

Carbon-nanorings ([10]CPP and [6]CPPA) as Fullerene (C_{60} and C_{70}) Receptors. A comprehensive dispersion-corrected DFT study

Iván González-Veloso, Jesús Rodríguez-Otero and Enrique M. Cabaleiro-Lago

Supplementary Information

Figure S1	2
Figure S2	3
Searching minima of complex $C_{60}@[10]CPP$	4
Searching minima of complex $C_{60}@[6]CPPA$	8
Searching minima of complex $C_{70}@[10]CPP$	10
Searching minima of complex $C_{70}@[6]CPPA$	13
Figure S3	16
Figure S4	17
Figure S5	18
Figure S6	19
Table S1	19
Table S2	19
Table S3	20
Figure S7	21
Geometry of complexes	22

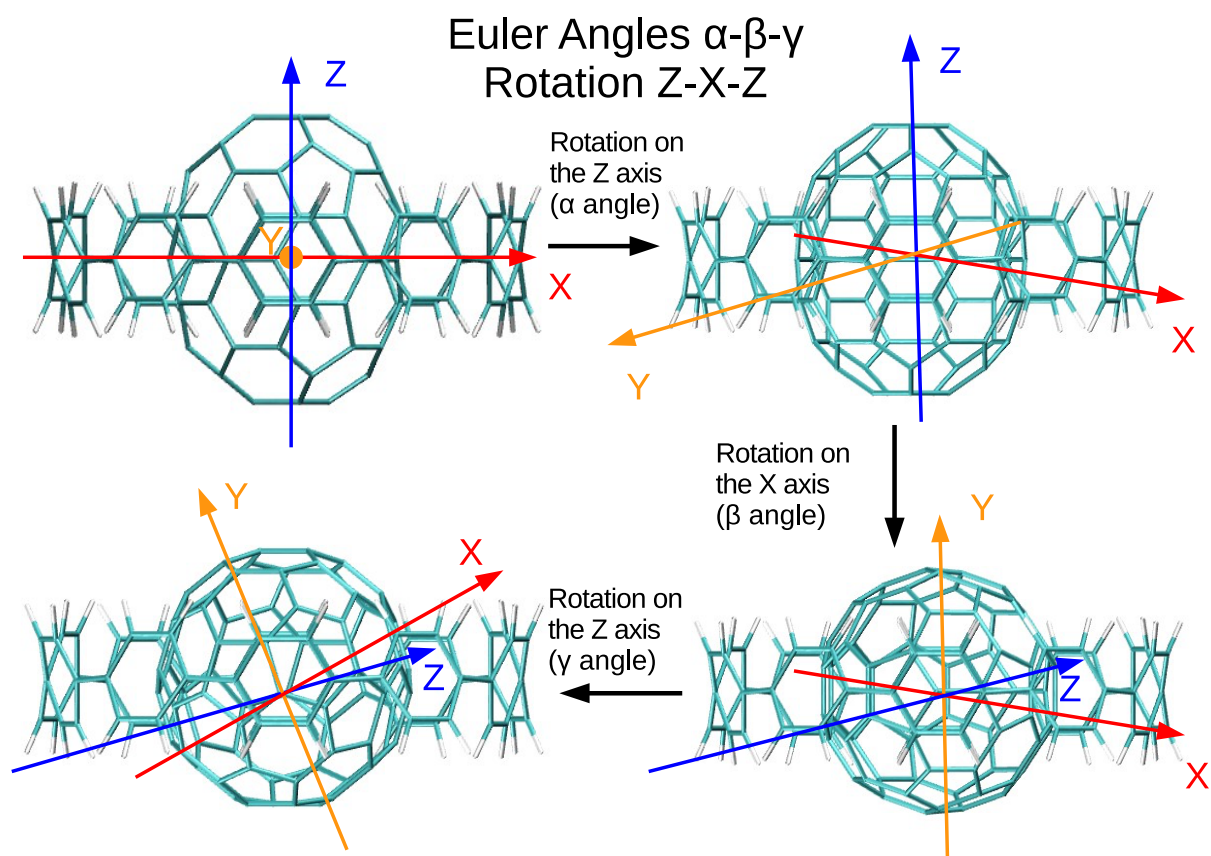


Figure S1. Description of the rotation through the three Euler angles.

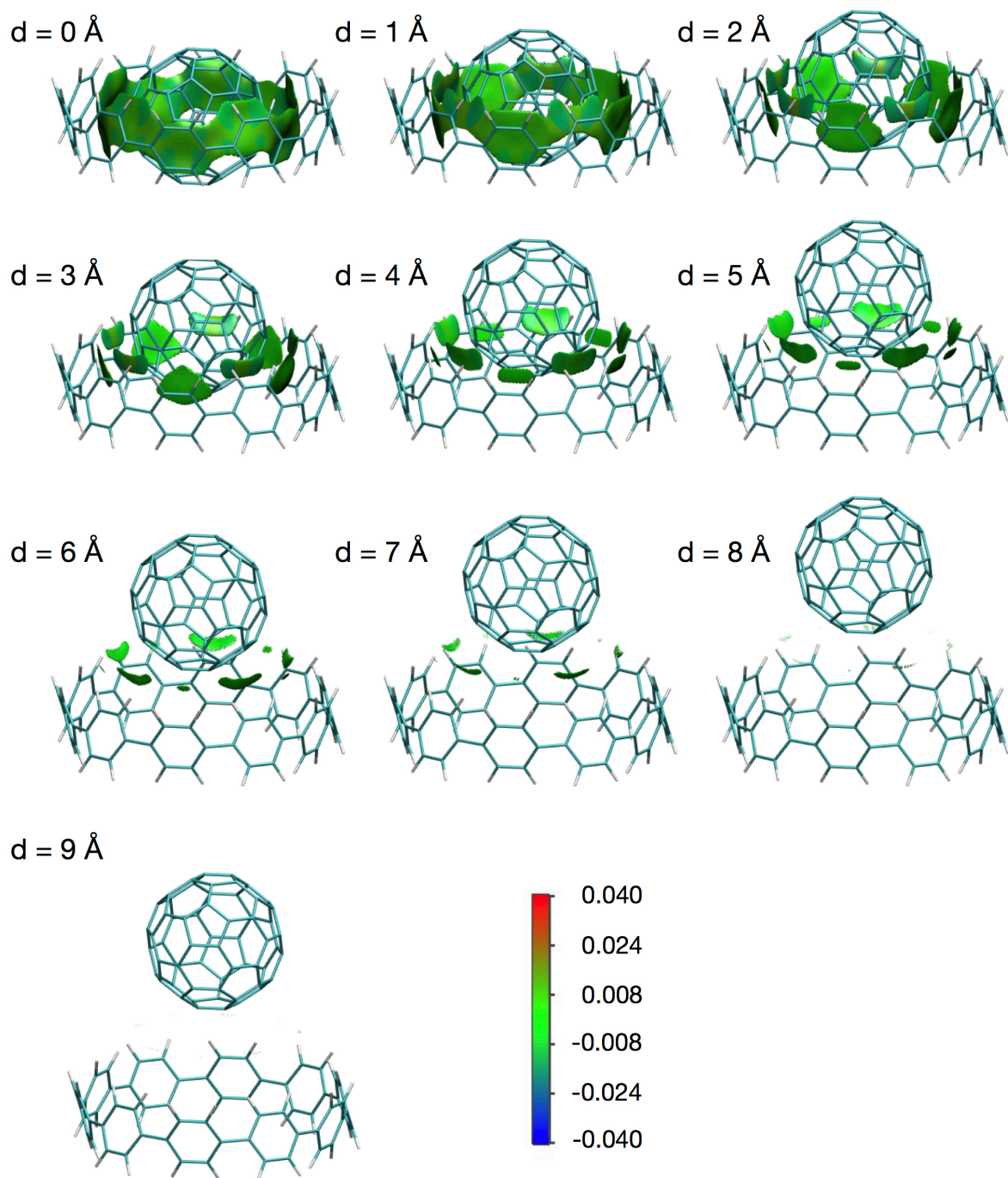
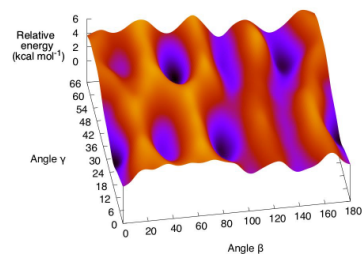


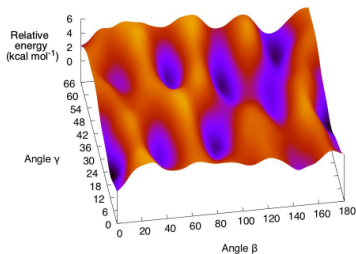
Figure S2. NCIPlot gradient isosurface (0.3 a.u.) corresponding to the vertical departure of C_{60} from [10]CPP (Fig. 4a shows the energetic profile). Shortly after 8 Å, the isosurface vanishes.

Searching minima of complex $C_{60}@[10]CPP$ with a systematic scanning procedure.

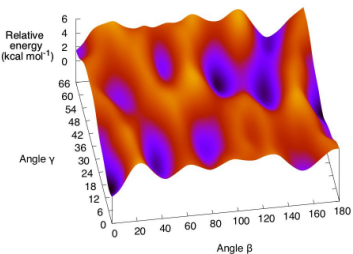
1) Scanning the three Euler angles:



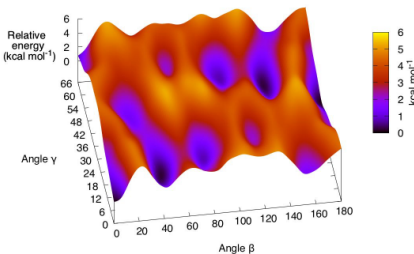
$\alpha = 0^\circ$



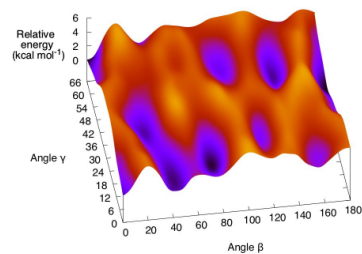
$\alpha = 6^\circ$



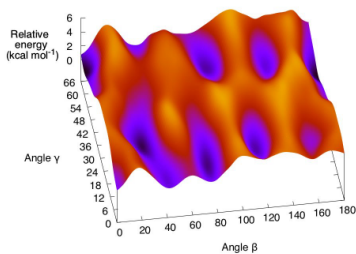
$\alpha = 12^\circ$



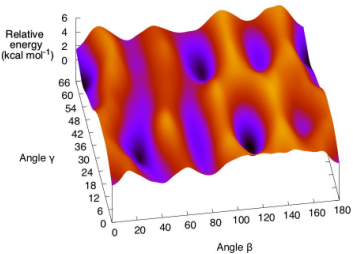
$\alpha = 18^\circ$



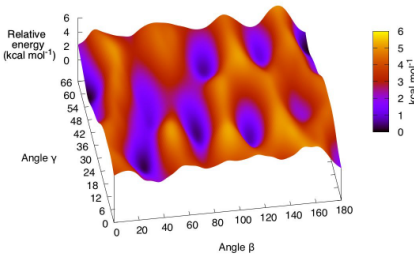
$\alpha = 24^\circ$



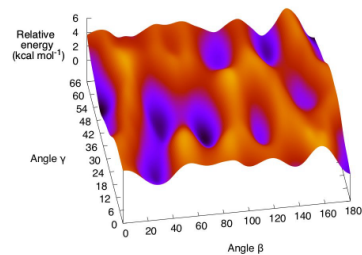
$\alpha = 30^\circ$



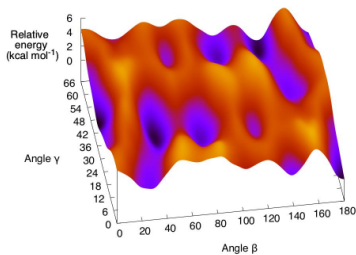
$\alpha = 36^\circ$



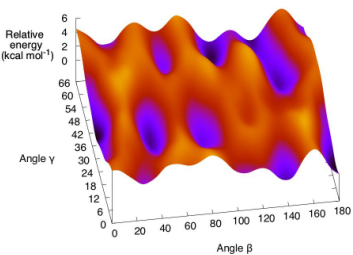
$\alpha = 42^\circ$



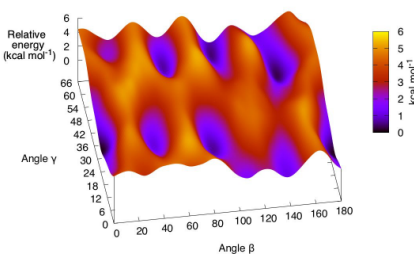
$\alpha = 48^\circ$



$\alpha = 54^\circ$

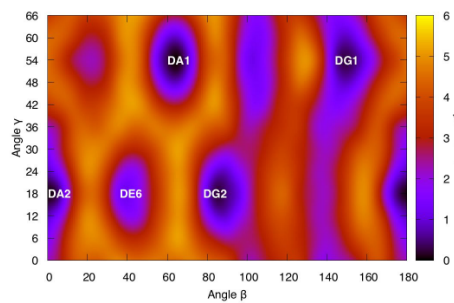


$\alpha = 60^\circ$

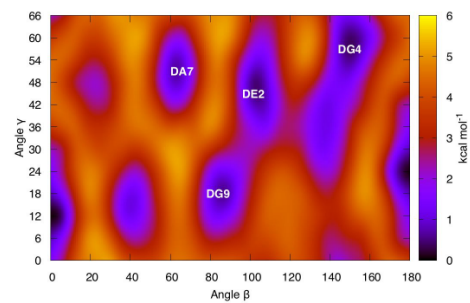


$\alpha = 66^\circ$

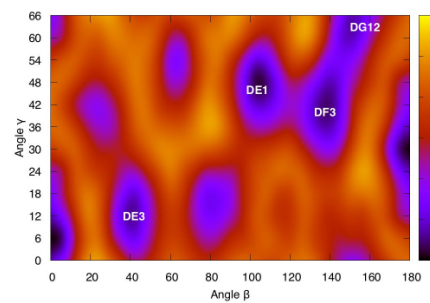
2) Looking for the minima:



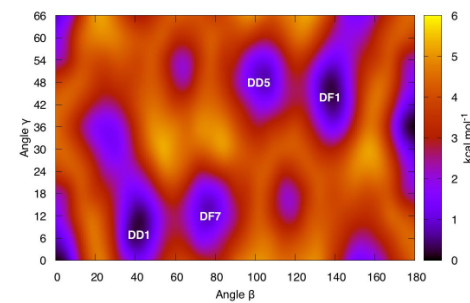
$$\alpha = 0^\circ$$



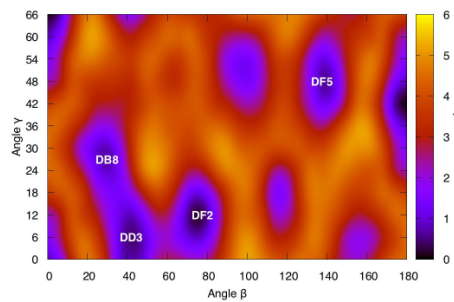
$$\alpha = 6^\circ$$



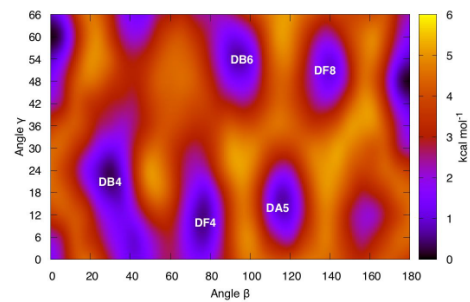
$$\alpha = 12^\circ$$



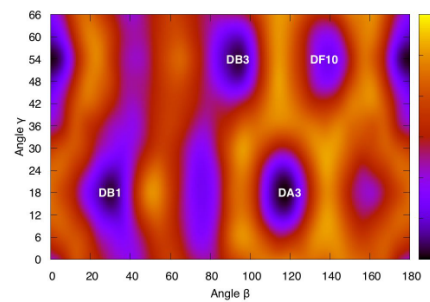
$$\alpha = 18^\circ$$



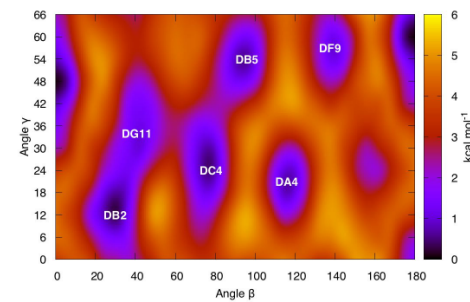
$$\alpha = 24^\circ$$



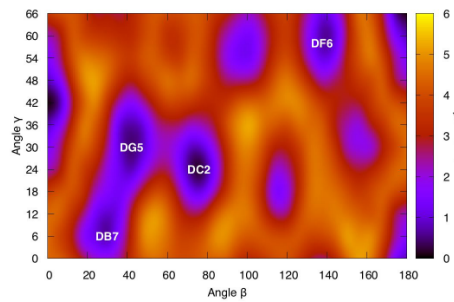
$$\alpha = 30^\circ$$



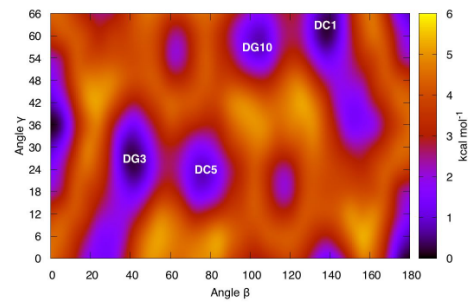
$$\alpha = 36^\circ$$



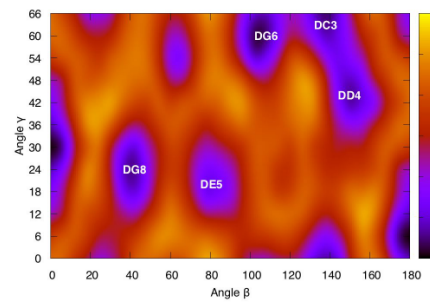
$$\alpha = 42^\circ$$



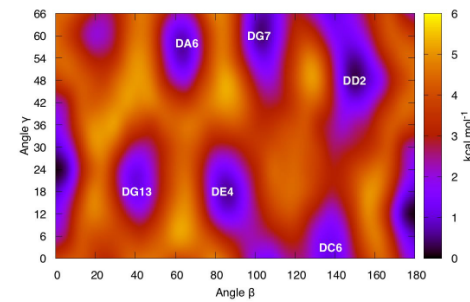
$$\alpha = 48^\circ$$



$$\alpha = 54^\circ$$

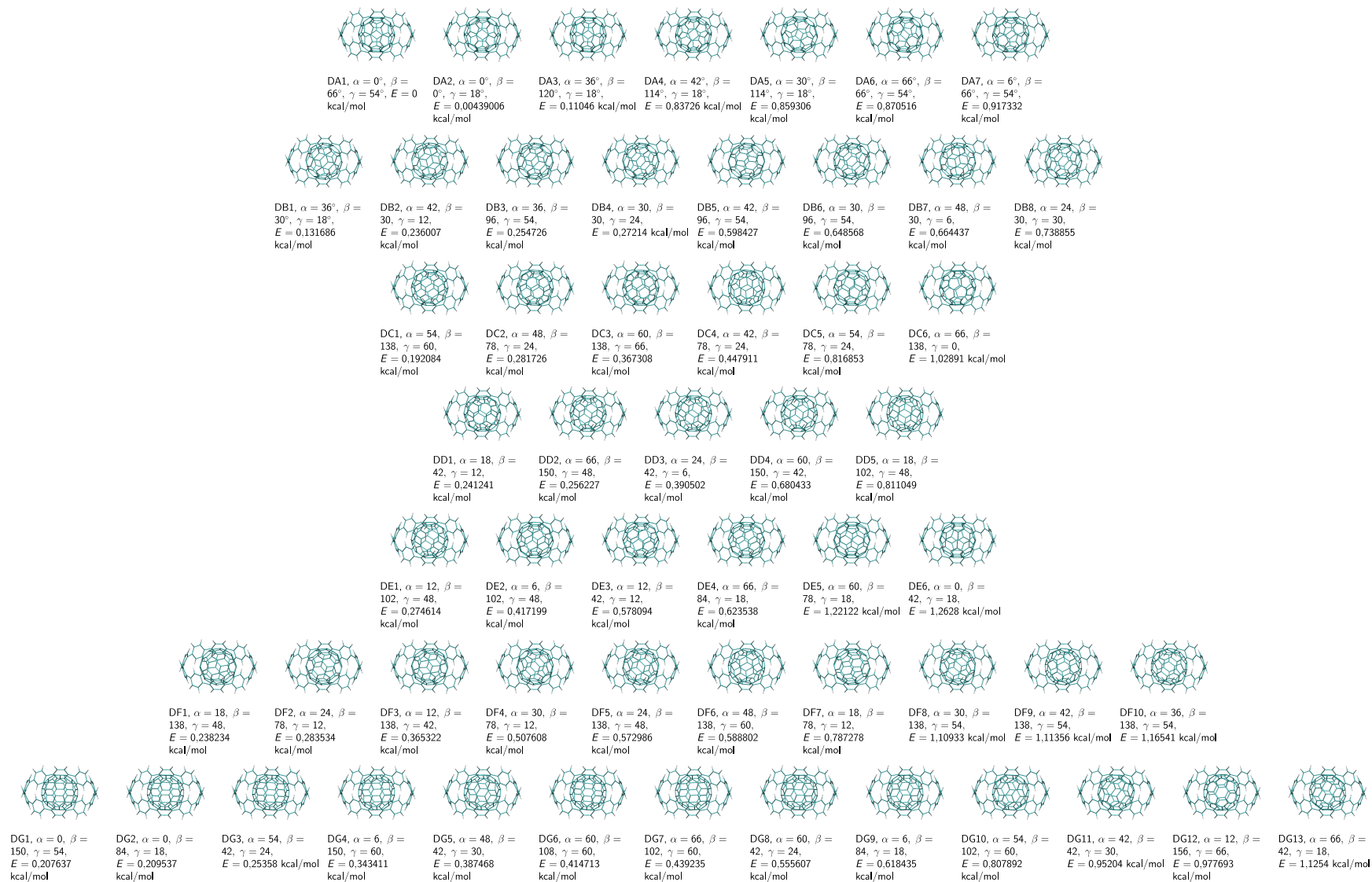


$$\alpha = 60^\circ$$



$$\alpha = 66^\circ$$

3) Classifying the minima in "families":



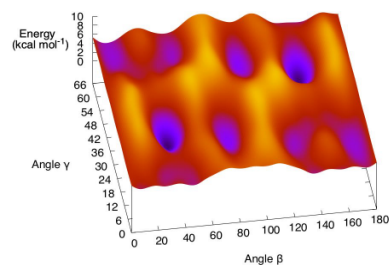
4) Optimization of the best structure of each family at the B97-D2/def2-TZVP level. Complexation energy calculation ($\Delta E_{\text{complex}}$).

	$\Delta E_{\text{complex}}$	E_{def}		Dispersion
		C_{60}	[10]CPP	
DA1	-49.78	0.11	0.23	-83.61
DB1	-49.27	0.08	0.39	-83.52
DC1	-49.24	0.08	0.42	-83.64
DD1	-49.23	0.10	0.42	-83.65
DE1	-49.23	0.11	0.43	-83.62
DF1	-49.26	0.07	0.40	-83.60
DG1	-49.23	0.13	0.40	-83.56

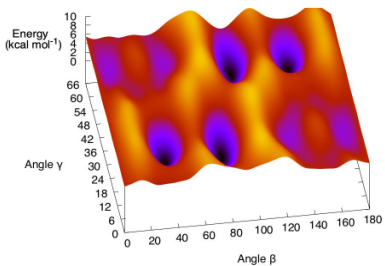
DA1 corresponds to minimum I of figure 3.

DB1-DG1 are virtually the same structure and correspond to minimum III of figure 3.

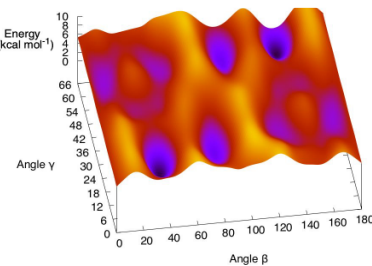
Searching minima of complex $C_{60}@[6]CPPA$ with a systematic scanning procedure.



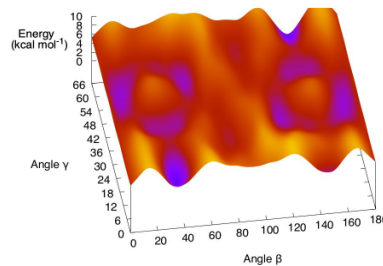
$$\alpha = 0^\circ$$



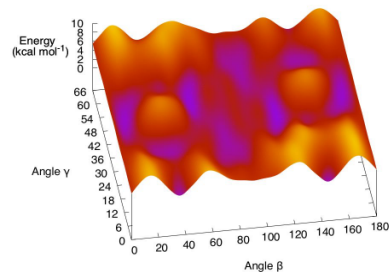
$$\alpha = 6^\circ$$



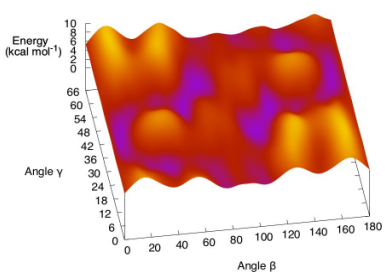
$$\alpha = 12^\circ$$



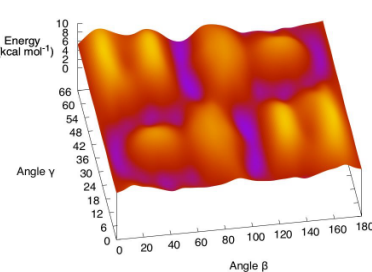
$$\alpha = 18^\circ$$



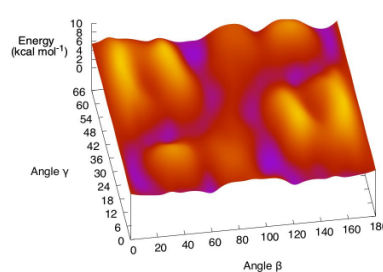
$$\alpha = 24^\circ$$



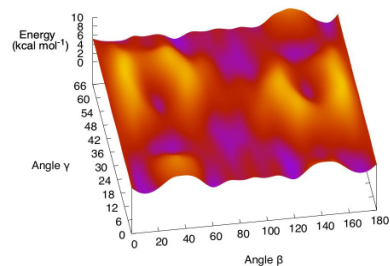
$$\alpha = 30^\circ$$



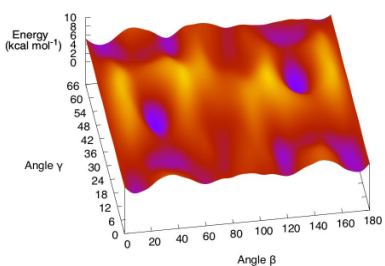
$$\alpha = 36^\circ$$



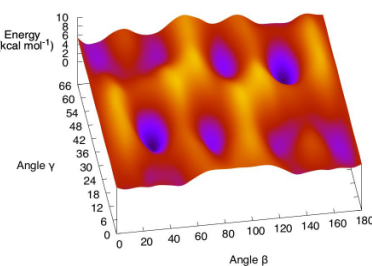
$$\alpha = 42^\circ$$



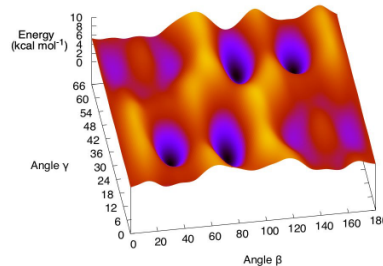
$$\alpha = 48^\circ$$



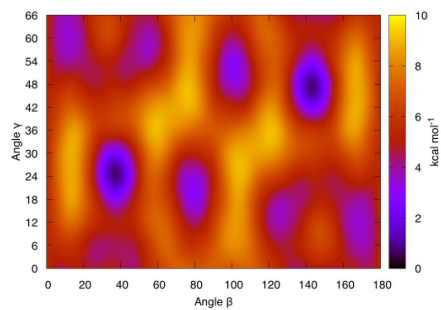
$$\alpha = 54^\circ$$



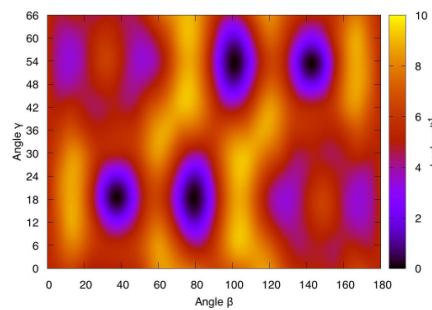
$$\alpha = 60^\circ$$



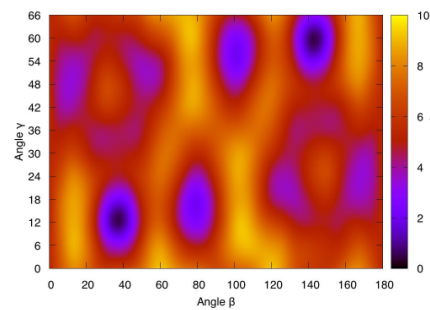
$$\alpha = 66^\circ$$



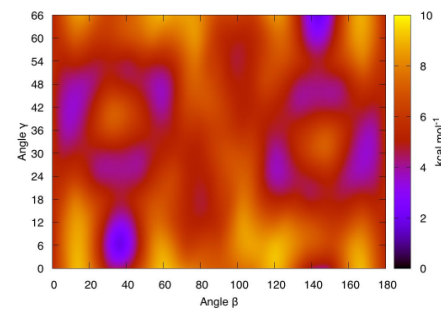
$$\alpha = 0^\circ$$



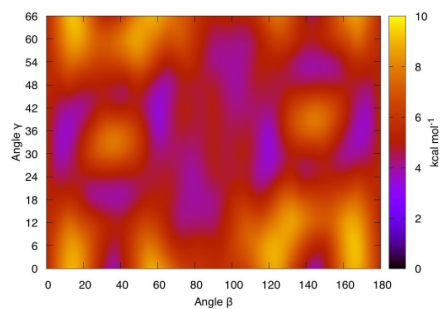
$$\alpha = 6^\circ$$



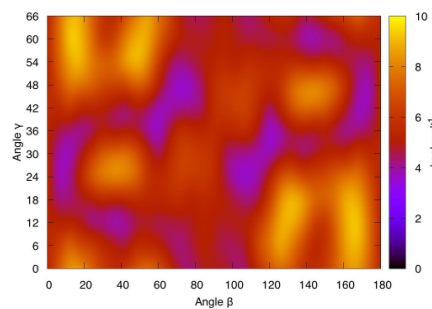
$$\alpha = 12^\circ$$



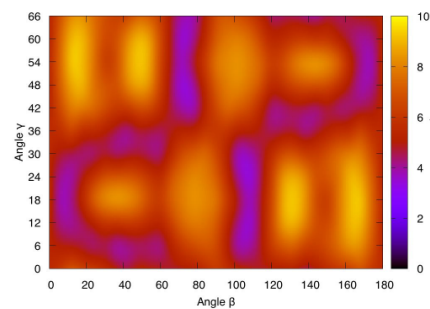
$$\alpha = 18^\circ$$



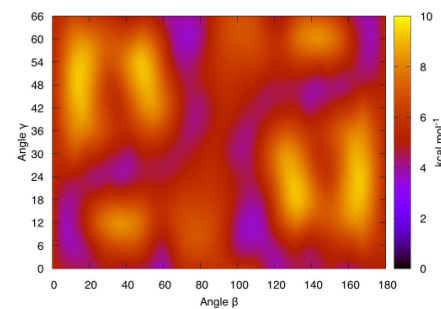
$$\alpha = 24^\circ$$



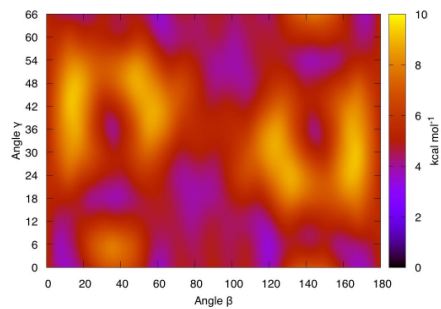
$$\alpha = 30^\circ$$



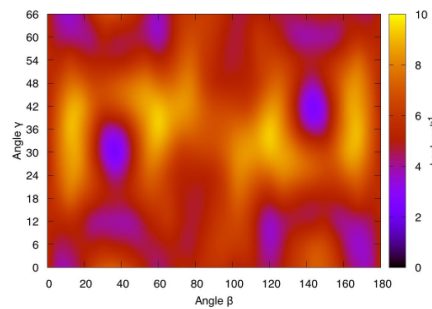
$$\alpha = 36^\circ$$



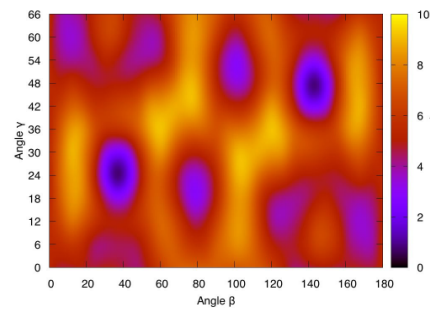
$$\alpha = 42^\circ$$



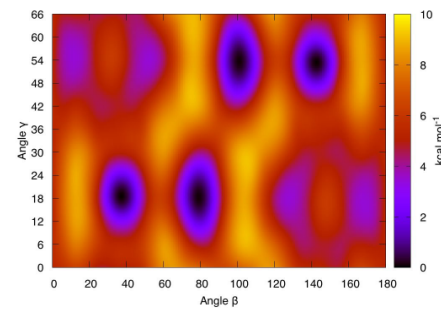
$$\alpha = 48^\circ$$



$$\alpha = 54^\circ$$



$$\alpha = 60^\circ$$

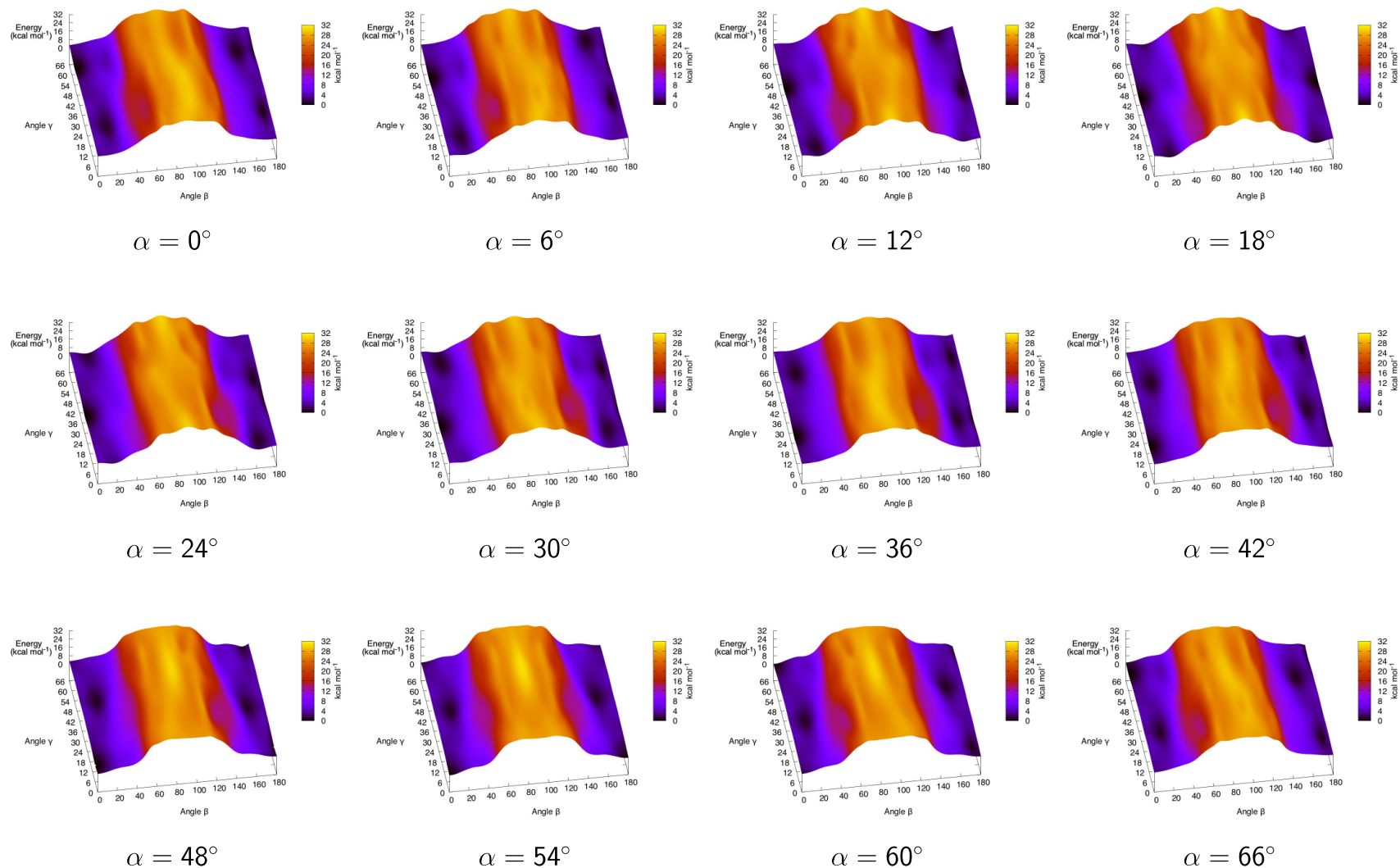


$$\alpha = 66^\circ$$

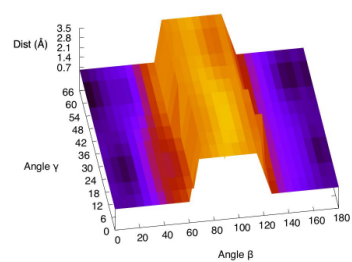
All the B97-D2/def2-TZVP optimizations from the minima led to minima II or III of figure 5.

