

Fullerene recognition with molecular tweezers made up of efficient buckybowls. A dispersion-corrected DFT study

Daniela Josa, Jesús Rodríguez-Otero and Enrique M. Cabaleiro-Lago

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Table S1. B97-D2/TZVP, B97-D3/TZVP, and B97-D3(BJ)/TZVP interaction energies (in kcal/mol).

D2: reference 47. D3: S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.*, 2010, 132, 154104. D3(BJ): S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.*, 2011, 32, 1456–1465.

	B97-D2/TZVP	B97-D3/TZVP ^a	B97-D3(BJ)/TZVP ^a
1a···C ₆₀	-39.92	-28.43	-39.46
1b···C ₆₀	-49.18	-35.08	-47.34
2a···C ₆₀	-47.26	-31.80	-43.82
2b···C ₆₀	-57.23	-38.84	-52.03
3a···C ₆₀	-72.86	-51.38	-71.64
3b···C ₆₀	-85.73	-60.18	-83.40
4a···C ₆₀	-63.83	-45.82	-61.86
4b···C ₆₀	-80.52	-56.73	-75.28
5a···C ₆₀	-77.53	-53.70	-74.58
5b···C ₆₀	-92.19	-64.91	-87.79
6a···C ₆₀	-103.72	-74.80	-102.14
6b···C ₆₀	-106.76	-77.27	-104.72

^a Calculated using the optimized B97-D2/TZVP geometries.



B97-D2/TZVP interaction energy vs. B97-D3/TZVP, and B97-D3(BJ)/TZVP interaction energies (in kcal/mol).

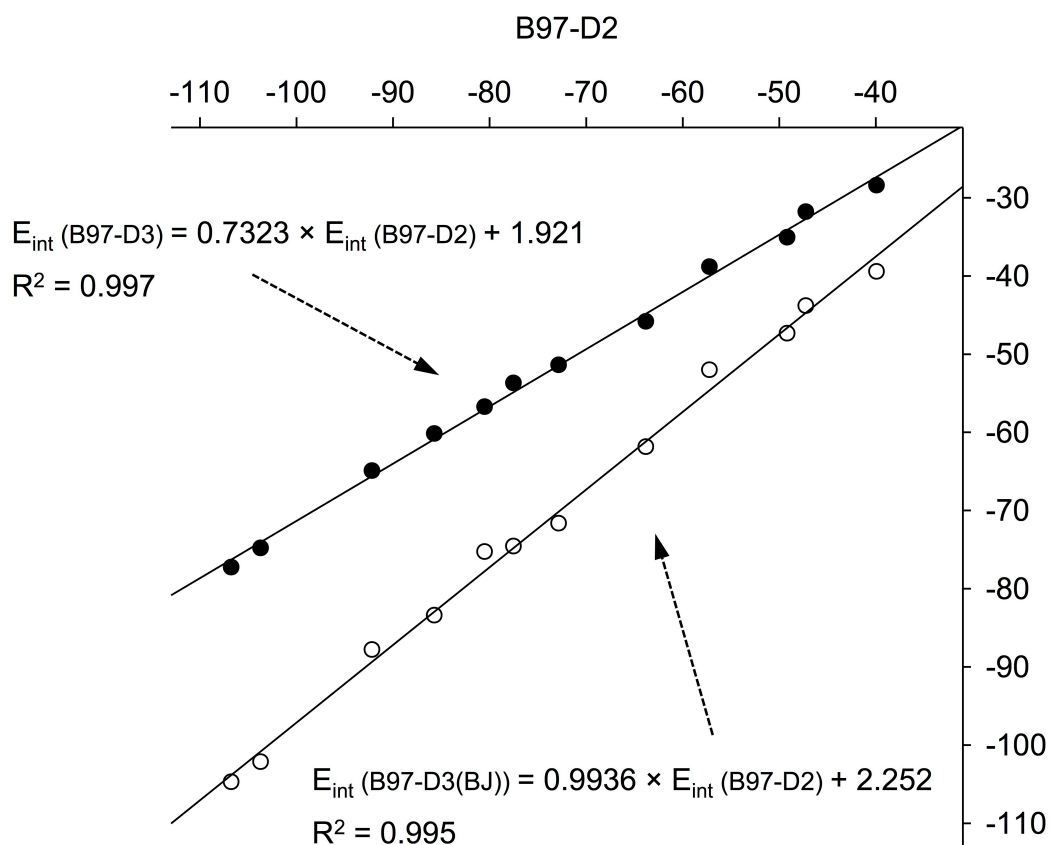


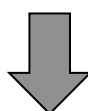
Table S2. B97-D2/TZVP interaction energies, BSSE and percentage of BSSE (kcal/mol).

	$E_{\text{int}}^{\text{a}}$	BSSE	% ^b	$E_{\text{int}}^{\text{c}}$
1a···C ₆₀	-44.53	4.61	10.4	-39.92
1b···C ₆₀	-54.47	5.29	9.7	-49.18
2a···C ₆₀	-52.96	5.70	10.8	-47.26
2b···C ₆₀	-63.86	6.63	10.4	-57.23
3a···C ₆₀	-81.32	8.46	10.4	-72.86
3b···C ₆₀	-95.35	9.62	10.1	-85.73
4a···C ₆₀	-71.14	7.31	10.3	-63.83
4b···C ₆₀	-89.59	9.07	10.1	-80.52
5a···C ₆₀	-86.68	9.15	10.6	-77.53
5b···C ₆₀	-102.59	10.40	10.1	-92.19
6a···C ₆₀	-115.48	11.76	10.2	-103.72
6b···C ₆₀	-118.29	11.53	9.7	-106.76

^a Without CP correction

^b $(-\text{BSSE}/E_{\text{int}}^{\text{a}}) \times 100$

^c With CP correction



Interaction energy with BSSE vs. interaction energy without BSSE (kcal/mol).

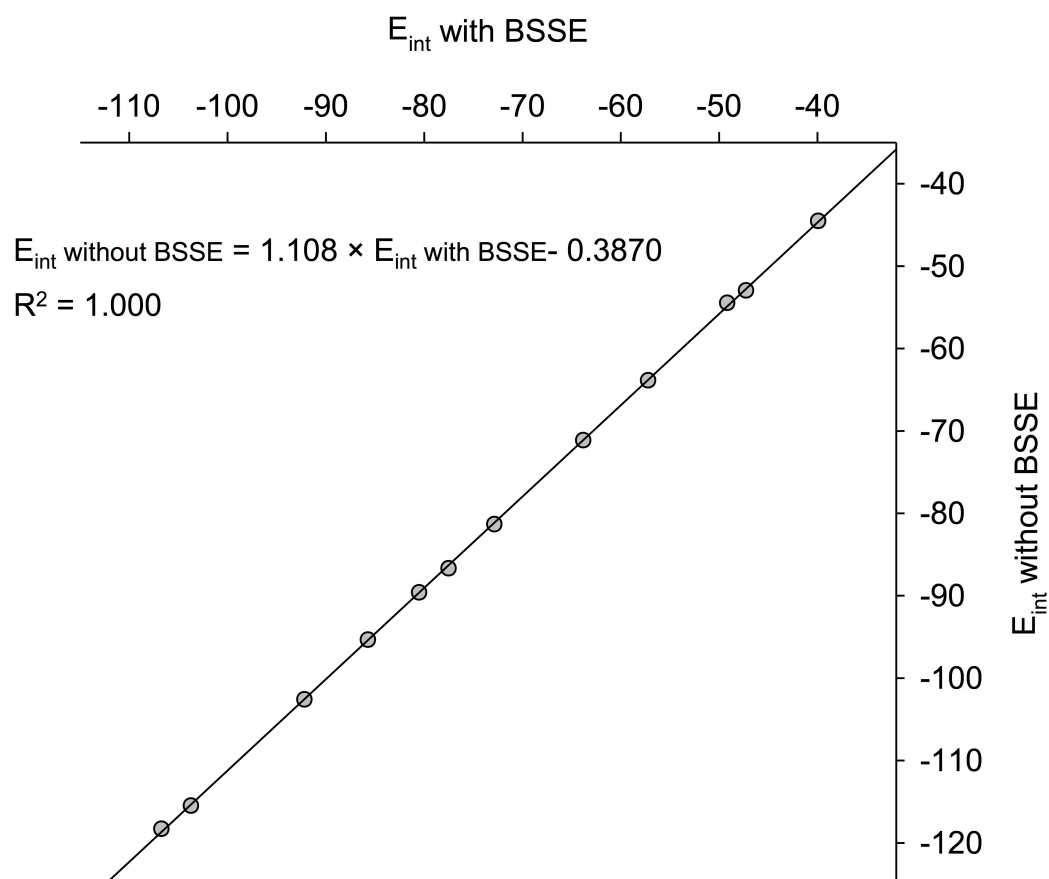


Figure S1. B97-D2/TZVP vs. B97-D2/TZVP//SCC-DFTB-D interaction energy (in kcal/mol).

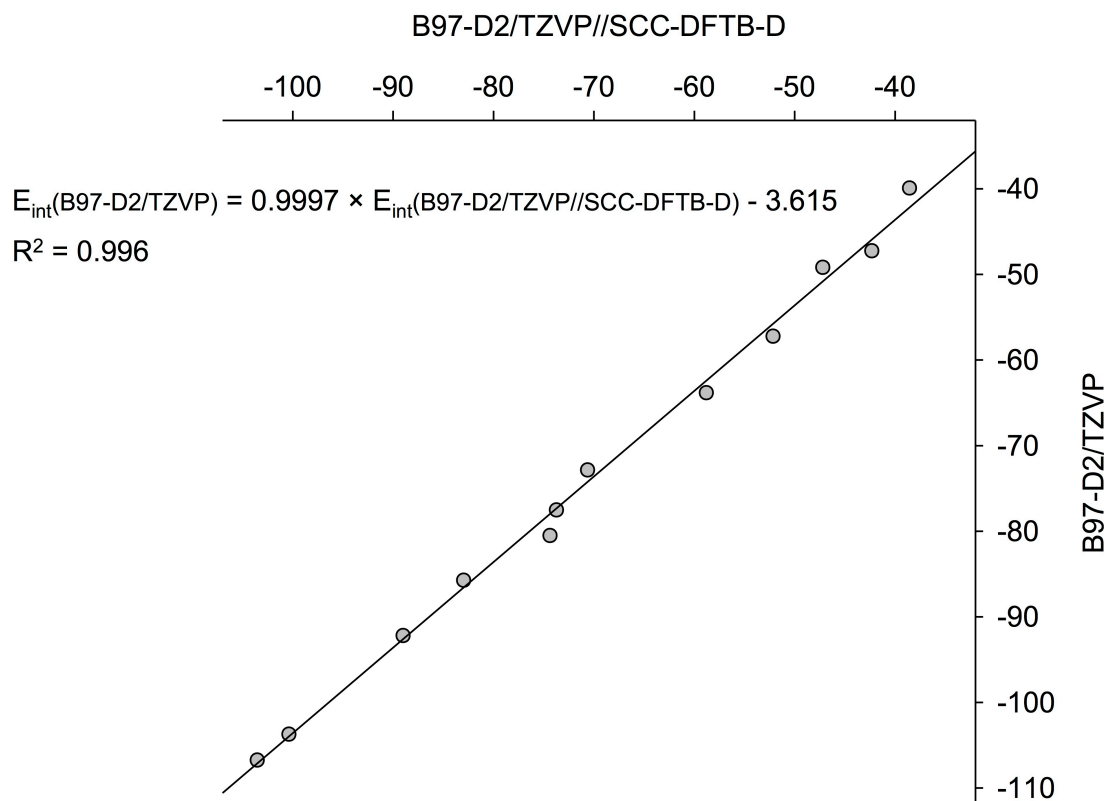
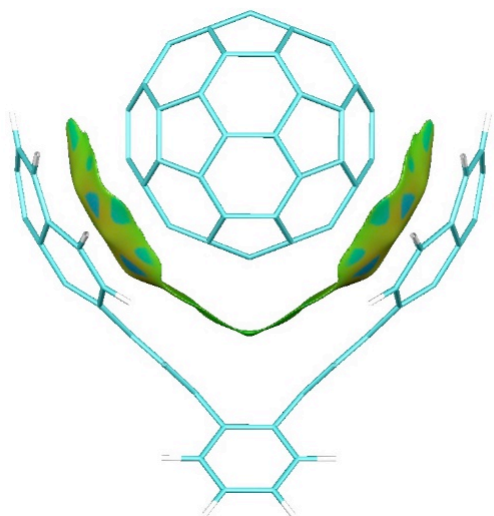


Table S3. Complexation energy (E_{complex}), deformation energy (E_{def}) in kcal/mol. Calculations were performed at the B97-D2/TZVP//SCC-DFTB-D level.

