3.753016
C	-2.545079	0.187675	3.621094
C	2.321856	-3.441260	2.156639
C	0.999369	-3.818594	2.511986
C	2.881750	-2.360575	2.902975
C	-3.698581	0.179479	2.736551
C	-3.959509	-0.913950	1.877902
C	-4.461650	-0.630680	0.523286
C	-3.917020	1.536346	2.322818
C	-4.403200	1.807772	1.048048
C	-4.679775	0.718439	0.152630
C	-2.889272	2.378544	2.882408
C	-2.327178	3.455503	2.132180
C	-1.005613	3.834779	2.489501
C	2.535651	-0.166104	3.629459
C	1.672328	0.936574	3.753107
C	0.253603	0.691710	4.054149
C	-0.673580	1.795898	3.887619
C	-2.057977	1.536095	3.707082
C	-0.205961	3.042800	3.377860
C	3.238940	2.164692	2.158958
C	2.116978	2.184460	3.121310
C	1.183673	3.242290	3.034739
C	3.291167	3.168018	1.161556
C	4.680266	-0.714896	0.169967
C	4.401024	-1.799469	1.070255
C	3.911190	-1.521400	2.342117
C	4.461217	0.636100	0.532939
C	3.955189	0.926457	1.884599
C	3.691689	-0.162435	2.748213
C	2.705539	3.214503	-2.361221
C	3.165382	1.916756	-2.767410
C	3.917310	1.087192	-1.902702
C	3.000085	3.692950	-1.088631
C	3.763930	2.874703	-0.187420
C	4.220048	1.584149	-0.550183
C	-0.951327	3.833654	-2.536702
C	0.389709	4.136714	-2.179027
C	1.400605	3.457290	-2.924229
C	1.230648	4.211263	1.976658
C	-0.114574	4.490197	1.547414
C	-0.447420	4.621205	0.174216
C	2.270545	4.173714	1.051609
C	1.995087	4.428522	-0.335611
C	0.660717	4.590262	-0.809052
C	-0.710416	8.145205	1.235022
C	0.685197	8.112650	1.244620
C	1.428282	8.370810	0.068178
C	0.718147	8.815292	-1.073846
C	-0.678626	8.844438	-1.084628
C	2.840241	7.936980	-0.004006
C	3.659364	7.854140	1.148155
C	4.825224	7.085348	1.146421
C	5.225445	6.369830	-0.008395
C	4.495278	6.589218	-1.200257
C	3.327814	7.354823	-1.197658
C	6.201436	5.261805	0.056621
C	6.307627	4.492763	1.240426
C	6.949713	3.253436	1.239897
C	7.512478	2.725709	0.054726
C	7.523670	3.553548	-1.093757
C	6.883786	4.794508	-1.092362
C	7.876465	1.295139	-0.010975
C	8.282373	0.571447	1.136142
C	8.319574	-0.824516	1.130862
C	7.949775	-1.559794	-0.021021
C	7.669837	-0.830697	-1.201964
C	7.635096	0.564393	-1.197449
C	7.638690	-3.003529	0.035930
C	7.116583	-3.563337	1.225926
C	6.474248	-4.803031	1.216221
C	6.327128	-5.538423	0.016778
C	6.994231	-5.054811	-1.134803
C	7.634001	-3.813786	-1.125765
C	5.308015	-6.607186	-0.061196
C	4.913234	-7.357333	1.073355
C	3.711010	-8.069229	1.080696
C	2.855110	-8.062687	-0.047340
C	3.327987	-7.444671	-1.228845
C	4.527604	-6.731138	-1.235176
C	1.427223	-8.436521	0.045463
C	0.715392	-8.144345	1.232717
C	-0.680133	-8.108147	1.242799
C	-1.424288	-8.366075	0.066989
C	-0.715656	-8.813563	-1.074788
C	0.681052	-8.846372	-1.086084

C	-2.835829	-7.930735	-0.004814
C	-3.654536	-7.847247	1.147562
C	-4.821029	-7.079344	1.145449
C	-5.222208	-6.365208	-0.009939
C	-4.491863	-6.584760	-1.201672
C	-3.323811	-7.349515	-1.198725
C	-6.199744	-5.258428	0.054345
C	-6.307326	-4.489076	1.237813
C	-6.951303	-3.250743	1.236748
C	-7.514761	-2.724254	0.051316
C	-7.524378	-3.552485	-1.096910
C	-6.882616	-4.792523	-1.094945
C	-7.880861	-1.294177	-0.014535
C	-8.288286	-0.571309	1.132591
C	-8.326133	0.824672	1.128047
C	-7.955401	1.560677	-0.023040
C	-7.674854	0.832374	-1.204346
C	-7.639579	-0.562787	-1.200579
C	-7.642659	3.004034	0.035382
C	-7.119085	3.561465	1.225886
C	-6.473779	4.799620	1.217245
C	-6.325117	5.535707	0.018458
C	-6.993711	5.054915	-1.133437
C	-7.636534	3.815456	-1.125459
C	-5.303799	6.602341	-0.058698
C	-4.908668	7.351888	1.076098
C	-3.706245	8.063447	1.083584
C	-3.322828	7.438270	-1.225751
C	-4.522667	6.725120	-1.232279
C	-2.850460	8.057193	-0.044509
C	-1.423369	8.433949	0.047610
H	-1.257934	7.816591	2.125987
H	1.202163	7.757749	2.143292
H	1.271597	9.088890	-1.980391
H	-1.207599	9.138176	-1.999666
H	3.344720	8.355612	2.071299
H	5.413203	6.995278	2.067574
H	4.773415	6.050213	-2.112424
H	2.716994	7.394733	-2.106909
H	5.782415	4.818310	2.144921
H	6.913795	2.634833	2.143820
H	8.009818	3.197968	-2.010210
H	6.874412	5.397357	-2.008259
H	8.536988	1.114793	2.053974
H	8.601877	-1.359550	2.045342
H	7.365426	-1.365965	-2.107930
H	7.304361	1.091695	-2.099417
H	7.100617	-2.965956	2.144022
H	5.967402	-5.145865	2.125599
H	6.959960	-5.637788	-2.062988
H	8.097469	-3.439961	-2.046594
H	5.534468	-7.335706	1.976959
H	3.399484	-8.597605	1.990141
H	2.684734	-7.414522	-2.115933
H	4.798425	-6.155766	-2.127695
H	1.264105	-7.816001	2.123019
H	-1.195870	-7.750842	2.141199
H	-1.270203	-9.086974	-1.980725
H	1.208913	-9.142580	-2.000954
H	-3.339413	-8.347864	2.071022
H	-5.408952	-6.989157	2.066621
H	-4.770539	-6.046622	-2.114204
H	-2.713047	-7.389674	-2.108004
H	-5.781749	-4.813446	2.142556
H	-6.916374	-2.631739	2.140453
H	-8.010915	-3.197954	-2.013590
H	-6.872292	-5.395740	-2.010612
H	-8.543300	-1.115277	2.049915
H	-8.609313	1.359069	2.042632
H	-7.370131	1.368255	-2.109816
H	-7.308145	-1.089453	-2.102658
H	-7.104226	2.963070	2.143317
H	-5.965782	5.140333	2.126796
H	-6.958191	5.638802	-2.060974
H	-8.101178	3.443638	-2.046512
H	-5.530152	7.330548	1.979539
H	-3.394798	8.591916	1.993004
H	-2.679294	7.407662	-2.112623
H	-4.793432	6.149511	-2.124693