Searching minima of complex $C_{70}@[10]CPP$ with a systematic scanning procedure.

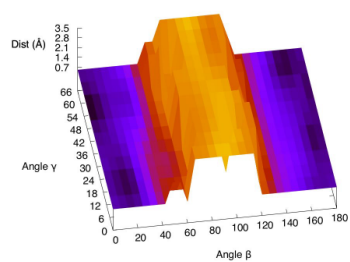
In this case (and in the next one), the search has been performed with a slightly more complicated procedure. This is because in these cases, our previous results indicate that it is likely the fullerene is not fully hosted in the CNR. For that reason, several different distances between the centre of the fullerene and that of the CNR have been tested. Thus, for each combination of the three Euler angles, four different "heights" have been tested: 0.5, 2.0, 3.5 and 5.0 Å, and the most favourable energy is chosen. Therefore, the number of calculations quadruples, reaching almost 18000 single points.



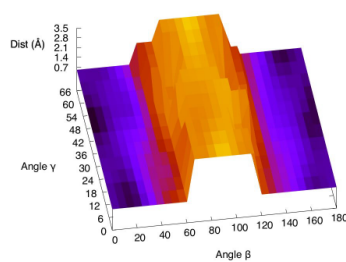
This Figure shows the preferred "height" for each combination of the three Euler angles:



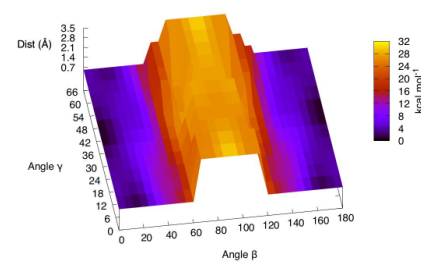
$$\alpha = 0^\circ$$



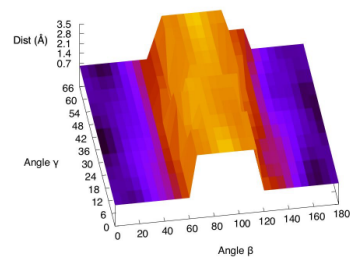
$$\alpha = 6^\circ$$



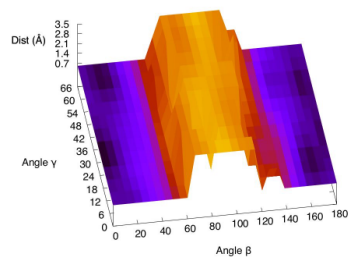
$$\alpha = 12^\circ$$



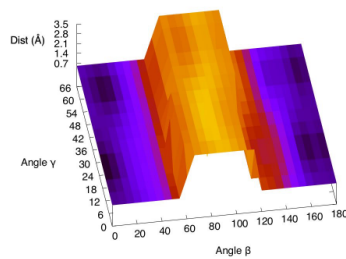
$$\alpha = 18^\circ$$



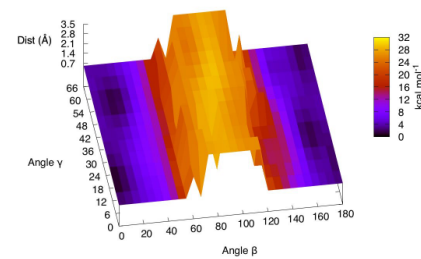
$$\alpha = 24^\circ$$



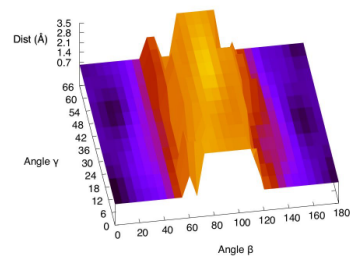
$$\alpha = 30^\circ$$



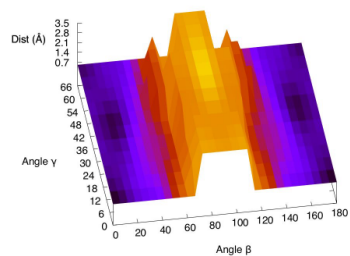
$$\alpha = 36^\circ$$



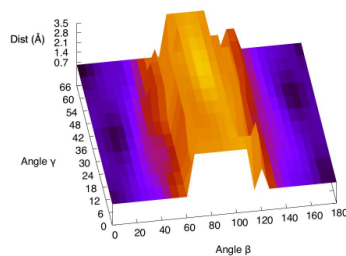
$$\alpha = 42^\circ$$



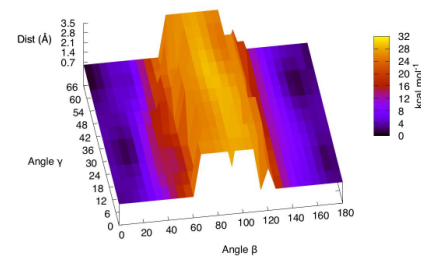
$$\alpha = 48^\circ$$



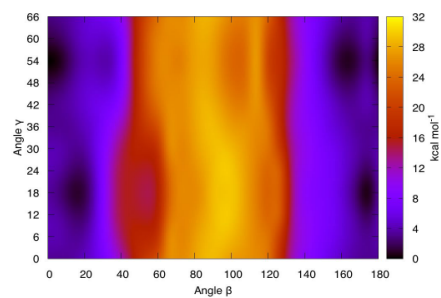
$$\alpha = 54^\circ$$



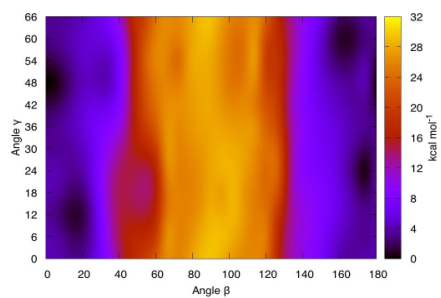
$$\alpha = 60^\circ$$



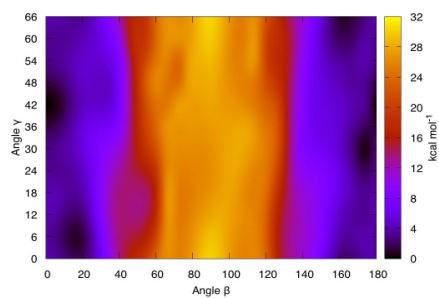
$$\alpha = 66^\circ$$



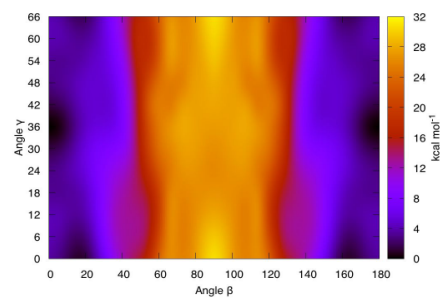
$$\alpha = 0^\circ$$



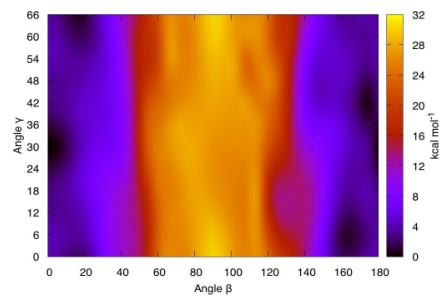
$$\alpha = 6^\circ$$



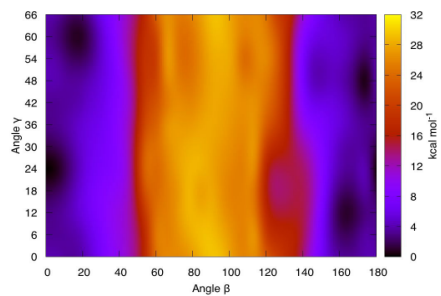
$$\alpha = 12^\circ$$



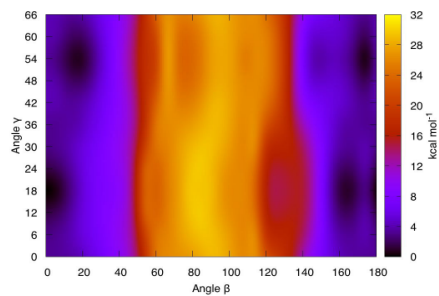
$$\alpha = 18^\circ$$



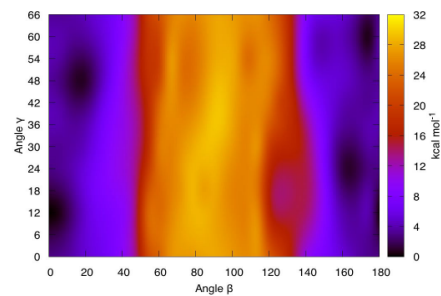
$$\alpha = 24^\circ$$



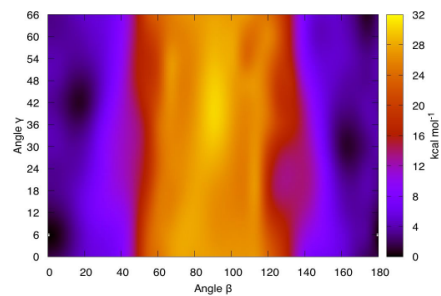
$$\alpha = 30^\circ$$



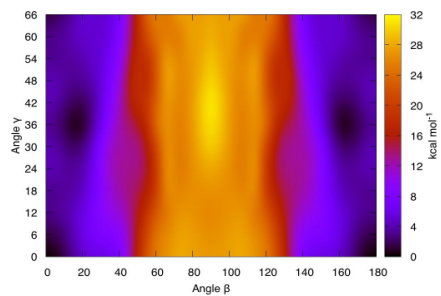
$$\alpha = 36^\circ$$



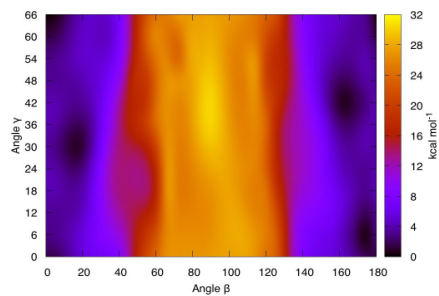
$$\alpha = 42^\circ$$



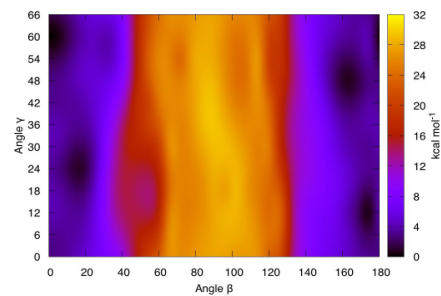
$$\alpha = 48^\circ$$



$$\alpha = 54^\circ$$



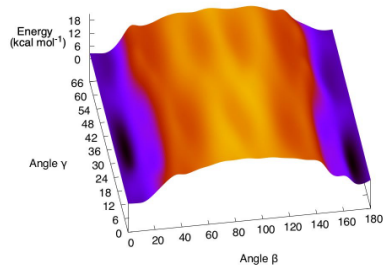
$$\alpha = 60^\circ$$



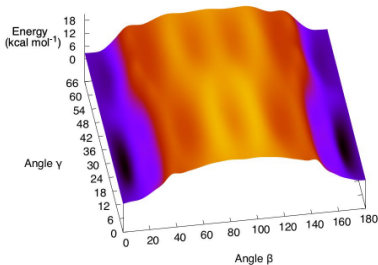
$$\alpha = 66^\circ$$

All the B97-D2/def2-TZVP optimizations from the minima led to minima I or III of figure 6

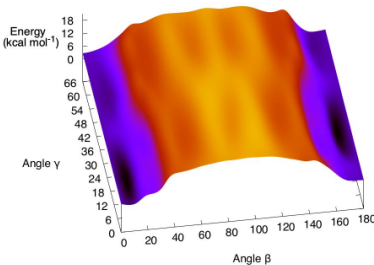
Searching minima of complex $C_{70}@[6]CPPA$ with a systematic scanning procedure.



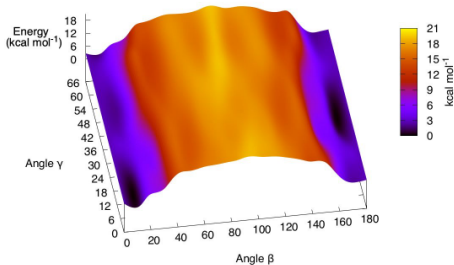
$$\alpha = 0^\circ$$



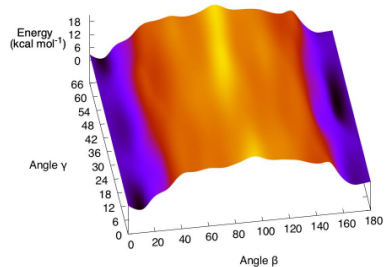
$$\alpha = 6^\circ$$



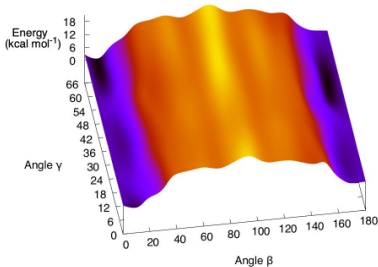
$$\alpha = 12^\circ$$



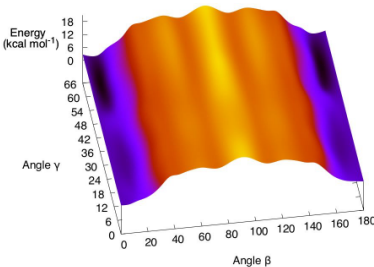
$$\alpha = 18^\circ$$



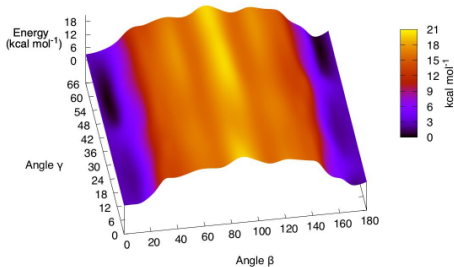
$$\alpha = 24^\circ$$



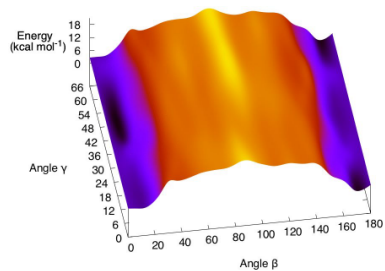
$$\alpha = 30^\circ$$



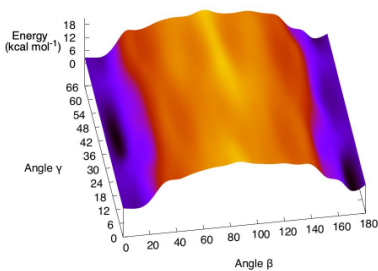
$$\alpha = 36^\circ$$



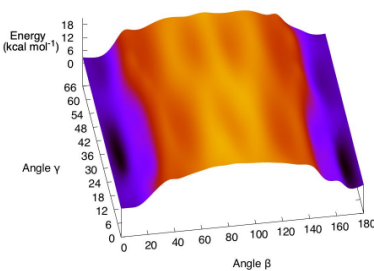
$$\alpha = 42^\circ$$



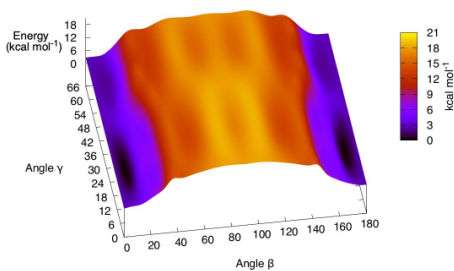
$$\alpha = 48^\circ$$



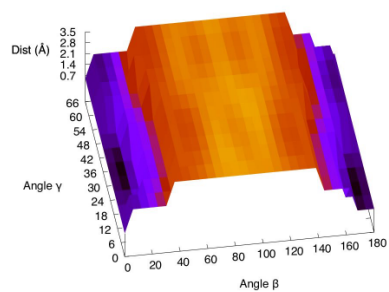
$$\alpha = 54^\circ$$



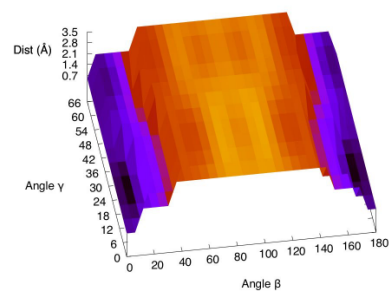
$$\alpha = 60^\circ$$



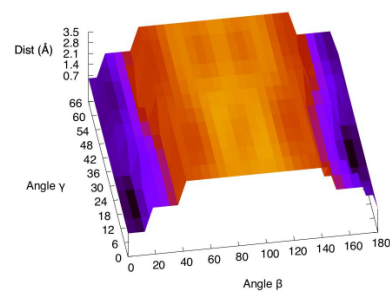
$$\alpha = 66^\circ$$



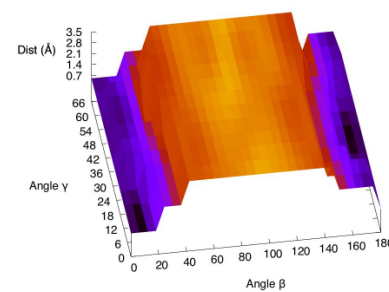
$$\alpha = 0^\circ$$



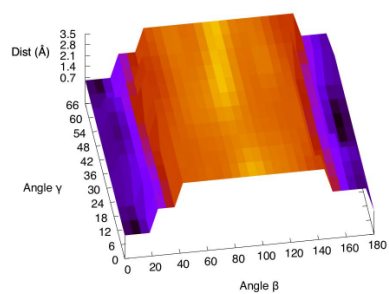
$$\alpha = 6^\circ$$



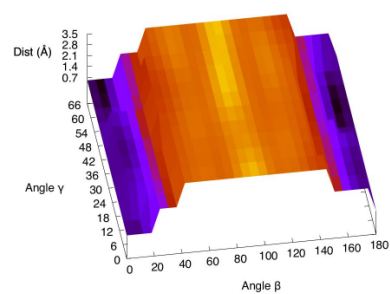
$$\alpha = 12^\circ$$



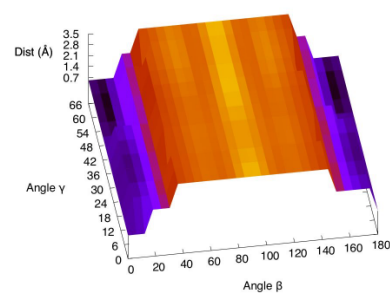
$$\alpha = 18^\circ$$



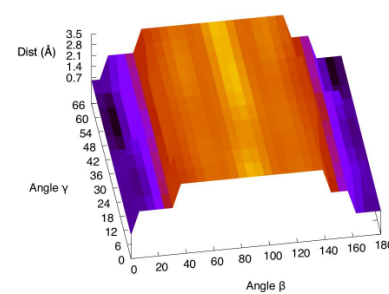
$$\alpha = 24^\circ$$



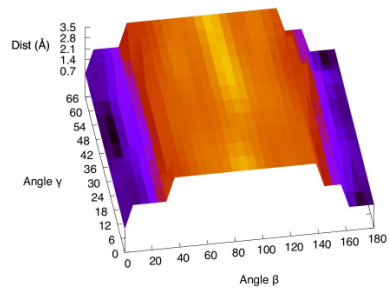
$$\alpha = 30^\circ$$



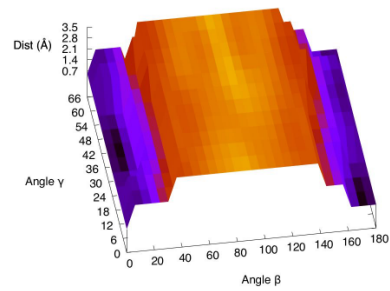
$$\alpha = 36^\circ$$



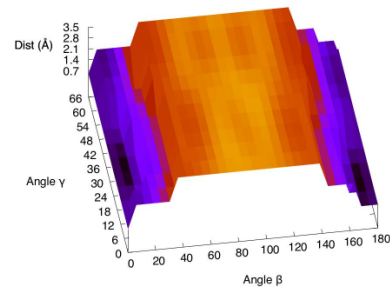
$$\alpha = 42^\circ$$



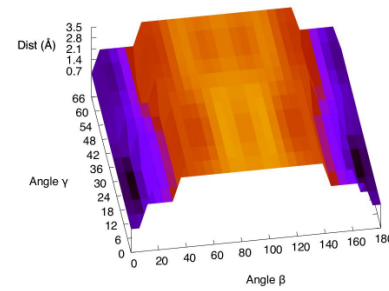
$$\alpha = 48^\circ$$



$$\alpha = 54^\circ$$

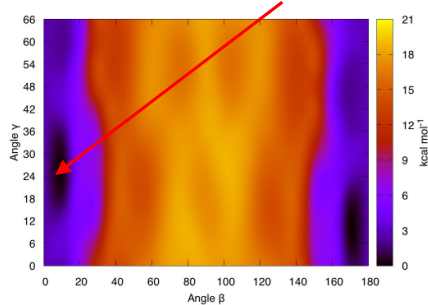


$$\alpha = 60^\circ$$

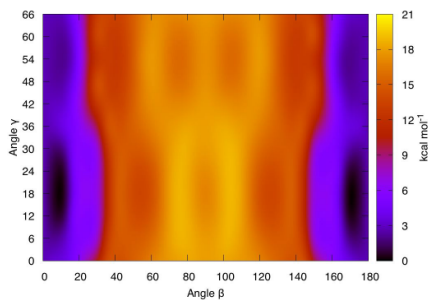


$$\alpha = 66^\circ$$

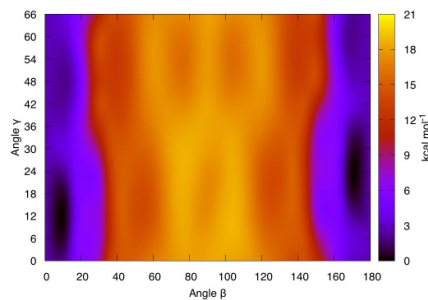
($\alpha = 0^\circ$, $\beta = 6^\circ$, $\gamma = 24^\circ$),



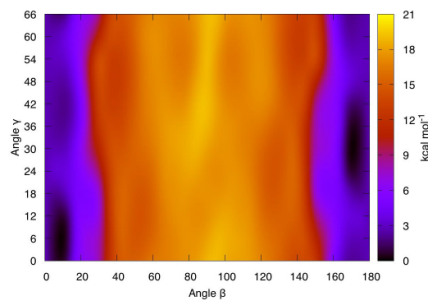
$\alpha = 0^\circ$



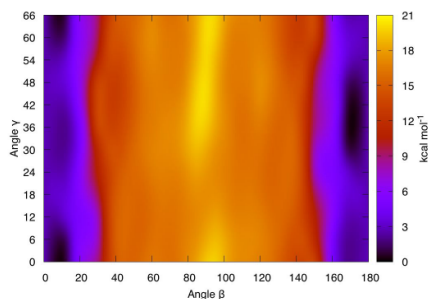
$\alpha = 6^\circ$



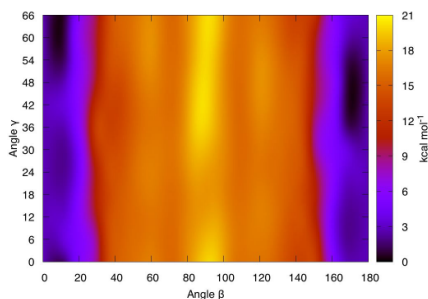
$\alpha = 12^\circ$



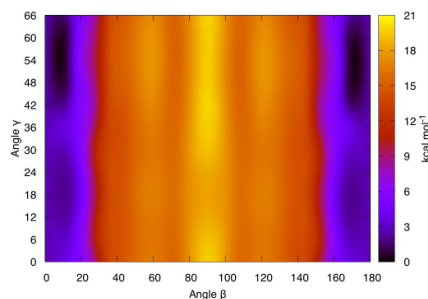
$\alpha = 18^\circ$



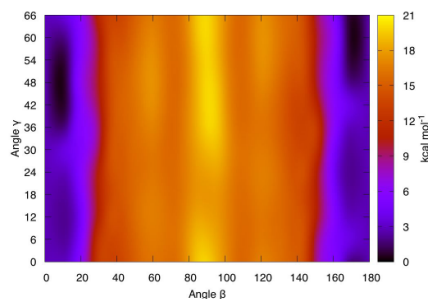
$\alpha = 24^\circ$



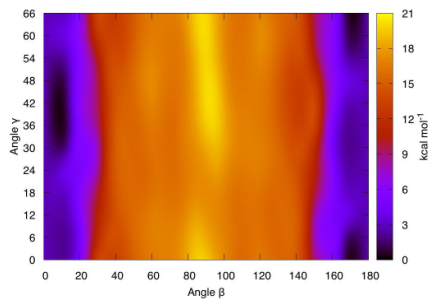
$\alpha = 30^\circ$



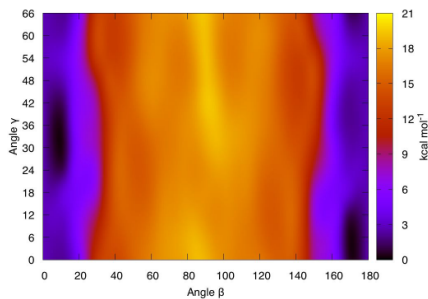
$\alpha = 36^\circ$



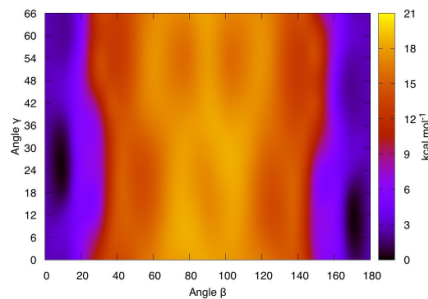
$\alpha = 42^\circ$



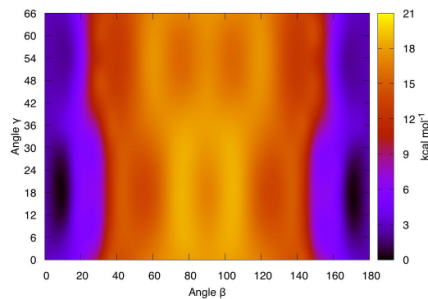
$\alpha = 48^\circ$



$\alpha = 54^\circ$



$\alpha = 60^\circ$



$\alpha = 66^\circ$

Optimization from the minimum $\alpha = 0^\circ$, $\beta = 6^\circ$, $\gamma = 24^\circ$, leads to a minimum, **I'**, more favourable than that obtained previously.