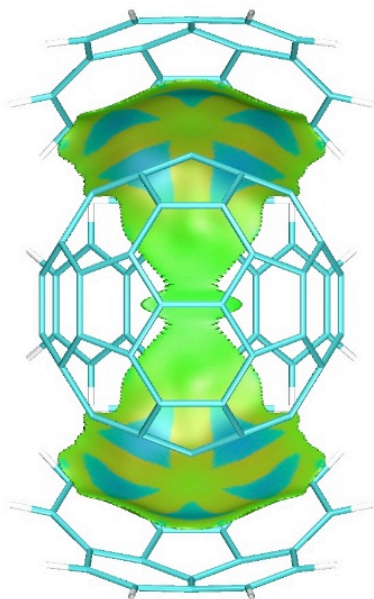
	E_{complex}	E_{def}
1a···C ₆₀	-37.86	0.69
1b···C ₆₀	-47.78	-0.59
2a···C ₆₀	-37.55	4.76
2b···C ₆₀	-45.69	6.46
3a···C ₆₀	-63.98	6.64
3b···C ₆₀	-76.55	6.43
4a···C ₆₀	-57.05	1.75
4b···C ₆₀	-73.97	0.40
5a···C ₆₀	-74.77	-1.05
5b···C ₆₀	-87.93	1.07
6a···C ₆₀	-94.92	5.46
6b···C ₆₀	-95.64	7.89

front

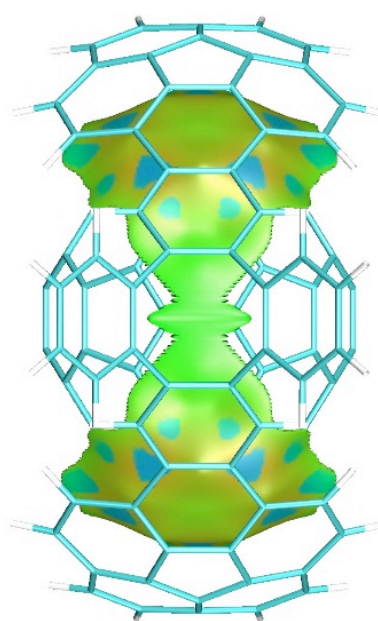


1a...C₆₀

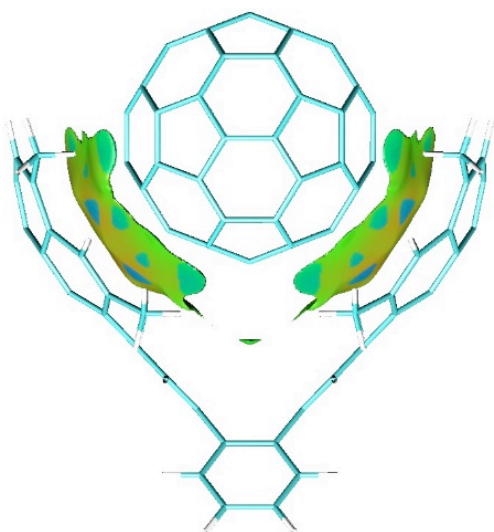
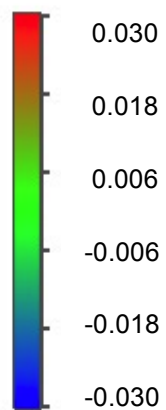
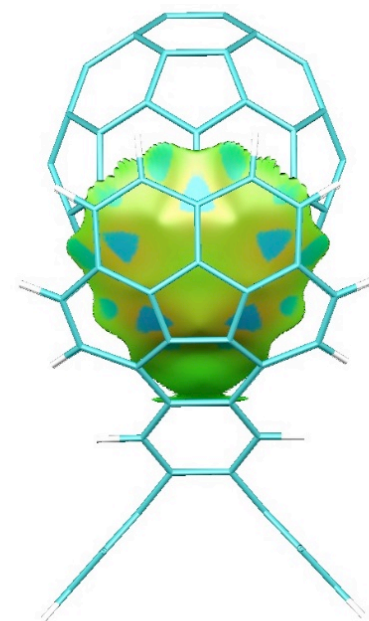
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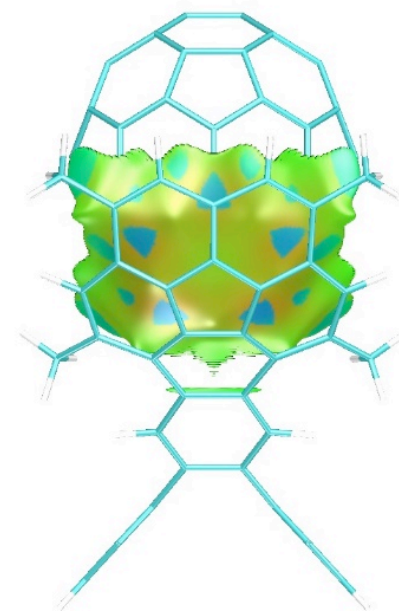
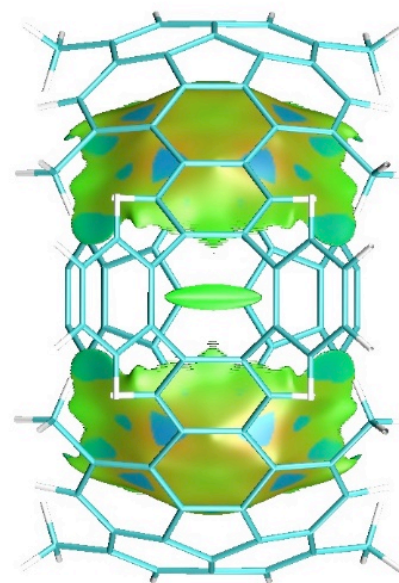
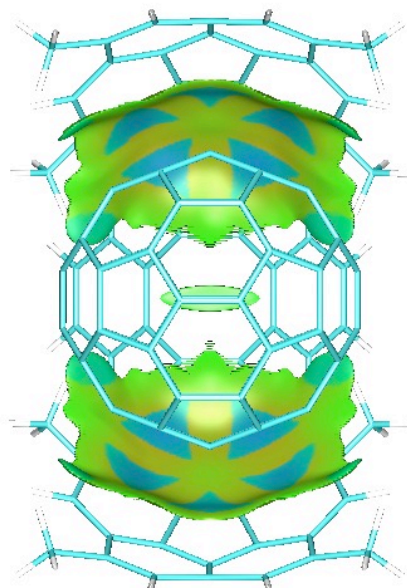
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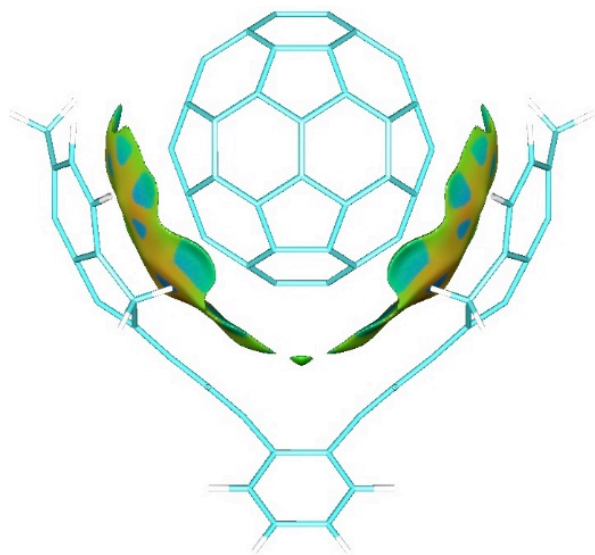


side

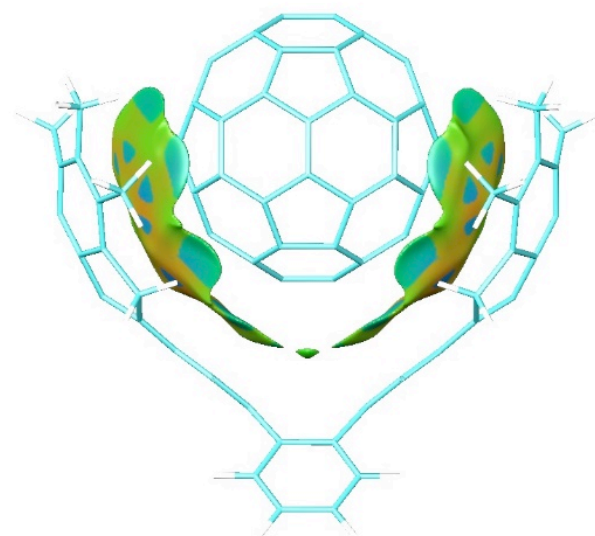
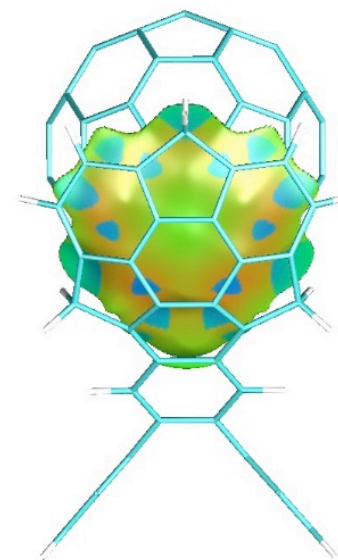
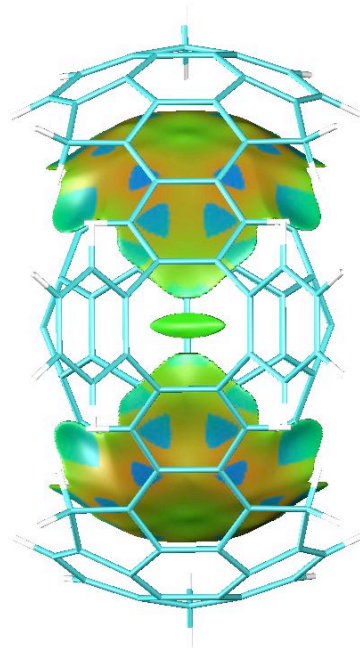
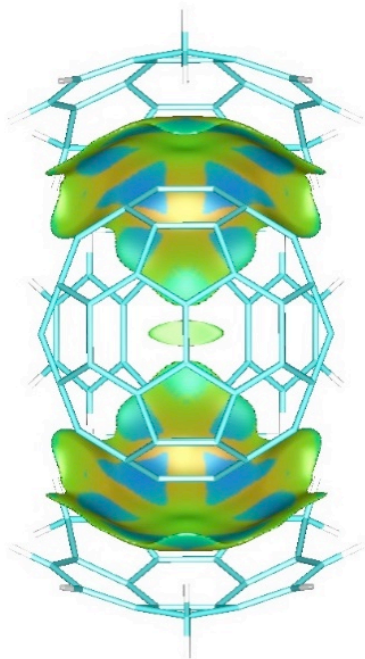


1b...C₆₀

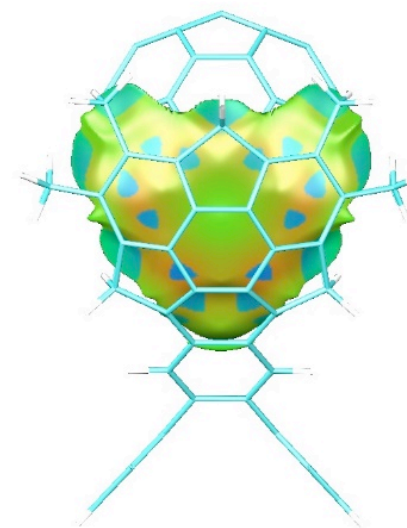
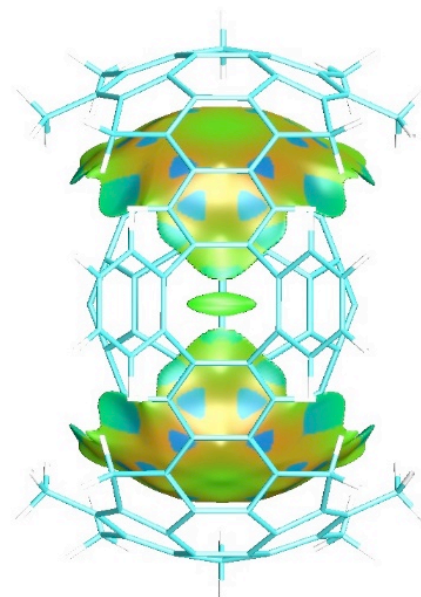
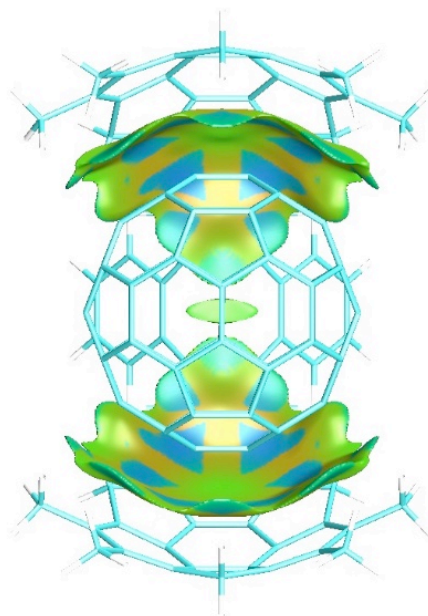


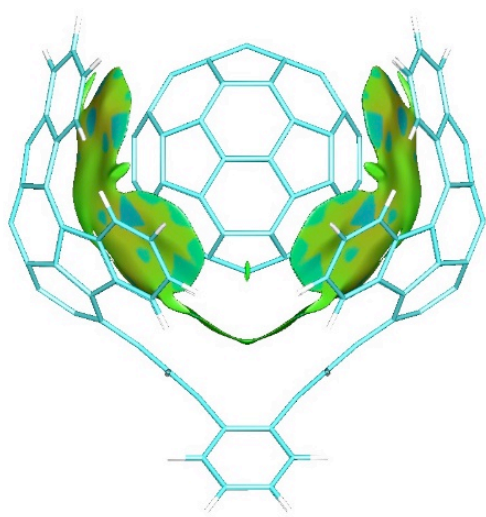


2a···**C₆₀**

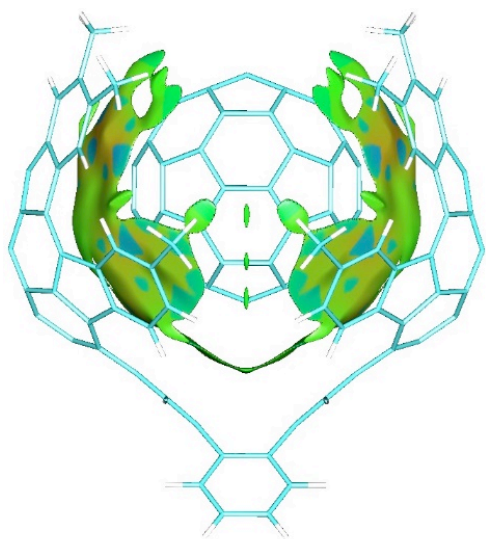
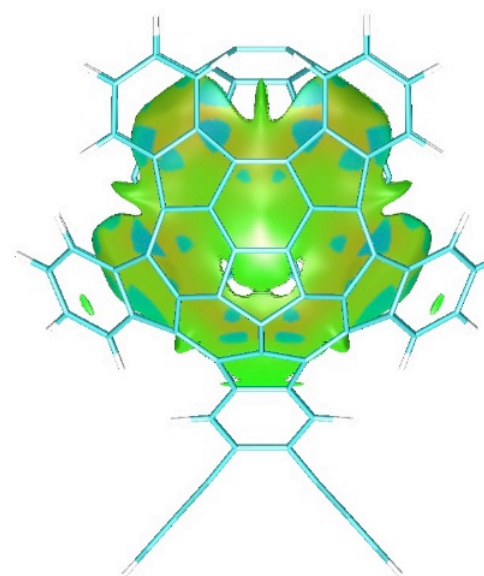
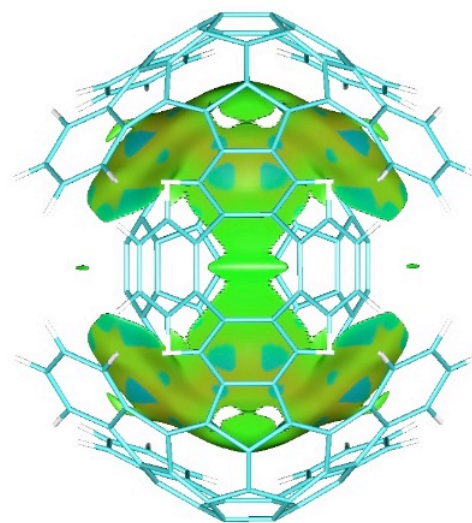
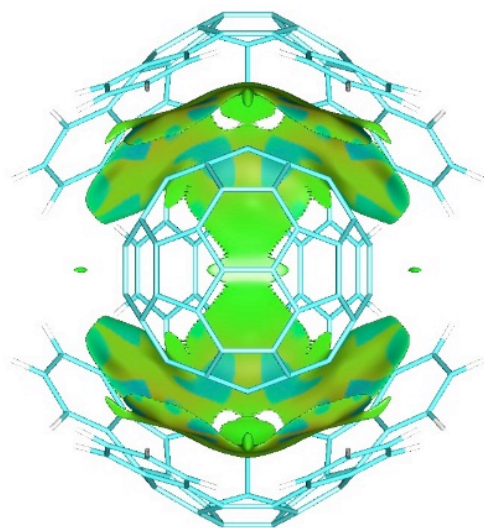


2b···**C₆₀**

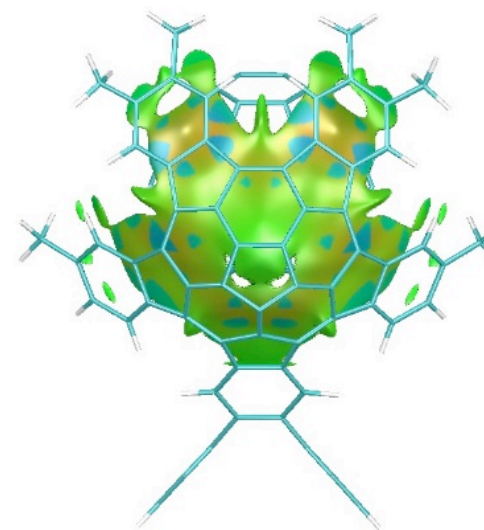
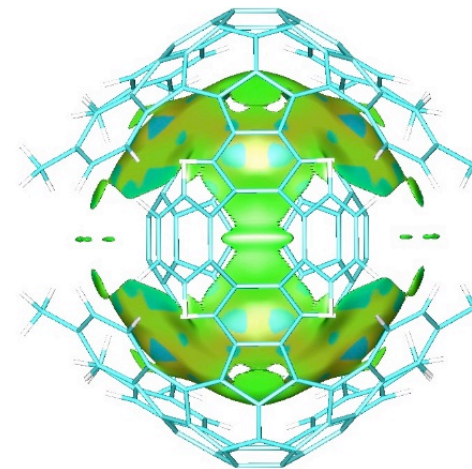
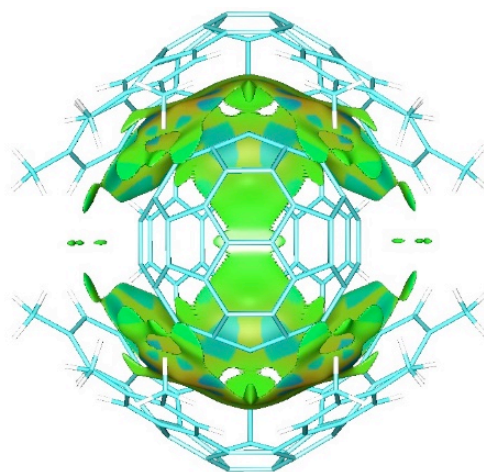


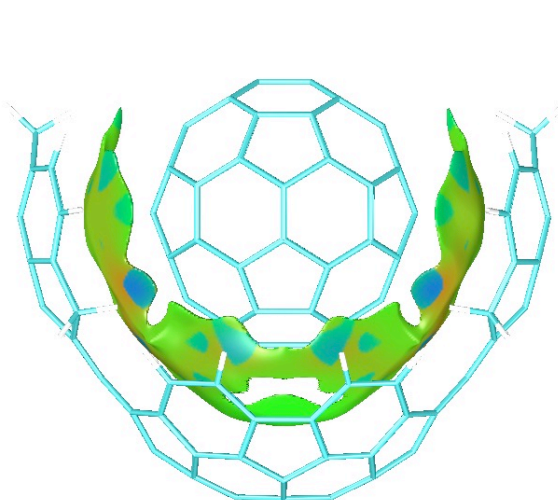


3a...C₆₀

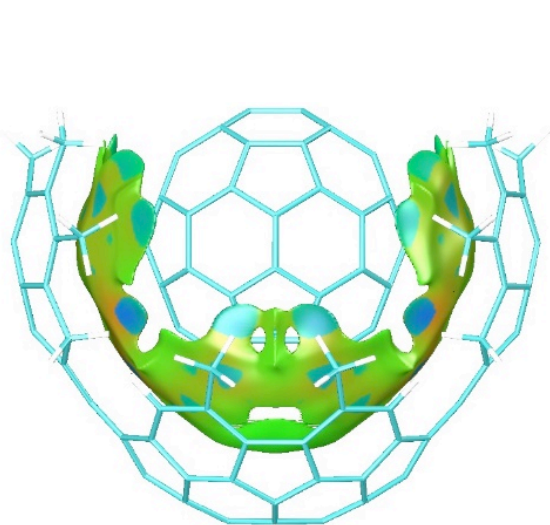
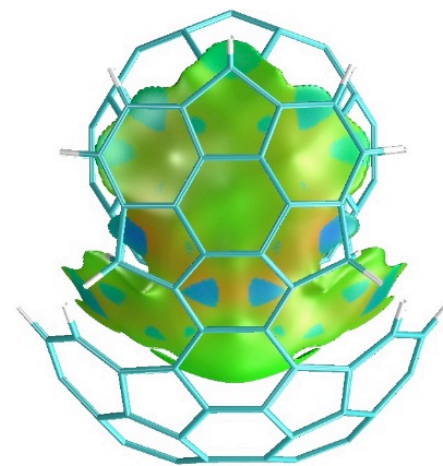
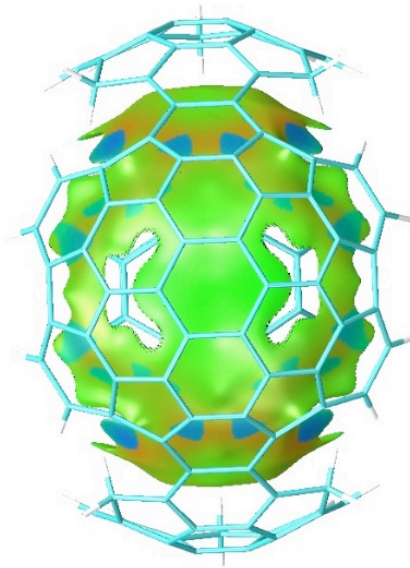
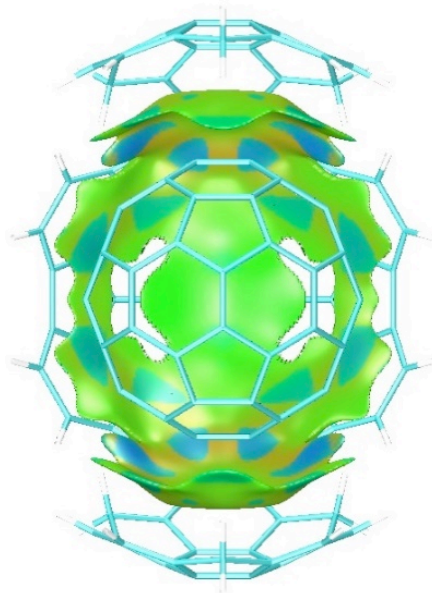


3b...C₆₀

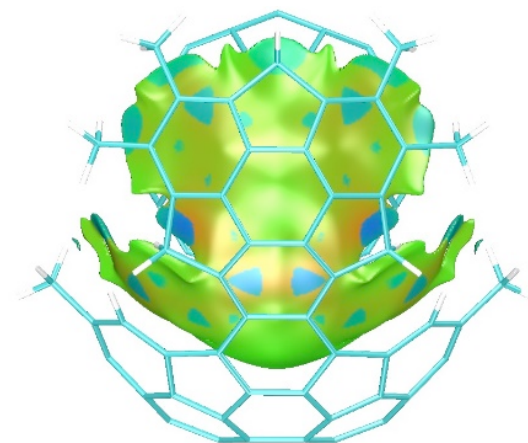
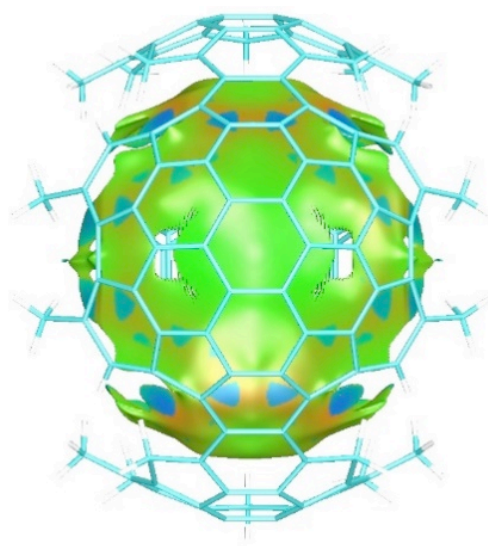
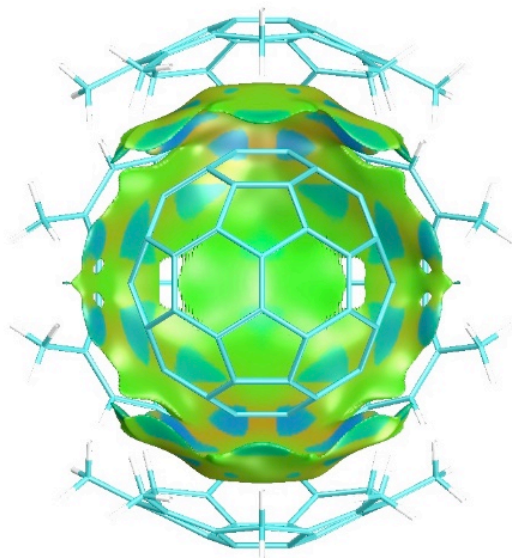