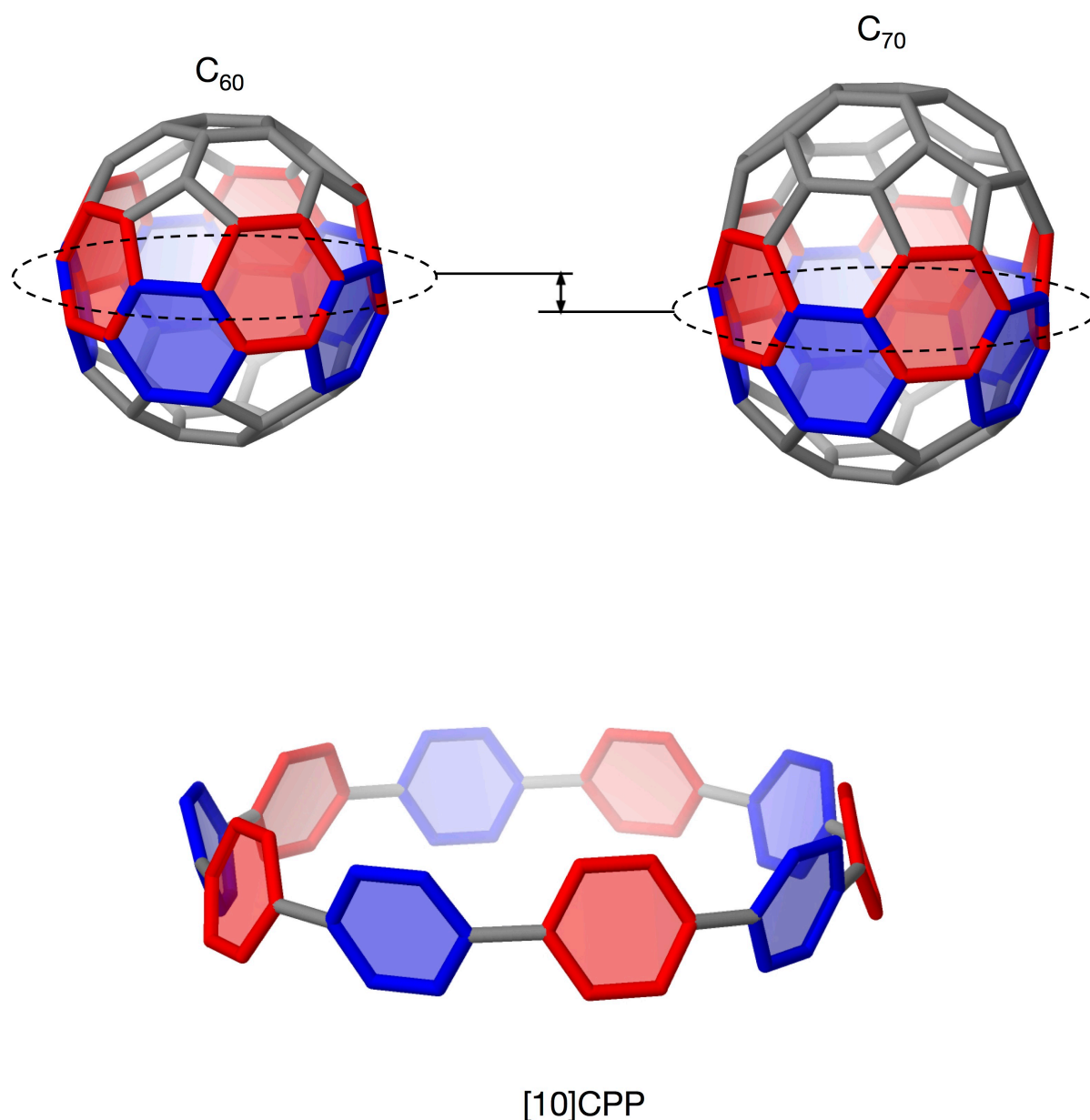
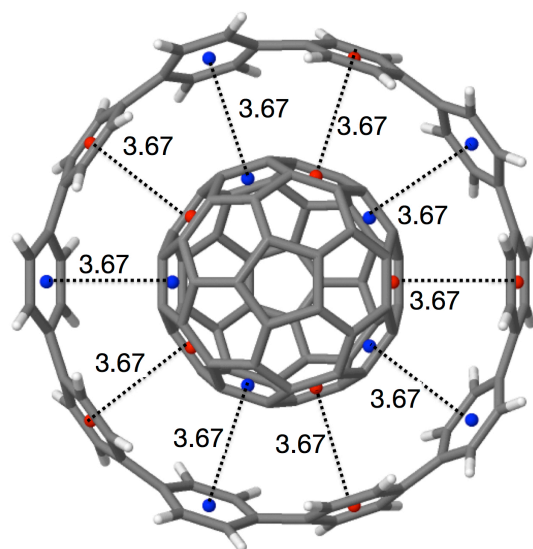
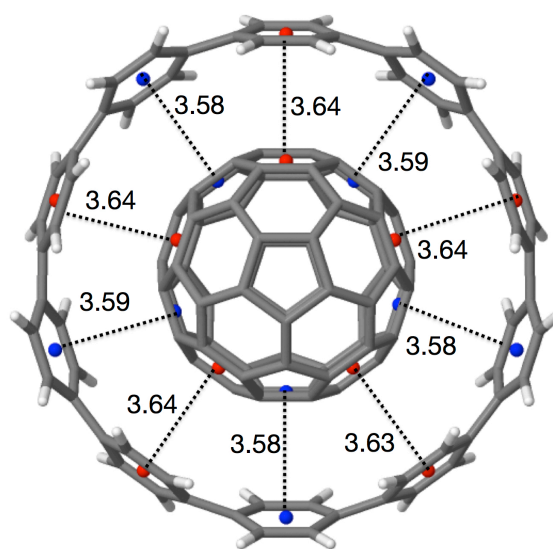


Figure S3. The best minimum (both for C_{60} and C_{70}) corresponds to a structure where each of the ten rings of [10]CPP is directly faced to a six-membered ring of the fullerene. Every six-membered ring of [10]CPP inclined outward (blue) is directly facing a six-membered ring of fullerene having the same disposition. The same happens with the rings inclined inward (red). So, the strong interaction that takes place, explains why C_{60} remains fully hosted in the CNR whereas C_{70} moves vertically from the centre of the CNR ($0.769 \text{ \AA}$): the interaction zone of C_{60} lies exactly at the middle of the fullerene, whereas it is slightly displaced in C_{70} .



C₆₀@[10]CPP

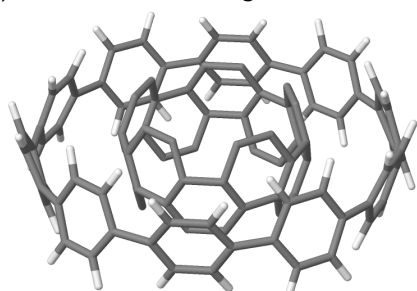


C₇₀@[10]CPP

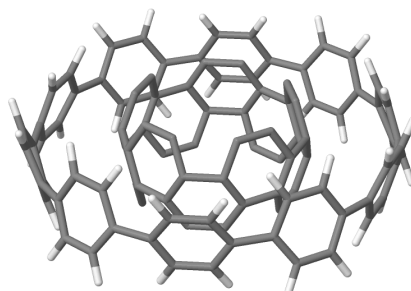
Figure S4. Distance between the centre of the six-membered ring of the CNR and the six-membered ring of the fullerene directly faced to it.

Computed dispersion between [10]CPP and the three "pieces" of C₆₀ and C₇₀ (kcal mol⁻¹)

1) With the central ring of the fullerene:



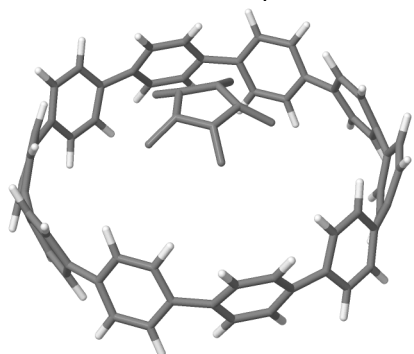
with C₆₀: -75.69



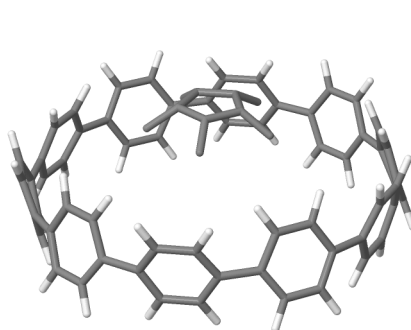
with C₇₀: -81.15

$\Delta = 5.46$

2) With the common "cap" of the fullerene:



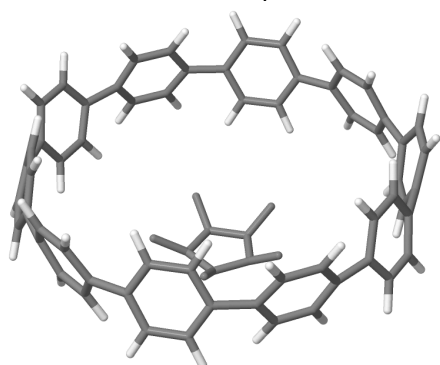
with C₆₀: -3.96



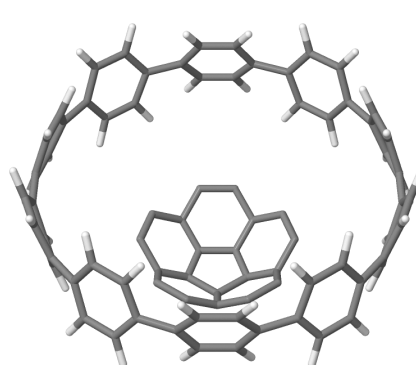
with C₇₀: -4.18

$\Delta = 0.22$

3) With the different "cap" of the fullerene:



with C₆₀: -3.96



with C₇₀: -8.40

$\Delta = 4.44$

with C₆₀: -83.61

TOTAL:

with C₇₀: -93.73

$\Delta = 10.12$

dispersion values of Table 1: $-83.61 - (-93.73) = 10.12$

Figure S5. The largest contribution to the difference of dispersion generated by C₆₀ and C₇₀ comes from the central region of the fullerene (5.46 kcal/mol, 54%). This is due to the fact that monomers are slightly closer for C₇₀, as shown in Figure S4. Although the dispersion is much more favourable for C₇₀ (10.12 kcal mol⁻¹), this is partially offset with a worse exchange+repulsion, so the final balance is only 3.53 kcal mol⁻¹ with regard to the interaction of C₆₀.

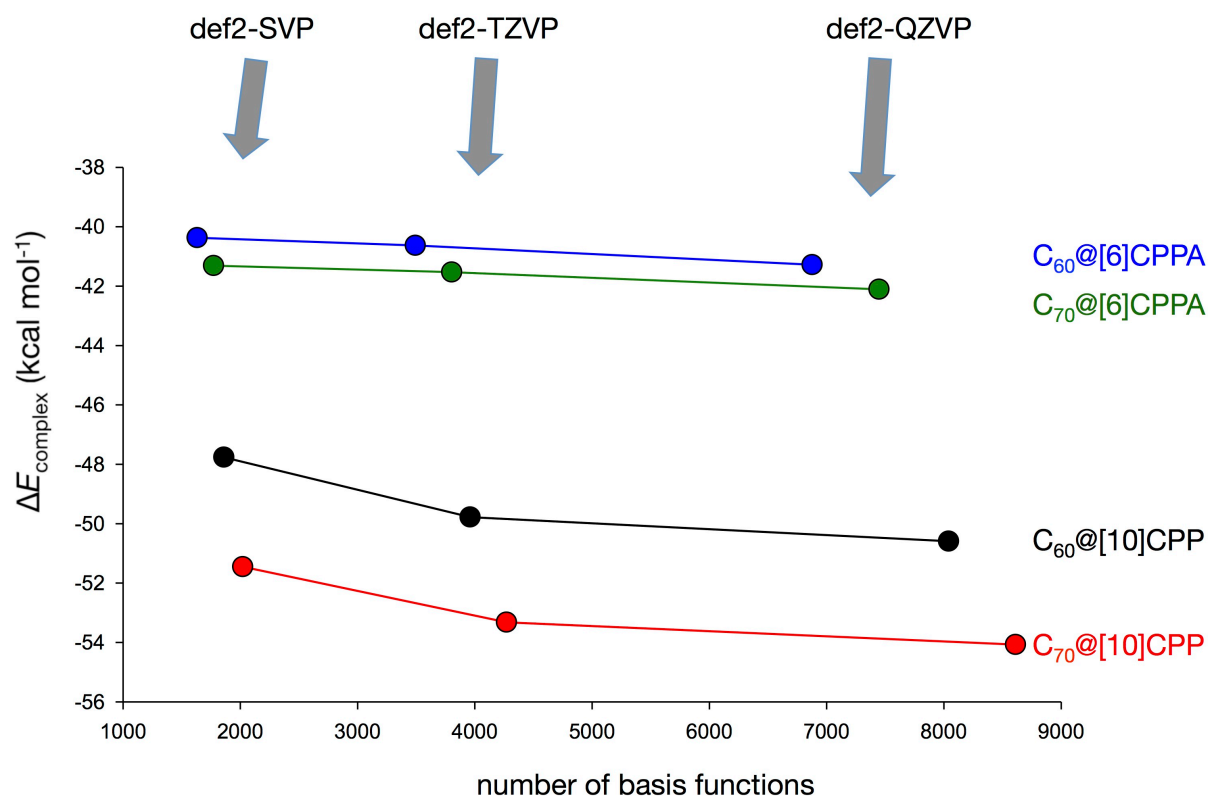


Figure S6. B97-D2 complexation energy (kcal mol⁻¹) obtained with different basis sets. Only the best complex of each case is shown.

Table S1. B97-D2 complexation energy (kcal mol⁻¹) obtained with different basis sets.

	def2-SVP	def2-TZVP	def2-QZVP ^a
C ₆₀ @[10]CPP	-47.76	-49.78	-50.59
C ₆₀ @[6]CPPA	-40.37	-40.63	-41.28
C ₇₀ @[10]CPP	-51.45	-53.32	-54.07
C ₇₀ @[6]CPPA	-41.31	-41.53	-42.11

^a Using def2-TZVP geometries. Auxiliary basis set for RI: def2-QZVPP.



Table S2. Differences between B97-D2 complexation energies (kcal mol⁻¹).

	def2-SVP	def2-TZVP	def2-QZVP	
C ₆₀ @[10]CPP - C ₆₀ @[6]CPPA	-7.39	-9.15	-9.31	difference between [10]CPP and [6]CPPA
C ₇₀ @[10]CPP - C ₇₀ @[6]CPPA	-10.14	-11.79	-11.96	
C ₇₀ @[10]CPP - C ₆₀ @[10]CPP	-3.69	-3.54	-3.48	difference between C ₆₀ and C ₇₀
C ₇₀ @[6]CPPA - C ₆₀ @[6]CPPA	-0.94	-0.90	-0.83	

Table S3. Complexation energy (kcal mol⁻¹) obtained with different methods. For hybrid functionals (B3LYP and PBE0) only single point calculations are performed, using the B97-D2 geometries. All the DFT-D calculations are performed with the def2-TZVP basis set. M06-2X with 6-31G/6-311G Pople basis set, plus diffuse functions (+) and polarization functions (d,p).

	B97-D2	BLYP-D2	B3LYP-D3(BJ)	TPSS-D3(BJ)	PBE0-D3(BJ)	M06-2X
C ₆₀ @[10]CPP	-49.78	-46.19	-49.58	-46.71	-44.65	-48.63 ^a (-39.31 ^b)
C ₆₀ @[6]CPPA	-40.63	-37.84	-38.80	-37.24	-34.43	-28.0 ^c
C ₇₀ @[10]CPP	-53.32	-49.76	-52.59	-49.78	-46.94	-39.74 ^d
C ₇₀ @[6]CPPA	-41.53	-38.58	-40.75	-38.10	-34.90	-31.38 ^e

^a Reference 25

^b Value obtained by us at the M06-2X/6-311+G(d,p)//B97-D2/def2-TZVP level.

^c Reference 24

^d Value obtained by us at the M06-2X/6-311+G(d,p) level using the geometry of Reference 21

^e Average value between -31.1 (Reference 24) and -31.66 (Reference 27)

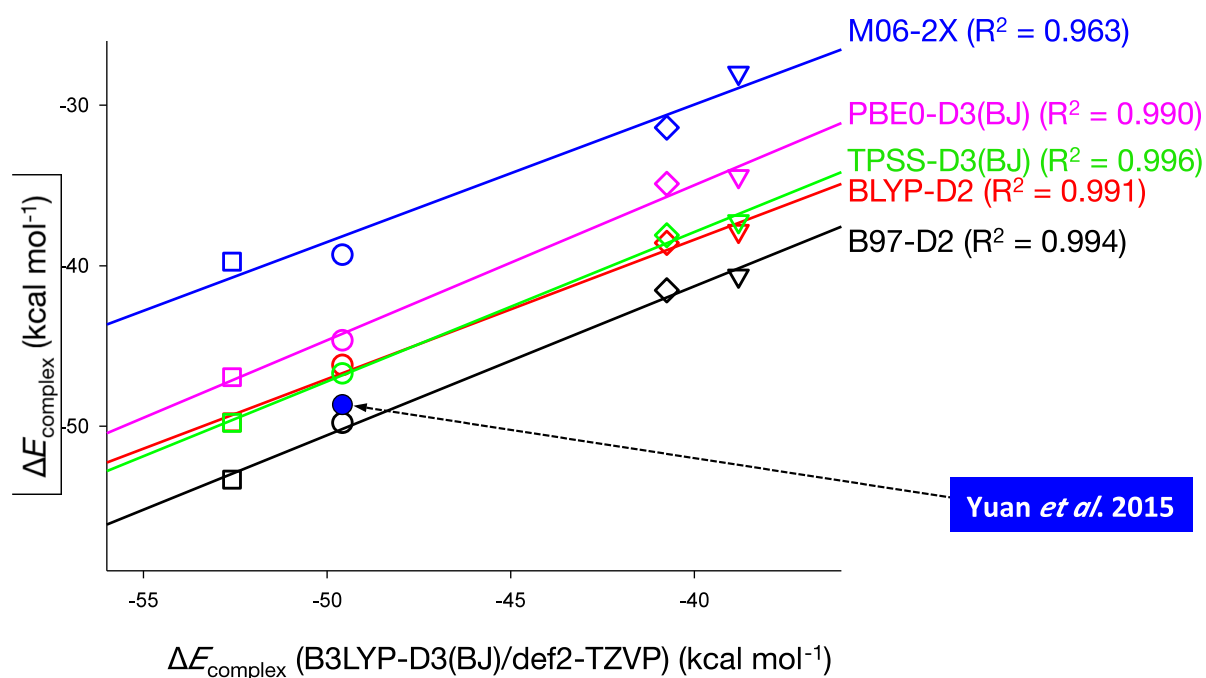


Figure S7. DFT vs. B3LYP-D3(BJ) complexation energy. (kcal mol⁻¹). The numeric data are included in Table S3.

B97-D2: $y = 0.9276x - 4.174$.

BLYP-D2: $y = 0.8674x - 3.685$.

TPSS-D3(BJ): $y = 0.9309x - 0.6674$

PBE0-D3(BJ): $y = 0.9660x + 3.657$

M06-2X: $y = 0.8396x + 3.608$.

Circles: C₆₀@[10]CPP

Triangles down: C₆₀@[6]CPPA

Squares: C₇₀@[10]CPP

Diamonds: C₇₀@[6]CPPA

Filled circle: C₆₀@[10]CPP M06-2X, obtained by Yuan et al. (reference 25), and very far from all the other M06-2X results.

Geometry of the optimized complexes (optimized complexes of Table 1 in red)

Table of Contents

Figure 2a.....	23
I.....	23
II.....	24
III.....	25
I opt C ₆₀ @[10]CPP I.....	27
III opt C ₆₀ @[10]CPP III.....	28
Figure 2b.....	29
I.....	29
II.....	30
III.....	31
I opt C ₆₀ @[6]CPPA I.....	33
II opt C ₆₀ @[6]CPPA II.....	34
III opt C ₆₀ @[6]CPPA III.....	35
Figure 2c.....	36
I.....	36
II.....	37
III.....	39
III opt C ₇₀ @[10]CPP IIIb.....	40
Figure 2d.....	42
I.....	42
II.....	43
II opt.....	44
Figure 4c1.....	45
Minimum.....	45
Minimum opt C ₇₀ @[10]CPP I.....	47
Figure 4c2.....	48
Minimum.....	48
Minimum opt C ₇₀ @[10]CPP IIIa.....	49
Figure 4d1.....	51
Minimum.....	51
Minimum opt C ₇₀ @[6]CPPA I.....	52
Figure 4d2.....	53
Minimum.....	53
Minimum opt C ₇₀ @[6]CPPA II.....	54
C70@[6]CPPA I'.....	56

Figure 2a**I**

C	0.998880	0.725730	3.327510
C	0.998880	-0.725730	3.327510
C	1.961100	-1.424820	2.592440
C	2.959980	-0.699090	1.829370
C	2.959980	0.699090	1.829370
C	1.961100	1.424820	2.592440
C	-0.381540	1.174250	3.327510
C	-1.234680	0.000000	3.327510
C	-0.381540	-1.174250	3.327510
C	-0.749070	-2.305410	2.592440
C	1.579560	-2.599070	1.829370
C	3.195780	-1.424820	0.594690
C	3.422930	-0.725730	-0.594690
C	3.422930	0.725730	-0.594690
C	3.195780	1.424820	0.594690
C	2.342640	2.599070	0.594690
C	1.579560	2.599070	1.829370
C	0.249810	3.031140	1.829370
C	-0.749070	2.305410	2.592440
C	-2.424050	0.000000	2.592440
C	-2.805590	1.174250	1.829370
C	-1.983750	2.305410	1.829370
C	-1.747950	3.031140	0.594690
C	-0.367540	3.479660	0.594690
C	0.367540	3.479660	-0.594690
C	1.747950	3.031140	-0.594690
C	1.983750	2.305410	-1.829370
C	2.805590	1.174250	-1.829370
C	2.342640	-2.599070	0.594690
C	0.381540	-1.174250	-3.327510
C	0.749070	-2.305410	-2.592440
C	-0.249810	-3.031140	-1.829370
C	-1.579560	-2.599070	-1.829370
C	-1.961100	-1.424820	-2.592440
C	-0.998880	0.725730	-3.327510
C	0.381540	1.174250	-3.327510
C	1.234680	0.000000	-3.327510
C	2.424050	0.000000	-2.592440
C	2.805590	-1.174250	-1.829370
C	1.983750	-2.305410	-1.829370
C	0.367540	-3.479660	-0.594690
C	-0.367540	-3.479660	0.594690
C	-1.747950	-3.031140	0.594690
C	-2.342640	-2.599070	-0.594690
C	-3.195780	-1.424820	-0.594690
C	-2.959980	-0.699090	-1.829370
C	-2.959980	0.699090	-1.829370
C	-1.961100	1.424820	-2.592440
C	0.749070	2.305410	-2.592440
C	-0.249810	3.031140	-1.829370
C	-1.579560	2.599070	-1.829370
C	-2.342640	2.599070	-0.594690
C	-3.195780	1.424820	-0.594690
C	-3.422930	0.725730	0.594690
C	-3.422930	-0.725730	0.594690
C	-2.805590	-1.174250	1.829370
C	-1.983750	-2.305410	1.829370
C	1.747950	-3.031140	-0.594690
C	0.249810	-3.031140	1.829370
C	-0.998880	-0.725730	-3.327510
C	6.230334	3.666470	1.090780
C	5.412312	4.792384	1.090780
C	4.646551	5.139019	-0.041650
C	4.889935	4.412176	-1.223530
C	5.707308	3.287155	-1.223530
C	6.323365	2.831070	-0.041650
C	3.451651	6.007168	0.041650
C	2.885350	6.628335	-1.090780
C	2.685172	6.014035	1.223530
C	1.561760	7.058397	-1.090780
C	1.362632	6.443756	1.223530
C	0.738499	6.888724	0.041650
C	6.779777	1.426385	0.041650
C	6.549451	0.695290	1.223530
C	7.195545	0.695853	-1.090780
C	6.549445	-0.695307	1.223530
C	7.195544	-0.695861	-1.090780
C	6.779778	-1.426401	0.041650
C	6.323364	-2.831089	-0.041650
C	6.230333	-3.666484	1.090780
C	5.707298	-3.287168	-1.223530
C	5.412299	-4.792408	1.090780
C	4.889923	-4.412186	-1.223530
C	4.646539	-5.139034	-0.041650
C	-0.738474	6.888731	-0.041650
C	-1.561731	7.058405	1.090780
C	-1.362613	6.443759	-1.223530
C	-2.885330	6.628344	1.090780
C	-2.685150	6.014038	-1.223530
C	-3.451638	6.007180	-0.041650
C	-4.646539	5.139034	0.041650
C	-5.412299	4.792408	-1.090780
C	-4.889923	4.412186	1.223530
C	-6.230333	3.666484	-1.090780
C	-5.707298	3.287168	1.223530
C	-6.323364	2.831089	0.041650
C	3.451638	-6.007180	0.041650
C	2.885330	-6.628344	-1.090780
C	2.685150	-6.014038	1.223530
C	1.561731	-7.058405	-1.090780
C	1.362613	-6.443759	1.223530
C	0.738474	-6.888731	0.041650
C	-0.738499	-6.888724	-0.041650
C	-1.561760	-7.058397	1.090780
C	-1.362632	-6.443756	-1.223530
C	-2.885350	-6.628335	1.090780
C	-2.685172	-6.014035	-1.223530
C	-3.451651	-6.007168	-0.041650
C	-6.779778	1.426401	-0.041650
C	-7.195544	0.695861	1.090780
C	-6.549445	0.695307	-1.223530
C	-7.195545	-0.695853	1.090780
C	-6.549451	-0.695290	-1.223530
C	-6.779777	-1.426385	-0.041650
C	-6.323365	-2.831070	0.041650
C	-6.230334	-3.666470	-1.090780
C	-5.707308	-3.287155	1.223530
C	-5.412312	-4.792384	-1.090780

C -4.889935 -4.412176 1.223530
 C -4.646551 -5.139019 0.041650
 H 6.757146 3.392764 2.002240
 H 5.314793 5.377997 2.002240
 H 4.327196 4.650961 -2.122380
 H 5.760505 2.678170 -2.122380
 H 3.472436 6.716551 -2.002240
 H 3.086165 5.552625 2.122380
 H 1.138658 7.474846 -2.002240
 H 0.767014 6.306164 2.122380
 H 6.234537 1.219238 2.122380
 H 7.460866 1.226928 -2.002240
 H 6.234529 -1.219260 2.122380
 H 7.460859 -1.226948 -2.002240
 H 6.757143 -3.392783 2.002240
 H 5.760502 -2.678184 -2.122380
 H 5.314786 -5.378011 2.002240
 H 4.327185 -4.650970 -2.122380
 H -1.138636 7.474850 2.002240
 H -0.766995 6.306165 -2.122380
 H -3.472411 6.716560 2.002240
 H -3.086146 5.552626 -2.122380
 H -5.314786 5.378011 -2.002240
 H -4.327185 4.650970 2.122380
 H -6.757143 3.392783 -2.002240
 H -5.760502 2.678184 2.122380
 H 3.472411 -6.716560 -2.002240
 H 3.086146 -5.552626 2.122380
 H 1.138636 -7.474850 -2.002240
 H 0.766995 -6.306165 2.122380
 H -1.138658 -7.474846 2.002240
 H -0.767014 -6.306164 -2.122380
 H -3.472436 -6.716551 2.002240
 H -3.086165 -5.552625 -2.122380
 H -7.460859 1.226948 2.002240
 H -6.234529 1.219260 -2.122380
 H -7.460866 -1.226928 2.002240
 H -6.234537 -1.219238 -2.122380
 H -6.757146 -3.392764 -2.002240
 H -5.760505 -2.678170 2.122380
 H -5.314793 -5.377997 -2.002240
 H -4.327196 -4.650961 2.122380

II

C 0.998880 0.725730 3.327510
 C 0.998880 -0.725730 3.327510
 C 1.961100 -1.424820 2.592440
 C 2.959980 -0.699090 1.829370
 C 2.959980 0.699090 1.829370
 C 1.961100 1.424820 2.592440
 C -0.381540 1.174250 3.327510
 C -1.234680 0.000000 3.327510
 C -0.381540 -1.174250 3.327510
 C -0.749070 -2.305410 2.592440
 C 1.579560 -2.599070 1.829370
 C 3.195780 -1.424820 0.594690
 C 3.422930 -0.725730 -0.594690
 C 3.422930 0.725730 -0.594690
 C 3.195780 1.424820 0.594690
 C 2.342640 2.599070 0.594690

C 1.579560 2.599070 1.829370
 C 0.249810 3.031140 1.829370
 C -0.749070 2.305410 2.592440
 C -2.424050 0.000000 2.592440
 C -2.805590 1.174250 1.829370
 C -1.983750 2.305410 1.829370
 C -1.747950 3.031140 0.594690
 C -0.367540 3.479660 0.594690
 C 0.367540 3.479660 -0.594690
 C 1.747950 3.031140 -0.594690
 C 1.983750 2.305410 -1.829370
 C 2.805590 1.174250 -1.829370
 C 2.342640 -2.599070 0.594690
 C 0.381540 -1.174250 -3.327510
 C 0.749070 -2.305410 -2.592440
 C -0.249810 -3.031140 -1.829370
 C -1.579560 -2.599070 -1.829370
 C -1.961100 -1.424820 -2.592440
 C -0.998880 0.725730 -3.327510
 C 0.381540 1.174250 -3.327510
 C 1.234680 0.000000 -3.327510
 C 2.424050 0.000000 -2.592440
 C 2.805590 -1.174250 -1.829370
 C 1.983750 -2.305410 -1.829370
 C 0.367540 -3.479660 -0.594690
 C -0.367540 -3.479660 0.594690
 C -1.747950 -3.031140 0.594690
 C -2.342640 -2.599070 -0.594690
 C -3.195780 -1.424820 -0.594690
 C -2.959980 -0.699090 -1.829370
 C -2.959980 0.699090 -1.829370
 C -1.961100 1.424820 -2.592440
 C 0.749070 2.305410 -2.592440
 C -0.249810 3.031140 -1.829370
 C -1.579560 2.599070 -1.829370
 C -2.342640 2.599070 -0.594690
 C -3.195780 1.424820 -0.594690
 C -3.422930 0.725730 0.594690
 C -3.422930 -0.725730 0.594690
 C -2.805590 -1.174250 1.829370
 C -1.983750 -2.305410 1.829370
 C 1.747950 -3.031140 -0.594690
 C 0.249810 -3.031140 1.829370
 C -0.998880 -0.725730 -3.327510
 C 7.195544 -0.695861 1.090780
 C 7.195545 0.695843 1.090780
 C 6.779779 1.426379 -0.041650
 C 6.549453 0.695293 -1.223530
 C 6.549451 -0.695307 -1.223530
 C 6.779771 -1.426396 -0.041650
 C 6.323369 2.831071 0.041650
 C 6.230335 3.666469 -1.090780
 C 5.707311 3.287152 1.223530
 C 5.412313 4.792383 -1.090780
 C 4.889937 4.412172 1.223530
 C 4.646549 5.139016 0.041650
 C 6.323363 -2.831083 0.041650
 C 5.707299 -3.287168 1.223530
 C 6.230330 -3.666478 -1.090780
 C 4.889921 -4.412183 1.223530
 C 5.412301 -4.792398 -1.090780

C 4.646538 -5.139036 0.041650
 C 3.451636 -6.007179 -0.041650
 C 2.885340 -6.628346 1.090780
 C 2.685152 -6.014041 -1.223530
 C 1.561735 -7.058409 1.090780
 C 1.362613 -6.443758 -1.223530
 C 0.738480 -6.888733 -0.041650
 C 3.451656 6.007165 -0.041650
 C 2.885359 6.628332 1.090780
 C 2.685169 6.014034 -1.223530
 C 1.561761 7.058398 1.090780
 C 1.362630 6.443751 -1.223530
 C 0.738497 6.888733 -0.041650
 C -0.738480 6.888733 0.041650
 C -1.561735 7.058409 -1.090780
 C -1.362613 6.443758 1.223530
 C -2.885340 6.628346 -1.090780
 C -2.685152 6.014041 1.223530
 C -3.451636 6.007179 0.041650
 C -0.738497 -6.888733 0.041650
 C -1.561761 -7.058398 -1.090780
 C -1.362630 -6.443751 1.223530
 C -2.885359 -6.628332 -1.090780
 C -2.685169 -6.014034 1.223530
 C -3.451656 -6.007165 0.041650
 C -4.646549 -5.139016 -0.041650
 C -5.412313 -4.792383 1.090780
 C -4.889937 -4.412172 -1.223530
 C -6.230335 -3.666469 1.090780
 C -5.707311 -3.287152 -1.223530
 C -6.323369 -2.831071 -0.041650
 C -4.646538 5.139036 -0.041650
 C -5.412301 4.792398 1.090780
 C -4.889921 4.412183 -1.223530
 C -6.230330 3.666478 1.090780
 C -5.707299 3.287168 -1.223530
 C -6.323363 2.831083 -0.041650
 C -6.779771 1.426396 0.041650
 C -7.195544 0.695861 -1.090780
 C -6.549451 0.695307 1.223530
 C -7.195545 -0.695843 -1.090780
 C -6.549453 -0.695293 1.223530
 C -6.779779 -1.426379 0.041650
 H 7.460863 -1.226946 2.002240
 H 7.460865 1.226934 2.002240
 H 6.234541 1.219244 -2.122380
 H 6.234536 -1.219254 -2.122380
 H 6.757150 3.392757 -2.002240
 H 5.760511 2.678166 2.122380
 H 5.314798 5.377991 -2.002240
 H 4.327198 4.650954 2.122380
 H 5.760497 -2.678184 2.122380
 H 6.757137 -3.392781 -2.002240
 H 4.327177 -4.650966 2.122380
 H 5.314779 -5.378005 -2.002240
 H 3.472415 -6.716568 2.002240
 H 3.086146 -5.552635 -2.122380
 H 1.138636 -7.474855 2.002240
 H 0.766994 -6.306169 -2.122380
 H 3.472430 6.716554 2.002240
 H 3.086158 5.552623 -2.122380

H 1.138655 7.474844 2.002240
 H 0.767007 6.306160 -2.122380
 H -1.138636 7.474855 -2.002240
 H -0.766994 6.306169 2.122380
 H -3.472415 6.716568 -2.002240
 H -3.086146 5.552635 2.122380
 H -1.138655 -7.474844 -2.002240
 H -0.767007 -6.306160 2.122380
 H -3.472430 -6.716554 -2.002240
 H -3.086158 -5.552623 2.122380
 H -5.314798 -5.377991 2.002240
 H -4.327198 -4.650954 -2.122380
 H -6.757150 -3.392757 2.002240
 H -5.760511 -2.678166 -2.122380
 H -5.314779 5.378005 2.002240
 H -4.327177 4.650966 -2.122380
 H -6.757137 3.392781 2.002240
 H -5.760497 2.678184 -2.122380
 H -7.460863 1.226946 -2.002240
 H -6.234536 1.219254 2.122380
 H -7.460865 -1.226934 -2.002240
 H -6.234541 -1.219244 2.122380

III

C 1.846444 2.966658 0.621568
 C 0.769128 3.457994 -0.217904
 C -0.538773 3.497280 0.274815
 C -0.819189 3.046733 1.625776
 C 0.218581 2.573432 2.434433
 C 1.576313 2.532644 1.922945
 C 2.762985 2.217021 -0.217910
 C 2.252127 2.245055 -1.576199
 C 1.019859 3.012015 -1.576199
 C -0.046523 2.621697 -2.391924
 C -1.645773 3.092090 -0.571991
 C -2.099503 2.363085 1.613905
 C -2.295064 1.231216 2.411136
 C -1.217747 0.739879 3.250608
 C 0.015583 1.398448 3.262035
 C 1.247850 0.631488 3.262035
 C 2.212438 1.332459 2.434427
 C 3.095347 0.610333 1.625769
 C 3.375763 1.060881 0.274808
 C 2.372795 1.115918 -2.391930
 C 3.008920 -0.084266 -1.880449
 C 3.501029 -0.111269 -0.571998
 C 3.298031 -1.286253 0.255603
 C 3.047304 -0.840278 1.613890
 C 2.118107 -1.515532 2.411131
 C 1.201570 -0.765899 3.250603
 C -0.078743 -1.449547 3.238732
 C -1.265794 -0.710728 3.238737
 C -2.610362 2.391119 0.255616
 C -2.762985 -2.217021 0.217910
 C -3.375763 -1.060881 -0.274808
 C -3.095347 -0.610333 -1.625769
 C -2.212438 -1.332459 -2.434427
 C -1.576313 -2.532644 -1.922945
 C -0.769128 -3.457994 0.217904
 C -1.019859 -3.012015 1.576199

C -2.252127 -2.245055 1.576199
 C -2.372795 -1.115918 2.391930
 C -3.008920 0.084266 1.880449
 C -3.501029 0.111269 0.571998
 C -3.047304 0.840278 -1.613890
 C -2.118107 1.515532 -2.411131
 C -1.201570 0.765899 -3.250603
 C -1.247850 -0.631488 -3.262035
 C -0.015583 -1.398448 -3.262035
 C -0.218581 -2.573432 -2.434433
 C 0.819189 -3.046733 -1.625776
 C 0.538773 -3.497280 -0.274815
 C 0.046523 -2.621697 2.391924
 C 1.404255 -2.662486 1.880436
 C 1.645773 -3.092090 0.571991
 C 2.610362 -2.391119 -0.255616
 C 2.099503 -2.363085 -1.613905
 C 2.295064 -1.231216 -2.411136
 C 1.217747 -0.739879 -3.250608
 C 1.265794 0.710728 -3.238737
 C 0.078743 1.449547 -3.238732
 C -3.298031 1.286253 -0.255603
 C -1.404255 2.662486 -1.880436
 C -1.846444 -2.966658 -0.621568
 C -5.109378 5.110009 -1.109926
 C -4.035229 5.994906 -1.108103
 C -3.209996 6.139782 0.026332
 C -3.630916 5.498489 1.207834
 C -4.704213 4.614292 1.206012
 C -5.411830 4.325878 0.022596
 C -1.835404 6.680574 -0.053970
 C -1.134440 7.141217 1.079784
 C -1.088582 6.493751 -1.233686
 C 0.254690 7.225745 1.083332
 C 0.299446 6.578211 -1.230141
 C 1.012095 6.853840 -0.046697
 C -6.205582 3.080368 -0.061386
 C -6.162787 2.313551 -1.242297
 C -6.794176 2.478661 1.070180
 C -6.511384 0.967356 -1.241698
 C -7.143058 1.131386 1.070779
 C -6.920735 0.318675 -0.060158
 C -6.831250 -1.155480 0.025033
 C -6.947641 -1.988793 -1.106770
 C -6.352290 -1.750105 1.208842
 C -6.437983 -3.283832 -1.103978
 C -5.843043 -3.044102 1.211631
 C -5.786542 -3.810081 0.030755
 C 2.441686 6.483687 0.040767
 C 3.284156 6.440294 -1.089408
 C 2.931245 5.897791 1.224595
 C 4.457677 5.692162 -1.085490
 C 4.103822 5.150254 1.228510
 C 4.847213 4.950141 0.048799
 C 5.786542 3.810081 -0.030755
 C 6.437983 3.283832 1.103978
 C 5.843043 3.044102 -1.211631
 C 6.947641 1.988793 1.106770
 C 6.352290 1.750105 -1.208842
 C 6.831250 1.155480 -0.025033
 C -4.847213 -4.950141 -0.048799

C -4.457677 -5.692162 1.085490
 C -4.103822 -5.150254 -1.228510
 C -3.284156 -6.440294 1.089408
 C -2.931245 -5.897791 -1.224595
 C -2.441686 -6.483687 -0.040767
 C -1.012095 -6.853840 0.046697
 C -0.254690 -7.225745 -1.083332
 C -0.299446 -6.578211 1.230141
 C 1.134440 -7.141217 -1.079784
 C 1.088582 -6.493751 1.233686
 C 1.835404 -6.680574 0.053970
 C 6.920735 -0.318675 0.060158
 C 7.143058 -1.131386 -1.070779
 C 6.511384 -0.967356 1.241698
 C 6.794176 -2.478661 -1.070180
 C 6.162787 -2.313551 1.242297
 C 6.205582 -3.080368 0.061386
 C 5.411830 -4.325878 -0.022596
 C 5.109378 -5.110009 1.109926
 C 4.704213 -4.614292 -1.206012
 C 4.035229 -5.994906 1.108103
 C 3.630916 -5.498489 -1.207834
 C 3.209996 -6.139782 -0.026332
 H -5.685589 4.976081 -2.022750
 H -3.791629 6.536349 -2.019536
 H -3.028645 5.589589 2.108164
 H -4.910732 4.039099 2.104971
 H -1.683054 7.374813 1.989547
 H -1.590080 6.146587 -2.133465
 H 0.766288 7.523856 1.995803
 H 0.843908 6.294692 -2.127248
 H -5.724226 2.740815 -2.140480
 H -6.920282 3.060314 1.980660
 H -6.335514 0.380179 -2.139431
 H -7.535426 0.684791 1.981716
 H -7.386624 -1.592794 -2.019830
 H -6.253488 -1.146220 2.107276
 H -6.487996 -3.876206 -2.014907
 H -5.360493 -3.415320 2.112168
 H 2.981360 6.948480 -2.002237
 H 2.317799 5.914911 2.121820
 H 5.050514 5.629365 -1.995328
 H 4.373986 4.604062 2.128686
 H 6.487996 3.876206 2.014907
 H 5.360493 3.415320 -2.112168
 H 7.386624 1.592794 2.019830
 H 6.253488 1.146220 -2.107276
 H -5.050514 -5.629365 1.995328
 H -4.373986 -4.604062 -2.128686
 H -2.981360 -6.948480 2.002237
 H -2.317799 -5.914911 -2.121820
 H -0.766288 -7.523856 -1.995803
 H -0.843908 -6.294692 2.127248
 H 1.683054 -7.374813 -1.989547
 H 1.590080 -6.146587 2.133465
 H 7.535426 -0.684791 -1.981716
 H 6.335514 -0.380179 2.139431
 H 6.920282 -3.060314 -1.980660
 H 5.724226 -2.740815 2.140480
 H 5.685589 -4.976081 2.022750
 H 4.910732 -4.039099 -2.104971

H 3.791629 -6.536349 2.019536
H 3.028645 -5.589589 -2.108164

I opt C₆₀@[10]CPP I

C 0.998711 0.725853 3.325808
C 0.998711 -0.725853 3.325808
C 1.961079 -1.425036 2.590476
C 2.960545 -0.699312 1.827499
C 2.960545 0.699312 1.827499
C 1.961079 1.425036 2.590476
C -0.382010 1.174362 3.325468
C -1.235231 0.000000 3.325268
C -0.382010 -1.174362 3.325468
C -0.749450 -2.305564 2.589814
C 1.579722 -2.599753 1.827243
C 3.195240 -1.425344 0.594072
C 3.422912 -0.725019 -0.592882
C 3.422912 0.725018 -0.592882
C 3.195240 1.425344 0.594072
C 2.342900 2.598455 0.593858
C 1.579722 2.599753 1.827243
C 0.249639 3.031889 1.826967
C -0.749450 2.305564 2.589814
C -2.424498 0.000000 2.589541
C -2.806251 1.174369 1.826424
C -1.984297 2.305856 1.826564
C -1.747271 3.031250 0.593208
C -0.368270 3.479357 0.593445
C 0.368271 3.479357 -0.593444
C 1.747272 3.031249 -0.593208
C 1.984297 2.305855 -1.826564
C 2.806251 1.174369 -1.826424
C 2.342899 -2.598455 0.593858
C 0.382010 -1.174362 -3.325468
C 0.749450 -2.305564 -2.589814
C -0.249639 -3.031889 -1.826967
C -1.579722 -2.599753 -1.827243
C -1.961079 -1.425036 -2.590476
C -0.998711 0.725853 -3.325808
C 0.382010 1.174362 -3.325468
C 1.235231 0.000000 -3.325268
C 2.424498 0.000000 -2.589541
C 2.806251 -1.174369 -1.826424
C 1.984297 -2.305856 -1.826564
C 0.368270 -3.479357 -0.593445
C -0.368271 -3.479357 0.593444
C -1.747272 -3.031249 0.593208
C -2.342900 -2.598455 -0.593858
C -3.195240 -1.425344 -0.594072
C -2.960545 -0.699312 -1.827499
C -2.960545 0.699312 -1.827499
C -1.961079 1.425036 -2.590476
C 0.749450 2.305564 -2.589814
C -0.249638 3.031889 -1.826967
C -1.579722 2.599753 -1.827243
C -2.342899 2.598455 -0.593858
C -3.195240 1.425344 -0.594072
C -3.422912 0.725019 0.592882
C -3.422912 -0.725018 0.592882
C -2.806251 -1.174369 1.826424

C -1.984297 -2.305855 1.826564
C 1.747271 -3.031250 -0.593208
C 0.249638 -3.031889 1.826967
C -0.998711 -0.725853 -3.325808
C 6.212108 3.653987 1.095145
C 5.394516 4.779165 1.095267
C 4.637180 5.129287 -0.040418
C 4.880159 4.404395 -1.222441
C 5.696468 3.280816 -1.222546
C 6.310904 2.825555 -0.040652
C 3.444896 5.995400 0.040738
C 2.878001 6.607370 -1.095063
C 2.680273 6.002375 1.222643
C 1.555218 7.036988 -1.095160
C 1.359455 6.431531 1.222625
C 0.736819 6.875088 0.040591
C 6.766073 1.423870 0.040238
C 6.537389 0.694413 1.222251
C 7.172257 0.695421 -1.095726
C 6.537387 -0.694433 1.222251
C 7.172256 -0.695441 -1.095727
C 6.766070 -1.423890 0.040238
C 6.310896 -2.825575 -0.040654
C 6.212098 -3.654004 1.095143
C 5.696459 -3.280829 -1.222548
C 5.394502 -4.779179 1.095266
C 4.880145 -4.404408 -1.222442
C 4.637167 -5.129299 -0.040420
C -0.736802 6.875090 -0.040592
C -1.555200 7.036992 1.095157
C -1.359437 6.431533 -1.222625
C -2.877983 6.607377 1.095062
C -2.680258 6.002380 -1.222643
C -3.444879 5.995408 -0.040738
C -4.637167 5.129299 0.040420
C -5.394502 4.779179 -1.095266
C -4.880145 4.404408 1.222442
C -6.212098 3.654004 -1.095143
C -5.696459 3.280829 1.222548
C -6.310896 2.825575 0.040654
C 3.444879 -5.995408 0.040738
C 2.877983 -6.607377 -1.095062
C 2.680258 -6.002380 1.222643
C 1.555200 -7.036992 -1.095157
C 1.359437 -6.431533 1.222625
C 0.736802 -6.875090 0.040592
C -0.736819 -6.875088 -0.040591
C -1.555218 -7.036988 1.095160
C -1.359455 -6.431531 -1.222625
C -2.878001 -6.607370 1.095063
C -2.680273 -6.002375 -1.222643
C -3.444896 -5.995400 -0.040738
C -6.766070 1.423890 -0.040238
C -7.172256 0.695441 1.095727
C -6.537387 0.694433 -1.222251
C -7.172257 -0.695421 1.095726
C -6.537389 -0.694413 -1.222251
C -6.766073 -1.423870 -0.040238
C -6.310904 -2.825555 0.040652
C -6.212108 -3.653987 -1.095145
C -5.696468 -3.280816 1.222546

C	-5.394516	-4.779165	-1.095267
C	-4.880159	-4.404395	1.222441
C	-4.637180	-5.129287	0.040418
H	6.733294	3.375535	2.008221
H	5.290636	5.360784	2.008338
H	4.312958	4.638691	-2.118970
H	5.744071	2.669141	-2.119236
H	3.463309	6.688203	-2.008130
H	3.078526	5.535770	2.119373
H	1.129207	7.446226	-2.008308
H	0.762916	6.287998	2.119234
H	6.217335	1.217397	2.119215
H	7.429778	1.226939	-2.008941
H	6.217335	-1.217416	2.119215
H	7.429775	-1.226961	-2.008941
H	6.733286	-3.375555	2.008220
H	5.744061	-2.669155	-2.119236
H	5.290620	-5.360797	2.008337
H	4.312943	-4.638700	-2.118971
H	-1.129188	7.446229	2.008307
H	-0.762899	6.287996	-2.119234
H	-3.463291	6.688211	2.008130
H	-3.078511	5.535775	-2.119373
H	-5.290620	5.360797	-2.008337
H	-4.312943	4.638700	2.118971
H	-6.733286	3.375555	-2.008220
H	-5.744061	2.669155	2.119236
H	3.463291	-6.688211	-2.008130
H	3.078511	-5.535775	2.119373
H	1.129188	-7.446229	-2.008307
H	0.762899	-6.287996	2.119234
H	-1.129207	-7.446226	2.008308
H	-0.762916	-6.287998	-2.119234
H	-3.463309	-6.688203	2.008130
H	-3.078526	-5.535770	-2.119373
H	-7.429775	1.226961	2.008941
H	-6.217335	1.217416	-2.119215
H	-7.429778	-1.226939	2.008941
H	-6.217335	-1.217397	-2.119215
H	-6.733294	-3.375535	-2.008221
H	-5.744071	-2.669141	2.119236
H	-5.290636	-5.360784	-2.008338
H	-4.312958	-4.638691	2.118970

III opt C₆₀@[10]CPP III

C	1.807742	2.898739	0.943290
C	0.776642	3.459611	0.091589
C	-0.553785	3.466156	0.516499
C	-0.904398	2.914553	1.812507
C	0.090650	2.376240	2.635035
C	1.473501	2.370617	2.192718
C	2.768631	2.215808	0.098112
C	2.330634	2.353684	-1.277249
C	1.099408	3.122269	-1.281240
C	0.076635	2.801978	-2.179358
C	-1.613873	3.131515	-0.414144
C	-2.179434	2.235325	1.679975
C	-2.419185	1.047398	2.377585
C	-1.386019	0.488573	3.229775
C	-0.154356	1.140767	3.356438

C	1.076688	0.371701	3.360426
C	2.083011	1.131555	2.641528
C	3.007393	0.471030	1.825517
C	3.355972	1.024169	0.529467
C	2.495473	1.291188	-2.171498
C	3.105265	0.052651	-1.723276
C	3.524512	-0.078242	-0.397117
C	3.275223	-1.311327	0.323548
C	2.956811	-0.973037	1.697120
C	1.990822	-1.707394	2.392170
C	1.031367	-1.021490	3.237710
C	-0.246470	-1.697747	3.106527
C	-1.432846	-0.956719	3.102706
C	-2.616371	2.368941	0.303921
C	-2.768631	-2.215808	-0.098112
C	-3.355972	-1.024169	-0.529467
C	-3.007393	-0.471030	-1.825517
C	-2.083011	-1.131555	-2.641528
C	-1.473501	-2.370617	-2.192718
C	-0.776642	-3.459611	-0.091589
C	-1.099408	-3.122269	1.281240
C	-2.330634	-2.353684	1.277249
C	-2.495473	-1.291188	2.171498
C	-3.105265	-0.052651	1.723276
C	-3.524512	0.078242	0.397117
C	-2.956811	0.973037	-1.697120
C	-1.990822	1.707394	-2.392170
C	-1.031367	1.021490	-3.237710
C	-1.076688	-0.371701	-3.360426
C	0.154356	-1.140767	-3.356438
C	-0.090650	-2.376240	-2.635035
C	0.904398	-2.914553	-1.812507
C	0.553785	-3.466156	-0.516499
C	-0.076635	-2.801978	2.179358
C	1.306043	-2.808330	1.737839
C	1.613873	-3.131515	0.414144
C	2.616371	-2.368941	-0.303921
C	2.179434	-2.235325	-1.679975
C	2.419185	-1.047398	-2.377585
C	1.386019	-0.488573	-3.229775
C	1.432846	0.956719	-3.102706
C	0.246470	1.697747	-3.106527
C	-3.275223	1.311327	-0.323548
C	-1.306043	2.808330	-1.737839
C	-1.807742	-2.898739	-0.943290
C	-5.050033	5.018817	-1.160161
C	-3.973702	5.897399	-1.183255
C	-3.166113	6.094485	-0.044069
C	-3.607909	5.513692	1.158862
C	-4.683075	4.633744	1.181458
C	-5.374039	4.290369	0.003051
C	-1.795899	6.635873	-0.134773
C	-1.097529	7.118922	0.990564
C	-1.052465	6.437718	-1.313974
C	0.288720	7.228961	0.985001
C	0.331546	6.546327	-1.319027
C	1.044391	6.859219	-0.145493
C	-6.170377	3.047901	-0.041263
C	-6.184866	2.271207	-1.216143
C	-6.705149	2.454973	1.121203
C	-6.534969	0.926611	-1.189524

C	-7.053662	1.110112	1.148284
C	-6.886698	0.288735	0.014351
C	-6.803558	-1.181702	0.113157
C	-6.945822	-2.023896	-1.008197
C	-6.311579	-1.765809	1.296001
C	-6.458099	-3.326252	-0.996468
C	-5.824002	-3.065732	1.307648
C	-5.803137	-3.848298	0.136899
C	2.479587	6.523307	-0.065553
C	3.299441	6.454093	-1.210624
C	2.998162	5.983565	1.126498
C	4.474309	5.711343	-1.208466
C	4.172959	5.241265	1.128621
C	4.885800	5.002387	-0.061308
C	5.803137	3.848298	-0.136899
C	6.458099	3.326252	0.996468
C	5.824002	3.065732	-1.307648
C	6.945822	2.023896	1.008197
C	6.311579	1.765809	-1.296001
C	6.803558	1.181702	-0.113157
C	-4.885800	-5.002387	0.061308
C	-4.474309	-5.711343	1.208466
C	-4.172959	-5.241265	-1.128621
C	-3.299441	-6.454093	1.210624
C	-2.998162	-5.983565	-1.126498
C	-2.479587	-6.523307	0.065553
C	-1.044391	-6.859219	0.145493
C	-0.288720	-7.228961	-0.985001
C	-0.331546	-6.546327	1.319027
C	1.097529	-7.118922	-0.990564
C	1.052465	-6.437718	1.313974
C	1.795899	-6.635873	0.134773
C	6.886698	-0.288735	-0.014351
C	7.053662	-1.110112	-1.148284
C	6.534969	-0.926611	1.189524
C	6.705149	-2.454973	-1.121203
C	6.184866	-2.271207	1.216143
C	6.170377	-3.047901	0.041263
C	5.374039	-4.290369	-0.003051
C	5.050033	-5.018817	1.160161
C	4.683075	-4.633744	-1.181458
C	3.973702	-5.897399	1.183255
C	3.607909	-5.513692	-1.158862
C	3.166113	-6.094485	0.044069
H	-5.611747	4.847319	-2.075078
H	-3.715394	6.394043	-2.115385
H	-3.017841	5.638103	2.062750
H	-4.897306	4.101630	2.103704
H	-1.644159	7.354699	1.900658
H	-1.548594	6.058564	-2.202813
H	0.800097	7.546722	1.890671
H	0.874797	6.248850	-2.211403
H	-5.783850	2.683745	-2.137443
H	-6.790223	3.041460	2.032802
H	-6.393927	0.333550	-2.088992
H	-7.403488	0.671791	2.079890
H	-7.389920	-1.632185	-1.920438
H	-6.178659	-1.151308	2.181954
H	-6.527641	-3.928058	-1.899715
H	-5.325634	-3.428057	-2.202480
H	2.974530	6.932392	-2.131652

H	2.400727	6.016563	2.033459
H	5.047875	5.621032	-2.127948
H	4.456984	4.717206	2.037090
H	6.527641	3.928058	1.899715
H	5.325634	3.428057	-2.202480
H	7.389920	1.632185	1.920438
H	6.178659	1.151308	-2.181954
H	-5.047875	-5.621032	2.127948
H	-4.456984	-4.717206	-2.037090
H	-2.974530	-6.932392	2.131652
H	-2.400727	-6.016563	-2.033459
H	-0.800097	-7.546722	-1.890671
H	-0.874797	-6.248850	2.211403
H	1.644159	-7.354699	-1.900658
H	1.548594	-6.058564	2.202813
H	7.403488	-0.671791	-2.079890
H	6.393927	-0.333550	2.088992
H	6.790223	-3.041460	-2.032802
H	5.783850	-2.683745	2.137443
H	5.611747	-4.847319	2.075078
H	4.897306	-4.101630	-2.103704
H	3.715394	-6.394043	2.115385
H	3.017841	-5.638103	-2.062750

Figure 2b

I

C	1.846440	2.966660	0.621570
C	0.769130	3.457990	-0.217900
C	-0.538770	3.497280	0.274820
C	-0.819190	3.046730	1.625780
C	0.218580	2.573430	2.434430
C	1.576310	2.532640	1.922950
C	2.762990	2.217020	-0.217910
C	2.252130	2.245060	-1.576200
C	1.019860	3.012020	-1.576200
C	-0.046520	2.621700	-2.391920
C	-1.645770	3.092090	-0.571990
C	-2.099500	2.363090	1.613910
C	-2.295060	1.231220	2.411140
C	-1.217750	0.739880	3.250610
C	0.015580	1.398450	3.262040
C	1.247850	0.631490	3.262040
C	2.212440	1.332460	2.434430
C	3.095350	0.610330	1.625770
C	3.375760	1.060880	0.274810
C	2.372800	1.115920	-2.391930
C	3.008920	-0.084270	-1.880450
C	3.501030	-0.111270	-0.572000
C	3.298030	-1.286250	0.255600
C	3.047300	-0.840280	1.613890
C	2.118110	-1.515530	2.411130
C	1.201570	-0.765900	3.250600
C	-0.078740	-1.449550	3.238730
C	-1.265790	-0.710730	3.238740
C	-2.610360	2.391120	0.255620
C	-2.762990	-2.217020	0.217910
C	-3.375760	-1.060880	-0.274810
C	-3.095350	-0.610330	-1.625770
C	-2.212440	-1.332460	-2.434430

C -1.576310 -2.532640 -1.922950
 C -0.769130 -3.457990 0.217900
 C -1.019860 -3.012020 1.576200
 C -2.252130 -2.245060 1.576200
 C -2.372800 -1.115920 2.391930
 C -3.008920 0.084270 1.880450
 C -3.501030 0.111270 0.572000
 C -3.047300 0.840280 -1.613890
 C -2.118110 1.515530 -2.411130
 C -1.201570 0.765900 -3.250600
 C -1.247850 -0.631490 -3.262040
 C -0.015580 -1.398450 -3.262040
 C -0.218580 -2.573430 -2.434430
 C 0.819190 -3.046730 -1.625780
 C 0.538770 -3.497280 -0.274820
 C 0.046520 -2.621700 2.391920
 C 1.404260 -2.662490 1.880440
 C 1.645770 -3.092090 0.571990
 C 2.610360 -2.391120 -0.255620
 C 2.099500 -2.363090 -1.613910
 C 2.295060 -1.231220 -2.411140
 C 1.217750 -0.739880 -3.250610
 C 1.265790 0.710730 -3.238740
 C 0.078740 1.449550 -3.238730
 C -3.298030 1.286250 -0.255600
 C -1.404260 2.662490 -1.880440
 C -1.846440 -2.966660 -0.621570
 C 6.565630 -0.236979 -0.014567
 C 6.465707 -0.962933 1.197131
 C 6.119170 -2.305874 1.189758
 C 5.858285 -2.977068 -0.029655
 C 6.117142 -2.292188 -1.241708
 C 6.463868 -0.949310 -1.234246
 C 5.153367 -4.205027 -0.035230
 C 4.295812 -5.076394 -0.036298
 C 3.079520 -5.801207 -0.032542
 C 2.400519 -6.072126 -1.245305
 C 2.411345 -6.072674 1.186099
 C 1.063549 -6.441608 -1.239537
 C 1.074622 -6.442596 1.191876
 C 0.351778 -6.555489 -0.020663
 C -1.064113 -6.558380 -0.013642
 C -2.247672 -6.252071 -0.005841
 C -3.484423 -5.562775 0.002584
 C -4.063154 -5.112561 -1.208903
 C -4.050334 -5.119053 1.222403
 C -5.052983 -4.141142 -1.201077
 C -5.040179 -4.147596 1.230238
 C -5.504229 -3.580486 0.018491
 C -6.216526 -2.356773 0.023807
 C -6.544297 -1.178964 0.021910
 C -6.566007 0.236718 0.021728
 C -6.452261 0.954682 1.237008
 C -6.477519 0.956957 -1.194315
 C -6.105366 2.297529 1.234621
 C -6.130359 2.299852 -1.196794
 C -5.857821 2.976637 0.016782
 C -5.152641 4.204422 0.012447
 C -4.295162 5.075779 0.011224
 C -3.079143 5.801014 0.011300
 C -2.406497 6.075988 -1.204094

C -2.404902 6.068980 1.227349
 C -1.069558 6.445860 -1.203962
 C -1.068238 6.439389 1.227454
 C -0.351704 6.556202 0.011614
 C 1.064299 6.559352 0.011074
 C 2.247792 6.252972 0.010723
 C 3.484422 5.563221 0.008886
 C 4.053760 5.115119 -1.207821
 C 4.059411 5.116965 1.223513
 C 5.043318 4.143390 -1.209336
 C 5.048985 4.145111 1.222027
 C 5.503639 3.580189 0.005699
 C 6.215626 2.356346 0.002474
 C 6.543458 1.178571 -0.006259
 H 6.583472 -0.436196 2.140511
 H 5.965329 -2.833312 2.127480
 H 5.961897 -2.809308 -2.184970
 H 6.580856 -0.412359 -2.171901
 H 2.915831 -5.908896 -2.188168
 H 2.935219 -5.909078 2.124247
 H 0.529336 -6.567599 -2.177739
 H 0.549264 -6.569514 2.134820
 H -3.666351 -5.477461 -2.152592
 H -3.643572 -5.489664 2.159667
 H -5.433277 -3.743505 -2.138366
 H -5.410722 -3.755867 2.173862
 H -6.559487 0.421737 2.178128
 H -6.605224 0.426327 -2.134169
 H -5.940676 2.818681 2.174027
 H -5.985507 2.823199 -2.138322
 H -2.926588 5.915389 -2.144804
 H -2.924020 5.902404 2.167644
 H -0.540273 6.574802 -2.144461
 H -0.538261 6.563673 2.168093
 H 3.649916 5.481856 -2.147791
 H 3.659985 5.485911 2.164568
 H 5.416387 3.747395 -2.150277
 H 5.426538 3.751386 2.162102

II

C 1.846440 2.966660 0.621570
 C 0.769130 3.457990 -0.217900
 C -0.538770 3.497280 0.274820
 C -0.819190 3.046730 1.625780
 C 0.218580 2.573430 2.434430
 C 1.576310 2.532640 1.922950
 C 2.762990 2.217020 -0.217910
 C 2.252130 2.245060 -1.576200
 C 1.019860 3.012020 -1.576200
 C -0.046520 2.621700 -2.391920
 C -1.645770 3.092090 -0.571990
 C -2.099500 2.363090 1.613910
 C -2.295060 1.231220 2.411140
 C -1.217750 0.739880 3.250610
 C 0.015580 1.398450 3.262040
 C 1.247850 0.631490 3.262040
 C 2.212440 1.332460 2.434430
 C 3.095350 0.610330 1.625770
 C 3.375760 1.060880 0.274810
 C 2.372800 1.115920 -2.391930

C 3.008920 -0.084270 -1.880450
 C 3.501030 -0.111270 -0.572000
 C 3.298030 -1.286250 0.255600
 C 3.047300 -0.840280 1.613890
 C 2.118110 -1.515530 2.411130
 C 1.201570 -0.765900 3.250600
 C -0.078740 -1.449550 3.238730
 C -1.265790 -0.710730 3.238740
 C -2.610360 2.391120 0.255620
 C -2.762990 -2.217020 0.217910
 C -3.375760 -1.060880 -0.274810
 C -3.095350 -0.610330 -1.625770
 C -2.212440 -1.332460 -2.434430
 C -1.576310 -2.532640 -1.922950
 C -0.769130 -3.457990 0.217900
 C -1.019860 -3.012020 1.576200
 C -2.252130 -2.245060 1.576200
 C -2.372800 -1.115920 2.391930
 C -3.008920 0.084270 1.880450
 C -3.501030 0.111270 0.572000
 C -3.047300 0.840280 -1.613890
 C -2.118110 1.515530 -2.411130
 C -1.201570 0.765900 -3.250600
 C -1.247850 -0.631490 -3.262040
 C -0.015580 -1.398450 -3.262040
 C -0.218580 -2.573430 -2.434430
 C 0.819190 -3.046730 -1.625780
 C 0.538770 -3.497280 -0.274820
 C 0.046520 -2.621700 2.391920
 C 1.404260 -2.662490 1.880440
 C 1.645770 -3.092090 0.571990
 C 2.610360 -2.391120 -0.255620
 C 2.099500 -2.363090 -1.613910
 C 2.295060 -1.231220 -2.411140
 C 1.217750 -0.739880 -3.250610
 C 1.265790 0.710730 -3.238740
 C 0.078740 1.449550 -3.238730
 C -3.298030 1.286250 -0.255600
 C -1.404260 2.662490 -1.880440
 C -1.846440 -2.966660 -0.621570
 C 6.171033 -2.254141 -0.032708
 C 5.854383 -2.916033 1.178424
 C 5.109814 -4.086155 1.170451
 C 4.651571 -4.641530 -0.049017
 C 5.106684 -4.067811 -1.260983
 C 5.851414 -2.897808 -1.252922
 C 3.601696 -5.591561 -0.054084
 C 2.516852 -6.155295 -0.053819
 C 1.136126 -6.468807 -0.047586
 C 0.403933 -6.514310 -1.258807
 C 0.419489 -6.522877 1.172557
 C -0.981761 -6.452595 -1.249825
 C -0.966105 -6.461657 1.181546
 C -1.691164 -6.343321 -0.029150
 C -3.038637 -5.908572 -0.018279
 C -4.069601 -5.251547 -0.006905
 C -5.032808 -4.213844 0.005677
 C -5.446802 -3.604493 -1.203713
 C -5.431185 -3.619330 1.227540
 C -6.087995 -2.374773 -1.192078
 C -6.072383 -2.389568 1.239185

C -6.341187 -1.704478 0.029357
 C -6.640477 -0.320563 0.038018
 C -6.588261 0.900887 0.038366
 C -6.171456 2.253996 0.039869
 C -5.838708 2.899325 1.255659
 C -5.867457 2.913994 -1.175583
 C -5.093849 4.069266 1.253870
 C -5.122332 4.083899 -1.177463
 C -4.651292 4.641001 0.036143
 C -3.601243 5.590805 0.031298
 C -2.516480 6.154557 0.028743
 C -1.135874 6.468548 0.026343
 C -0.413895 6.524565 -1.190561
 C -0.409113 6.512707 1.240860
 C 0.971903 6.463220 -1.193642
 C 0.976589 6.451957 1.237752
 C 1.691435 6.343994 0.020102
 C 3.039108 5.909444 0.015712
 C 4.070005 5.252358 0.011788
 C 5.032970 4.214247 0.005793
 C 5.433261 3.614502 -1.212972
 C 5.444635 3.609810 1.218338
 C 6.074115 2.384557 -1.218297
 C 6.085466 2.379742 1.213043
 C 6.340589 1.704330 -0.005165
 C 6.639548 0.320385 -0.011734
 C 6.587377 -0.901033 -0.022713
 H 6.131256 -2.453289 2.122085
 H 4.802615 -4.542056 2.107982
 H 4.797138 -4.509829 -2.204412
 H 6.126502 -2.421472 -2.190275
 H 0.942357 -6.516477 -2.202881
 H 0.970371 -6.530979 2.109462
 H -1.530856 -6.405534 -2.186714
 H -1.502864 -6.421850 2.125770
 H -5.184283 -4.072324 -2.148896
 H -5.156759 -4.099305 2.163267
 H -6.328899 -1.877272 -2.127870
 H -6.301636 -1.904337 2.184264
 H -6.103268 2.423776 2.196454
 H -6.154978 2.450611 -2.115694
 H -4.774083 4.512207 2.193422
 H -4.824955 4.538694 -2.118781
 H -0.960258 6.534354 -2.130036
 H -0.952197 6.512873 2.182372
 H 1.513027 6.424121 -2.135429
 H 1.521133 6.404577 2.177088
 H 5.160406 4.089895 -2.151418
 H 5.180866 4.082304 2.160899
 H 6.304459 1.894483 -2.160703
 H 6.324978 1.886804 2.151633

III

C 0.998880 0.725730 3.327510
 C 0.998880 -0.725730 3.327510
 C 1.961100 -1.424820 2.592440
 C 2.959980 -0.699090 1.829370
 C 2.959980 0.699090 1.829370
 C 1.961100 1.424820 2.592440
 C -0.381540 1.174250 3.327510