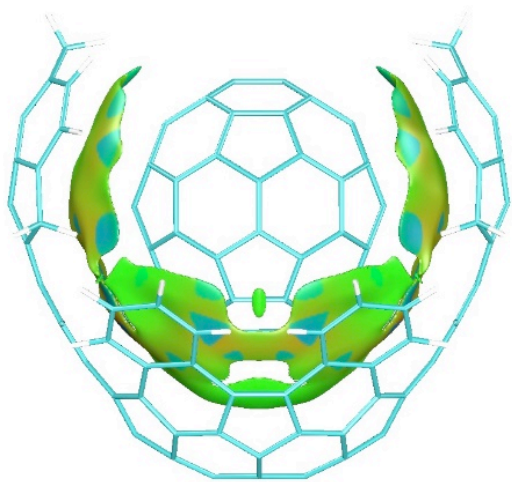


4a···**C₆₀**

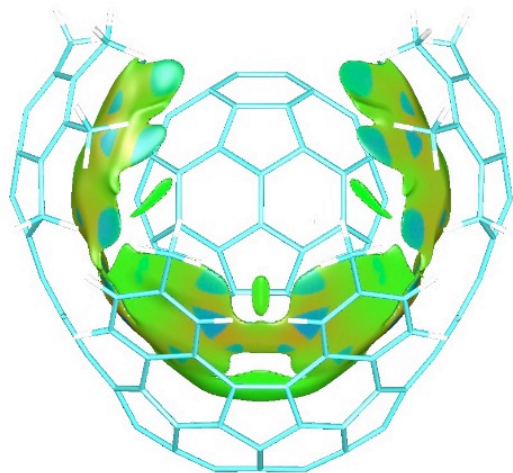
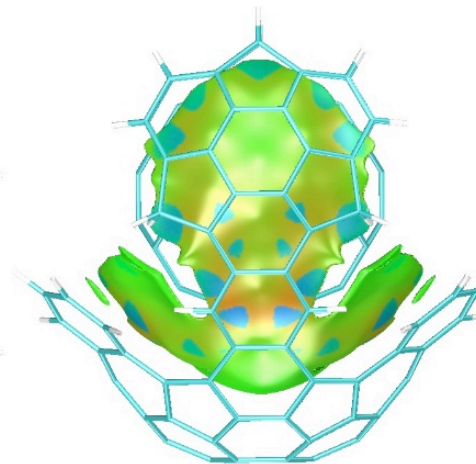
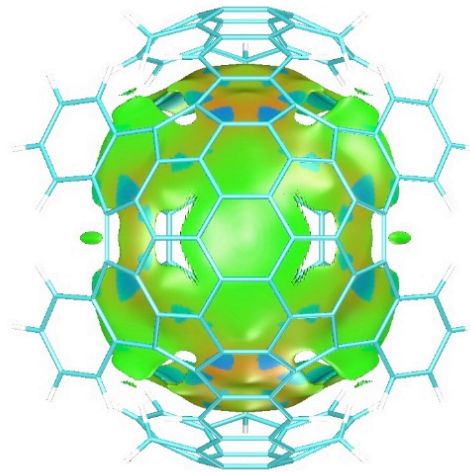
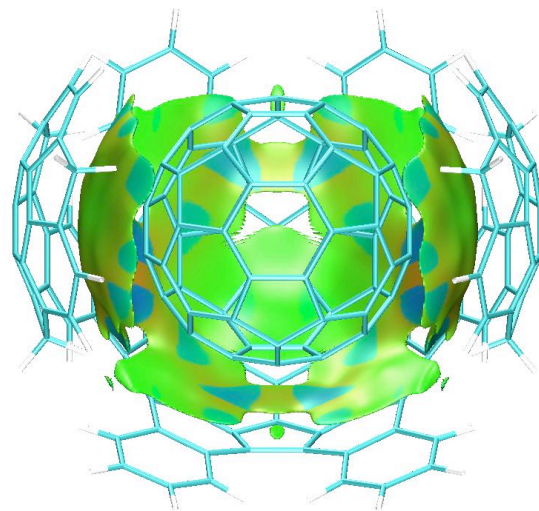


4b···**C₆₀**

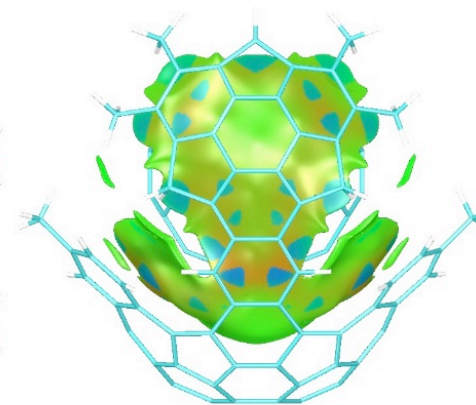
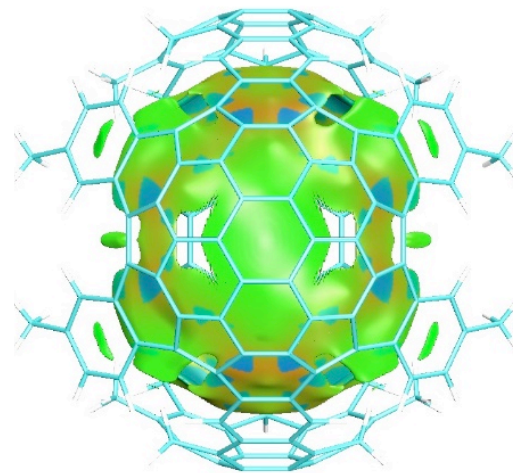
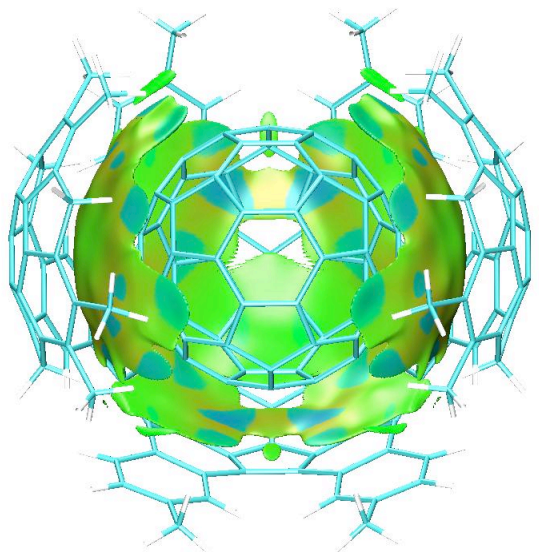


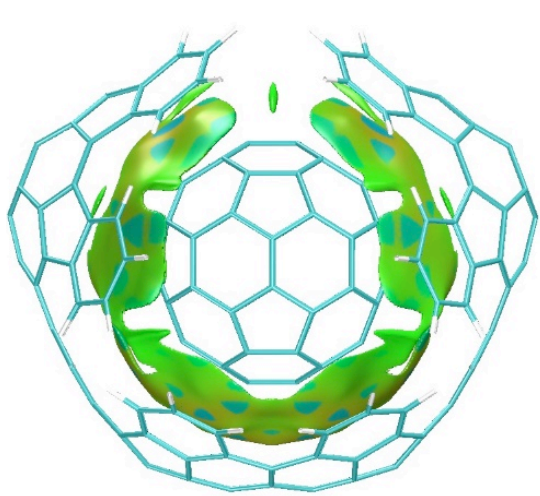


5a···C₆₀

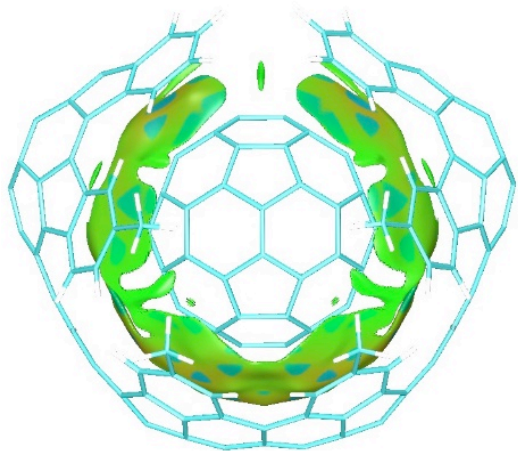
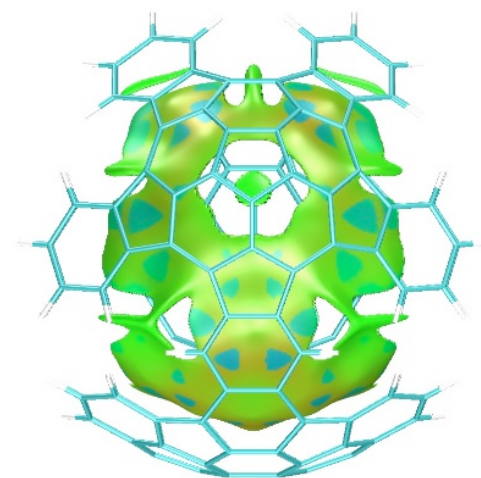
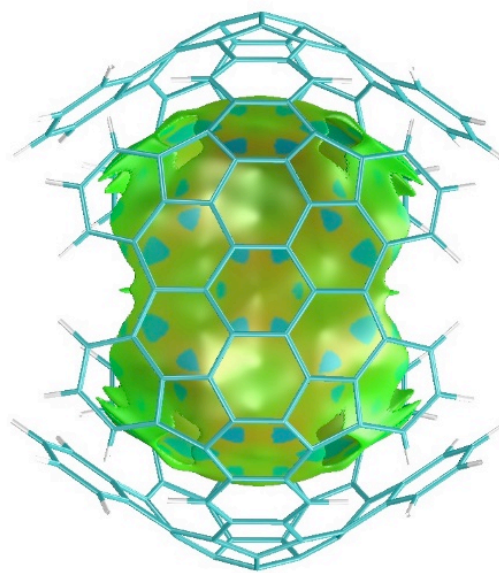
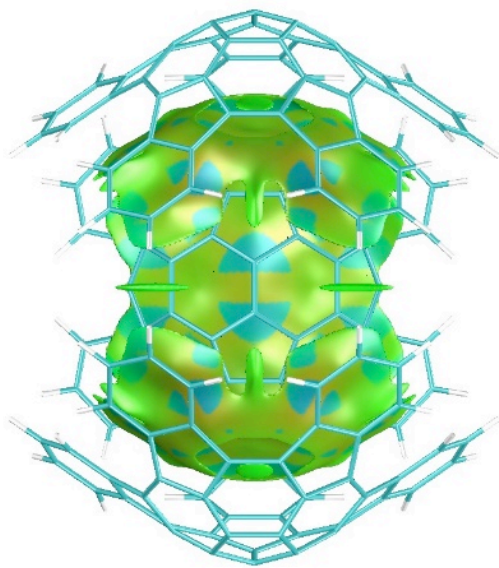


5b···C₆₀

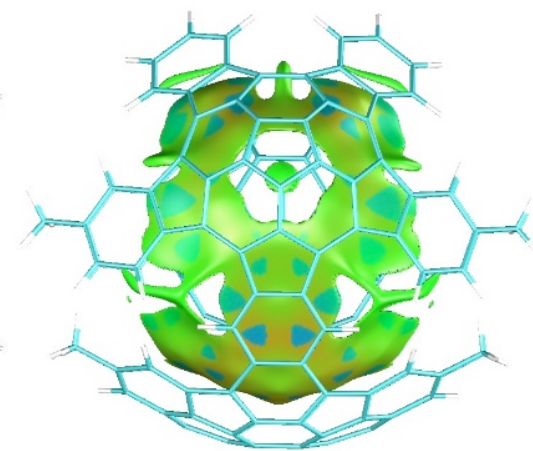
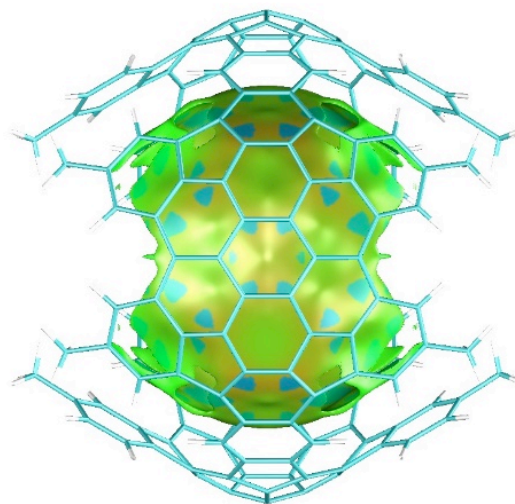
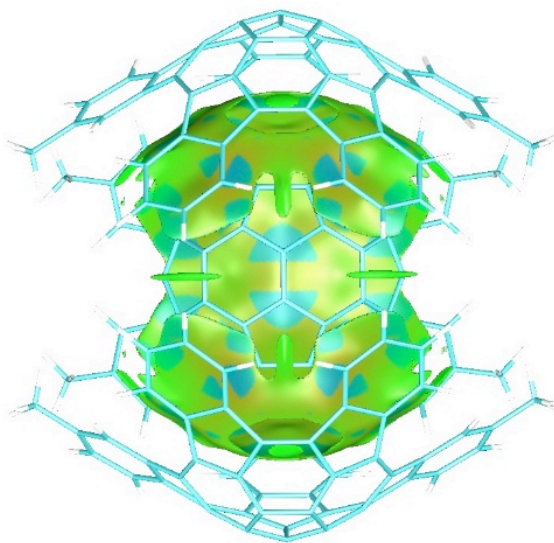




6a...C₆₀



6b...C₆₀



B97-D2/TZVP optimized geometries of complexes included in this work.