C	-1.234680	0.000000	3.327510	C	6.434951	-1.315213	-0.011040
C	-0.381540	-1.174250	3.327510	C	6.216120	-2.010836	-1.224900
C	-0.749070	-2.305410	2.592440	C	6.215066	-2.004009	1.206520
C	1.579560	-2.599070	1.829370	C	5.650506	-3.277370	-1.221690
C	3.195780	-1.424820	0.594690	C	5.649948	-3.270632	1.209740
C	3.422930	-0.725730	-0.594690	C	5.281308	-3.899536	-0.004380
C	3.422930	0.725730	-0.594690	C	4.382659	-4.993714	-0.000980
C	3.195780	1.424820	0.594690	C	3.393286	-5.711922	0.003070
C	2.342640	2.599070	0.594690	C	2.074602	-6.227492	0.006710
C	1.579560	2.599070	1.829370	C	1.363224	-6.386938	-1.207310
C	0.249810	3.031140	1.829370	C	1.368025	-6.382354	1.224030
C	-0.749070	2.305410	2.592440	C	-0.016005	-6.532510	-1.204300
C	-2.424050	0.000000	2.592440	C	-0.011244	-6.527915	1.227050
C	-2.805590	1.174250	1.829370	C	-0.739838	-6.524510	0.012790
C	-1.983750	2.305410	1.829370	C	-2.137122	-6.295449	0.013410
C	-1.747950	3.031140	0.594690	C	-3.254312	-5.798935	0.007910
C	-0.367540	3.479660	0.594690	C	-4.360294	-4.914954	0.004350
C	0.367540	3.479660	-0.594690	C	-4.845997	-4.370984	1.218230
C	1.747950	3.031140	-0.594690	C	-4.855458	-4.387846	-1.213150
C	1.983750	2.305410	-1.829370	C	-5.661257	-3.248971	1.213580
C	2.805590	1.174250	-1.829370	C	-5.670585	-3.265599	-1.217890
C	2.342640	-2.599070	0.594690	C	-6.023485	-2.625322	-0.005210
C	0.381540	-1.174250	-3.327510	C	-6.522012	-1.300108	-0.010620
C	0.749070	-2.305410	-2.592440	C	-6.648673	-0.084176	-0.011690
C	-0.249810	-3.031140	-1.829370	C	-6.434490	1.315391	-0.010200
C	-1.579560	-2.599070	-1.829370	C	-6.214476	2.009866	-1.224510
C	-1.961100	-1.424820	-2.592440	C	-6.216420	2.005462	1.206940
C	-0.998880	0.725730	-3.327510	C	-5.649203	3.276622	-1.221820
C	0.381540	1.174250	-3.327510	C	-5.651736	3.272347	1.209600
C	1.234680	0.000000	-3.327510	C	-5.281780	3.900051	-0.004670
C	2.424050	0.000000	-2.592440	C	-4.383281	4.994477	-0.001590
C	2.805590	-1.174250	-1.829370	C	-3.393922	5.712586	0.001810
C	1.983750	-2.305410	-1.829370	C	-2.074987	6.227769	0.004760
C	0.367540	-3.479660	-0.594690	C	-1.362860	6.382487	-1.209430
C	-0.367540	-3.479660	0.594690	C	-1.369053	6.386845	1.221900
C	-1.747950	-3.031140	0.594690	C	0.016415	6.527650	-1.206130
C	-2.342640	-2.599070	-0.594690	C	0.010328	6.531941	1.225230
C	-3.195780	-1.424820	-0.594690	C	0.739609	6.523855	0.011400
C	-2.959980	-0.699090	-1.829370	C	2.136788	6.294470	0.012870
C	-2.959980	0.699090	-1.829370	C	3.254028	5.798031	0.007740
C	-1.961100	1.424820	-2.592440	H	4.517860	4.800464	2.158390
C	0.749070	2.305410	-2.592440	H	5.973937	2.798417	2.149400
C	-0.249810	3.031140	-1.829370	H	5.968071	2.813128	-2.163090
C	-1.579560	2.599070	-1.829370	H	4.512642	4.815698	-2.154060
C	-2.342640	2.599070	-0.594690	H	6.421301	-1.508970	-2.166820
C	-3.195780	1.424820	-0.594690	H	6.418940	-1.496215	2.145620
C	-3.422930	0.725730	0.594690	H	5.411042	-3.769214	-2.160960
C	-3.422930	-0.725730	0.594690	H	5.410362	-3.757145	2.151630
C	-2.805590	-1.174250	1.829370	H	1.900448	-6.312523	-2.149120
C	-1.983750	-2.305410	1.829370	H	1.909519	-6.304799	2.163200
C	1.747950	-3.031140	-0.594690	H	-0.561510	-6.572450	-2.143490
C	0.249810	-3.031140	1.829370	H	-0.552457	-6.565000	2.168800
C	-0.998880	-0.725730	-3.327510	H	-4.506302	-4.793249	2.160320
C	4.360230	4.914494	0.002810	H	-4.524108	-4.823527	-2.152080
C	4.852544	4.374930	1.215950	H	-5.961763	-2.790787	2.152180
C	5.668137	3.253139	1.210840	H	-5.978936	-2.820413	-2.160270
C	6.024157	2.625413	-0.007660	H	-6.418247	1.506899	-2.166170
C	5.664653	3.261458	-1.220650	H	-6.421432	1.498532	2.146290
C	4.849229	4.383355	-1.215450	H	-5.408688	3.767450	-2.161260
C	6.523019	1.300294	-0.012160	H	-5.413659	3.759836	2.151300
C	6.649648	0.084298	-0.013380	H	-1.899500	6.304720	-2.151290

H -1.911058 6.312982 2.161060
H 0.562517 6.563969 -2.145180
H 0.551061 6.572254 2.167190

I opt C₆₀@[6]CPPA I

C 1.838771 2.948882 0.621154
C 0.767550 3.439012 -0.218687
C -0.533469 3.476135 0.273891
C -0.815693 3.037871 1.626541
C 0.219179 2.572506 2.440805
C 1.575875 2.529215 1.927023
C 2.746877 2.201240 -0.217427
C 2.245919 2.236729 -1.576965
C 1.018940 3.007440 -1.578560
C -0.046511 2.621596 -2.398927
C -1.634360 3.076621 -0.572283
C -2.096830 2.360568 1.615924
C -2.295646 1.231211 2.417605
C -1.219106 0.740167 3.259958
C 0.015788 1.398773 3.270826
C 1.248365 0.632320 3.271719
C 2.212560 1.332831 2.441427
C 3.091565 0.608990 1.628392
C 3.358930 1.052675 0.275371
C 2.372405 1.114454 -2.398178
C 3.005694 -0.085896 -1.884218
C 3.481916 -0.113728 -0.571684
C 3.277312 -1.280600 0.255331
C 3.037931 -0.839191 1.615128
C 2.116623 -1.515675 2.417555
C 1.201242 -0.766429 3.259399
C -0.078709 -1.450510 3.248138
C -1.266443 -0.710385 3.247224
C -2.595456 2.380896 0.255625
C -2.746425 -2.201127 0.217092
C -3.358722 -1.052889 -0.275769
C -3.091512 -0.609197 -1.628744
C -2.212371 -1.332966 -2.441586
C -1.575660 -2.529200 -1.927104
C -0.767337 -3.438845 0.218459
C -1.018746 -3.007339 1.578055
C -2.245532 -2.236675 1.576481
C -2.372185 -1.114629 2.397773
C -3.005523 0.085673 1.883859
C -3.481625 0.113511 0.571313
C -3.038066 0.839020 -1.615580
C -2.116655 1.515565 -2.417972
C -1.201171 0.766204 -3.259745
C -1.248249 -0.632531 -3.271899
C -0.015717 -1.398911 -3.270976
C -0.219045 -2.572494 -2.440896
C 0.815630 -3.037639 -1.626612
C 0.533397 -3.475796 -0.274186
C 0.046575 -2.621576 2.398395
C 1.401188 -2.660094 1.884341
C 1.634290 -3.076438 0.571927
C 2.595307 -2.380870 -0.256000
C 2.096700 -2.360537 -1.616062
C 2.295653 -1.231387 -2.417832
C 1.219157 -0.740371 -3.260166

C 1.266586 0.710173 -3.247558
C 0.078801 1.450329 -3.248567
C -3.277373 1.280426 -0.255697
C -1.401228 2.660109 -1.884876
C -1.838419 -2.948803 -0.621425
C 6.587123 -0.235354 -0.014417
C 6.488447 -0.966898 1.193451
C 6.144496 -2.312520 1.185342
C 5.884272 -2.990372 -0.030503
C 6.141568 -2.299505 -1.239687
C 6.483038 -0.953819 -1.231365
C 5.168505 -4.216841 -0.034360
C 4.305545 -5.085310 -0.034810
C 3.091116 -5.821525 -0.031188
C 2.407780 -6.094850 -1.240374
C 2.416902 -6.096576 1.184362
C 1.070105 -6.468802 -1.233976
C 1.080380 -6.472391 1.190838
C 0.352980 -6.587955 -0.018676
C -1.067051 -6.579728 -0.013124
C -2.250450 -6.265820 -0.006602
C -3.495694 -5.583217 0.001086
C -4.080101 -5.130693 -1.207855
C -4.066643 -5.136345 1.216940
C -5.076033 -4.163361 -1.201526
C -5.061435 -4.167063 1.223389
C -5.532436 -3.599320 0.014701
C -6.236361 -2.366052 0.021420
C -6.556874 -1.184389 0.023847
C -6.587175 0.235433 0.024358
C -6.474149 0.960605 1.236527
C -6.497167 0.960290 -1.188305
C -6.132467 2.306196 1.234711
C -6.153145 2.305998 -1.190393
C -5.884096 2.990433 0.019817
C -5.168486 4.216924 0.014300
C -4.305663 5.085605 0.012025
C -3.091216 5.821729 0.011522
C -2.412417 6.097909 -1.201326
C -2.412501 6.093687 1.223793
C -1.075818 6.473723 -1.202171
C -1.074832 6.467287 1.223014
C -0.353149 6.587869 0.010457
C 1.066898 6.579819 0.011236
C 2.250342 6.265962 0.011705
C 3.495591 5.583298 0.009603
C 4.069939 5.134713 -1.204090
C 4.076373 5.132422 1.221004
C 5.064614 4.165454 -1.206252
C 5.072225 4.164895 1.218961
C 5.532084 3.599340 0.004690
C 6.236241 2.366109 -0.000270
C 6.556692 1.184522 -0.006473
H 6.594145 -0.443070 2.139531
H 5.980435 -2.832280 2.125358
H 5.978245 -2.809060 -2.185457
H 6.584496 -0.417571 -2.170825
H 2.914075 -5.919724 -2.185679
H 2.932122 -5.921254 2.124668
H 0.537831 -6.581523 -2.174499
H 0.557316 -6.589433 2.135993

H -3.676578 -5.482636 -2.153144
H -3.654686 -5.492205 2.157216
H -5.446249 -3.763707 -2.141706
H -5.419093 -3.768591 2.168859
H -6.568163 0.429621 2.179744
H -6.610410 0.431300 -2.130649
H -5.961294 2.820990 2.176293
H -5.996572 2.820669 -2.134522
H -2.924032 5.923607 -2.143943
H -2.922575 5.917251 2.166951
H -0.549061 6.592319 -2.145235
H -0.545905 6.578348 2.165746
H 3.660294 5.488980 -2.146092
H 3.670160 5.486012 2.164658
H 5.424847 3.765250 -2.150106
H 5.439815 3.766778 2.160935

II opt C₆₀@[6]CPPA II

C 1.844135 2.949686 0.620230
C 0.771686 3.437171 -0.219135
C -0.528971 3.479502 0.272931
C -0.810555 3.041897 1.626014
C 0.225473 2.574526 2.440044
C 1.582578 2.530950 1.926426
C 2.752046 2.199510 -0.219722
C 2.250458 2.234777 -1.579351
C 1.022397 3.002036 -1.578960
C -0.043240 2.621544 -2.399665
C -1.632437 3.080992 -0.573519
C -2.089044 2.361896 1.614749
C -2.292392 1.236128 2.417994
C -1.215938 0.743274 3.257528
C 0.020369 1.400471 3.268443
C 1.251203 0.631035 3.268120
C 2.216524 1.329959 2.439501
C 3.090270 0.603436 1.625076
C 3.359733 1.048369 0.271928
C 2.374933 1.110253 -2.400381
C 3.008903 -0.090714 -1.887327
C 3.484499 -0.117931 -0.574731
C 3.278054 -1.285735 0.253631
C 3.039839 -0.844055 1.613807
C 2.116658 -1.520054 2.417104
C 1.202208 -0.768243 3.257081
C -0.079514 -1.449437 3.245939
C -1.266814 -0.707242 3.246133
C -2.591017 2.383352 0.254941
C -2.751781 -2.199357 0.219115
C -3.359495 -1.048340 -0.272544
C -3.090098 -0.603392 -1.625671
C -2.216413 -1.329885 -2.440021
C -1.582387 -2.530866 -1.926986
C -0.771503 -3.437130 0.218473
C -1.022309 -3.002039 1.578230
C -2.250163 -2.234652 1.578673
C -2.374659 -1.110259 2.399544
C -3.008609 0.090700 1.886550
C -3.484166 0.117904 0.574054
C -3.039647 0.844007 -1.614439
C -2.116496 1.519929 -2.417622

C -1.202003 0.768235 -3.257599
C -1.251072 -0.631027 -3.268669
C -0.020247 -1.400425 -3.269060
C -0.225313 -2.574494 -2.440624
C 0.810713 -3.041896 -1.626733
C 0.529127 -3.479543 -0.273624
C 0.043382 -2.621669 2.399051
C 1.400545 -2.665433 1.885589
C 1.632679 -3.081242 0.572798
C 2.591333 -2.383529 -0.255703
C 2.089318 -2.362083 -1.615456
C 2.292672 -1.236147 -2.418798
C 1.216092 -0.743282 -3.258258
C 1.266988 0.707329 -3.246864
C 0.079648 1.449386 -3.246531
C -3.277831 1.285697 -0.254365
C -1.400332 2.665286 -1.886196
C -1.843965 -2.949617 -0.620813
C 6.189264 -2.258461 -0.026621
C 5.869072 -2.928128 1.180176
C 5.126262 -4.100271 1.168359
C 4.666024 -4.653061 -0.051165
C 5.124078 -4.071019 -1.258847
C 5.870950 -2.901366 -1.247159
C 3.607030 -5.597690 -0.061050
C 2.521651 -6.162793 -0.061042
C 1.140351 -6.488267 -0.050610
C 0.400307 -6.531146 -1.257990
C 0.424112 -6.546646 1.169213
C -0.986122 -6.472492 -1.245734
C -0.962107 -6.483096 1.181471
C -1.695046 -6.363619 -0.025016
C -3.042689 -5.919100 -0.009669
C -4.075463 -5.262871 -0.000391
C -5.049259 -4.230504 0.006497
C -5.468271 -3.626243 -1.203151
C -5.446767 -3.624574 1.223886
C -6.106680 -2.394049 -1.196504
C -6.089114 -2.394678 1.230718
C -6.359443 -1.712971 0.019709
C -6.648598 -0.323683 0.023182
C -6.596546 0.898796 0.029728
C -6.189292 2.258240 0.037785
C -5.861408 2.905327 1.253462
C -5.878557 2.923901 -1.173651
C -5.114649 4.075025 1.255061
C -5.135855 4.096152 -1.171972
C -4.666228 4.653149 0.041885
C -3.607368 5.597995 0.042609
C -2.522036 6.163069 0.039928
C -1.140639 6.488333 0.032233
C -0.419864 6.545216 -1.184879
C -0.405032 6.532697 1.242302
C 0.966461 6.481984 -1.191759
C 0.981339 6.473974 1.235399
C 1.694967 6.363829 0.017592
C 3.042584 5.919414 0.008272
C 4.075478 5.263015 0.005215
C 5.049031 4.230537 0.003338
C 5.450190 3.622925 -1.212103
C 5.464374 3.627929 1.215139

C 6.092594 2.393034 -1.215272
 C 6.102760 2.395636 1.212014
 C 6.359166 1.712877 -0.002488
 C 6.648268 0.323546 -0.003872
 C 6.596339 -0.899021 -0.011956
 H 6.133828 -2.465045 2.126800
 H 4.812721 -4.551510 2.105793
 H 4.807006 -4.500834 -2.205039
 H 6.136745 -2.420008 -2.184381
 H 0.933725 -6.519190 -2.204501
 H 0.973770 -6.547209 2.106544
 H -1.533405 -6.415675 -2.182682
 H -1.492725 -6.432971 2.128279
 H -5.201384 -4.091900 -2.147939
 H -5.162090 -4.091183 2.162877
 H -6.336745 -1.898960 -2.135931
 H -6.305900 -1.902811 2.175013
 H -6.119185 2.427179 2.194509
 H -6.151169 2.457521 -2.116327
 H -4.789540 4.507964 2.197065
 H -4.830378 4.544241 -2.113562
 H -0.965813 6.544670 -2.124374
 H -0.942088 6.521731 2.186721
 H 1.500787 6.431251 -2.136450
 H 1.525026 6.417644 2.174484
 H 5.168087 4.088222 -2.152589
 H 5.194977 4.094969 2.158580
 H 6.312001 1.899760 -2.158254
 H 6.330074 1.901785 2.152767

III opt C₆₀@[6]CPPA III

C 1.282696 0.935687 3.182926
 C 1.277564 -0.512977 3.279835
 C 2.170670 -1.267537 2.511243
 C 3.095305 -0.600552 1.613684
 C 3.101967 0.791147 1.521303
 C 2.180168 1.575352 2.320708
 C -0.091763 1.395594 3.270632
 C -0.946300 0.231750 3.421202
 C -0.099678 -0.948577 3.426942
 C -0.532347 -2.122130 2.800923
 C 1.720589 -2.483995 1.860735
 C 3.209792 -1.401842 0.412770
 C 3.344493 -0.792216 -0.834173
 C 3.350756 0.651938 -0.931873
 C 3.220623 1.424358 0.223025
 C 2.379672 2.595981 0.217381
 C 1.736085 2.694388 1.511994
 C 0.415244 3.134281 1.595618
 C -0.516741 2.478081 2.493030
 C -2.193815 0.193969 2.789604
 C -2.632461 1.317575 1.982168
 C -1.810229 2.437583 1.836979
 C -1.670847 3.062349 0.537203
 C -0.301270 3.491611 0.388987
 C 0.324939 3.416858 -0.854658
 C 1.695089 2.959564 -0.943002
 C 1.827836 2.162070 -2.144874
 C 2.642950 1.025546 -2.139366
 C 2.363159 -2.560630 0.564439

C 0.091937 -1.394822 -3.271175
 C 0.517170 -2.477558 -2.493630
 C -0.414957 -3.133909 -1.596001
 C -1.735929 -2.693830 -1.512368
 C -2.180081 -1.574675 -2.321053
 C -1.277340 0.513928 -3.280245
 C 0.099918 0.949674 -3.427428
 C 0.946575 -0.230778 -3.421734
 C 2.194090 -0.193064 -2.790015
 C 2.632901 -1.316652 -1.982556
 C 1.810642 -2.437008 -1.837358
 C 0.301671 -3.491038 -0.389259
 C -0.324541 -3.416013 0.854441
 C -1.694932 -2.958538 0.942880
 C -2.379558 -2.595255 -0.217564
 C -3.220508 -1.423512 -0.223206
 C -3.101726 -0.790367 -1.521520
 C -3.094881 0.601314 -1.613798
 C -2.170341 1.268379 -2.511432
 C 0.532660 2.123305 -2.801437
 C -0.394894 2.904300 -2.003225
 C -1.720194 2.484888 -1.861000
 C -2.362722 2.561388 -0.564630
 C -3.209483 1.402636 -0.412908
 C -3.344153 0.792930 0.833954
 C -3.350484 -0.650938 0.931722
 C -2.642736 -1.024417 2.138974
 C -1.827478 -2.161004 2.144605
 C 1.671280 -3.061686 -0.537425
 C 0.395136 -2.903196 2.002985
 C -1.282421 -0.934959 -3.183461
 C 4.364009 4.932715 0.203422
 C 4.837702 4.380526 1.418166
 C 5.654534 3.257595 1.419832
 C 6.035846 2.635068 0.206615
 C 5.692643 3.282710 -1.005828
 C 4.876149 4.404471 -1.007434
 C 6.524808 1.302796 0.197680
 C 6.648905 0.085407 0.175876
 C 6.457306 -1.320449 0.141534
 C 6.272545 -1.993806 -1.090585
 C 6.205804 -2.042154 1.332958
 C 5.711570 -3.263571 -1.132950
 C 5.641436 -3.309813 1.291241
 C 5.306251 -3.917120 0.055630
 C 4.404635 -5.012609 0.011174
 C 3.415263 -5.732275 -0.024530
 C 2.095514 -6.253356 -0.067394
 C 1.412167 -6.383566 -1.301841
 C 1.351633 -6.441450 1.122332
 C 0.032344 -6.532797 -1.340736
 C -0.028952 -6.587308 1.082776
 C -0.729369 -6.553967 -0.147706
 C -2.126110 -6.302912 -0.180426
 C -3.245605 -5.808444 -0.203014
 C -4.363551 -4.933820 -0.210945
 C -4.873409 -4.409173 1.002378
 C -4.841291 -4.378804 -1.422967
 C -5.689837 -3.287391 1.006125
 C -5.658940 -3.256128 -1.419172
 C -6.036475 -2.636167 -0.203412

C -6.525633 -1.303736 -0.189782
 C -6.650157 -0.086363 -0.165469
 C -6.458573 1.319719 -0.131529
 C -6.210682 2.040935 -1.324050
 C -6.269915 1.994344 1.099282
 C -5.645369 3.308345 -1.285113
 C -5.707695 3.263723 1.138892
 C -5.305160 3.916121 -0.051159
 C -4.403253 5.011712 -0.010100
 C -3.414407 5.732294 0.022735
 C -2.094820 6.254211 0.063882
 C -1.351107 6.438704 -1.126445
 C -1.411273 6.387889 1.297735
 C 0.029529 6.584077 -1.087296
 C -0.031291 6.535833 1.336159
 C 0.730201 6.553297 0.142935
 C 2.126650 6.301485 0.173720
 C 3.246208 5.807296 0.193205
 H 4.480596 4.789176 2.359460
 H 5.931917 2.793396 2.362320
 H 5.999758 2.837555 -1.948381
 H 4.548550 4.831016 -1.951540
 H 6.490060 -1.468739 -2.016770
 H 6.368401 -1.555020 2.290565
 H 5.494510 -3.726406 -2.091914
 H 5.367384 -3.809460 2.216746
 H 1.969584 -6.273467 -2.228190
 H 1.861172 -6.379114 2.080193
 H -0.483368 -6.536517 -2.297134
 H -0.592966 -6.636320 2.010471
 H -4.543627 -4.839509 1.944059
 H -4.487708 -4.785590 -2.366533
 H -5.994874 -2.845816 1.950897
 H -5.941130 -2.790881 -2.359800
 H -6.377457 1.553921 -2.280934
 H -6.485602 1.471130 2.026870
 H -5.375540 3.807786 -2.211920
 H -5.487958 3.727462 2.096726
 H -1.860026 6.373382 -2.084303
 H -1.968740 6.281559 2.224470
 H 0.593590 6.630013 -2.014911
 H 0.483929 6.541597 2.292635

Figure 2c

I

C 0.676962 -3.402637 -1.207902
 C 1.415402 -3.270710 0.000002
 C 2.614777 -2.421385 0.000001
 C 2.984481 -1.768743 -1.207904
 C 2.265587 -1.994777 -2.440518
 C 1.128892 -2.799542 -2.440516
 C 3.445307 -0.407722 -1.207959
 C 3.011684 0.208466 -2.440670
 C 2.597627 1.538374 -2.440832
 C 2.604756 2.291874 -1.208036
 C 3.111232 1.738548 0.000002
 C 1.452461 3.150680 -1.208078
 C 0.777506 3.477911 0.000002
 C -0.692257 3.495894 0.000002

C -1.375001 3.185296 -1.208098
 C -0.660557 2.945754 -2.440890
 C 0.732427 2.928705 -2.440859
 C -2.548025 2.354935 -1.208090
 C -2.559236 1.601481 -2.440892
 C -3.005761 0.282014 -2.440746
 C -3.454417 -0.323372 -1.208008
 C -3.539036 0.421991 0.000001
 C -3.067928 1.814193 0.000002
 C -2.673300 -2.356869 0.000001
 C -1.494931 -3.235200 0.000002
 C -0.759898 -3.385097 -1.207924
 C -1.196920 -2.771158 -2.440547
 C -2.313687 -1.938848 -2.440564
 C -3.026939 -1.695351 -1.207936
 C 3.548094 0.335328 0.000001
 C 3.445301 -0.407720 1.207973
 C 2.604752 2.291868 1.208051
 C 3.011669 0.208454 2.440672
 C 2.597610 1.538376 2.440833
 C 1.452457 3.150675 1.208092
 C 0.732432 2.928687 2.440862
 C -0.660564 2.945736 2.440892
 C -1.374997 3.185290 1.208112
 C -2.548022 2.354929 1.208104
 C -2.559219 1.601482 2.440893
 C -3.005747 0.282002 2.440747
 C -3.454411 -0.323370 1.208022
 C -3.026933 -1.695348 1.207950
 C -2.313681 -1.938831 2.440565
 C -1.196905 -2.771148 2.440548
 C -0.759899 -3.385091 1.207936
 C 0.676962 -3.402630 1.207915
 C 1.128877 -2.799532 2.440517
 C 2.265581 -1.994760 2.440519
 C 2.984474 -1.768741 1.207919
 C 1.444643 1.937940 3.218326
 C -1.396771 1.972674 3.218349
 C -2.307601 -0.718821 3.218046
 C -0.029489 -2.416693 3.217899
 C 2.289364 -0.775005 3.218007
 C 2.289361 -0.775003 -3.218029
 C 1.444641 1.937937 -3.218349
 C -1.396769 1.972672 -3.218373
 C -2.307597 -0.718820 -3.218069
 C -0.029489 -2.416689 -3.217922
 C 0.737281 0.989008 -3.964990
 C -0.712757 1.006714 -3.964961
 C -1.177611 -0.366921 -3.964766
 C -0.015007 -1.233481 -3.964697
 C 1.168429 -0.395594 -3.964800
 C -0.015007 -1.233453 3.964688
 C -1.177584 -0.366913 3.964755
 C -0.712741 1.006690 3.964950
 C 0.737264 0.988983 3.964979
 C 1.168402 -0.395585 3.964790
 C -4.792388 -5.412309 1.090780
 C -3.666474 -6.230332 1.090780
 C -2.831076 -6.323367 -0.041650
 C -3.287156 -5.707309 -1.223530
 C -4.412176 -4.889934 -1.223530

C -5.139019 -4.646545 -0.041650
 C -1.426385 -6.779778 0.041650
 C -0.695848 -7.195545 -1.090780
 C -0.695298 -6.549453 1.223530
 C 0.695855 -7.195544 -1.090780
 C 0.695302 -6.549451 1.223530
 C 1.426390 -6.779772 0.041650
 C -6.007167 -3.451651 0.041650
 C -6.014036 -2.685164 1.223530
 C -6.628334 -2.885354 -1.090780
 C -6.443752 -1.362625 1.223530
 C -7.058399 -1.561755 -1.090780
 C -6.888733 -0.738492 0.041650
 C -6.888733 0.738485 -0.041650
 C -7.058408 1.561741 1.090780
 C -6.443757 1.362618 -1.223530
 C -6.628343 2.885345 1.090780
 C -6.014039 2.685157 -1.223530
 C -6.007177 3.451641 -0.041650
 C 2.831078 -6.323366 -0.041650
 C 3.666473 -6.230333 1.090780
 C 3.287164 -5.707302 -1.223530
 C 4.792394 -5.412304 1.090780
 C 4.412179 -4.889925 -1.223530
 C 5.139033 -4.646542 -0.041650
 C 6.007177 -3.451641 0.041650
 C 6.628343 -2.885345 -1.090780
 C 6.014039 -2.685157 1.223530
 C 7.058408 -1.561741 -1.090780
 C 6.443757 -1.362618 1.223530
 C 6.888733 -0.738485 0.041650
 C -5.139033 4.646542 0.041650
 C -4.792394 5.412304 -1.090780
 C -4.412179 4.889925 1.223530
 C -3.666473 6.230333 -1.090780
 C -3.287164 5.707302 1.223530
 C -2.831078 6.323366 0.041650
 C -1.426390 6.779772 -0.041650
 C -0.695855 7.195544 1.090780
 C -0.695302 6.549451 -1.223530
 C 0.695848 7.195545 1.090780
 C 0.695298 6.549453 -1.223530
 C 1.426385 6.779778 -0.041650
 C 6.888733 0.738492 -0.041650
 C 7.058399 1.561755 1.090780
 C 6.443752 1.362625 -1.223530
 C 6.628334 2.885354 1.090780
 C 6.014036 2.685164 -1.223530
 C 6.007167 3.451651 -0.041650
 C 5.139019 4.646545 0.041650
 C 4.792388 5.412309 -1.090780
 C 4.412176 4.889934 1.223530
 C 3.666474 6.230332 -1.090780
 C 3.287156 5.707309 1.223530
 C 2.831076 6.323367 0.041650
 H -5.377995 -5.314794 2.002240
 H -3.392762 -6.757147 2.002240
 H -2.678170 -5.760509 -2.122380
 H -4.650957 -4.327194 -2.122380
 H -1.226940 -7.460864 -2.002240
 H -1.219249 -6.234540 2.122380

H 1.226940 -7.460864 -2.002240
 H 1.219249 -6.234537 2.122380
 H -5.552626 -3.086153 2.122380
 H -6.716557 -3.472425 -2.002240
 H -6.306160 -0.767002 2.122380
 H -7.474844 -1.138649 -2.002240
 H -7.474854 1.138642 2.002240
 H -6.306169 0.766999 -2.122380
 H -6.716565 3.472421 2.002240
 H -5.552632 3.086151 -2.122380
 H 3.392776 -6.757140 2.002240
 H 2.678179 -5.760499 -2.122380
 H 5.378001 -5.314784 2.002240
 H 4.650963 -4.327180 -2.122380
 H 6.716565 -3.472421 -2.002240
 H 5.552632 -3.086151 2.122380
 H 7.474854 -1.138642 -2.002240
 H 6.306169 -0.766999 2.122380
 H -5.378001 5.314784 -2.002240
 H -4.650963 4.327180 2.122380
 H -3.392776 6.757140 -2.002240
 H -2.678179 5.760499 2.122380
 H -1.226940 7.460864 2.002240
 H -1.219249 6.234537 -2.122380
 H 1.226940 7.460864 2.002240
 H 1.219249 6.234540 -2.122380
 H 7.474844 1.138649 2.002240
 H 6.306160 0.767002 -2.122380
 H 6.716557 3.472425 2.002240
 H 5.552626 3.086153 -2.122380
 H 5.377995 5.314794 -2.002240
 H 4.650957 4.327194 2.122380
 H 3.392762 6.757147 -2.002240
 H 2.678170 5.760509 2.122380

II

C 0.676962 -3.402637 -1.207902
 C 1.415402 -3.270710 0.000002
 C 2.614777 -2.421385 0.000001
 C 2.984481 -1.768743 -1.207904
 C 2.265587 -1.994777 -2.440518
 C 1.128892 -2.799542 -2.440516
 C 3.445307 -0.407722 -1.207959
 C 3.011684 0.208466 -2.440670
 C 2.597627 1.538374 -2.440832
 C 2.604756 2.291874 -1.208036
 C 3.111232 1.738548 0.000002
 C 1.452461 3.150680 -1.208078
 C 0.777506 3.477911 0.000002
 C -0.692257 3.495894 0.000002
 C -1.375001 3.185296 -1.208098
 C -0.660557 2.945754 -2.440890
 C 0.732427 2.928705 -2.440859
 C -2.548025 2.354935 -1.208090
 C -2.559236 1.601481 -2.440892
 C -3.005761 0.282014 -2.440746
 C -3.454417 -0.323372 -1.208008
 C -3.539036 0.421991 0.000001
 C -3.067928 1.814193 0.000002
 C -2.673300 -2.356869 0.000001