1a...C₆₀:

C	-2.42244700	-1.38365000	-3.64814800
C	-1.52149300	-0.70829500	-4.47530300
C	-1.52149300	0.70829500	-4.47530300
C	-2.42244700	1.38365000	-3.64814800
C	1.52149300	0.70829500	-4.47530300
C	2.42244700	1.38365000	-3.64814800
C	1.52149300	-0.70829500	-4.47530300
C	2.42244700	-1.38365000	-3.64814800
C	0.70548000	-1.50733300	-5.42893700
C	-0.70548000	-1.50733300	-5.42893700
C	1.38653600	-2.34613100	-6.33012700
C	-1.38653600	-2.34613100	-6.33012700
C	0.69876300	-3.16420900	-7.22682600
C	-0.69876300	-3.16420900	-7.22682600
C	0.70548000	1.50733300	-5.42893700
C	1.38653600	2.34613100	-6.33012700
C	-0.70548000	1.50733300	-5.42893700
C	0.69876300	3.16420900	-7.22682600
C	-1.38653600	2.34613100	-6.33012700
C	-0.69876300	3.16420900	-7.22682600
C	-4.86333500	-3.25436900	-0.33345900
C	-5.73988100	-2.37260200	0.39876200
C	-4.15993500	-2.82326600	-1.45764600
C	-5.96776300	-1.14722600	-0.21829500
C	-6.17026500	-2.43931800	1.77932800
C	-4.27177400	-1.47578200	-1.96129400
C	-6.40381700	0.00000000	0.48865000
C	-5.25475800	-0.71389000	-1.35981200
C	-6.59308200	-1.31018600	2.47433800
C	-3.35622400	-0.72684000	-2.83232300
C	-5.96776300	1.14722600	-0.21829500
C	-6.63191600	0.00000000	1.85866500
C	-5.25475800	0.71389000	-1.35981200
C	-3.35622400	0.72684000	-2.83232300
C	-5.73988100	2.37260200	0.39876200
C	-6.59308200	1.31018600	2.47433800
C	-4.27177400	1.47578200	-1.96129400
C	-4.86333500	3.25436900	-0.33345900
C	-6.17026500	2.43931800	1.77932800
C	-4.15993500	2.82326600	-1.45764600
C	6.17026500	2.43931800	1.77932800
C	5.73988100	2.37260200	0.39876200
C	6.59308200	1.31018600	2.47433800
C	5.96776300	1.14722600	-0.21829500
C	4.86333500	3.25436900	-0.33345900
C	6.63191600	0.00000000	1.85866500
C	5.25475800	0.71389000	-1.35981200
C	6.40381700	0.00000000	0.48865000
C	4.15993500	2.82326600	-1.45764600
C	6.59308200	-1.31018600	2.47433800
C	5.25475800	-0.71389000	-1.35981200
C	4.27177400	1.47578200	-1.96129400
C	5.96776300	-1.14722600	-0.21829500
C	6.17026500	-2.43931800	1.77932800
C	4.27177400	-1.47578200	-1.96129400
C	3.35622400	0.72684000	-2.83232300
C	5.73988100	-2.37260200	0.39876200
C	4.15993500	-2.82326600	-1.45764600
C	3.35622400	-0.72684000	-2.83232300
C	4.86333500	-3.25436900	-0.33345900
H	-2.42056900	-2.47111100	-3.66604700
H	-2.42056900	2.47111100	-3.66604700
H	2.42056900	2.47111100	-3.66604700
H	2.42056900	-2.47111100	-3.66604700
H	2.47451100	-2.34227000	-6.32132600
H	-2.47451100	-2.34227000	-6.32132600
H	1.25075100	-3.79539300	-7.92041500
H	-1.25075100	-3.79539300	-7.92041500
H	2.47451100	2.34227000	-6.32132600
H	1.25075100	3.79539300	-7.92041500
H	-2.47451100	2.34227000	-6.32132600

H	-1.25075100	3.79539300	-7.92041500
H	-4.65204200	-4.24791100	0.05883200
H	-3.42674700	-3.49982100	-1.89196400
H	-6.06335900	-3.37473100	2.32671200
H	-6.80117800	-1.40526400	3.53913600
H	-6.80117800	1.40526400	3.53913600
H	-4.65204200	4.24791100	0.05883200
H	-6.06335900	3.37473100	2.32671200
H	-3.42674700	3.49982100	-1.89196400
H	6.06335900	3.37473100	2.32671200
H	6.80117800	1.40526400	3.53913600
H	4.65204200	4.24791100	0.05883200
H	3.42674700	3.49982100	-1.89196400
H	6.80117800	-1.40526400	3.53913600
H	6.06335900	-3.37473100	2.32671200
H	3.42674700	-3.49982100	-1.89196400
H	4.65204200	-4.24791100	0.05883200
C	3.46780500	0.00000000	2.19111300
C	3.01980900	1.17108200	1.46715700
C	3.47635800	0.00000000	3.58708800
C	3.01980900	-1.17108200	1.46715700
C	2.59649100	2.30528400	2.16208000
C	2.29767800	0.72453600	0.29473900
C	2.29767800	0.72453600	0.29473900
C	3.03215100	1.17521600	4.31328200
C	3.03215100	-1.17521600	4.31328200
C	2.59649100	-2.30528400	2.16208000
C	2.29767800	-0.72453600	0.29473900
C	1.42552000	3.03358000	1.71133600
C	2.59970200	2.30701500	3.61343300
C	1.17201600	1.42402600	-0.14468300
C	2.30634200	0.72663500	5.48811700
C	2.30634200	-0.72663500	5.48811700
C	2.59970200	-2.30701500	3.61343300
C	1.42552000	-3.03358000	1.71133600
C	1.17201600	-1.42402600	-0.14468300
C	0.69942100	3.48308600	2.88636700
C	0.72622700	2.60076800	0.57868100
C	1.42542000	3.03361200	4.06226100
C	0.00000000	0.69964400	-0.59919600
C	1.17479400	1.42610400	5.92015000
C	1.17479400	-1.42610400	5.92015000
C	1.42542000	-3.03361200	4.06226100
C	0.69942100	-3.48308600	2.88636700
C	0.72622700	-2.60076800	0.57868100
C	0.00000000	-0.69964400	-0.59919600
C	-0.69942100	3.48308600	2.88636700
C	-0.72622700	2.60076800	0.57868100
C	0.72628300	2.60135800	5.19419700
C	-1.17201600	1.42402600	-0.14468300
C	0.00000000	0.69943000	6.36907200
C	0.72628300	-2.60135800	5.19419700
C	0.00000000	-0.69943000	6.36907200
C	-0.69942100	-3.48308600	2.88636700
C	-0.72622700	-2.60076800	0.57868100
C	-1.17201600	-1.42402600	-0.14468300
C	-1.42542000	3.03361200	4.06226100
C	-1.42552000	3.03358000	1.71133600
C	-0.72628300	2.60135800	5.19419700
C	-2.29767800	0.72453600	0.29473900
C	-1.17479400	1.42610400	5.92015000
C	-0.72628300	-2.60135800	5.19419700
C	-1.17479400	-1.42610400	5.92015000
C	-1.42542000	-3.03361200	4.06226100
C	-1.42552000	-3.03358000	1.71133600
C	-2.29767800	-0.72453600	0.29473900
C	-2.59970200	2.30701500	3.61343300
C	-2.59649100	2.30528400	2.16208000
C	-3.01980900	1.17108200	1.46715700
C	-2.30634200	0.72663500	5.48811700
C	-2.30634200	-0.72663500	5.48811700
C	-2.59970200	-2.30701500	3.61343300
C	-2.59649100	-2.30528400	2.16208000
C	-3.01980900	-1.17108200	1.46715700
C	-3.03215100	1.17521600	4.31328200
C	-3.46780500	0.00000000	2.19111300
C	-3.03215100	-1.17521600	4.31328200

C	-3.47635800	0.00000000	3.58708800	H	-6.81885300	-1.39619600	3.42909200
				H	-6.81885300	1.39619600	3.42909200
1b...C₆₀:				H	-4.55373500	4.23028300	0.05042300
C	-2.36037000	-1.37547500	-3.81415600	H	6.81885300	1.39619600	3.42909200
C	-1.50002800	-0.70475700	-4.68493200	H	4.55373500	4.23028300	0.05042300
C	-1.50002800	0.70475700	-4.68493200	H	6.81885300	-1.39619600	3.42909200
C	-2.36037000	1.37547500	-3.81415600	H	4.55373500	-4.23028300	0.05042300
C	1.50002800	0.70475700	-4.68493200	C	3.46793300	0.00000000	2.24750800
C	2.36037000	1.37547500	-3.81415600	C	3.02120500	1.17132900	1.52359800
C	1.50002800	-0.70475700	-4.68493200	C	3.47717300	0.00000000	3.64318100
C	2.36037000	-1.37547500	-3.81415600	C	3.02120500	-1.17132900	1.52359800
C	0.70552800	-1.50571600	-5.65461400	C	2.59690500	2.30486300	2.21861800
C	-0.70552800	-1.50571600	-5.65461400	C	2.29850000	0.72458700	0.35037000
C	1.38854300	-2.34354900	-6.55312100	C	3.03305400	1.17516400	4.36956500
C	-1.38854300	-2.34354900	-6.55312100	C	3.03305400	-1.17516400	4.36956500
C	0.69898000	-3.16211000	-7.44900700	C	2.59690500	-2.30486300	2.21861800
C	-0.69898000	-3.16211000	-7.44900700	C	2.29850000	-0.72458700	0.35037000
C	0.70552800	1.50571600	-5.65461400	C	1.42576800	3.03349300	1.76816400
C	1.38854300	2.34354900	-6.55312100	C	2.59982000	2.30658900	3.66971100
C	-0.70552800	1.50571600	-5.65461400	C	1.17154000	1.42304500	-0.08677200
C	0.69898000	3.16211000	-7.44900700	C	2.30686500	0.72664100	5.54426000
C	-1.38854300	2.34354900	-6.55312100	C	2.30686500	-0.72664100	5.54426000
C	-0.69898000	3.16211000	-7.44900700	C	2.59982000	-2.30658900	3.66971100
C	-4.74916300	-3.24118400	-0.35959100	C	1.42576800	-3.03349300	1.76816400
C	-5.64244700	-2.36357800	0.33937200	C	1.17154000	-1.42304500	-0.08677200
C	-3.99313400	-2.85179600	-1.47277800	C	0.69968700	3.48296900	2.94272700
C	-5.84310600	-1.14308200	-0.28949500	C	0.72563700	2.59925200	0.63706300
C	-6.11978600	-2.45020600	1.71278000	C	1.42568700	3.03328900	4.11843400
C	-4.10168600	-1.49207000	-1.99735600	C	0.00000000	0.69961800	-0.54196600
C	-6.31109000	0.00000000	0.39465400	C	1.17494700	1.42587700	5.97613800
C	-5.08499500	-0.71748800	-1.40508700	C	1.17494700	-1.42587700	5.97613800
C	-6.57304300	-1.30718600	2.37086600	C	1.42568700	-3.03328900	4.11843400
C	-3.22015100	-0.73185600	-2.90629400	C	0.69968700	-3.48296900	2.94272700
C	-5.84310600	1.14308200	-0.28949500	C	0.72563700	-2.59925200	0.63706300
C	-6.59042000	0.00000000	1.75290600	C	0.00000000	-0.69961800	-0.54196600
C	-5.08499500	0.71748800	-1.40508700	C	-0.69968700	3.48296900	2.94272700
C	-3.22015100	0.73185600	-2.90629400	C	-0.72563700	2.59925200	0.63706300
C	-5.64244700	2.36357800	0.33937200	C	0.72624700	2.60105400	5.25027800
C	-6.57304300	1.30718600	2.37086600	C	-1.17154000	1.42304500	-0.08677200
C	-4.10168600	1.49207000	-1.99735600	C	0.00000000	0.69935600	6.42498500
C	-4.74916300	3.24118400	-0.35959100	C	0.72624700	-2.60105400	5.25027800
C	-6.11978600	2.45020600	1.71278000	C	0.00000000	-0.69935600	6.42498500
C	-3.99313400	2.85179600	-1.47277800	C	-0.69968700	-3.48296900	2.94272700
C	6.11978600	2.45020600	1.71278000	C	-0.72563700	-2.59925200	0.63706300
C	5.64244700	2.36357800	0.33937200	C	-1.17154000	-1.42304500	-0.08677200
C	6.57304300	1.30718600	2.37086600	C	-1.42568700	3.03328900	4.11843400
C	5.84310600	1.14308200	-0.28949500	C	-1.42576800	3.03349300	1.76816400
C	4.74916300	3.24118400	-0.35959100	C	-0.72624700	2.60105400	5.25027800
C	6.59042000	0.00000000	1.75290600	C	-2.29850000	0.72458700	0.35037000
C	5.08499500	0.71748800	-1.40508700	C	-1.17494700	1.42587700	5.97613800
C	6.31109000	0.00000000	0.39465400	C	-0.72624700	-2.60105400	5.25027800
C	3.99313400	2.85179600	-1.47277800	C	-1.17494700	-1.42587700	5.97613800
C	6.57304300	-1.30718600	2.37086600	C	-1.42568700	-3.03328900	4.11843400
C	5.08499500	-0.71748800	-1.40508700	C	-1.42576800	-3.03349300	1.76816400
C	4.10168600	1.49207000	-1.99735600	C	-2.29850000	-0.72458700	0.35037000
C	5.84310600	-1.14308200	-0.28949500	C	-2.59982000	2.30658900	3.66971100
C	6.11978600	-2.45020600	1.71278000	C	-2.59690500	2.30486300	2.21861800
C	4.10168600	-1.49207000	-1.99735600	C	-3.02120500	1.17132900	1.52359800
C	3.22015100	0.73185600	-2.90629400	C	-2.30686500	0.72664100	5.54426000
C	5.64244700	-2.36357800	0.33937200	C	-2.30686500	-0.72664100	5.54426000
C	3.99313400	-2.85179600	-1.47277800	C	-2.59982000	-2.30658900	3.66971100
C	3.22015100	-0.73185600	-2.90629400	C	-2.59690500	-2.30486300	2.21861800
C	4.74916300	-3.24118400	-0.35959100	C	-3.02120500	-1.17132900	1.52359800
H	-2.37865300	-2.45370100	-3.88413600	C	-3.03305400	1.17516400	4.36956500
H	-2.37865300	2.45370100	-3.88413600	C	-3.46793300	0.00000000	2.24750800
H	2.37865300	2.45370100	-3.88413600	C	-3.03305400	-1.17516400	4.36956500
H	2.37865300	-2.45370100	-3.88413600	C	-3.47717300	0.00000000	3.64318100
H	2.47675500	-2.34035000	-6.54316100	C	-5.97923900	3.75377500	2.45782500
H	-2.47675500	-2.34035000	-6.54316100	H	-4.92548500	4.06663100	2.48781300
H	1.25016400	-3.79434800	-8.14234800	H	-6.54283500	4.55757900	1.96299000
H	-1.25016400	-3.79434800	-8.14234800	H	-6.33646100	3.66240500	3.48972000
H	2.47675500	2.34035000	-6.54316100	C	-5.97923900	-3.75377500	2.45782500
H	1.25016400	3.79434800	-8.14234800	H	-6.54283500	-4.55757900	1.96299000
H	-2.47675500	2.34035000	-6.54316100	H	-4.92548500	-4.06663100	2.48781300
H	-1.25016400	3.79434800	-8.14234800	H	-6.33646100	-3.66240500	3.48972000
H	-4.55373500	-4.23028300	0.05042300	C	-2.98226800	-3.84611800	-1.99618100