C	-1.494931	-3.235200	0.000002	C	-6.549447	0.695294	1.223530
C	-0.759898	-3.385097	-1.207924	C	-7.195546	0.695847	-1.090780
C	-1.196920	-2.771158	-2.440547	C	-6.779781	1.426387	0.041650
C	-2.313687	-1.938848	-2.440564	C	-6.323369	2.831077	-0.041650
C	-3.026939	-1.695351	-1.207936	C	-6.230340	3.666472	1.090780
C	3.548094	0.335328	0.000001	C	-5.707305	3.287157	-1.223530
C	3.445301	-0.407720	1.207973	C	-5.412308	4.792397	1.090780
C	2.604752	2.291868	1.208051	C	-4.889931	4.412176	-1.223530
C	3.011669	0.208454	2.440672	C	-4.646549	5.139025	-0.041650
C	2.597610	1.538376	2.440833	C	0.738487	-6.888729	-0.041650
C	1.452457	3.150675	1.208092	C	1.561744	-7.058402	1.090780
C	0.732432	2.928687	2.440862	C	1.362625	-6.443756	-1.223530
C	-0.660564	2.945736	2.440892	C	2.885343	-6.628339	1.090780
C	-1.374997	3.185290	1.208112	C	2.685161	-6.014033	-1.223530
C	-2.548022	2.354929	1.208104	C	3.451650	-6.007173	-0.041650
C	-2.559219	1.601482	2.440893	C	4.646549	-5.139025	0.041650
C	-3.005747	0.282002	2.440747	C	5.412308	-4.792397	-1.090780
C	-3.454411	-0.323370	1.208022	C	4.889931	-4.412176	1.223530
C	-3.026933	-1.695348	1.207950	C	6.230340	-3.666472	-1.090780
C	-2.313681	-1.938831	2.440565	C	5.707305	-3.287157	1.223530
C	-1.196905	-2.771148	2.440548	C	6.323369	-2.831077	0.041650
C	-0.759899	-3.385091	1.207936	C	-3.451650	6.007173	0.041650
C	0.676962	-3.402630	1.207915	C	-2.885343	6.628339	-1.090780
C	1.128877	-2.799532	2.440517	C	-2.685161	6.014033	1.223530
C	2.265581	-1.994760	2.440519	C	-1.561744	7.058402	-1.090780
C	2.984474	-1.768741	1.207919	C	-1.362625	6.443756	1.223530
C	1.444643	1.937940	3.218326	C	-0.738487	6.888729	0.041650
C	-1.396771	1.972674	3.218349	C	0.738486	6.888726	-0.041650
C	-2.307601	-0.718821	3.218046	C	1.561747	7.058400	1.090780
C	-0.029489	-2.416693	3.217899	C	1.362620	6.443758	-1.223530
C	2.289364	-0.775005	3.218007	C	2.885337	6.628340	1.090780
C	2.289361	-0.775003	-3.218029	C	2.685160	6.014040	-1.223530
C	1.444641	1.937937	-3.218349	C	3.451639	6.007175	-0.041650
C	-1.396769	1.972672	-3.218373	C	6.779781	-1.426387	-0.041650
C	-2.307597	-0.718820	-3.218069	C	7.195546	-0.695847	1.090780
C	-0.029489	-2.416689	-3.217922	C	6.549447	-0.695294	-1.223530
C	0.737281	0.989008	-3.964990	C	7.195544	0.695867	1.090780
C	-0.712757	1.006714	-3.964961	C	6.549450	0.695303	-1.223530
C	-1.177611	-0.366921	-3.964766	C	6.779775	1.426398	-0.041650
C	-0.015007	-1.233481	-3.964697	C	6.323359	2.831083	0.041650
C	1.168429	-0.395594	-3.964800	C	6.230327	3.666482	-1.090780
C	-0.015007	-1.233453	3.964688	C	5.707302	3.287166	1.223530
C	-1.177584	-0.366913	3.964755	C	5.412302	4.792395	-1.090780
C	-0.712741	1.006690	3.964950	C	4.889927	4.412186	1.223530
C	0.737264	0.988983	3.964979	C	4.646541	5.139028	0.041650
C	1.168402	-0.395585	3.964790	H	-6.757139	-3.392777	2.002240
C	-6.230327	-3.666482	1.090780	H	-5.314782	-5.378007	2.002240
C	-5.412302	-4.792395	1.090780	H	-4.327187	-4.650969	-2.122380
C	-4.646541	-5.139028	-0.041650	H	-5.760500	-2.678181	-2.122380
C	-4.889927	-4.412186	-1.223530	H	-3.472423	-6.716558	-2.002240
C	-5.707302	-3.287166	-1.223530	H	-3.086154	-5.552631	2.122380
C	-6.323359	-2.831083	-0.041650	H	-1.138643	-7.474849	-2.002240
C	-3.451639	-6.007175	0.041650	H	-0.767002	-6.306165	2.122380
C	-2.885337	-6.628340	-1.090780	H	-6.234535	-1.219250	2.122380
C	-2.685160	-6.014040	1.223530	H	-7.460863	-1.226942	-2.002240
C	-1.561747	-7.058400	-1.090780	H	-6.234531	1.219248	2.122380
C	-1.362620	-6.443758	1.223530	H	-7.460861	1.226934	-2.002240
C	-0.738486	-6.888726	0.041650	H	-6.757149	3.392770	2.002240
C	-6.779775	-1.426398	0.041650	H	-5.760507	2.678173	-2.122380
C	-6.549450	-0.695303	1.223530	H	-5.314796	5.378001	2.002240
C	-7.195544	-0.695867	-1.090780	H	-4.327194	4.650962	-2.122380

H 1.138650 -7.474847 2.002240
H 0.767008 -6.306163 -2.122380
H 3.472424 -6.716553 2.002240
H 3.086156 -5.552620 -2.122380
H 5.314796 -5.378001 -2.002240
H 4.327194 -4.650962 2.122380
H 6.757149 -3.392770 -2.002240
H 5.760507 -2.678173 2.122380
H -3.472424 6.716553 -2.002240
H -3.086156 5.552620 2.122380
H -1.138650 7.474847 -2.002240
H -0.767008 6.306163 2.122380
H 1.138643 7.474849 2.002240
H 0.767002 6.306165 -2.122380
H 3.472423 6.716558 2.002240
H 3.086154 5.552631 -2.122380
H 7.460861 -1.226934 2.002240
H 6.234531 -1.219248 -2.122380
H 7.460863 1.226942 2.002240
H 6.234535 1.219250 -2.122380
H 6.757139 3.392777 -2.002240
H 5.760500 2.678181 2.122380
H 5.314782 5.378007 -2.002240
H 4.327187 4.650969 2.122380

III

C -1.207784 -3.402658 -0.676867
C 0.000115 -3.270724 -1.415307
C 0.000108 -2.421416 -2.614695
C -1.207797 -1.768781 -2.984404
C -2.440416 -1.994827 -2.265514
C -2.440410 -2.799575 -1.128806
C -1.207870 -0.407766 -3.445247
C -2.440587 0.208415 -3.011626
C -2.440761 1.538319 -2.597589
C -1.207978 2.291831 -2.604724
C 0.000067 1.738518 -3.111187
C -1.208029 3.150653 -1.452433
C 0.000046 3.477902 -0.777484
C 0.000043 3.495896 0.692285
C -1.208054 3.185301 1.375026
C -2.440840 2.945732 0.660586
C -2.440808 2.928668 -0.732403
C -1.208037 2.354943 2.548054
C -2.440830 1.601481 2.559279
C -2.440677 0.282015 3.005813
C -1.207932 -0.323347 3.454481
C 0.000069 0.422025 3.539095
C 0.000056 1.814220 3.067971
C 0.000099 -2.356843 2.673383
C 0.000109 -3.235185 1.495022
C -1.207807 -3.385104 0.759991
C -2.440444 -2.771172 1.197003
C -2.440464 -1.938851 2.313765
C -1.207848 -1.695331 3.027014
C 0.000082 0.335294 -3.548033
C 1.208059 -0.407742 -3.445233
C 1.208111 2.291856 -2.604710
C 2.440752 0.208444 -3.011608
C 2.440898 1.538378 -2.597561

C 1.208140 3.150677 -1.452429
C 2.440911 2.928707 -0.732395
C 2.440939 2.945771 0.660594
C 1.208155 3.185315 1.375030
C 1.208152 2.354967 2.548058
C 2.440949 1.601530 2.559268
C 2.440822 0.282054 3.005811
C 1.208097 -0.323323 3.454475
C 1.208041 -1.695307 3.027008
C 2.440665 -1.938782 2.313763
C 2.440655 -2.771113 1.197001
C 1.208052 -3.385070 0.759995
C 1.208025 -3.402624 -0.676863
C 2.440629 -2.799516 -1.128787
C 2.440623 -1.994758 -2.265495
C 1.208022 -1.768757 -2.984390
C 3.218393 1.937957 -1.444594
C 3.218407 1.972716 1.396815
C 3.218133 -0.718764 2.307672
C 3.218004 -2.416657 0.029579
C 3.218101 -0.774990 -2.289286
C -3.217938 -0.775055 -2.289297
C -3.218286 1.937893 -1.444604
C -3.218312 1.972651 1.396804
C -3.217986 -0.718829 2.307661
C -3.217815 -2.416721 0.029568
C -3.964918 0.988962 -0.737236
C -3.964891 1.006677 0.712803
C -3.964688 -0.366947 1.177667
C -3.964607 -1.233519 0.015075
C -3.964714 -0.395641 -1.168372
C 3.964782 -1.233410 0.015088
C 3.964841 -0.366858 1.177650
C 3.965018 1.006736 0.712796
C 3.965051 0.989012 -0.737203
C 3.964875 -0.395562 -1.168329
C -5.331875 -4.881719 1.090780
C -4.297636 -5.812950 1.090780
C -3.476539 -5.992799 -0.041650
C -3.865725 -5.332442 -1.223530
C -4.899143 -4.401948 -1.223530
C -5.596563 -4.083917 -0.041650
C -2.127250 -6.593540 0.041650
C -1.444176 -7.083391 -1.090780
C -1.376094 -6.440895 1.223530
C -0.060095 -7.228863 -1.090780
C 0.006889 -6.586251 1.223530
C 0.709897 -6.891730 0.041650
C -6.335055 -2.804823 0.041650
C -6.261767 -2.041816 1.223530
C -6.893625 -2.176698 -1.090780
C -6.550886 -0.681605 1.223530
C -7.182980 -0.815396 -1.090780
C -6.928189 -0.014377 0.041650
C -6.773803 1.454508 -0.041650
C -6.856495 2.290990 1.090780
C -6.266025 2.028709 -1.223530
C -6.290432 3.562390 1.090780
C -5.700418 3.299086 -1.223530
C -5.613474 4.060653 -0.041650
C 2.154597 -6.584654 -0.041650

C 2.995141 -6.579454 1.090780
 C 2.672581 -6.019639 -1.223530
 C 4.200401 -5.883597 1.090780
 C 3.876872 -5.324335 -1.223530
 C 4.625184 -5.158263 -0.041650
 C 5.613474 -4.060653 0.041650
 C 6.290432 -3.562390 -1.090780
 C 5.700418 -3.299086 1.223530
 C 6.856495 -2.290990 -1.090780
 C 6.266025 -2.028709 1.223530
 C 6.773803 -1.454508 0.041650
 C -4.625184 5.158263 0.041650
 C -4.200401 5.883597 -1.090780
 C -3.876872 5.324335 1.223530
 C -2.995141 6.579454 -1.090780
 C -2.672581 6.019639 1.223530
 C -2.154597 6.584654 0.041650
 C -0.709897 6.891730 -0.041650
 C 0.060095 7.228863 1.090780
 C -0.006889 6.586251 -1.223530
 C 1.444176 7.083391 1.090780
 C 1.376094 6.440895 -1.223530
 C 2.127250 6.593540 -0.041650
 C 6.928189 0.014377 -0.041650
 C 7.182980 0.815396 1.090780
 C 6.550886 0.681605 -1.223530
 C 6.893625 2.176698 1.090780
 C 6.261767 2.041816 -1.223530
 C 6.335055 2.804823 -0.041650
 C 5.596563 4.083917 0.041650
 C 5.331875 4.881719 -1.090780
 C 4.899143 4.401948 1.223530
 C 4.297636 5.812950 -1.090780
 C 3.865725 5.332442 1.223530
 C 3.476539 5.992799 0.041650
 H -5.904081 -4.723525 2.002240
 H -4.080491 -6.365490 2.002240
 H -3.265636 -5.449007 -2.122380
 H -5.077794 -3.817332 -2.122380
 H -2.000091 -7.291743 -2.002240
 H -1.864257 -6.072941 2.122380
 H 0.440346 -7.548243 -2.002240
 H 0.560883 -6.327829 2.122380
 H -5.844799 -2.488839 2.122380
 H -7.042730 -2.751331 -2.002240
 H -6.351788 -0.103627 2.122380
 H -7.552918 -0.351077 -2.002240
 H -7.314886 1.913739 2.002240
 H -6.191450 1.421972 -2.122380
 H -6.316804 4.155471 2.002240
 H -5.199624 3.649653 -2.122380
 H 2.667876 -7.074765 2.002240
 H 2.061372 -6.008888 -2.122380
 H 4.792994 -5.847823 2.002240
 H 4.173171 -4.789634 -2.122380
 H 6.316804 -4.155471 -2.002240
 H 5.199624 -3.649653 2.122380
 H 7.314886 -1.913739 -2.002240
 H 6.191450 -1.421972 2.122380
 H -4.792994 5.847823 -2.002240
 H -4.173171 4.789634 2.122380

H -2.667876 7.074765 -2.002240
 H -2.061372 6.008888 2.122380
 H -0.440346 7.548243 2.002240
 H -0.560883 6.327829 -2.122380
 H 2.000091 7.291743 2.002240
 H 1.864257 6.072941 -2.122380
 H 7.552918 0.351077 2.002240
 H 6.351788 0.103627 -2.122380
 H 7.042730 2.751331 2.002240
 H 5.844799 2.488839 -2.122380
 H 5.904081 4.723525 -2.002240
 H 5.077794 3.817332 2.122380
 H 4.080491 6.365490 -2.002240
 H 3.265636 5.449007 2.122380

III opt C₇₀@[10]CPP IIIb

C -0.872631 -3.516473 -0.607602
 C 0.290909 -3.392092 -1.407513
 C 0.179277 -2.750499 -2.724335
 C -1.094905 -2.276684 -3.139303
 C -2.276275 -2.498346 -2.340448
 C -2.160749 -3.101529 -1.092026
 C -1.239073 -1.007494 -3.800084
 C -2.512916 -0.447960 -3.411869
 C -2.627492 0.925310 -3.199060
 C -1.474448 1.778206 -3.369598
 C -0.232584 1.266292 -3.837665
 C -1.524466 2.796570 -2.354773
 C -0.336208 3.325217 -1.782856
 C -0.296634 3.550289 -0.334011
 C -1.444562 3.241448 0.434650
 C -2.661046 2.789662 -0.184127
 C -2.704118 2.570931 -1.556859
 C -1.338459 2.614447 1.721831
 C -2.494135 1.769848 1.898886
 C -2.357829 0.540564 2.542001
 C -1.062308 0.124366 3.028976
 C 0.072222 0.979807 2.951326
 C -0.074289 2.275836 2.273696
 C 0.314212 -1.886358 2.506805
 C 0.365869 -2.923649 1.467248
 C -0.836874 -3.286990 0.808622
 C -2.108604 -2.732939 1.201967
 C -2.162827 -1.750581 2.188460
 C -0.942129 -1.292108 2.810593
 C -0.110182 -0.181455 -4.061045
 C 1.166769 -0.787902 -3.898769
 C 0.930250 1.998147 -3.468267
 C 2.346481 -0.003507 -3.611517
 C 2.229236 1.369342 -3.398747
 C 0.877830 3.016154 -2.453540
 C 2.140904 3.014800 -1.756238
 C 2.170425 3.227483 -0.381799
 C 0.946996 3.458667 0.338236
 C 1.060343 2.835130 1.624659
 C 2.357460 2.207254 1.697186
 C 2.500720 0.981247 2.342030
 C 1.344630 0.342768 2.929744
 C 1.463630 -1.073076 2.709462
 C 2.691983 -1.308251 1.985994

C	2.733316	-2.287489	0.998493	C	6.909357	-1.649116	0.446933
C	1.557772	-3.068436	0.709421	C	-4.510102	5.151928	0.551758
C	1.516594	-3.292439	-0.706053	C	-4.004160	5.833357	-0.577282
C	2.668888	-2.659015	-1.292740	C	-3.758249	5.277884	1.736991
C	2.573839	-2.056163	-2.542403	C	-2.755297	6.449539	-0.563586
C	1.308542	-2.057446	-3.239896	C	-2.511425	5.892735	1.750843
C	2.991737	2.005969	-2.347152	C	-1.930942	6.427695	0.582054
C	3.052134	2.456359	0.457538	C	-0.475194	6.707269	0.534201
C	3.348369	-0.039037	1.765150	C	0.292715	6.872314	1.706802
C	3.433021	-2.041634	-0.238982	C	0.253259	6.584334	-0.667422
C	3.231721	-0.790456	-2.780666	C	1.674616	6.720084	1.702364
C	-3.170313	-1.375526	-2.516707	C	1.637899	6.430954	-0.671710
C	-3.401302	1.419701	-2.082756	C	2.382592	6.389886	0.525350
C	-3.324463	1.882712	0.721319	C	7.185408	-0.190276	0.439256
C	-3.051781	-0.620545	2.030301	C	7.292387	0.557798	1.633622
C	-2.935468	-2.621488	0.026086	C	7.074524	0.563250	-0.745753
C	-4.023973	0.525479	-1.208846	C	7.056193	1.927299	1.660972
C	-3.984755	0.763713	0.218540	C	6.835472	1.935334	-0.717992
C	-3.844598	-0.511273	0.883458	C	6.692349	2.640401	0.496030
C	-3.789906	-1.535322	-0.134707	C	5.928453	3.912951	0.558176
C	-3.909021	-0.897409	-1.429104	C	5.576881	4.653915	-0.592222
C	4.064423	-0.820960	-0.459572	C	5.269514	4.285209	1.748596
C	4.014983	0.202691	0.560086	C	4.518530	5.560019	-0.586873
C	3.863368	1.475205	-0.104316	C	4.213594	5.189258	1.753873
C	3.833092	1.243407	-1.532438	C	3.739934	5.789572	0.569178
C	3.960569	-0.179723	-1.753862	H	-6.103162	-4.548346	2.166458
C	-5.600619	-4.719572	1.218163	H	-4.261829	-6.121635	2.107902
C	-4.543853	-5.621598	1.184963	H	-3.799673	-5.419467	-2.112864
C	-3.788170	-5.836595	0.010616	H	-5.620911	-3.838028	-2.053523
C	-4.313857	-5.268968	-1.168288	H	-2.206708	-6.877400	-2.045343
C	-5.367971	-4.358130	-1.133852	H	-2.157995	-6.031898	2.176698
C	-5.967291	-3.965915	0.080735	H	0.208068	-7.146070	-2.011090
C	-2.409219	-6.383834	0.055059	H	0.227892	-6.294079	2.210571
C	-1.685408	-6.755410	-1.099040	H	-6.375618	-2.477135	2.331082
C	-1.668234	-6.325350	1.253138	H	-7.236216	-2.440219	-1.889067
C	-0.299423	-6.908496	-1.079388	H	-6.797996	-0.118476	2.445886
C	-0.286824	-6.476776	1.272369	H	-7.663785	-0.055868	-1.772225
C	0.456438	-6.701282	0.095682	H	-7.253330	1.940421	2.479056
C	-6.690845	-2.674571	0.196245	H	-6.633396	1.801247	-1.779449
C	-6.703397	-1.979379	1.423530	H	-6.091966	4.068351	2.571190
C	-7.143457	-1.945700	-0.925453	H	-5.477110	3.910616	-1.686245
C	-6.946504	-0.612243	1.490314	H	2.247619	-6.835839	2.210819
C	-7.387491	-0.575471	-0.858379	H	2.107733	-6.134387	-2.033552
C	-7.196611	0.156236	0.334699	H	4.417429	-5.764697	2.314601
C	-6.970099	1.623433	0.351728	H	4.278080	-5.077430	-1.931149
C	-6.867338	2.359046	1.553223	H	6.264476	-4.220277	-1.715830
C	-6.562669	2.299039	-0.817492	H	5.170030	-3.803731	2.428177
C	-6.200397	3.578782	1.606804	H	7.407239	-2.074660	-1.619088
C	-5.894787	3.518072	-0.764330	H	6.295013	-1.686279	2.523800
C	-5.595981	4.144569	0.461837	H	-4.570509	5.832123	-1.505025
C	1.926621	-6.493443	0.092951	H	-4.086668	4.771770	2.640044
C	2.673200	-6.443192	1.291326	H	-2.392627	6.910180	-1.479211
C	2.613174	-6.098554	-1.072468	H	-1.928152	5.837877	2.665149
C	3.919193	-5.829970	1.350884	H	-0.203847	7.069374	2.653351
C	3.866068	-5.488083	-1.013785	H	-0.277434	6.471782	-1.608283
C	4.507513	-5.231398	0.214387	H	2.204894	6.805848	2.646995
C	5.557403	-4.188034	0.332000	H	2.123090	6.202684	-1.616097
C	6.273483	-3.678565	-0.773108	H	7.491661	0.049259	2.573218
C	5.696122	-3.470470	1.539047	H	7.018042	0.054809	-1.703807
C	6.928293	-2.448749	-0.717575	H	7.081522	2.432864	2.622449
C	6.346899	-2.245302	1.594571	H	6.607663	2.427802	-1.658421

H	6.093153	4.473160	-1.531436
H	5.488126	3.764134	2.675487
H	4.253566	6.048302	-1.521216
H	3.670179	5.322833	2.684198

Figure 2d

I

C	0.676962	-3.402637	-1.207902
C	1.415402	-3.270710	0.000002
C	2.614777	-2.421385	0.000001
C	2.984481	-1.768743	-1.207904
C	2.265587	-1.994777	-2.440518
C	1.128892	-2.799542	-2.440516
C	3.445307	-0.407722	-1.207959
C	3.011684	0.208466	-2.440670
C	2.597627	1.538374	-2.440832
C	2.604756	2.291874	-1.208036
C	3.111232	1.738548	0.000002
C	1.452461	3.150680	-1.208078
C	0.777506	3.477911	0.000002
C	-0.692257	3.495894	0.000002
C	-1.375001	3.185296	-1.208098
C	-0.660557	2.945754	-2.440890
C	0.732427	2.928705	-2.440859
C	-2.548025	2.354935	-1.208090
C	-2.559236	1.601481	-2.440892
C	-3.005761	0.282014	-2.440746
C	-3.454417	-0.323372	-1.208008
C	-3.539036	0.421991	0.000001
C	-3.067928	1.814193	0.000002
C	-2.673300	-2.356869	0.000001
C	-1.494931	-3.235200	0.000002
C	-0.759898	-3.385097	-1.207924
C	-1.196920	-2.771158	-2.440547
C	-2.313687	-1.938848	-2.440564
C	-3.026939	-1.695351	-1.207936
C	3.548094	0.335328	0.000001
C	3.445301	-0.407720	1.207973
C	2.604752	2.291868	1.208051
C	3.011669	0.208454	2.440672
C	2.597610	1.538376	2.440833
C	1.452457	3.150675	1.208092
C	0.732432	2.928687	2.440862
C	-0.660564	2.945736	2.440892
C	-1.374997	3.185290	1.208112
C	-2.548022	2.354929	1.208104
C	-2.559219	1.601482	2.440893
C	-3.005747	0.282002	2.440747
C	-3.454411	-0.323370	1.208022
C	-3.026933	-1.695348	1.207950
C	-2.313681	-1.938831	2.440565
C	-1.196905	-2.771148	2.440548
C	-0.759899	-3.385091	1.207936
C	0.676962	-3.402630	1.207915
C	1.128877	-2.799532	2.440517
C	2.265581	-1.994760	2.440519
C	2.984474	-1.768741	1.207919
C	1.444643	1.937940	3.218326
C	-1.396771	1.972674	3.218349

C	-2.307601	-0.718821	3.218046
C	-0.029489	-2.416693	3.217899
C	2.289364	-0.775005	3.218007
C	2.289361	-0.775003	-3.218029
C	1.444641	1.937937	-3.218349
C	-1.396769	1.972672	-3.218373
C	-2.307597	-0.718820	-3.218069
C	-0.029489	-2.416689	-3.217922
C	0.737281	0.989008	-3.964990
C	-0.712757	1.006714	-3.964961
C	-1.177611	-0.366921	-3.964766
C	-0.015007	-1.233481	-3.964697
C	1.168429	-0.395594	-3.964800
C	-0.015007	-1.233453	3.964688
C	-1.177584	-0.366913	3.964755
C	-0.712741	1.006690	3.964950
C	0.737264	0.988983	3.964979
C	1.168402	-0.395585	3.964790
C	4.431771	-4.850079	0.002810
C	3.843699	-5.283292	1.215950
C	2.642796	-5.977150	1.210840
C	1.981292	-6.265600	-0.007660
C	2.651434	-5.974554	-1.220650
C	3.852424	-5.280876	-1.215450
C	0.611285	-6.623207	-0.012160
C	-0.611285	-6.622028	-0.013380
C	-1.980686	-6.262209	-0.011040
C	-2.649622	-5.971860	-1.224900
C	-2.642722	-5.971525	1.206520
C	-3.850091	-5.276947	-1.221690
C	-3.843331	-5.277097	1.209740
C	-4.430253	-4.844734	-0.004380
C	-5.424496	-3.836628	-0.000980
C	-6.035345	-2.777597	0.003070
C	-6.410242	-1.412243	0.006710
C	-6.494450	-0.688095	-1.207310
C	-6.490393	-0.693349	1.224030
C	-6.495047	0.698794	-1.204300
C	-6.490974	0.693580	1.227050
C	-6.411425	1.417826	0.012790
C	-6.037552	2.783509	0.013410
C	-5.426973	3.842675	0.007910
C	-4.432221	4.850190	0.004350
C	-3.840458	5.276369	1.218230
C	-3.856240	5.287541	-1.213150
C	-2.639370	5.969872	1.213580
C	-2.654932	5.980887	-1.217890
C	-1.981273	6.264922	-0.005210
C	-0.611205	6.622186	-0.010620
C	0.611305	6.621045	-0.011690
C	1.980815	6.261732	-0.010200
C	2.648486	5.970326	-1.224510
C	2.644309	5.972720	1.206940
C	3.849211	5.275730	-1.221820
C	3.845224	5.278695	1.209600
C	4.430815	4.845150	-0.004670
C	5.425320	3.837168	-0.001590
C	6.036072	2.778161	0.001810
C	6.410558	1.412597	0.004760
C	6.489985	0.688199	-1.209430
C	6.494967	0.693902	1.221900

C 6.490170 -0.698694 -1.206130
 C 6.495074 -0.693089 1.225230
 C 6.410797 -1.417530 0.011400
 C 6.036614 -2.783074 0.012870
 C 5.426104 -3.842298 0.007740
 H 4.301888 -4.994925 2.158390
 H 2.158598 -6.233740 2.149400
 H 2.173842 -6.229444 -2.163090
 H 4.317584 -4.991328 -2.154060
 H -2.171955 -6.228379 -2.166820
 H -2.159023 -6.227364 2.145620
 H -4.314208 -4.987380 -2.160960
 H -4.302133 -4.987965 2.151630
 H -6.476602 -1.230155 -2.149120
 H -6.469868 -1.239984 2.163200
 H -6.477743 1.245486 -2.143490
 H -6.471280 1.235704 2.168800
 H -4.295920 4.982677 2.160320
 H -4.324172 5.003549 -2.152080
 H -2.152283 6.220835 2.152180
 H -2.179951 6.241011 -2.160270
 H 2.169576 6.225559 -2.166170
 H 2.161588 6.229600 2.146290
 H 4.312207 4.985224 -2.161260
 H 4.305154 4.990964 2.151300
 H 6.468742 1.230028 -2.151290
 H 6.478167 1.240659 2.161060
 H 6.469203 -1.245601 -2.145180
 H 6.478641 -1.235073 2.167190

II

C -1.207784 -3.402658 -0.676867
 C 0.000115 -3.270724 -1.415307
 C 0.000108 -2.421416 -2.614695
 C -1.207797 -1.768781 -2.984404
 C -2.440416 -1.994827 -2.265514
 C -2.440410 -2.799575 -1.128806
 C -1.207870 -0.407766 -3.445247
 C -2.440587 0.208415 -3.011626
 C -2.440761 1.538319 -2.597589
 C -1.207978 2.291831 -2.604724
 C 0.000067 1.738518 -3.111187
 C -1.208029 3.150653 -1.452433
 C 0.000046 3.477902 -0.777484
 C 0.000043 3.495896 0.692285
 C -1.208054 3.185301 1.375026
 C -2.440840 2.945732 0.660586
 C -2.440808 2.928668 -0.732403
 C -1.208037 2.354943 2.548054
 C -2.440830 1.601481 2.559279
 C -2.440677 0.282015 3.005813
 C -1.207932 -0.323347 3.454481
 C 0.000069 0.422025 3.539095
 C 0.000056 1.814220 3.067971
 C 0.000099 -2.356843 2.673383
 C 0.000109 -3.235185 1.495022
 C -1.207807 -3.385104 0.759991
 C -2.440444 -2.771172 1.197003
 C -2.440464 -1.938851 2.313765
 C -1.207848 -1.695331 3.027014

C 0.000082 0.335294 -3.548033
 C 1.208059 -0.407742 -3.445233
 C 1.208111 2.291856 -2.604710
 C 2.440752 0.208444 -3.011608
 C 2.440898 1.538378 -2.597561
 C 1.208140 3.150677 -1.452429
 C 2.440911 2.928707 -0.732395
 C 2.440939 2.945771 0.660594
 C 1.208155 3.185315 1.375030
 C 1.208152 2.354967 2.548058
 C 2.440949 1.601530 2.559268
 C 2.440822 0.282054 3.005811
 C 1.208097 -0.323323 3.454475
 C 1.208041 -1.695307 3.027008
 C 2.440665 -1.938782 2.313763
 C 2.440655 -2.771113 1.197001
 C 1.208052 -3.385070 0.759995
 C 1.208025 -3.402624 -0.676863
 C 2.440629 -2.799516 -1.128787
 C 2.440623 -1.994758 -2.265495
 C 1.208022 -1.768757 -2.984390
 C 3.218393 1.937957 -1.444594
 C 3.218407 1.972716 1.396815
 C 3.218133 -0.718764 2.307672
 C 3.218004 -2.416657 0.029579
 C 3.218101 -0.774990 -2.289286
 C -3.217938 -0.775055 -2.289297
 C -3.218286 1.937893 -1.444604
 C -3.218312 1.972651 1.396804
 C -3.217986 -0.718829 2.307661
 C -3.217815 -2.416721 0.029568
 C -3.964918 0.988962 -0.737236
 C -3.964891 1.006677 0.712803
 C -3.964688 -0.366947 1.177667
 C -3.964607 -1.233519 0.015075
 C -3.964714 -0.395641 -1.168372
 C 3.964782 -1.233410 0.015088
 C 3.964841 -0.366858 1.177650
 C 3.965018 1.006736 0.712796
 C 3.965051 0.989012 -0.737203
 C 3.964875 -0.395562 -1.168329
 C 5.982192 2.716107 0.002810
 C 6.212477 2.022948 1.215950
 C 6.501277 0.666407 1.210840
 C 6.571192 -0.051855 -0.007660
 C 6.501477 0.675424 -1.220650
 C 6.212876 2.031993 -1.215450
 C 6.487942 -1.465316 -0.012160
 C 6.109025 -2.627686 -0.013380
 C 5.343649 -3.818873 -0.011040
 C 4.860798 -4.365347 -1.224900
 C 4.862612 -4.358681 1.206520
 C 3.828931 -5.292321 -1.221690
 C 3.831163 -5.285938 1.209740
 C 3.238592 -5.710527 -0.004380
 C 1.972588 -6.344586 -0.000980
 C 0.776628 -6.598279 0.003070
 C -0.637750 -6.532910 0.006710
 C -1.352477 -6.389222 -1.207310
 C -1.346226 -6.386987 1.224030
 C -2.671673 -5.961217 -1.204300

C -2.665455 -5.958955 1.227050
 C -3.329672 -5.659495 0.012790
 C -4.512981 -4.881902 0.013410
 C -5.331628 -3.973906 0.007910
 C -5.982437 -2.716502 0.004350
 C -6.204892 -2.022005 1.218230
 C -6.220394 -2.033562 -1.213150
 C -6.493296 -0.665398 1.213580
 C -6.508581 -0.676794 -1.217890
 C -6.570542 0.051664 -0.005210
 C -6.486946 1.465077 -0.010620
 C -6.108085 2.627401 -0.011690
 C -5.343155 3.818849 -0.010200
 C -4.859690 4.363792 -1.224510
 C -4.863258 4.360560 1.206940
 C -3.828046 5.291107 -1.221820
 C -3.832098 5.288232 1.209600
 C -3.238814 5.711189 -0.004670
 C -1.972847 6.345536 -0.001590
 C -0.776939 6.599144 0.001810
 C 0.637511 6.533319 0.004760
 C 1.350999 6.385008 -1.209430
 C 1.347114 6.391508 1.221900
 C 2.670070 5.956610 -1.206130
 C 2.666255 5.963006 1.225230
 C 3.329196 5.658989 0.011400
 C 4.512277 4.881144 0.012870
 C 5.331001 3.973196 0.007740
 H 6.079813 2.547822 2.158390
 H 6.595682 0.126617 2.149400
 H 6.596308 0.142442 -2.163090
 H 6.081242 2.563861 -2.154060
 H 5.252369 -3.990327 -2.166820
 H 5.255401 -3.977714 2.145620
 H 3.410117 -5.644241 -2.160960
 H 3.414404 -5.632938 2.151630
 H -0.831432 -6.539753 -2.149120
 H -0.820004 -6.536387 2.163200
 H -3.186261 -5.775824 -2.143490
 H -3.174960 -5.772700 2.168800
 H -6.066319 -2.545931 2.160320
 H -6.094901 -2.566350 -2.152080
 H -6.581458 -0.124599 2.152180
 H -6.609197 -0.144678 -2.160270
 H -5.250422 3.987193 -2.166170
 H -5.256735 3.980845 2.146290
 H -3.408684 5.641672 -2.161260
 H -3.416322 5.636738 2.151300
 H 0.829124 6.532239 -2.151290
 H 0.821926 6.544488 2.161060
 H 3.183731 5.767666 -2.145180
 H 3.176635 5.779894 2.167190

II opt

C -1.203993 -3.343304 -0.674487
 C -0.013419 -3.232606 -1.425105
 C -0.013724 -2.414459 -2.643635
 C -1.221499 -1.769331 -3.022302
 C -2.445191 -1.987081 -2.288246
 C -2.427038 -2.760439 -1.132229

C -1.223651 -0.409404 -3.491877
 C -2.455238 0.207664 -3.052210
 C -2.448728 1.536640 -2.627147
 C -1.216901 2.286530 -2.634224
 C -0.012979 1.735691 -3.150389
 C -1.206803 3.120347 -1.459912
 C -0.011247 3.426430 -0.776399
 C -0.011394 3.442170 0.688103
 C -1.206282 3.152924 1.379303
 C -2.411966 2.893547 0.656015
 C -2.412877 2.878305 -0.730146
 C -1.216895 2.349832 2.574528
 C -2.448495 1.600087 2.586125
 C -2.455612 0.282344 3.044844
 C -1.224190 -0.323735 3.499955
 C -0.013279 0.421982 3.583903
 C -0.013343 1.812196 3.104873
 C -0.014149 -2.350088 2.703188
 C -0.013739 -3.199785 1.505882
 C -1.204733 -3.328249 0.757644
 C -2.428597 -2.734091 1.200501
 C -2.446105 -1.931123 2.336491
 C -1.222142 -1.695200 3.064967
 C -0.012733 0.333871 -3.594273
 C 1.198098 -0.408867 -3.489197
 C 1.192325 2.283175 -2.630268
 C 2.428990 0.206261 -3.047730
 C 2.424951 1.533789 -2.623432
 C 1.183565 3.110497 -1.457086
 C 2.396415 2.878721 -0.731559
 C 2.395017 2.893620 0.657357
 C 1.182487 3.142878 1.376415
 C 1.191499 2.346475 2.570905
 C 2.423933 1.597559 2.583089
 C 2.428305 0.281104 3.040933
 C 1.197558 -0.323103 3.497612
 C 1.194643 -1.695970 3.063740
 C 2.416393 -1.935398 2.336783
 C 2.394278 -2.735696 1.198726
 C 1.174468 -3.340135 0.760784
 C 1.174021 -3.355317 -0.676884
 C 2.393804 -2.762902 -1.129684
 C 2.416070 -1.991325 -2.287447
 C 1.194987 -1.770099 -3.020617
 C 3.179969 1.919882 -1.453060
 C 3.178506 1.954231 1.403344
 C 3.194832 -0.719045 2.328263
 C 3.146091 -2.373858 0.029793
 C 3.195090 -0.776052 -2.309914
 C -3.221632 -0.770268 -2.316158
 C -3.198868 1.917786 -1.454652
 C -3.197624 1.951621 1.404148
 C -3.222169 -0.713490 2.333393
 C -3.178589 -2.372750 0.029221
 C -3.924005 0.977722 -0.737587
 C -3.923669 0.995039 0.711187
 C -3.926993 -0.358976 1.179230
 C -3.906213 -1.204630 0.014292
 C -3.926781 -0.387721 -1.171350
 C 3.891917 -1.215210 0.015066
 C 3.909499 -0.367775 1.180780