H	-3.21734200	-4.16840200	-3.02074500
H	-1.97354600	-3.41345300	-2.00885100
H	-2.96001500	-4.73931200	-1.36181600
C	-2.98226800	3.84611800	-1.99618100
H	-1.97354600	3.41345300	-2.00885100
H	-3.21734200	4.16840200	-3.02074500
H	-2.96001500	4.73931200	-1.36181600
C	5.97923900	-3.75377500	2.45782500
H	4.92548500	-4.06663100	2.48781300
H	6.54283500	-4.55757900	1.96299000
H	6.33646100	-3.66240500	3.48972000
C	5.97923900	3.75377500	2.45782500
H	6.54283500	4.55757900	1.96299000
H	4.92548500	4.06663100	2.48781300
H	6.33646100	3.66240500	3.48972000
C	2.98226800	3.84611800	-1.99618100
H	3.21734200	4.16840200	-3.02074500
H	1.97354600	3.41345300	-2.00885100
H	2.96001500	4.73931200	-1.36181600
C	2.98226800	-3.84611800	-1.99618100
H	1.97354600	-3.41345300	-2.00885100
H	3.21734200	-4.16840200	-3.02074500
H	2.96001500	-4.73931200	-1.36181600

2a...C₆₀:

C	2.48995200	1.39021100	-3.55429900
C	1.54736800	0.71414700	-4.32106500
C	1.54736800	-0.71414700	-4.32106500
C	2.48995200	-1.39021100	-3.55429900
C	-1.54736800	-0.71414700	-4.32106500
C	-2.48995200	-1.39021100	-3.55429900
C	-1.54736800	0.71414700	-4.32106500
C	-2.48995200	1.39021100	-3.55429900
C	-0.70644900	1.50313600	-5.26354700
C	0.70644900	1.50313600	-5.26354700
C	-1.38388600	2.32337200	-6.18662800
C	1.38388600	2.32337200	-6.18662800
C	-0.69850900	3.12249600	-7.10136200
C	0.69850900	3.12249600	-7.10136200
C	-0.70644900	-1.50313600	-5.26354700
C	-1.38388600	-2.32337200	-6.18662800
C	0.70644900	-1.50313600	-5.26354700
C	-0.69850900	-3.12249600	-7.10136200
C	1.38388600	-2.32337200	-6.18662800
C	0.69850900	-3.12249600	-7.10136200
C	5.41676900	0.70224200	-1.37370700
C	6.00102300	1.41145500	-0.27585200
C	5.41676900	-0.70224200	-1.37370700
C	6.55756000	0.71516000	0.78835600
C	6.55756000	-0.71516000	0.78835600
C	6.00102300	-1.41145500	-0.27585200
C	6.11727500	2.54262300	2.24454400
C	5.54528500	3.26160500	1.14773200
C	3.49266500	0.73809300	-2.79865600
C	3.49266500	-0.73809300	-2.79865600
C	6.11727500	-2.54262300	2.24454400
C	5.54528500	-3.26160500	1.14773200
C	5.40945300	2.66665000	-0.11924400
C	4.43190000	1.45058700	-1.98695600
C	4.45359600	2.86056200	-1.33265200
C	5.40945300	-2.66665000	-0.11924400
C	4.43190000	-1.45058700	-1.98695600
C	4.45359600	-2.86056200	-1.33265200
C	6.56493600	1.21840200	2.09125500
C	6.56493600	-1.21840200	2.09125500
C	6.76327000	0.00000000	3.04172000
C	-5.41676900	-0.70224200	-1.37370700
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C	-6.55756000	-0.71516000	0.78835600
C	-6.55756000	0.71516000	0.78835600
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C	-6.11727500	-2.54262300	2.24454400
C	-5.54528500	-3.26160500	1.14773200
C	-3.49266500	-0.73809300	-2.79865600
C	-3.49266500	0.73809300	-2.79865600

C	-6.11727500	2.54262300	2.24454400
C	-5.54528500	3.26160500	1.14773200
C	-5.40945300	-2.66665000	-0.11924400
C	-4.43190000	-1.45058700	-1.98695600
C	-4.45359600	-2.86056200	-1.33265200
C	-5.40945300	2.66665000	-0.11924400
C	-4.43190000	1.45058700	-1.98695600
C	-4.45359600	2.86056200	-1.33265200
C	-6.56493600	-1.21840200	2.09125500
C	-6.56493600	1.21840200	2.09125500
C	-6.76327000	0.00000000	3.04172000
H	2.48893600	2.47822700	-3.57355300
H	2.48893600	-2.47822700	-3.57355300
H	-2.48893600	-2.47822700	-3.57355300
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H	-2.47179200	2.31450100	-6.18275600
H	2.47179200	2.31450100	-6.18275600
H	-1.25244000	3.73423100	-7.81085400
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H	6.06493900	3.00480700	3.22914900
H	5.08767100	4.22575800	1.36358600
H	6.06493900	-3.00480700	3.22914900
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H	4.81107900	3.63711900	-2.02632500
H	3.45101800	3.16015700	-1.00340200
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H	4.81107900	-3.63711900	-2.02632500
H	7.75909800	0.00000000	3.51026100
H	6.02120200	0.00000000	3.84926200
H	-6.06493900	-3.00480700	3.22914900
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H	-4.81107900	3.63711900	-2.02632500
H	-7.75909800	0.00000000	3.51026100
H	-6.02120200	0.00000000	3.84926200
C	2.30537600	-2.60166800	3.31440300
C	2.30128500	-2.59785000	1.86323100
C	3.01912900	-1.42041800	1.41763300
C	3.47211000	-0.69816200	2.58644500
C	3.02960300	-1.42483600	3.76166600
C	1.17420100	-3.03512000	4.01458600
C	1.17418500	-3.03600500	1.16196700
C	2.58614000	-0.72361400	0.29158100
C	3.47211000	0.69816200	2.58644500
C	2.60105200	-0.72678400	4.89517300
C	2.60105200	0.72678400	4.89517300
C	3.02960300	1.42483600	3.76166600
C	3.01912900	1.42041800	1.41763300
C	2.58614000	0.72361400	0.29158100
C	0.72546400	-2.31015800	-0.01478100
C	1.41781900	-1.17262700	-0.43578800
C	0.00000000	-3.48554900	1.88835600
C	0.00000000	-3.48586300	3.28880400
C	0.72608700	-2.30804300	5.18965000
C	1.42575300	-1.17545300	5.62035100
C	2.30128500	2.59785000	1.86323100
C	2.30537600	2.60166800	3.31440300
C	0.69666200	0.00000000	-0.88620700
C	1.41781900	1.17262700	-0.43578800
C	-1.17418500	-3.03600500	1.16196700
C	-0.72608700	-2.30804300	5.18965000
C	-1.17420100	-3.03512000	4.01458600
C	1.42575300	1.17545300	5.62035100
C	0.69952500	0.00000000	6.06803900
C	0.72546400	2.31015800	-0.01478100
C	1.17418500	3.03600500	1.16196700
C	1.17420100	3.03512000	4.01458600
C	0.72608700	2.30804300	5.18965000

C	-0.69952500	0.00000000	6.06803900	C	-6.10419600	-2.53913900	1.88036100
C	-1.42575300	-1.17545300	5.62035100	C	-5.53769400	-3.27110900	0.76619600
C	-2.30537600	-2.60166800	3.31440300	C	-3.51572000	-0.73803400	-3.18033000
C	-2.30128500	-2.59785000	1.86323100	C	-3.51572000	0.73803400	-3.18033000
C	-1.41781900	-1.17262700	-0.43578800	C	-6.10419600	2.53913900	1.88036100
C	-0.69666200	0.00000000	-0.88620700	C	-5.53769400	3.27110900	0.76619600
C	-2.58614000	-0.72361400	0.29158100	C	-5.42804900	-2.66033200	-0.49742400
C	-3.01912900	-1.42041800	1.41763300	C	-4.45904400	-1.45062700	-2.37445200
C	-3.02960300	-1.42483600	3.76166600	C	-4.47561500	-2.85821300	-1.71487300
C	-2.60105200	-0.72678400	4.89517300	C	-5.42804900	2.66033200	-0.49742400
C	-1.42575300	1.17545300	5.62035100	C	-4.45904400	1.45062700	-2.37445200
C	-0.72608700	2.30804300	5.18965000	C	-4.47561500	2.85821300	-1.71487300
C	0.00000000	3.48586300	3.28880400	C	-6.55901700	-1.21879400	1.70333500
C	0.00000000	3.48554900	1.88835600	C	-6.55901700	1.21879400	1.70333500
C	-0.72546400	2.31015800	-0.01478100	C	-6.74479400	0.00000000	2.65760000
C	-1.41781900	1.17262700	-0.43578800	C	2.50218100	2.47654100	-3.94181500
C	-1.17420100	3.03512000	4.01458600	H	2.50218100	-2.47654100	-3.94181500
C	-2.60105200	0.72678400	4.89517300	H	-2.50218100	-2.47654100	-3.94181500
C	-2.58614000	0.72361400	0.29158100	H	-2.50218100	2.47654100	-3.94181500
C	-1.17418500	3.03600500	1.16196700	H	-2.47027300	2.35521900	-6.50713900
C	-3.01912900	1.42041800	1.41763300	H	2.47027300	2.35521900	-6.50713900
C	-2.30128500	2.59785000	1.86323100	H	-1.25349800	3.83295800	-8.08183100
C	-3.47211000	-0.69816200	2.58644500	H	1.25349800	3.83295800	-8.08183100
C	-3.47211000	0.69816200	2.58644500	H	-2.47027300	-2.35521900	-6.50713900
C	-0.72546400	-2.31015800	-0.01478100	H	-1.25349800	-3.83295800	-8.08183100
C	-2.30537600	2.60166800	3.31440300	H	2.47027300	-2.35521900	-6.50713900
C	-3.02960300	1.42483600	3.76166600	H	1.25349800	-3.83295800	-8.08183100
				H	4.82832100	3.64010700	-2.40539800
				H	3.47012600	3.15038700	-1.38714200
				H	3.47012600	-3.15038700	-1.38714200
				H	4.82832100	-3.64010700	-2.40539800
				H	7.72989900	0.00000000	3.14917200
				H	5.98718500	0.00000000	3.45077500
				H	-4.82832100	-3.64010700	-2.40539800
				H	-3.47012600	-3.15038700	-1.38714200
				H	-3.47012600	3.15038700	-1.38714200
				H	-4.82832100	3.64010700	-2.40539800
				H	-7.72989900	0.00000000	3.14917200
				H	-5.98718500	0.00000000	3.45077500
				C	2.30297400	-2.59757200	2.91591700
				C	2.29988700	-2.59409700	1.46521200
				C	3.02287900	-1.42122600	1.01842000
				C	3.47585600	-0.69806700	2.18888500
				C	3.02867400	-1.42205900	3.36322800
				C	1.17368100	-3.03296800	3.61666600
				C	1.17384700	-3.03397600	0.76423600
				C	2.58822000	-0.72395500	-0.10685800
				C	3.47585600	0.69806700	2.18888500
				C	2.60206400	-0.72619800	4.49841500
				C	2.60206400	0.72619800	4.49841500
				C	3.02867400	1.42205900	3.36322800
				C	3.02287900	1.42122600	1.01842000
				C	2.58822000	0.72395500	-0.10685800
				C	0.72541800	-2.30939700	-0.41233000
				C	1.41894100	-1.17235000	-0.83320900
				C	0.00000000	-3.48343000	1.49092400
				C	0.00000000	-3.48473100	2.89112000
				C	0.72594200	-2.30669800	4.79254700
				C	1.42620700	-1.17490300	5.22369600
				C	2.29988700	2.59409700	1.46521200
				C	2.30297400	2.59757200	2.91591700
				C	0.69675700	0.00000000	-1.28237800
				C	1.41894100	1.17235000	-0.83320900
				C	-1.17384700	-3.03397600	0.76423600
				C	-0.72594200	-2.30669800	4.79254700
				C	-1.17368100	-3.03296800	3.61666600
				C	1.42620700	1.17490300	5.22369600
				C	0.69984000	0.00000000	5.67168500
				C	0.72541800	2.30939700	-0.41233000
				C	1.17384700	3.03397600	0.76423600
				C	1.17368100	3.03296800	3.61666600
				C	0.72594200	2.30669800	4.79254700
				C	-0.69984000	0.00000000	5.67168500
				C	-1.42620700	-1.17490300	5.22369600
				C	-2.30297400	-2.59757200	2.91591700
				C	-2.29988700	-2.59409700	1.46521200