C	3.898557	0.988647	0.709351
C	3.899334	0.971113	-0.734480
C	3.909734	-0.396857	-1.171463
C	6.238972	2.867949	0.002658
C	6.539169	2.166786	1.201693
C	6.878162	0.811094	1.197695
C	6.944632	0.059064	-0.005867
C	6.876922	0.818186	-1.204961
C	6.538193	2.173944	-1.200682
C	6.839156	-1.378380	-0.009347
C	6.463994	-2.553118	-0.010884
C	5.699456	-3.776224	-0.009993
C	5.187889	-4.336802	-1.210661
C	5.191317	-4.334633	1.193282
C	4.105701	-5.220965	-1.207409
C	4.109102	-5.218699	1.195459
C	3.458994	-5.614638	-0.004498
C	2.131159	-6.176809	-0.001431
C	0.919810	-6.406815	0.002230
C	-0.522057	-6.409860	0.005479
C	-1.278036	-6.317337	-1.194332
C	-1.273111	-6.314063	1.207839
C	-2.631074	-5.967203	-1.192164
C	-2.626157	-5.963319	1.210113
C	-3.332940	-5.682199	0.010028
C	-4.580550	-4.956798	0.010725
C	-5.484944	-4.118194	0.009233
C	-6.261013	-2.900603	0.006224
C	-6.545524	-2.193414	1.205350
C	-6.546576	-2.200483	-1.196688
C	-6.863457	-0.831553	1.201140
C	-6.864256	-0.838570	-1.200184
C	-6.924947	-0.076713	-0.001714
C	-6.795749	1.361361	-0.005492
C	-6.396747	2.529864	-0.007706
C	-5.627291	3.749723	-0.007674
C	-5.131043	4.328701	-1.208026
C	-5.134996	4.328932	1.194126
C	-4.078691	5.248553	-1.206302
C	-4.082034	5.248110	1.195810
C	-3.436861	5.649415	-0.004247
C	-2.099976	6.188004	-0.001527
C	-0.888941	6.416337	0.003148
C	0.552860	6.434876	0.005834
C	1.304750	6.331838	-1.194930
C	1.304609	6.345072	1.207879
C	2.657080	5.985055	-1.193188
C	2.657201	5.997617	1.210010
C	3.359964	5.710553	0.009780
C	4.583874	4.948519	0.010410
C	5.454358	4.075770	0.006646
H	6.383358	2.662696	2.156077
H	6.980551	0.295711	2.149040
H	6.978205	0.308422	-2.159442
H	6.381639	2.675461	-2.151976
H	5.568076	-3.980596	-2.164526
H	5.574209	-3.975972	2.145174
H	3.684898	-5.534138	-2.159163
H	3.691149	-5.529608	2.149202
H	-0.768990	-6.426744	-2.148239
H	-0.760287	-6.420742	2.160032

H	-3.132139	-5.813984	-2.144273
H	-3.123266	-5.807338	2.163868
H	-6.393429	-2.689394	2.160475
H	-6.395482	-2.702136	-2.148965
H	-6.955978	-0.315851	2.153200
H	-6.957484	-0.328498	-2.155182
H	-5.509326	3.971039	-2.161916
H	-5.516523	3.971351	2.146756
H	-3.664036	5.567833	-2.158817
H	-3.669881	5.566749	2.149647
H	0.791666	6.429488	-2.148010
H	0.791328	6.452391	2.159903
H	3.154896	5.818878	-2.144902
H	3.154640	5.840714	2.163566

Figure 4c1

Minimum

C	0.676962	-3.402637	-0.457902
C	1.415402	-3.270710	0.750002
C	2.614777	-2.421385	0.750001
C	2.984481	-1.768743	-0.457904
C	2.265587	-1.994777	-1.690518
C	1.128892	-2.799542	-1.690516
C	3.445307	-0.407722	-0.457959
C	3.011684	0.208466	-1.690670
C	2.597627	1.538374	-1.690832
C	2.604756	2.291874	-0.458036
C	3.111232	1.738548	0.750002
C	1.452461	3.150680	-0.458078
C	0.777506	3.477911	0.750002
C	-0.692257	3.495894	0.750002
C	-1.375001	3.185296	-0.458098
C	-0.660557	2.945754	-1.690890
C	0.732427	2.928705	-1.690859
C	-2.548025	2.354935	-0.458090
C	-2.559236	1.601481	-1.690892
C	-3.005761	0.282014	-1.690746
C	-3.454417	-0.323372	-0.458008
C	-3.539036	0.421991	0.750001
C	-3.067928	1.814193	0.750002
C	-2.673300	-2.356869	0.750001
C	-1.494931	-3.235200	0.750002
C	-0.759898	-3.385097	-0.457924
C	-1.196920	-2.771158	-1.690547
C	-2.313687	-1.938848	-1.690564
C	-3.026939	-1.695351	-0.457936
C	3.548094	0.335328	0.750001
C	3.445301	-0.407720	1.957973
C	2.604752	2.291868	1.958051
C	3.011669	0.208454	3.190672
C	2.597610	1.538376	3.190833
C	1.452457	3.150675	1.958092
C	0.732432	2.928687	3.190862
C	-0.660564	2.945736	3.190892
C	-1.374997	3.185290	1.958112
C	-2.548022	2.354929	1.958104
C	-2.559219	1.601482	3.190893
C	-3.005747	0.282002	3.190747
C	-3.454411	-0.323370	1.958022

C	-3.026933	-1.695348	1.957950	C	7.058408	-1.561741	-1.090780
C	-2.313681	-1.938831	3.190565	C	6.443757	-1.362618	1.223530
C	-1.196905	-2.771148	3.190548	C	6.888733	-0.738485	0.041650
C	-0.759899	-3.385091	1.957936	C	-5.139033	4.646542	0.041650
C	0.676962	-3.402630	1.957915	C	-4.792394	5.412304	-1.090780
C	1.128877	-2.799532	3.190517	C	-4.412179	4.889925	1.223530
C	2.265581	-1.994760	3.190519	C	-3.666473	6.230333	-1.090780
C	2.984474	-1.768741	1.957919	C	-3.287164	5.707302	1.223530
C	1.444643	1.937940	3.968326	C	-2.831078	6.323366	0.041650
C	-1.396771	1.972674	3.968349	C	-1.426390	6.779772	-0.041650
C	-2.307601	-0.718821	3.968046	C	-0.695855	7.195544	1.090780
C	-0.029489	-2.416693	3.967899	C	-0.695302	6.549451	-1.223530
C	2.289364	-0.775005	3.968007	C	0.695848	7.195545	1.090780
C	2.289361	-0.775003	-2.468029	C	0.695298	6.549453	-1.223530
C	1.444641	1.937937	-2.468349	C	1.426385	6.779778	-0.041650
C	-1.396769	1.972672	-2.468373	C	6.888733	0.738492	-0.041650
C	-2.307597	-0.718820	-2.468069	C	7.058399	1.561755	1.090780
C	-0.029489	-2.416689	-2.467922	C	6.443752	1.362625	-1.223530
C	0.737281	0.989008	-3.214990	C	6.628334	2.885354	1.090780
C	-0.712757	1.006714	-3.214961	C	6.014036	2.685164	-1.223530
C	-1.177611	-0.366921	-3.214766	C	6.007167	3.451651	-0.041650
C	-0.015007	-1.233481	-3.214697	C	5.139019	4.646545	0.041650
C	1.168429	-0.395594	-3.214800	C	4.792388	5.412309	-1.090780
C	-0.015007	-1.233453	4.714688	C	4.412176	4.889934	1.223530
C	-1.177584	-0.366913	4.714755	C	3.666474	6.230332	-1.090780
C	-0.712741	1.006690	4.714950	C	3.287156	5.707309	1.223530
C	0.737264	0.988983	4.714979	C	2.831076	6.323367	0.041650
C	1.168402	-0.395585	4.714790	H	-5.377995	-5.314794	2.002240
C	-4.792388	-5.412309	1.090780	H	-3.392762	-6.757147	2.002240
C	-3.666474	-6.230332	1.090780	H	-2.678170	-5.760509	-2.122380
C	-2.831076	-6.323367	-0.041650	H	-4.650957	-4.327194	-2.122380
C	-3.287156	-5.707309	-1.223530	H	-1.226940	-7.460864	-2.002240
C	-4.412176	-4.889934	-1.223530	H	-1.219249	-6.234540	2.122380
C	-5.139019	-4.646545	-0.041650	H	1.226940	-7.460864	-2.002240
C	-1.426385	-6.779778	0.041650	H	1.219249	-6.234537	2.122380
C	-0.695848	-7.195545	-1.090780	H	-5.552626	-3.086153	2.122380
C	-0.695298	-6.549453	1.223530	H	-6.716557	-3.472425	-2.002240
C	0.695855	-7.195544	-1.090780	H	-6.306160	-0.767002	2.122380
C	0.695302	-6.549451	1.223530	H	-7.474844	-1.138649	-2.002240
C	1.426390	-6.779772	0.041650	H	-7.474854	1.138642	2.002240
C	-6.007167	-3.451651	0.041650	H	-6.306169	0.766999	-2.122380
C	-6.014036	-2.685164	1.223530	H	-6.716565	3.472421	2.002240
C	-6.628334	-2.885354	-1.090780	H	-5.552632	3.086151	-2.122380
C	-6.443752	-1.362625	1.223530	H	3.392776	-6.757140	2.002240
C	-7.058399	-1.561755	-1.090780	H	2.678179	-5.760499	-2.122380
C	-6.888733	-0.738492	0.041650	H	5.378001	-5.314784	2.002240
C	-6.888733	0.738485	-0.041650	H	4.650963	-4.327180	-2.122380
C	-7.058408	1.561741	1.090780	H	6.716565	-3.472421	-2.002240
C	-6.443757	1.362618	-1.223530	H	5.552632	-3.086151	2.122380
C	-6.628343	2.885345	1.090780	H	7.474854	-1.138642	-2.002240
C	-6.014039	2.685157	-1.223530	H	6.306169	-0.766999	2.122380
C	-6.007177	3.451641	-0.041650	H	-5.378001	5.314784	-2.002240
C	2.831078	-6.323366	-0.041650	H	-4.650963	4.327180	2.122380
C	3.666473	-6.230333	1.090780	H	-3.392776	6.757140	-2.002240
C	3.287164	-5.707302	-1.223530	H	-2.678179	5.760499	2.122380
C	4.792394	-5.412304	1.090780	H	-1.226940	7.460864	2.002240
C	4.412179	-4.889925	-1.223530	H	-1.219249	6.234537	-2.122380
C	5.139033	-4.646542	-0.041650	H	1.226940	7.460864	2.002240
C	6.007177	-3.451641	0.041650	H	1.219249	6.234540	-2.122380
C	6.628343	-2.885345	-1.090780	H	7.474844	1.138649	2.002240
C	6.014039	-2.685157	1.223530	H	6.306160	0.767002	-2.122380

H 6.716557 3.472425 2.002240
H 5.552626 3.086153 -2.122380
H 5.377995 5.314794 -2.002240
H 4.650957 4.327194 2.122380
H 3.392762 6.757147 -2.002240
H 2.678170 5.760509 2.122380

Minimum opt C₇₀@[10]CPP I

C 0.685597 -3.401267 -0.764397
C 1.424088 -3.263937 0.441406
C 2.618818 -2.413514 0.441468
C 2.990021 -1.760455 -0.764337
C 2.271880 -1.989634 -1.995986
C 1.137061 -2.797607 -1.996120
C 3.446728 -0.399843 -0.764334
C 3.012425 0.216276 -1.996048
C 2.594685 1.545264 -1.995983
C 2.598439 2.298889 -0.764146
C 3.104839 1.743838 0.441638
C 1.445372 3.153712 -0.764158
C 0.767096 3.476506 0.441693
C -0.699329 3.490932 0.441751
C -1.383598 3.180932 -0.764080
C -0.667897 2.944535 -1.995884
C 0.725296 2.931177 -1.995933
C -2.553012 2.348483 -0.764135
C -2.563677 1.594958 -1.996026
C -3.006849 0.274115 -1.995950
C -3.453036 -0.333528 -0.764194
C -3.536609 0.412969 0.441663
C -3.069872 1.803169 0.441709
C -2.663574 -2.362778 0.441532
C -1.485489 -3.236205 0.441480
C -0.749690 -3.387406 -0.764326
C -1.189547 -2.775128 -1.995981
C -2.308826 -1.945628 -1.996002
C -3.022398 -1.702765 -0.764265
C 3.544275 0.344866 0.441536
C 3.443004 -0.398051 1.647657
C 2.596720 2.295150 1.647868
C 3.012410 0.215692 2.880626
C 2.594718 1.545289 2.880865
C 1.442283 3.150348 1.647822
C 0.725592 2.930726 2.880875
C -0.668124 2.944341 2.881020
C -1.380663 3.177927 1.648000
C -2.551011 2.344498 1.647881
C -2.563491 1.594951 2.880997
C -3.006973 0.273657 2.880894
C -3.449519 -0.331768 1.647877
C -3.018258 -1.702216 1.647673
C -2.309008 -1.945654 2.880618
C -1.189394 -2.775641 2.880570
C -0.750420 -3.383736 1.647664
C 0.686242 -3.397218 1.647525
C 1.136788 -2.797925 2.880482
C 2.272185 -1.989763 2.880506
C 2.986265 -1.760088 1.647698
C 1.440783 1.942116 3.659369
C -1.402097 1.969554 3.659493

C -2.306464 -0.725605 3.659185
C -0.022747 -2.418386 3.658891
C 2.293018 -0.769916 3.658999
C 2.292322 -0.769332 -2.773233
C 1.440215 1.941873 -2.773299
C -1.401685 1.969162 -2.773304
C -2.305711 -0.725068 -2.773228
C -0.022747 -2.417477 -2.773275
C 0.735251 0.990912 -3.520151
C -0.715014 1.004882 -3.520092
C -1.176356 -0.370138 -3.520024
C -0.011348 -1.233788 -3.520071
C 1.170037 -0.392727 -3.520128
C -0.011348 -1.234327 4.404678
C -1.176516 -0.370510 4.404654
C -0.715060 1.004695 4.404804
C 0.735445 0.990693 4.404865
C 1.170279 -0.393178 4.404758
C -4.778806 -5.388528 0.787803
C -3.653392 -6.206717 0.787442
C -2.821482 -6.305657 -0.346601
C -3.269624 -5.675429 -1.523332
C -4.392233 -4.858840 -1.522920
C -5.129825 -4.627485 -0.345982
C -1.426805 -6.785095 -0.273296
C -0.697273 -7.153708 -1.422902
C -0.697161 -6.623836 0.919020
C 0.692356 -7.154766 -1.422552
C 0.692168 -6.625830 0.919511
C 1.422053 -6.787776 -0.272560
C -6.016715 -3.449240 -0.272657
C -6.086746 -2.704497 0.919178
C -6.592790 -2.869798 -1.422396
C -6.514760 -1.382806 0.918489
C -7.021859 -1.548074 -1.422972
C -6.895637 -0.739858 -0.273872
C -6.871341 0.734598 -0.347691
C -7.033196 1.556220 0.786598
C -6.411739 1.355549 -1.525004
C -6.602669 2.879247 0.786662
C -5.981537 2.675450 -1.524780
C -5.987863 3.448101 -0.347558
C 2.816849 -6.308446 -0.345792
C 3.649177 -6.209558 0.787978
C 3.264969 -5.678510 -1.522719
C 4.774782 -5.391656 0.787678
C 4.388426 -4.863092 -1.523121
C 5.126126 -4.631394 -0.346423
C 6.012969 -3.453138 -0.273148
C 6.589905 -2.873972 -1.422579
C 6.083876 -2.708819 0.918868
C 7.020274 -1.552727 -1.422574
C 6.515076 -1.388212 0.919085
C 6.895732 -0.744939 -0.273070
C -5.140590 4.655098 -0.274071
C -4.766949 5.382371 -1.423431
C -4.454273 4.951253 0.918155
C -3.642357 6.198898 -1.423198
C -3.329407 5.766683 0.918201
C -2.835059 6.328149 -0.273685
C -1.425137 6.760638 -0.346604

C	-0.693921	7.167597	0.788170
C	-0.692049	6.516599	-1.523767
C	0.697484	7.167269	0.788534
C	0.696156	6.515713	-1.523288
C	1.429001	6.759624	-0.345854
C	6.871057	0.729575	-0.346815
C	7.033621	1.551716	0.786987
C	6.410971	1.350233	-1.524085
C	6.603568	2.874864	0.786447
C	5.982319	2.670590	-1.524684
C	5.989199	3.443673	-0.347900
C	5.142110	4.650782	-0.274400
C	4.769295	5.379040	-1.423398
C	4.456197	4.947356	0.917938
C	3.645576	6.196721	-1.422671
C	3.333338	5.765493	0.918860
C	2.838974	6.327148	-0.272858
H	-5.363210	-5.292756	1.699915
H	-3.381645	-6.733125	1.699446
H	-2.656566	-5.715654	-2.419186
H	-4.619432	-4.287317	-2.418306
H	-1.227033	-7.376233	-2.346085
H	-1.217122	-6.347051	1.831455
H	1.222135	-7.377508	-2.345650
H	1.212317	-6.350973	1.832427
H	-5.663142	-3.113494	1.831855
H	-6.641275	-3.443085	-2.345140
H	-6.410866	-0.802083	1.830357
H	-7.398155	-1.113374	-2.345994
H	-7.448744	1.134864	1.699012
H	-6.261779	0.760053	-2.421083
H	-6.691263	3.464550	1.698995
H	-5.509424	3.068445	-2.420786
H	3.377800	-6.735753	1.700203
H	2.651445	-5.718200	-2.418217
H	5.359123	-5.295350	1.699697
H	4.616011	-4.292430	-2.418896
H	6.638272	-3.447018	-2.345441
H	5.659246	-3.117221	1.831193
H	7.396219	-1.117867	-2.345598
H	6.413430	-0.808095	1.831523
H	-5.326984	5.251913	-2.346401
H	-4.712611	4.421573	1.830538
H	-3.345001	6.691538	-2.345960
H	-2.745714	5.847245	1.830670
H	-1.223200	7.432032	1.700653
H	-1.211746	6.190848	-2.420398
H	1.226359	7.431916	1.701195
H	1.215866	6.189071	-2.419544
H	7.449524	1.130912	1.699445
H	6.259769	0.754376	-2.419593
H	6.692061	3.460430	1.698537
H	5.510529	3.063613	-2.420775
H	5.329304	5.248728	-2.346371
H	4.713608	4.416779	1.829969
H	3.348126	6.689354	-2.345374
H	2.750538	5.847619	1.831728

Minimum

C	-1.207784	-3.402658	2.823132
C	0.000115	-3.270724	2.084692
C	0.000108	-2.421416	0.885304
C	-1.207797	-1.768781	0.515595
C	-2.440416	-1.994827	1.234485
C	-2.440410	-2.799575	2.371193
C	-1.207870	-0.407766	0.054752
C	-2.440587	0.208415	0.488373
C	-2.440761	1.538319	0.902410
C	-1.207978	2.291831	0.895275
C	0.000067	1.738518	0.388812
C	-1.208029	3.150653	2.047566
C	0.000046	3.477902	2.722515
C	0.000043	3.495896	4.192285
C	-1.208054	3.185301	4.875026
C	-2.440840	2.945732	4.160586
C	-2.440808	2.928668	2.767596
C	-1.208037	2.354943	6.048054
C	-2.440830	1.601481	6.059279
C	-2.440677	0.282015	6.505813
C	-1.207932	-0.323347	6.954481
C	0.000069	0.422025	7.039095
C	0.000056	1.814220	6.567971
C	0.000099	-2.356843	6.173383
C	0.000109	-3.235185	4.995022
C	-1.207807	-3.385104	4.259991
C	-2.440444	-2.771172	4.697003
C	-2.440464	-1.938851	5.813765
C	-1.207848	-1.695331	6.527014
C	0.000082	0.335294	-0.048033
C	1.208059	-0.407742	0.054766
C	1.208111	2.291856	0.895289
C	2.440752	0.208444	0.488391
C	2.440898	1.538378	0.902438
C	1.208140	3.150677	2.047570
C	2.440911	2.928707	2.767604
C	2.440939	2.945771	4.160594
C	1.208155	3.185315	4.875030
C	1.208152	2.354967	6.048058
C	2.440949	1.601530	6.059268
C	2.440822	0.282054	6.505811
C	1.208097	-0.323323	6.954475
C	1.208041	-1.695307	6.527008
C	2.440665	-1.938782	5.813763
C	2.440655	-2.771113	4.697001
C	1.208052	-3.385070	4.259995
C	1.208025	-3.402624	2.823136
C	2.440629	-2.799516	2.371212
C	2.440623	-1.994758	1.234504
C	1.208022	-1.768757	0.515609
C	3.218393	1.937957	2.055405
C	3.218407	1.972716	4.896815
C	3.218133	-0.718764	5.807672
C	3.218004	-2.416657	3.529579
C	3.218101	-0.774990	1.210713
C	-3.217938	-0.775055	1.210702
C	-3.218286	1.937893	2.055395
C	-3.218312	1.972651	4.896804
C	-3.217986	-0.718829	5.807661

Figure 4c2

C -3.217815 -2.416721 3.529568
 C -3.964918 0.988962 2.762763
 C -3.964891 1.006677 4.212803
 C -3.964688 -0.366947 4.677667
 C -3.964607 -1.233519 3.515075
 C -3.964714 -0.395641 2.331627
 C 3.964782 -1.233410 3.515088
 C 3.964841 -0.366858 4.677650
 C 3.965018 1.006736 4.212796
 C 3.965051 0.989012 2.762796
 C 3.964875 -0.395562 2.331670
 C -5.416260 -4.787921 1.090780
 C -4.398431 -5.737061 1.090780
 C -3.580598 -5.931212 -0.041650
 C -3.958200 -5.264164 -1.223530
 C -4.975222 -4.315776 -1.223530
 C -5.666985 -3.985622 -0.041650
 C -2.242000 -6.555410 0.041650
 C -1.567578 -7.057107 -1.090780
 C -1.488293 -6.415898 1.223530
 C -0.186247 -7.226713 -1.090780
 C -0.108057 -6.585368 1.223530
 C 0.589512 -6.903070 0.041650
 C -6.383041 -2.693833 0.041650
 C -6.296448 -1.932222 1.223530
 C -6.930564 -2.056056 -1.090780
 C -6.561783 -0.567173 1.223530
 C -7.196117 -0.689912 -1.090780
 C -6.927385 0.106537 0.041650
 C -6.747386 1.572506 -0.041650
 C -6.815467 2.410303 1.090780
 C -6.229665 2.137757 -1.223530
 C -6.227301 3.671630 1.090780
 C -5.641973 3.398069 -1.223530
 C -5.541751 4.158004 -0.041650
 C 2.039351 -6.621254 -0.041650
 C 2.879857 -6.630724 1.090780
 C 2.567117 -6.065365 -1.223530
 C 4.097078 -5.956008 1.090780
 C 3.783359 -5.391185 -1.223530
 C 4.534456 -5.238198 -0.041650
 C 5.541751 -4.158004 0.041650
 C 6.227301 -3.671630 -1.090780
 C 5.641973 -3.398069 1.223530
 C 6.815467 -2.410303 -1.090780
 C 6.229665 -2.137757 1.223530
 C 6.747386 -1.572506 0.041650
 C -4.534456 5.238198 0.041650
 C -4.097078 5.956008 -1.090780
 C -3.783359 5.391185 1.223530
 C -2.879857 6.630724 -1.090780
 C -2.567117 6.065365 1.223530
 C -2.039351 6.621254 0.041650
 C -0.589512 6.903070 -0.041650
 C 0.186247 7.226713 1.090780
 C 0.108057 6.585368 -1.223530
 C 1.567578 7.057107 1.090780
 C 1.488293 6.415898 -1.223530
 C 2.242000 6.555410 -0.041650
 C 6.927385 -0.106537 -0.041650
 C 7.196117 0.689912 1.090780

C 6.561783 0.567173 -1.223530
 C 6.930564 2.056056 1.090780
 C 6.296448 1.932222 -1.223530
 C 6.383041 2.693833 -0.041650
 C 5.666985 3.985622 0.041650
 C 5.416260 4.787921 -1.090780
 C 4.975222 4.315776 1.223530
 C 4.398431 5.737061 -1.090780
 C 3.958200 5.264164 1.223530
 C 3.580598 5.931212 0.041650
 H -5.985619 -4.619765 2.002240
 H -4.190962 -6.293307 2.002240
 H -3.360237 -5.391184 -2.122380
 H -5.143642 -3.728131 -2.122380
 H -2.127045 -7.255726 -2.002240
 H -1.969961 -6.039480 2.122380
 H 0.308544 -7.554778 -2.002240
 H 0.450362 -6.336654 2.122380
 H -5.887345 -2.386455 2.122380
 H -7.089675 -2.628000 -2.002240
 H -6.352629 0.007242 2.122380
 H -7.557895 -0.219207 -2.002240
 H -7.280373 2.041110 2.002240
 H -6.165690 1.529811 -2.122380
 H -6.243319 4.265081 2.002240
 H -5.135136 3.739843 -2.122380
 H 2.543998 -7.120249 2.002240
 H 1.956188 -6.043949 -2.122380
 H 4.690205 -5.930581 2.002240
 H 4.088945 -4.861736 -2.122380
 H 6.243319 -4.265081 -2.002240
 H 5.135136 -3.739843 2.122380
 H 7.280373 -2.041110 -2.002240
 H 6.165690 -1.529811 2.122380
 H -4.690205 5.930581 -2.002240
 H -4.088945 4.861736 2.122380
 H -2.543998 7.120249 -2.002240
 H -1.956188 6.043949 2.122380
 H -0.308544 7.554778 2.002240
 H -0.450362 6.336654 -2.122380
 H 2.127045 7.255726 2.002240
 H 1.969961 6.039480 -2.122380
 H 7.557895 0.219207 2.002240
 H 6.352629 -0.007242 -2.122380
 H 7.089675 2.628000 2.002240
 H 5.887345 2.386455 -2.122380
 H 5.985619 4.619765 -2.002240
 H 5.143642 3.728131 2.122380
 H 4.190962 6.293307 -2.002240
 H 3.360237 5.391184 2.122380

Minimum opt C₇₀@[10]CPP IIIa

C -0.834781 -3.449326 0.196132
 C 0.378167 -3.201048 -0.493418
 C 0.341760 -2.352077 -1.690836
 C -0.910492 -1.819918 -2.106046
 C -2.138811 -2.172550 -1.435625
 C -2.100222 -2.978611 -0.301974
 C -1.029825 -0.460228 -2.559430
 C -2.334776 0.025004 -2.170297

C -2.483976 1.342616 -1.743224
 C -1.334470 2.216485 -1.695357
 C -0.058341 1.792731 -2.159161
 C -1.463460 3.049731 -0.532176
 C -0.325922 3.487389 0.194136
 C -0.386732 3.493589 1.660638
 C -1.581074 3.055594 2.293153
 C -2.746879 2.693541 1.526735
 C -2.685280 2.687167 0.138021
 C -1.545927 2.220942 3.463912
 C -2.695672 1.347271 3.419586
 C -2.581604 0.029294 3.858593
 C -1.312749 -0.454136 4.352588
 C -0.189947 0.408153 4.490361
 C -0.311445 1.798802 4.029004
 C 0.125180 -2.346565 3.604360
 C 0.259533 -3.203148 2.417301
 C -0.894098 -3.452900 1.629947
 C -2.197477 -2.981061 2.022127
 C -2.328724 -2.172711 3.149412
 C -1.157128 -1.815236 3.914887
 C 0.101074 0.400959 -2.607851
 C 1.373680 -0.219244 -2.461445
 C 1.065050 2.456043 -1.595870
 C 2.519225 0.512186 -1.970292
 C 2.366238 1.830194 -1.543959
 C 0.930181 3.289371 -0.433722
 C 2.141976 3.176569 0.333992
 C 2.089776 3.188314 1.723532
 C 0.816722 3.300042 2.391207
 C 0.855310 2.463744 3.560074
 C 2.156283 1.837915 3.614932
 C 2.272145 0.520216 4.053520
 C 1.090233 -0.211061 4.449488
 C 1.245393 -1.571620 4.012615
 C 2.522401 -1.681461 3.345667
 C 2.645565 -2.494597 2.220384
 C 1.502229 -3.226455 1.728810
 C 1.559294 -3.222374 0.294032
 C 2.737860 -2.494775 -0.102770
 C 2.707510 -1.686109 -1.235741
 C 1.492288 -1.579532 -2.008692
 C 3.044389 2.285732 -0.353694
 C 2.935198 2.296784 2.484526
 C 3.172375 -0.389643 3.379322
 C 3.416674 -2.043444 1.087452
 C 3.357033 -0.395478 -1.218508
 C -3.034440 -1.039053 -1.483483
 C -3.333572 1.642819 -0.613463
 C -3.454397 1.648144 2.225964
 C -3.223716 -1.035975 3.120103
 C -2.955720 -2.692527 0.825087
 C -4.005174 0.619221 0.056233
 C -4.066930 0.620658 1.502428
 C -3.944739 -0.746285 1.956722
 C -3.807272 -1.590587 0.788836
 C -3.849455 -0.748036 -0.385993
 C 4.040293 -0.795815 1.111507
 C 3.919181 0.049409 2.279039
 C 3.801063 1.419574 1.823085
 C 3.854275 1.413596 0.375113

C 4.009889 0.045280 -0.063874
 C -5.603813 -4.702969 0.511529
 C -4.552683 -5.620019 0.509573
 C -3.726931 -5.793875 -0.621335
 C -4.116912 -5.108319 -1.789354
 C -5.161635 -4.195384 -1.787460
 C -5.892004 -3.905415 -0.617152
 C -2.383732 -6.418547 -0.570518
 C -1.692825 -6.777757 -1.748969
 C -1.632494 -6.433232 0.620460
 C -0.311373 -6.915949 -1.765069
 C -0.244657 -6.571984 0.604738
 C 0.464128 -6.707015 -0.603352
 C -6.687778 -2.656973 -0.559434
 C -6.807799 -1.927397 0.639481
 C -7.107636 -1.991178 -1.732565
 C -7.062266 -0.557355 0.632657
 C -7.365493 -0.626753 -1.738761
 C -7.215712 0.156854 -0.572389
 C -6.934909 1.611148 -0.641393
 C -6.871140 2.436028 0.502692
 C -6.442642 2.175179 -1.836233
 C -6.207079 3.659799 0.487469
 C -5.775657 3.393126 -1.850524
 C -5.560589 4.139543 -0.672292
 C 1.910320 -6.399459 -0.685499
 C 2.784983 -6.466049 0.418819
 C 2.422255 -5.806754 -1.857375
 C 4.044529 -5.869041 0.389369
 C 3.675041 -5.210670 -1.886154
 C 4.503284 -5.166930 -0.745514
 C 5.636539 -4.214062 -0.714271
 C 6.197137 -3.690598 -1.901595
 C 6.015559 -3.577941 0.482087
 C 6.857738 -2.470218 -1.911018
 C 6.676374 -2.350942 0.472330
 C 6.993518 -1.698503 -0.733711
 C -4.512291 5.187161 -0.635883
 C -3.950351 5.721016 -1.816297
 C -3.840731 5.504738 0.562600
 C -2.698400 6.322962 -1.818465
 C -2.582747 6.100646 0.560791
 C -1.924919 6.426653 -0.641226
 C -0.458172 6.629026 -0.686497
 C 0.317062 6.915020 0.458252
 C 0.257574 6.314566 -1.858874
 C 1.702824 6.768047 0.461092
 C 1.637945 6.166409 -1.855863
 C 2.402772 6.325346 -0.681215
 C 7.152710 -0.226279 -0.783551
 C 7.431584 0.566058 0.351099
 C 6.749332 0.468313 -1.942691
 C 7.167989 1.934945 0.368996
 C 6.488961 1.830610 -1.925787
 C 6.613166 2.595655 -0.748005
 C 5.932272 3.908249 -0.667743
 C 5.556758 4.614907 -1.831250
 C 5.380594 4.369018 0.543778
 C 4.513687 5.531093 -1.815879
 C 4.338584 5.293448 0.559355
 C 3.787076 5.799822 -0.635214

H	-6.171774	-4.561242	1.428142
H	-4.332412	-6.164775	1.424816
H	-3.511503	-5.187337	-2.687195
H	-5.324255	-3.605506	-2.684463
H	-2.240567	-6.890887	-2.681174
H	-2.115984	-6.181379	1.560288
H	0.182828	-7.134635	-2.708338
H	0.301596	-6.423331	1.532355
H	-6.543575	-2.397181	1.582693
H	-7.159130	-2.535420	-2.672038
H	-6.981144	-0.019959	1.572535
H	-7.612508	-0.150086	-2.683586
H	-7.291957	2.088240	1.442595
H	-6.457643	1.596674	-2.754999
H	-6.139550	4.221631	1.415328
H	-5.308920	3.702095	-2.780771
H	2.457255	-6.955403	1.333190
H	1.784873	-5.705579	-2.731098
H	4.664032	-5.909659	1.282322
H	3.962286	-4.665824	-2.780596
H	6.046901	-4.211822	-2.843645
H	5.647139	-3.956235	1.431539
H	7.206984	-2.073608	-2.860870
H	6.793997	-1.824444	1.415192
H	-4.472502	5.611497	-2.762969
H	-4.234379	5.150988	1.510149
H	-2.289945	6.665078	-2.765597
H	-2.054274	6.184289	1.505902
H	-0.174706	7.215151	1.380102
H	-0.278867	6.062763	-2.768738
H	2.244508	6.955686	1.384859
H	2.112229	5.804794	-2.763126
H	7.803235	0.095387	1.258134
H	6.505806	-0.083847	-2.845186
H	7.341081	2.488242	1.288975
H	6.055823	2.276365	-2.816070
H	6.039279	4.389801	-2.778827
H	5.655979	3.887239	1.477686
H	4.214001	5.994670	-2.752251
H	3.848622	5.498262	1.506278

Figure 4d1

Minimum

C	0.676962	-3.402637	0.792098
C	1.415402	-3.270710	2.000002
C	2.614777	-2.421385	2.000001
C	2.984481	-1.768743	0.792096
C	2.265587	-1.994777	-0.440518
C	1.128892	-2.799542	-0.440516
C	3.445307	-0.407722	0.792041
C	3.011684	0.208466	-0.440670
C	2.597627	1.538374	-0.440832
C	2.604756	2.291874	0.791964
C	3.111232	1.738548	2.000002
C	1.452461	3.150680	0.791922
C	0.777506	3.477911	2.000002
C	-0.692257	3.495894	2.000002
C	-1.375001	3.185296	0.791902
C	-0.660557	2.945754	-0.440890

C	0.732427	2.928705	-0.440859
C	-2.548025	2.354935	0.791910
C	-2.559236	1.601481	-0.440892
C	-3.005761	0.282014	-0.440746
C	-3.454417	-0.323372	0.791992
C	-3.539036	0.421991	2.000001
C	-3.067928	1.814193	2.000002
C	-2.673300	-2.356869	2.000001
C	-1.494931	-3.235200	2.000002
C	-0.759898	-3.385097	0.792076
C	-1.196920	-2.771158	-0.440547
C	-2.313687	-1.938848	-0.440564
C	-3.026939	-1.695351	0.792064
C	3.548094	0.335328	2.000001
C	3.445301	-0.407720	3.207973
C	2.604752	2.291868	3.208051
C	3.011669	0.208454	4.440672
C	2.597610	1.538376	4.440833
C	1.452457	3.150675	3.208092
C	0.732432	2.928687	4.440862
C	-0.660564	2.945736	4.440892
C	-1.374997	3.185290	3.208112
C	-2.548022	2.354929	3.208104
C	-2.559219	1.601482	4.440893
C	-3.005747	0.282002	4.440747
C	-3.454411	-0.323370	3.208022
C	-3.026933	-1.695348	3.207950
C	-2.313681	-1.938831	4.440565
C	-1.196905	-2.771148	4.440548
C	-0.759899	-3.385091	3.207936
C	0.676962	-3.402630	3.207915
C	1.128877	-2.799532	4.440517
C	2.265581	-1.994760	4.440519
C	2.984474	-1.768741	3.207919
C	1.444643	1.937940	5.218326
C	-1.396771	1.972674	5.218349
C	-2.307601	-0.718821	5.218046
C	-0.029489	-2.416693	5.217899
C	2.289364	-0.775005	5.218007
C	2.289361	-0.775003	-1.218029
C	1.444641	1.937937	-1.218349
C	-1.396769	1.972672	-1.218373
C	-2.307597	-0.718820	-1.218069
C	-0.029489	-2.416689	-1.217922
C	0.737281	0.989008	-1.964990
C	-0.712757	1.006714	-1.964961
C	-1.177611	-0.366921	-1.964766
C	-0.015007	-1.233481	-1.964697
C	1.168429	-0.395594	-1.964800
C	-0.015007	-1.233453	5.964688
C	-1.177584	-0.366913	5.964755
C	-0.712741	1.006690	5.964950
C	0.737264	0.988983	5.964979
C	1.168402	-0.395585	5.964790
C	4.431771	-4.850079	0.002810
C	3.843699	-5.283292	1.215950
C	2.642796	-5.977150	1.210840
C	1.981292	-6.265600	-0.007660
C	2.651434	-5.974554	-1.220650
C	3.852424	-5.280876	-1.215450
C	0.611285	-6.623207	-0.012160

C -0.611285 -6.622028 -0.013380
 C -1.980686 -6.262209 -0.011040
 C -2.649622 -5.971860 -1.224900
 C -2.642722 -5.971525 1.206520
 C -3.850091 -5.276947 -1.221690
 C -3.843331 -5.277097 1.209740
 C -4.430253 -4.844734 -0.004380
 C -5.424496 -3.836628 -0.000980
 C -6.035345 -2.777597 0.003070
 C -6.410242 -1.412243 0.006710
 C -6.494450 -0.688095 -1.207310
 C -6.490393 -0.693349 1.224030
 C -6.495047 0.698794 -1.204300
 C -6.490974 0.693580 1.227050
 C -6.411425 1.417826 0.012790
 C -6.037552 2.783509 0.013410
 C -5.426973 3.842675 0.007910
 C -4.432221 4.850190 0.004350
 C -3.840458 5.276369 1.218230
 C -3.856240 5.287541 -1.213150
 C -2.639370 5.969872 1.213580
 C -2.654932 5.980887 -1.217890
 C -1.981273 6.264922 -0.005210
 C -0.611205 6.622186 -0.010620
 C 0.611305 6.621045 -0.011690
 C 1.980815 6.261732 -0.010200
 C 2.648486 5.970326 -1.224510
 C 2.644309 5.972720 1.206940
 C 3.849211 5.275730 -1.221820
 C 3.845224 5.278695 1.209600
 C 4.430815 4.845150 -0.004670
 C 5.425320 3.837168 -0.001590
 C 6.036072 2.778161 0.001810
 C 6.410558 1.412597 0.004760
 C 6.489985 0.688199 -1.209430
 C 6.494967 0.693902 1.221900
 C 6.490170 -0.698694 -1.206130
 C 6.495074 -0.693089 1.225230
 C 6.410797 -1.417530 0.011400
 C 6.036614 -2.783074 0.012870
 C 5.426104 -3.842298 0.007740
 H 4.301888 -4.994925 2.158390
 H 2.158598 -6.233740 2.149400
 H 2.173842 -6.229444 -2.163090
 H 4.317584 -4.991328 -2.154060
 H -2.171955 -6.228379 -2.166820
 H -2.159023 -6.227364 2.145620
 H -4.314208 -4.987380 -2.160960
 H -4.302133 -4.987965 2.151630
 H -6.476602 -1.230155 -2.149120
 H -6.469868 -1.239984 2.163200
 H -6.477743 1.245486 -2.143490
 H -6.471280 1.235704 2.168800
 H -4.295920 4.982677 2.160320
 H -4.324172 5.003549 -2.152080
 H -2.152283 6.220835 2.152180
 H -2.179951 6.241011 -2.160270
 H 2.169576 6.225559 -2.166170
 H 2.161588 6.229600 2.146290
 H 4.312207 4.985224 -2.161260
 H 4.305154 4.990964 2.151300

H 6.468742 1.230028 -2.151290
 H 6.478167 1.240659 2.161060
 H 6.469203 -1.245601 -2.145180
 H 6.478641 -1.235073 2.167190

Minimum opt C₇₀@[6]CPPA I

C 0.673654 -3.376300 -0.158718
 C 1.410857 -3.232682 1.046883
 C 2.609768 -2.387189 1.037483
 C 2.976547 -1.748412 -0.177134
 C 2.263778 -1.992433 -1.408818
 C 1.128250 -2.795108 -1.399588
 C 3.433863 -0.391932 -0.193046
 C 3.009543 0.208099 -1.435016
 C 2.597960 1.536104 -1.453189
 C 2.597163 2.298399 -0.227313
 C 3.107969 1.766041 0.986787
 C 1.447610 3.149128 -0.237604
 C 0.775555 3.495424 0.963985
 C -0.688869 3.514251 0.962511
 C -1.367200 3.185030 -0.240511
 C -0.656447 2.939607 -1.471535
 C 0.733421 2.921865 -1.470001
 C -2.537659 2.363132 -0.232423
 C -2.555340 1.600976 -1.458305
 C -3.000278 0.283644 -1.440972
 C -3.441733 -0.305565 -0.199826
 C -3.531762 0.453694 0.997223
 C -3.064016 1.843526 0.980646
 C -2.670878 -2.321028 1.032333
 C -1.493463 -3.195954 1.044075
 C -0.757805 -3.358115 -0.160134
 C -1.195066 -2.765859 -1.401867
 C -2.310075 -1.934972 -1.413375
 C -3.018657 -1.673041 -0.183017
 C 3.540378 0.364828 1.004244
 C 3.445452 -0.362493 2.220513
 C 2.607163 2.338144 2.186997
 C 3.011325 0.268751 3.444971
 C 2.598283 1.599852 3.428942
 C 1.452723 3.195756 2.175295
 C 0.731560 2.990051 3.409632
 C -0.662340 3.007630 3.408251
 C -1.375740 3.231472 2.172464
 C -2.551334 2.402948 2.181841
 C -2.563384 1.664714 3.423760
 C -3.009923 0.344464 3.439024
 C -3.457482 -0.275755 2.213756
 C -3.030841 -1.649119 2.230995
 C -2.318524 -1.877586 3.466978
 C -1.200912 -2.710202 3.477677
 C -0.763231 -3.338986 2.253246
 C 0.674911 -3.357095 2.254626
 C 1.125978 -2.739477 3.479962
 C 2.264118 -1.935139 3.471454
 C 2.984200 -1.724623 2.236809
 C 1.443055 2.008425 4.199542
 C -1.399816 2.044160 4.196689
 C -2.311607 -0.647268 4.228504
 C -0.033436 -2.346023 4.250863

C 2.286776 -0.705077 4.233066
 C 2.291203 -0.784874 -2.203931
 C 1.448086 1.927413 -2.239151
 C -1.394387 1.963261 -2.242029
 C -2.305432 -0.727035 -2.208459
 C -0.028128 -2.425711 -2.185473
 C 0.740928 0.971213 -2.977537
 C -0.710059 0.989481 -2.978959
 C -1.175363 -0.384671 -2.961038
 C -0.012623 -1.251636 -2.948584
 C 1.171510 -0.414192 -2.958666
 C -0.019130 -1.153132 4.982603
 C -1.181466 -0.286439 4.971212
 C -0.716161 1.086964 4.955211
 C 0.734050 1.068748 4.956690
 C 1.164643 -0.315926 4.973580
 C 4.413620 -4.867812 -1.012238
 C 3.909257 -5.444453 0.177179
 C 2.716354 -6.153951 0.169212
 C 1.979519 -6.311673 -1.027870
 C 2.564390 -5.868832 -2.239256
 C 3.754768 -5.160884 -2.231326
 C 0.611756 -6.675954 -1.008188
 C -0.610859 -6.675571 -1.009036
 C -1.978053 -6.309174 -1.030904
 C -2.557012 -5.856104 -2.241392
 C -2.719927 -6.159722 0.164080
 C -3.746255 -5.146400 -2.233068
 C -3.911859 -5.448493 0.172418
 C -4.410274 -4.861988 -1.014644
 C -5.400770 -3.851597 -0.981389
 C -6.019633 -2.797256 -0.970447
 C -6.406827 -1.435601 -0.991722
 C -6.263495 -0.698441 -2.192788
 C -6.721481 -0.730728 0.193181
 C -6.273060 0.686078 -2.176827
 C -6.731664 0.657963 0.208817
 C -6.426665 1.394344 -0.959566
 C -6.054481 2.759682 -0.908692
 C -5.443288 3.818498 -0.898888
 C -4.442668 4.820340 -0.920910
 C -3.958647 5.416703 0.267036
 C -3.749079 5.074220 -2.129641
 C -2.752814 6.105083 0.272343
 C -2.546123 5.760327 -2.123496
 C -1.983462 6.223934 -0.909049
 C -0.610278 6.570097 -0.874140
 C 0.612672 6.570439 -0.877972
 C 1.986116 6.225970 -0.919486
 C 2.542507 5.757869 -2.135058
 C 2.761928 6.112090 0.258044
 C 3.744874 5.070559 -2.144615
 C 3.967297 5.422708 0.249358
 C 4.444085 4.820408 -0.938399
 C 5.442824 3.816620 -0.917070
 C 6.051928 2.756589 -0.924891
 C 6.422216 1.390593 -0.971135
 C 6.270650 0.678345 -2.186358
 C 6.726491 0.657942 0.199824
 C 6.263764 -0.706182 -2.198301
 C 6.718623 -0.730777 0.188190

C 6.406902 -1.439737 -0.995020
 C 6.021531 -2.801889 -0.970511
 C 5.403540 -3.856760 -0.980746
 H 4.419659 -5.252113 1.116847
 H 2.292822 -6.513586 1.102847
 H 2.023719 -6.013134 -3.170692
 H 4.149447 -4.750380 -3.156848
 H -2.012523 -5.993917 -3.171593
 H -2.300998 -6.527195 1.096751
 H -4.136422 -4.728288 -3.157095
 H -4.426305 -5.263062 1.111303
 H -6.056637 -1.230136 -3.117667
 H -6.863745 -1.284163 1.117478
 H -6.073399 1.241452 -3.089155
 H -6.884149 1.188352 1.144904
 H -4.494236 5.253764 1.198313
 H -4.127571 4.649068 -3.055312
 H -2.346838 6.477862 1.208525
 H -1.979920 5.872000 -3.044192
 H 1.971761 5.866353 -3.053316
 H 2.361103 6.489030 1.194764
 H 4.118220 4.641581 -3.070582
 H 4.507488 5.263104 1.178544
 H 6.071328 1.230691 -3.100580
 H 6.877378 1.191259 1.134494
 H 6.059010 -1.240921 -3.121860
 H 6.860161 -1.281191 1.114374

Figure 4d2

Minimum

C -1.207784 -3.402658 3.323132
 C 0.000115 -3.270724 2.584692
 C 0.000108 -2.421416 1.385304
 C -1.207797 -1.768781 1.015595
 C -2.440416 -1.994827 1.734485
 C -2.440410 -2.799575 2.871193
 C -1.207870 -0.407766 0.554752
 C -2.440587 0.208415 0.988373
 C -2.440761 1.538319 1.402410
 C -1.207978 2.291831 1.395275
 C 0.000067 1.738518 0.888812
 C -1.208029 3.150653 2.547566
 C 0.000046 3.477902 3.222515
 C 0.000043 3.495896 4.692285
 C -1.208054 3.185301 5.375026
 C -2.440840 2.945732 4.660586
 C -2.440808 2.928668 3.267596
 C -1.208037 2.354943 6.548054
 C -2.440830 1.601481 6.559279
 C -2.440677 0.282015 7.005813
 C -1.207932 -0.323347 7.454481
 C 0.000069 0.422025 7.539095
 C 0.000056 1.814220 7.067971
 C 0.000099 -2.356843 6.673383
 C 0.000109 -3.235185 5.495022
 C -1.207807 -3.385104 4.759991
 C -2.440444 -2.771172 5.197003
 C -2.440464 -1.938851 6.313765
 C -1.207848 -1.695331 7.027014

C 0.000082 0.335294 0.451966
 C 1.208059 -0.407742 0.554766
 C 1.208111 2.291856 1.395289
 C 2.440752 0.208444 0.988391
 C 2.440898 1.538378 1.402438
 C 1.208140 3.150677 2.547570
 C 2.440911 2.928707 3.267604
 C 2.440939 2.945771 4.660594
 C 1.208155 3.185315 5.375030
 C 1.208152 2.354967 6.548058
 C 2.440949 1.601530 6.559268
 C 2.440822 0.282054 7.005811
 C 1.208097 -0.323323 7.454475
 C 1.208041 -1.695307 7.027008
 C 2.440665 -1.938782 6.313763
 C 2.440655 -2.771113 5.197001
 C 1.208052 -3.385070 4.759995
 C 1.208025 -3.402624 3.323136
 C 2.440629 -2.799516 2.871212
 C 2.440623 -1.994758 1.734504
 C 1.208022 -1.768757 1.015609
 C 3.218393 1.937957 2.555405
 C 3.218407 1.972716 5.396815
 C 3.218133 -0.718764 6.307672
 C 3.218004 -2.416657 4.029579
 C 3.218101 -0.774990 1.710713
 C -3.217938 -0.775055 1.710702
 C -3.218286 1.937893 2.555395
 C -3.218312 1.972651 5.396804
 C -3.217986 -0.718829 6.307661
 C -3.217815 -2.416721 4.029568
 C -3.964918 0.988962 3.262763
 C -3.964891 1.006677 4.712803
 C -3.964688 -0.366947 5.177667
 C -3.964607 -1.233519 4.015075
 C -3.964714 -0.395641 2.831627
 C 3.964782 -1.233410 4.015088
 C 3.964841 -0.366858 5.177650
 C 3.965018 1.006736 4.712796
 C 3.965051 0.989012 3.262796
 C 3.964875 -0.395562 2.831670
 C 5.933878 2.820097 0.002810
 C 6.176226 2.131062 1.215950
 C 6.488656 0.779769 1.210840
 C 6.571096 0.062835 -0.007660
 C 6.488699 0.788788 -1.220650
 C 6.176467 2.140113 -1.215450
 C 6.512527 -1.351863 -0.012160
 C 6.153954 -2.520668 -0.013380
 C 5.409484 -3.725032 -0.011040
 C 4.936243 -4.279849 -1.224900
 C 4.937941 -4.273153 1.206520
 C 3.920712 -5.224691 -1.221690
 C 3.922832 -5.218270 1.209740
 C 3.337761 -5.653136 -0.004380
 C 2.083016 -6.309193 -0.000980
 C 0.891665 -6.583720 0.003070
 C -0.523637 -6.543045 0.006710
 C -1.240764 -6.411853 -1.207310
 C -1.234553 -6.409509 1.224030
 C -2.567228 -6.006936 -1.204300

C -2.561051 -6.004566 1.227050
 C -3.230393 -5.716744 0.012790
 C -4.427092 -4.959921 0.013410
 C -5.261462 -4.066351 0.007910
 C -5.934116 -2.820496 0.004350
 C -6.168658 -2.129987 1.218230
 C -6.183956 -2.141813 -1.213150
 C -6.480694 -0.778620 1.213580
 C -6.495778 -0.790281 -1.217890
 C -6.570443 -0.063014 -0.005210
 C -6.511527 1.351641 -0.010620
 C -6.153009 2.520400 -0.011690
 C -5.408989 3.725016 -0.010200
 C -4.935109 4.278314 -1.224510
 C -4.938619 4.275020 1.206940
 C -3.919805 5.223493 -1.221820
 C -3.923807 5.220547 1.209600
 C -3.337995 5.653794 -0.004670
 C -2.083291 6.310139 -0.001590
 C -0.891991 6.584580 0.001810
 C 0.523392 6.543450 0.004760
 C 1.239359 6.407614 -1.209430
 C 1.235361 6.414045 1.221900
 C 2.565707 6.002302 -1.206130
 C 2.561780 6.008630 1.225230
 C 3.229926 5.716229 0.011400
 C 4.426403 4.959151 0.012870
 C 5.260847 4.065629 0.007740
 H 6.034421 2.653541 2.158390
 H 6.592468 0.241708 2.149400
 H 6.592817 0.257542 -2.163090
 H 6.035570 2.669603 -2.154060
 H 5.321210 -3.898053 -2.166820
 H 5.324021 -3.885389 2.145620
 H 3.508103 -5.583866 -2.160960
 H 3.512193 -5.572490 2.151630
 H -0.717171 -6.553268 -2.149120
 H -0.705803 -6.549702 2.163200
 H -3.084973 -5.830552 -2.143490
 H -3.073729 -5.827231 2.168800
 H -6.020963 -2.651415 2.160320
 H -6.049183 -2.672329 -2.152080
 H -6.578281 -0.239442 2.152180
 H -6.605665 -0.260003 -2.160270
 H -5.319209 3.894953 -2.166170
 H -5.325409 3.888496 2.146290
 H -3.506626 5.581323 -2.161260
 H -3.514177 5.576256 2.151300
 H 0.714995 6.545714 -2.151290
 H 0.707584 6.557836 2.161060
 H 3.082586 5.822351 -2.145180
 H 3.075278 5.834454 2.167190

Minimum opt C₇₀@[6]CPPA II

C -1.187267 -3.365823 0.603871
 C 0.025063 -3.220412 -0.118957
 C 0.037779 -2.352498 -1.302832
 C -1.166893 -1.693048 -1.672428
 C -2.403266 -1.931767 -0.967040
 C -2.412342 -2.756058 0.153131

C -1.163251 -0.322061 -2.105560
 C -2.400656 0.284813 -1.668982
 C -2.402702 1.603397 -1.221528
 C -1.170932 2.357168 -1.199909
 C 0.040813 1.816075 -1.708503
 C -1.181244 3.183317 -0.025334
 C 0.015814 3.491853 0.670340
 C 0.000454 3.486975 2.138728
 C -1.214698 3.163245 2.802103
 C -2.437943 2.937928 2.068184
 C -2.417674 2.944216 0.676217
 C -1.227466 2.307629 3.956898
 C -2.459906 1.553860 3.937332
 C -2.464119 0.224037 4.354357
 C -1.235832 -0.390858 4.802338
 C -0.028732 0.352543 4.915783
 C -0.024153 1.755196 4.476915
 C -0.018776 -2.407101 3.989946
 C -0.005987 -3.259437 2.792261
 C -1.204712 -3.389857 2.040274
 C -2.442199 -2.787491 2.477519
 C -2.456545 -1.981648 3.614384
 C -1.230990 -1.753593 4.345115
 C 0.046136 0.423243 -2.179609
 C 1.254041 -0.322395 -2.079414
 C 1.242156 2.354999 -1.171931
 C 2.480590 0.284313 -1.615576
 C 2.474639 1.603567 -1.169759
 C 1.226707 3.177312 0.003041
 C 2.448987 2.942597 0.729035
 C 2.440554 2.938969 2.121027
 C 1.201400 3.164007 2.828246
 C 1.189545 2.308138 3.983074
 C 2.422683 1.554241 3.989777
 C 2.418319 0.224460 4.406412
 C 1.180669 -0.390717 4.828175
 C 1.185590 -1.753089 4.370934
 C 2.426260 -1.980672 3.665847
 C 2.436402 -2.786899 2.529383
 C 1.209448 -3.392618 2.065932
 C 1.222303 -3.369033 0.629620
 C 2.455833 -2.755721 0.205735
 C 2.471554 -1.932571 -0.915235
 C 1.249274 -1.693911 -1.647191
 C 3.232849 1.972796 0.003047
 C 3.211812 1.951372 2.844126
 C 3.203499 -0.760657 3.695029
 C 3.221163 -2.401651 1.377708
 C 3.246781 -0.713553 -0.902917
 C -3.181174 -0.713899 -0.972002
 C -3.185694 1.972541 -0.065292
 C -3.224466 1.951095 2.774671
 C -3.233672 -0.761474 3.626633
 C -3.204124 -2.405448 1.308966
 C -3.939647 1.011960 0.611214
 C -3.962159 0.999584 2.060373
 C -3.966585 -0.383531 2.494801
 C -3.946615 -1.221744 1.313239
 C -3.931872 -0.359384 0.151101
 C 3.970404 -1.222098 1.396948
 C 3.960664 -0.382901 2.579246

C 3.963567 0.999850 2.144843
 C 3.971320 1.011939 0.695564
 C 3.976335 -0.359432 0.234260
 C 6.082603 2.794157 -1.433389
 C 6.781871 2.224900 -0.344798
 C 7.119959 0.875567 -0.346839
 C 6.770673 0.047542 -1.437954
 C 6.222280 0.658765 -2.593245
 C 5.885565 2.000220 -2.590698
 C 6.714604 -1.365643 -1.352771
 C 6.309664 -2.519370 -1.322458
 C 5.503451 -3.683858 -1.343574
 C 4.728591 -3.938151 -2.503644
 C 5.273960 -4.482222 -0.200165
 C 3.680624 -4.840854 -2.472044
 C 4.217541 -5.385958 -0.167031
 C 3.353842 -5.528479 -1.277093
 C 2.084643 -6.150444 -1.187855
 C 0.888005 -6.399224 -1.158926
 C -0.526199 -6.339637 -1.207057
 C -1.127508 -5.819106 -2.380306
 C -1.352090 -6.589016 -0.087420
 C -2.459859 -5.448082 -2.388792
 C -2.691792 -6.215466 -0.095746
 C -3.256693 -5.577989 -1.224044
 C -4.490310 -4.882314 -1.187689
 C -5.355850 -4.019189 -1.222737
 C -6.059484 -2.793775 -1.318036
 C -6.690826 -2.184008 -0.210400
 C -5.944532 -2.046078 -2.517374
 C -7.039402 -0.838291 -0.246083
 C -6.297322 -0.708629 -2.554993
 C -6.773657 -0.054219 -1.392057
 C -6.734177 1.361298 -1.355294
 C -6.359255 2.525319 -1.349974
 C -5.558346 3.693184 -1.383688
 C -4.768800 3.924405 -2.537627
 C -5.332914 4.502022 -0.246552
 C -3.706018 4.809286 -2.501460
 C -4.264448 5.391100 -0.210261
 C -3.384146 5.507289 -1.310732
 C -2.107489 6.114099 -1.219504
 C -0.907798 6.350038 -1.201124
 C 0.506124 6.290934 -1.263001
 C 1.101239 5.805760 -2.453929
 C 1.340184 6.513614 -0.142791
 C 2.434641 5.437404 -2.480915
 C 2.681081 6.146640 -0.170884
 C 3.239872 5.538892 -1.319123
 C 4.479673 4.853862 -1.304328
 C 5.368718 4.014483 -1.342188
 H 6.969443 2.827664 0.539581
 H 7.569314 0.429463 0.536316
 H 5.983662 0.040522 -3.454432
 H 5.381924 2.435336 -3.449628
 H 4.918825 -3.357240 -3.402084
 H 5.875498 -4.320828 0.689956
 H 3.046135 -4.968064 -3.345060
 H 3.996798 -5.926672 0.749408
 H -0.509713 -5.647644 -3.257737
 H -0.911796 -7.004043 0.815255

H -2.889085 -4.982730 -3.271907
H -3.293406 -6.338904 0.800736
H -6.816899 -2.751191 0.707534
H -5.498067 -2.515114 -3.389997
H -7.432652 -0.357908 0.645764
H -6.125118 -0.126188 -3.456008
H -4.953886 3.333220 -3.430325
H -5.945330 4.355625 0.639012
H -3.058400 4.916577 -3.367432
H -4.048098 5.939767 0.702122
H 0.478481 5.657418 -3.331975
H 0.905783 6.906154 0.772599
H 2.859103 4.998137 -3.379578
H 3.289875 6.251684 0.722770

C70@[6]CPPA I'

C 0.312957 -2.802418 -3.553716
C 1.488751 -2.951411 -2.722257
C 0.214706 -1.728174 -4.445177
C 2.530927 -2.031037 -2.815271
C 3.187559 -1.570379 -1.614543
C 2.852429 -2.094216 -0.338265
C 3.120123 -1.260947 0.778728
C -2.138765 -1.382899 -3.791693
C -2.029338 -2.488559 -2.864073
C -1.036196 -1.003663 -4.566050
C -0.827008 -3.183383 -2.747039
C -0.352562 -3.574141 -1.441317
C -1.122120 -3.345752 -0.271725
C -0.407930 -3.264999 0.951818
C 1.758200 -3.057480 -0.240812
C 1.074297 -3.431784 -1.426079
C 1.016403 -3.122536 0.967214
C -1.528753 1.372936 -4.127509
C -2.662571 0.975937 -3.320534
C -0.724810 0.402449 -4.737180
C -2.960248 -0.375690 -3.154626
C -3.363513 -0.866292 -1.858009
C -3.547830 0.010644 -0.756471
C -3.403620 -0.559210 0.535008
C -2.384055 -2.619759 -0.394498
C -2.790289 -2.170663 -1.678583
C -2.833909 -1.857965 0.714922
C 1.299809 1.656636 -4.097074
C 0.464651 2.652139 -3.460130
C 0.718078 0.547225 -4.721712
C -0.922092 2.513221 -3.475119
C -1.687396 2.824711 -2.289878
C -1.066481 3.346630 -1.124887
C -1.731390 3.107850 0.106398
C -3.237701 1.431601 -0.931041
C -2.763374 1.875552 -2.194127
C -2.801370 2.167230 0.202313
C 2.438162 -0.923561 -3.742779
C 3.029304 0.225363 -3.090504
C 1.299044 -0.769255 -4.541187
C 2.472424 1.491009 -3.265385
C 2.368166 2.390043 -2.139007
C 2.894683 2.046824 -0.865608

C 2.297337 2.679140 0.256446
C 0.390376 3.491750 -1.109192
C 1.127261 3.106345 -2.259522
C 1.063661 3.387369 0.136017
C 3.478112 0.715838 -0.681380
C 3.493998 -0.178143 -1.784572
C 3.424683 0.126001 0.608072
C 1.149263 2.465341 2.291087
C 2.353022 2.101418 1.578328
C 2.907684 0.839458 1.750993
C 0.534359 1.548021 3.151081
C -1.676420 2.181680 2.261064
C -1.030979 3.116515 1.367303
C 0.349558 3.254553 1.381764
C -0.909550 1.403062 3.135773
C -2.286823 -0.570488 2.598378
C -3.064520 0.239805 1.687403
C -2.768134 1.586943 1.523658
C -1.220680 -0.003198 3.307401
C 0.163546 -1.989329 2.836229
C -0.938914 -2.564577 2.096604
C -2.139109 -1.870234 1.980019
C 0.030554 -0.727548 3.428549
C 2.287230 -0.111238 2.646464
C 2.413972 -1.413241 2.028092
C 1.373776 -2.332828 2.121222
C 1.115185 0.231386 3.331888
C 6.214162 2.174442 0.707304
C 6.201372 1.423824 1.908438
C 6.362671 0.047143 1.886178
C 6.549141 -0.643097 0.662550
C 6.734200 0.125832 -0.510104
C 6.567656 1.504857 -0.488683
C 6.325437 -2.042740 0.608156
C 5.843732 -3.167039 0.579019
C 4.974282 -4.287661 0.580160
C 4.573724 -4.927518 -0.617528
C 4.310386 -4.646991 1.778774
C 3.465611 -5.766132 -0.640236
C 3.205941 -5.483801 1.755639
C 2.710515 -6.000640 0.533342
C 1.388809 -6.513400 0.488682
C 0.173654 -6.657602 0.496171
C -1.231176 -6.469393 0.551110
C -2.025824 -6.416763 -0.618462
C -1.827740 -6.084119 1.776681
C -3.297459 -5.857286 -0.589631
C -3.096281 -5.526030 1.806266
C -3.830062 -5.328393 0.610932
C -4.938331 -4.443173 0.612636
C -5.672532 -3.464692 0.635562
C -6.217840 -2.155829 0.676032
C -6.211418 -1.431774 1.894320
C -6.566388 -1.461427 -0.506077
C -6.378828 -0.055705 1.903913
C -6.730223 -0.081908 -0.496917
C -6.556477 0.661085 0.694863
C -6.334327 2.061610 0.671275
C -5.858605 3.188824 0.665798
C -4.994034 4.313384 0.684538
C -4.557443 4.934876 -0.510033

C	-4.365917	4.689631	1.897285
C	-3.442485	5.763532	-0.512675
C	-3.254385	5.517615	1.894299
C	-2.717459	6.007848	0.678346
C	-1.389773	6.507319	0.653171
C	-0.174386	6.650369	0.659866
C	1.233300	6.477105	0.694707
C	2.001536	6.410419	-0.492249
C	1.864344	6.125976	1.913545
C	3.279199	5.865521	-0.483913
C	3.138854	5.580848	1.922252
C	3.842945	5.361817	0.712688
C	4.946124	4.469873	0.695741
C	5.672043	3.484955	0.694007
H	5.968586	1.926420	2.843100
H	6.253791	-0.524820	2.803698
H	6.912429	-0.381757	-1.454064
H	6.618719	2.069137	-1.415947
H	5.087911	-4.686959	-1.544067
H	4.623922	-4.190491	2.713553
H	3.116738	-6.173921	-1.584955
H	2.655051	-5.677635	2.671862
H	-1.596368	-6.732803	-1.565079
H	-1.243018	-6.146517	2.690454
H	-3.857699	-5.741478	-1.513542
H	-3.502855	-5.155593	2.743239
H	-5.980675	-1.955360	2.818343
H	-6.609853	-2.004110	-1.446305
H	-6.279794	0.495153	2.835110
H	-6.902097	0.447648	-1.430129
H	-5.045844	4.683414	-1.447533
H	-4.709333	4.248112	2.828851
H	-3.063211	6.154809	-1.452657
H	-2.729769	5.722106	2.823479
H	1.545689	6.702415	-1.434290
H	1.302399	6.202088	2.840476
H	3.817310	5.736235	-1.418959
H	3.571923	5.232682	2.855918