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C	-1.41894100	-1.17235000	-0.83320900	C	-5.68890600	-3.08890800	0.10188800
C	-0.69675700	0.00000000	-1.28237800	C	-2.41938200	5.30590500	1.70721500
C	-2.58822000	-0.72395500	-0.10685800	C	-2.94709700	4.16443900	2.32444400
C	-3.02287900	-1.42122600	1.01842000	C	-4.04354900	3.51388000	1.75986400
C	-3.02867400	-1.42205900	3.36322800	C	-4.59756400	3.99358800	0.51807500
C	-2.60206400	-0.72619800	4.49841500	C	-4.07474800	5.14815700	-0.06343100
C	-1.42620700	1.17490300	5.22369600	C	-2.98744000	5.80181300	0.53241600
C	-0.72594200	2.30669800	4.79254700	C	-2.43750600	1.39899400	4.55535800
C	0.00000000	3.48473100	2.89112000	C	-1.51563000	0.70490800	5.36401800
C	0.00000000	3.48343000	1.49092400	C	-1.51563000	-0.70490800	5.36401800
C	-0.72541800	2.30939700	-0.41233000	C	-2.43750600	-1.39899400	4.55535800
C	-1.41894100	1.17235000	-0.83320900	C	-3.35532400	-0.71939400	3.76631300
C	-1.17368100	3.03296800	3.61666600	C	-3.35532400	0.71939400	3.76631300
C	-2.60206400	0.72619800	4.49841500	C	-2.98744000	-5.80181300	0.53241600
C	-2.58822000	0.72395500	-0.10685800	C	-4.07474800	-5.14815700	-0.06343100
C	-1.17384700	3.03397600	0.76423600	C	-4.59756400	-3.99358800	0.51807500
C	-3.02287900	1.42122600	1.01842000	C	-4.04354900	-3.51388000	1.75986400
C	-2.29988700	2.59409700	1.46521200	C	-2.94709700	-4.16443900	2.32444400
C	-3.47585600	-0.69806700	2.18888500	C	-2.41938200	-5.30590500	1.70721500
C	-3.47585600	0.69806700	2.18888500	C	-6.17944700	-1.74133400	-3.33275600
C	-0.72541800	-2.30939700	-0.41233000	C	-5.84695100	-2.90299800	-2.54761800
C	-2.30297400	2.59757200	2.91591700	C	-5.26924300	-4.00973600	-3.16776900
C	-3.02867400	1.42205900	3.36322800	C	-5.01082100	-3.98849000	-4.54456100
C	6.05486600	3.14990200	3.26074100	C	-5.34195000	-2.86785100	-5.30725000
H	5.03120700	3.43730600	3.53791100	C	-5.93211900	-1.74885400	-4.70484000
H	6.42775600	2.44610700	4.01253400	C	-5.26924300	4.00973600	-3.16776900
H	6.66692900	4.06223900	3.31362100	C	-5.84695100	2.90299800	-2.54761800
C	4.92671600	4.63021300	1.01256300	C	-6.17944700	1.74133400	-3.33275600
H	4.18448800	4.60041300	1.82162100	C	-5.93211900	1.74885400	-4.70484000
H	5.69423100	5.35998900	1.31018000	C	-5.34195000	2.86785100	-5.30725000
H	4.43291200	5.00564000	0.10988400	C	-5.01082100	3.98849000	-4.54456100
C	6.05486600	-3.14990200	3.26074100	H	-1.56589400	5.81079100	2.15444000
H	6.42775600	-2.44610700	4.01253400	H	-2.49931600	3.80372700	3.24184200
H	5.03120700	-3.43730600	3.53791100	H	-4.51823400	5.57024600	-0.95657800
H	6.66692900	-4.06223900	3.31362100	H	-2.58479100	6.70110500	0.07155600
C	4.92671600	-4.63021300	1.01256300	H	-2.47035300	2.47939800	4.63792200
H	5.69423100	-5.35998900	1.31018000	H	-2.47035300	-2.47939800	4.63792200
H	4.18448800	-4.60041300	1.82162100	H	-2.58479100	-6.70110500	0.07155600
H	4.43291200	-5.00564000	0.10988400	H	-4.51823400	-5.57024600	-0.95657800
C	-6.05486600	-3.14990200	3.26074100	H	-2.49931600	-3.80372700	3.24184200
H	-5.03120700	-3.43730600	3.53791100	H	-1.56589400	-5.81079100	2.15444000
H	-6.42775600	-2.44610700	4.01253400	H	-5.02681100	-4.89888000	-2.60137400
H	-6.66692900	-4.06223900	3.31362100	H	-4.55623900	-4.85532900	-5.01891400
C	-4.92671600	-4.63021300	1.01256300	H	-5.15004200	-2.86137200	-6.37786300
H	-4.18448800	-4.60041300	1.82162100	H	-6.21189900	-0.90704200	-5.32406300
H	-5.69423100	-5.35998900	1.31018000	H	-5.02681100	4.89888000	-2.60137400
H	-4.43291200	-5.00564000	0.10988400	H	-6.21189900	0.90704200	-5.32406300
C	-6.05486600	3.14990200	3.26074100	H	-5.15004200	2.86137200	-6.37786300
H	-6.42775600	2.44610700	4.01253400	H	-4.55623900	4.85532900	-5.01891400
H	-5.03120700	3.43730600	3.53791100	C	2.59361200	-2.30168800	-2.71065900
H	-6.66692900	4.06223900	3.31362100	C	2.59193700	-2.29880800	-1.26068500
C	-4.92671600	4.63021300	1.01256300	C	3.02763500	-1.17188400	-0.56129900
H	-5.69423100	5.35998900	1.31018000	C	3.47732200	0.00000000	-1.28602700
H	-4.18448800	4.60041300	1.82162100	C	3.46557800	0.00000000	-2.68223100
H	-4.43291200	5.00564000	0.10988400	C	3.02047100	-1.17073900	-3.40772700
				C	0.69947800	-3.47992900	-1.98527000
				C	1.42244800	-3.02524700	-0.81242900
				C	0.72529600	-2.59396900	0.31898600
				C	2.30429800	-0.72466600	0.61245600
				C	3.02763500	1.17188400	-0.56129900
				C	2.59193700	2.29880800	-1.26068500
				C	2.59361200	2.30168800	-2.71065900
				C	3.02047100	1.17073900	-3.40772700
				C	2.30153200	0.72597400	-4.58503100
				C	2.30153200	-0.72597400	-4.58503100
				C	1.17388600	-1.42757900	-5.02277900
				C	-0.69947800	-3.47992900	-1.98527000
				C	-1.42443400	-3.03210300	-3.16135300
				C	-0.72593300	-2.60383100	-4.29606900
				C	-1.17388600	-1.42757900	-5.02277900
				C	0.00000000	-0.70056400	-5.47242900
				C	0.00000000	0.70056400	-5.47242900
				C	1.17388600	1.42757900	-5.02277900
				C	0.72593300	2.60383100	-4.29606900
				C	1.42443400	3.03210300	-3.16135300
				C	2.30429800	0.72466600	0.61245600

3a...C ₆₀ :			
C	-7.27769700	-0.71448800	-0.02863400
C	-7.27769700	0.71448800	-0.02863400
C	-6.75483100	1.15560800	1.22328200
C	-6.43554800	0.00000000	1.99405900
C	-6.75483100	-1.15560800	1.22328200
C	-6.92355400	-1.38966200	-1.17728400
C	-6.92355400	1.38966200	-1.17728400
C	-5.90748500	2.24391100	1.26009800
C	-5.29495700	0.00000000	2.76385800
C	-5.90748500	-2.24391100	1.26009800
C	-4.80232100	-2.32884100	2.19732400
C	-4.50689200	-1.19669700	2.97997400
C	-4.50689200	1.19669700	2.97997400
C	-4.80232100	2.32884100	2.19732400
C	-6.19488300	2.64607600	-1.13810300
C	-5.68890600	3.08890800	0.10188800
C	-6.74153000	0.70527700	-2.44471800
C	-6.74153000	-0.70527700	-2.44471800
C	-6.19488300	-2.64607600	-1.13810300

C	-2.45641700	-1.39786200	5.16861600	C	-3.01568700	1.16921600	-2.74947200
C	-3.38528800	-0.71949800	4.39097900	C	-0.72586400	2.60615900	-3.64164900
C	-3.38528800	0.71949800	4.39097900	C	-1.17342600	1.42875200	-4.36856200
C	-2.92544500	-5.75903300	1.11141200	C	-2.29875800	0.72579800	-3.92712700
C	-4.03641900	-5.11283100	0.54109400	C	-2.29875800	-0.72579800	-3.92712700
C	-4.59339800	-3.98409900	1.13735000	C	-3.01568700	-1.16921600	-2.74947200
C	-4.05991300	-3.50925700	2.38895900	C	-2.59092400	-2.30076500	-2.05328500
C	-2.96469000	-4.15961100	2.95415400	C	-2.58997000	-2.29810800	-0.60403900
C	-2.40421500	-5.27146600	2.31511500	C	-1.42229200	-3.02590400	-0.15576200
C	-6.13097800	-1.73551900	-2.71845100	C	-0.72490700	-2.59345800	0.97515500
C	-5.80702000	-2.89340400	-1.93253700	C	1.17373000	1.42281000	1.70443700
C	-5.17272600	-3.97153900	-2.54539700	C	1.17373000	-1.42281000	1.70443700
C	-4.81763700	-3.93933500	-3.90189200	C	-2.58997000	2.29810800	-0.60403900
C	-5.14468600	-2.80790600	-4.67590800	C	0.72586400	-2.60615900	-3.64164900
C	-5.81588500	-1.73239300	-4.07546600	C	1.42356800	-3.03232100	-2.50499200
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C	-5.80702000	2.89340400	-1.93253700	C	-0.72490700	2.59345800	0.97515500
C	-6.13097800	1.73551900	-2.71845100	C	7.27958400	0.71502000	0.56881200
C	-5.81588500	1.73239300	-4.07546600	C	6.76856000	1.15577000	1.82654800
C	-5.14468600	2.80790600	-4.67590800	C	6.45658700	0.00000000	2.60081300
C	-4.81763700	3.93933500	-3.90189200	C	6.76856000	-1.15577000	1.82654800
H	-1.54444600	5.76715300	2.76287400	C	7.27958400	-0.71502000	0.56881200
H	-2.53664800	3.81897000	3.88843900	C	6.91732100	1.39124100	-0.57676100
H	-4.46273000	5.52586800	-0.36512900	C	5.92357100	2.24587800	1.87330900
H	-2.48754200	2.47807000	5.25142700	C	5.32324700	0.00000000	3.38254900
H	-2.48754200	-2.47807000	5.25142700	C	5.92357100	-2.24587800	1.87330900
H	-4.46273000	-5.52586800	-0.36512900	C	6.91732100	-1.39124100	-0.57676100
H	-2.53664800	-3.81897000	3.88843900	C	6.18474300	-2.64658500	-0.53006300
H	-1.54444600	-5.76715300	2.76287400	C	5.69025500	-3.08851400	0.71570400
H	-4.93305800	-4.86293500	-1.98094300	C	4.82759000	-2.33068900	2.82238100
H	-6.08695200	-0.89275300	-4.70216800	C	4.53706700	-1.19685800	3.60528200
H	-4.93305800	4.86293500	-1.98094300	C	4.82759000	2.33068900	2.82238100
H	-6.08695200	0.89275300	-4.70216800	C	4.53706700	1.19685800	3.60528200
C	2.59092400	-2.30076500	-2.05328500	C	5.69025500	3.08851400	0.71570400
C	2.58997000	-2.29810800	-0.60403900	C	6.18474300	2.64658500	-0.53006300
C	3.02606500	-1.17177200	0.09522600	C	6.72076700	0.70559600	-1.84292300
C	3.47511000	0.00000000	-0.62919500	C	6.72076700	-0.70559600	-1.84292300
C	3.46082000	0.00000000	-2.02456300	C	1.52252900	-0.70503900	5.96521400
C	3.01568700	-1.16921600	-2.74947200	C	2.45641700	-1.39786200	5.16861600
C	0.69971500	-3.48190800	-1.32861700	C	3.38528800	-0.71949800	4.39097900
C	1.42229200	-3.02590400	-0.15576200	C	3.38528800	0.71949800	4.39097900
C	0.72490700	-2.59345800	0.97515500	C	2.45641700	1.39786200	5.16861600
C	2.30364600	-0.72467300	1.26918500	C	1.52252900	0.70503900	5.96521400
C	3.02606500	1.17177200	0.09522600	C	2.96469000	-4.15961100	2.95415400
C	2.58997000	2.29810800	-0.60403900	C	2.40421500	-5.27146600	2.31511500
C	2.59092400	2.30076500	-2.05328500	C	2.92544500	-5.75903300	1.11141200
C	3.01568700	1.16921600	-2.74947200	C	4.03641900	-5.11283100	0.54109400
C	2.29875800	0.72579800	-3.92712700	C	4.59339800	-3.98409900	1.13735000
C	2.29875800	-0.72579800	-3.92712700	C	4.05991300	-3.50925700	2.38895900
C	1.17342600	-1.42875200	-4.36856200	C	5.14468600	-2.80790600	-4.67590800
C	-0.69971500	-3.48190800	-1.32861700	C	5.81588500	-1.73239300	-4.07546600
C	-1.42356800	-3.03232100	-2.50499200	C	6.13097800	-1.73551900	-2.71845100
C	-0.72586400	-2.60615900	-3.64164900	C	5.80702000	-2.89340400	-1.93253700
C	-1.17342600	-1.42875200	-4.36856200	C	5.17272600	-3.97153900	-2.54539700
C	0.00000000	-0.70116600	-4.81853100	C	4.81763700	-3.93933500	-3.90189200
C	0.00000000	0.70116600	-4.81853100	C	5.80702000	2.89340400	-1.93253700
C	1.17342600	1.42875200	-4.36856200	C	6.13097800	1.73551900	-2.71845100
C	0.72586400	2.60615900	-3.64164900	C	5.81588500	1.73239300	-4.07546600
C	1.42356800	3.03232100	-2.50499200	C	5.14468600	2.80790600	-4.67590800
C	2.30364600	0.72467300	1.26918500	C	4.81763700	3.93933500	-3.90189200
C	-1.17373000	1.42281000	1.70443700	C	5.17272600	3.97153900	-2.54539700
C	-2.30364600	0.72467300	1.26918500	C	2.96469000	4.15961100	2.95415400
C	-3.02606500	1.17177200	0.09522600	C	4.05991300	3.50925700	2.38895900
C	-2.59092400	2.30076500	-2.05328500	C	4.59339800	3.98409900	1.13735000
C	-1.42356800	3.03232100	-2.50499200	C	4.03641900	5.11283100	0.54109400
C	-0.69971500	3.48190800	-1.32861700	C	2.92544500	5.75903300	1.11141200
C	0.69971500	3.48190800	-1.32861700	C	2.40421500	5.27146600	2.31511500
C	1.42229200	3.02590400	-0.15576200	H	2.48754200	-2.47807000	5.25142700
C	0.72490700	2.59345800	0.97515500	H	2.48754200	2.47807000	5.25142700
C	0.00000000	0.69949600	2.15802800	H	2.53664800	-3.81897000	3.88843900
C	0.00000000	-0.69949600	2.15802800	H	1.54444600	-5.76715300	2.76287400
C	-1.17373000	-1.42281000	1.70443700	H	4.46273000	-5.52586800	-0.36512900
C	-2.30364600	-0.72467300	1.26918500	H	6.08695200	-0.89275300	-4.70216800
C	-3.02606500	-1.17177200	0.09522600	H	4.93305800	-4.86293500	-1.98094300
C	-3.47511000	0.00000000	-0.62919500	H	6.08695200	0.89275300	-4.70216800
C	-3.46082000	0.00000000	-2.02456300	H	4.93305800	4.86293500	-1.98094300

H	2.53664800	3.81897000	3.88843900	C	6.99716600	0.71511800	1.87543900
H	4.46273000	5.52586800	-0.36512900	C	6.99716600	-0.71511800	1.87543900
H	1.54444600	5.76715300	2.76287400	C	6.71911400	-1.40772300	0.70388300
C	-0.70537100	-1.50267900	6.91849800	C	6.17156500	2.53212100	3.17576800
C	0.70537100	-1.50267900	6.91849800	C	5.90436900	3.25365100	1.97240300
C	0.70537100	1.50267900	6.91849800	C	4.85307300	0.78414100	-2.36354900
C	-0.70537100	1.50267900	6.91849800	C	4.85307300	-0.78414100	-2.36354900
C	-1.38602800	2.34238700	7.82039400	C	6.17156500	-2.53212100	3.17576800
C	1.38602800	2.34238700	7.82039400	C	5.90436900	-3.25365100	1.97240300
C	-1.38602800	-2.34238700	7.82039400	C	6.11622700	2.66470600	0.71509600
C	1.38602800	-2.34238700	7.82039400	C	5.58185400	1.45176200	-1.32851400
C	-0.69897500	3.16261600	8.71502100	C	5.46305800	2.85298000	-0.66928700
C	0.69897500	3.16261600	8.71502100	C	6.11622700	-2.66470600	0.71509600
C	-0.69897500	-3.16261600	8.71502100	C	5.58185400	-1.45176200	-1.32851400
C	0.69897500	-3.16261600	8.71502100	C	5.46305800	-2.85298000	-0.66928700
H	2.47410800	2.33701800	7.81420600	C	6.66156200	1.21564200	3.13560900
H	1.25157000	3.79405000	9.40795300	C	6.66156200	-1.21564200	3.13560900
H	-1.25157000	3.79405000	9.40795300	C	6.58351900	0.00000000	4.10037000
H	-2.47410800	2.33701800	7.81420600	H	5.85824500	2.98345900	4.11582100
H	-2.47410800	-2.33701800	7.81420600	H	5.40193400	4.21575900	2.06073200
H	2.47410800	-2.33701800	7.81420600	H	5.85824500	-2.98345900	4.11582100
H	1.25157000	-3.79405000	9.40795300	H	5.40193400	-4.21575900	2.06073200
H	-1.25157000	-3.79405000	9.40795300	H	5.90673600	3.65700300	-1.27415900
C	4.75079200	2.73035700	-6.12977200	H	4.41123100	3.09194000	-0.50987900
H	5.12966000	1.81172900	-6.59222700	H	4.41123100	-3.09194000	-0.50987900
H	3.65584300	2.73851600	-6.23478600	H	5.90673600	-3.65700300	-1.27415900
H	5.13279500	3.58993900	-6.69834700	H	7.39438400	0.00000000	4.84454900
C	4.06128000	5.09383100	-4.50992200	H	5.63527400	0.00000000	4.65377000
H	4.58012200	5.49712100	-5.39113100	C	-6.39338400	-0.70112100	-0.50086000
H	3.06545800	4.76972400	-4.84593000	C	-6.71911400	-1.40772300	0.70388300
H	3.92842400	5.90396100	-3.78367500	C	-6.39338400	0.70112100	-0.50086000
C	4.75079200	-2.73035700	-6.12977200	C	-6.99716600	-0.71511800	1.87543900
H	3.65584300	-2.73851600	-6.23478600	C	-6.99716600	0.71511800	1.87543900
H	5.12966000	-1.81172900	-6.59222700	C	-6.71911400	1.40772300	0.70388300
H	5.13279500	-3.58993900	-6.69834700	C	-6.17156500	-2.53212100	3.17576800
C	4.06128000	-5.09383100	-4.50992200	C	-5.90436900	-3.25365100	1.97240300
H	3.06545800	-4.76972400	-4.84593000	C	-4.85307300	-0.78414100	-2.36354900
H	4.58012200	-5.49712100	-5.39113100	C	-4.85307300	0.78414100	-2.36354900
H	3.92842400	-5.90396100	-3.78367500	C	-6.17156500	2.53212100	3.17576800
C	-4.75079200	-2.73035700	-6.12977200	C	-5.90436900	3.25365100	1.97240300
H	-5.12966000	-1.81172900	-6.59222700	C	-6.11622700	-2.66470600	0.71509600
H	-3.65584300	-2.73851600	-6.23478600	C	-5.58185400	-1.45176200	-1.32851400
H	-5.13279500	-3.58993900	-6.69834700	C	-5.46305800	-2.85298000	-0.66928700
C	-4.06128000	-5.09383100	-4.50992200	C	-6.11622700	2.66470600	0.71509600
H	-4.58012200	-5.49712100	-5.39113100	C	-5.58185400	1.45176200	-1.32851400
H	-3.06545800	-4.76972400	-4.84593000	C	-5.46305800	2.85298000	-0.66928700
H	-3.92842400	-5.90396100	-3.78367500	C	-6.66156200	-1.21564200	3.13560900
C	-4.75079200	2.73035700	-6.12977200	C	-6.66156200	1.21564200	3.13560900
H	-3.65584300	2.73851600	-6.23478600	C	-6.58351900	0.00000000	4.10037000
H	-5.12966000	1.81172900	-6.59222700	H	-5.85824500	-2.98345900	4.11582100
H	-5.13279500	3.58993900	-6.69834700	H	-5.40193400	-4.21575900	2.06073200
C	-4.06128000	5.09383100	-4.50992200	H	-5.85824500	2.98345900	4.11582100
H	-3.06545800	4.76972400	-4.84593000	H	-5.40193400	4.21575900	2.06073200
H	-4.58012200	5.49712100	-5.39113100	H	-5.90673600	-3.65700300	-1.27415900
H	-3.92842400	5.90396100	-3.78367500	H	-4.41123100	-3.09194000	-0.50987900
C	2.27833900	-6.92270100	0.40016800	H	-4.41123100	3.09194000	-0.50987900
H	1.71787700	-7.55652400	1.09817200	H	-5.90673600	3.65700300	-1.27415900
H	1.57219600	-6.55730500	-0.36091400	H	-7.39438400	0.00000000	4.84454900
H	3.02518800	-7.54251500	-0.11278200	H	-5.63527400	0.00000000	4.65377000
C	-2.27833900	-6.92270100	0.40016800	C	2.30624900	-2.60009100	2.71480200
H	-1.57219600	-6.55730500	-0.36091400	C	2.30150100	-2.59627200	1.26304200
H	-1.71787700	-7.55652400	1.09817200	C	3.01791900	-1.41708900	0.81931000
H	-3.02518800	-7.54251500	-0.11278200	C	3.47559900	-0.69781900	1.98833200
C	2.27833900	6.92270100	0.40016800	C	3.03219900	-1.42500800	3.16214000
H	1.57219600	6.55730500	-0.36091400	C	1.17470600	-3.03303400	3.41377300
H	1.71787700	7.55652400	1.09817200	C	1.17271300	-3.02768200	0.56085500
H	3.02518800	7.54251500	-0.11278200	C	2.58319900	-0.72279400	-0.30917700
C	-2.27833900	6.92270100	0.40016800	C	3.47559900	0.69781900	1.98833200
H	-1.71787700	7.55652400	1.09817200	C	2.60233400	-0.72675500	4.29446200
H	-1.57219600	6.55730500	-0.36091400	C	2.60233400	0.72675500	4.29446200
H	-3.02518800	7.54251500	-0.11278200	C	3.03219900	1.42500800	3.16214000
				C	3.01791900	1.41708900	0.81931000
				C	2.58319900	0.72279400	-0.30917700
				C	0.72373000	-2.30192400	-0.61438000
				C	1.42165800	-1.17321200	-1.04970200
				C	0.00000000	-3.47927500	1.28679900
4a...C ₆₀ :							
C	6.39338400	0.70112100	-0.50086000				
C	6.71911400	1.40772300	0.70388300				
C	6.39338400	-0.70112100	-0.50086000				

C	0.00000000	-3.48131000	2.68674300	C	-4.01582800	1.48360000	-3.29561700
C	0.72611800	-2.30723600	4.58897200	C	4.01582800	1.48360000	-3.29561700
C	1.42629700	-1.17495000	5.01947000	C	4.01582800	-1.48360000	-3.29561700
C	2.30150100	2.59627200	1.26304200	C	0.75175900	-4.31025300	-3.47860300
C	2.30624900	2.60009100	2.71480200	C	1.74714600	-4.61783700	-2.54833800
C	0.70021600	0.00000000	-1.50888000	C	2.99095900	-3.90267000	-2.50624500
C	1.42165800	1.17321200	-1.04970200	C	3.26773200	-2.81325900	-3.35308900
C	-1.17271300	-3.02768200	0.56085500	C	-0.75175900	-4.31025300	-3.47860300
C	-0.72611800	-2.30723600	4.58897200	C	-1.74714600	-4.61783700	-2.54833800
C	-1.17470600	-3.03303400	3.41377300	C	-2.99095900	-3.90267000	-2.50624500
C	1.42629700	1.17495000	5.01947000	C	-3.26773200	-2.81325900	-3.35308900
C	0.69978200	0.00000000	5.46676100	H	3.65065000	-4.18380000	-1.69929000
C	0.72373000	2.30192400	-0.61438000	H	1.55845900	-5.31927500	-1.73751300
C	1.17271300	3.02768200	0.56085500	H	-1.55845900	-5.31927500	-1.73751300
C	1.17470600	3.03303400	3.41377300	H	-3.65065000	-4.18380000	-1.69929000
C	0.72611800	2.30723600	4.58897200	H	3.65065000	4.18380000	-1.69929000
C	-0.69978200	0.00000000	5.46676100	H	1.55845900	5.31927500	-1.73751300
C	-1.42629700	-1.17495000	5.01947000	H	-1.55845900	5.31927500	-1.73751300
C	-2.30624900	-2.60009100	2.71480200	H	-3.65065000	4.18380000	-1.69929000
C	-2.30150100	-2.59627200	1.26304200				
C	-1.42165800	-1.17321200	-1.04970200				
C	-0.70021600	0.00000000	-1.50888000	4b...C₆₀:	6.41274500	0.70158400	-0.80607500
C	-2.58319900	-0.72279400	-0.30917700	C	6.70701300	1.40758600	0.40706000
C	-3.01791900	-1.41708900	0.81931000	C	6.41274500	-0.70158400	-0.80607500
C	-3.03219900	-1.42500800	3.16214000	C	6.95002000	0.71503600	1.58331400
C	-2.60233400	-0.72675500	4.29446200	C	6.95002000	-0.71503600	1.58331400
C	-1.42629700	1.17495000	5.01947000	C	6.70701300	-1.40758600	0.40706000
C	-0.72611800	2.30723600	4.58897200	C	6.05711700	2.52842200	2.87735100
C	0.00000000	3.48131000	2.68674300	C	5.82108000	3.25944800	1.65266400
C	0.00000000	3.47927500	1.28679900	C	4.88994400	0.78501100	-2.68572400
C	-0.72373000	2.30192400	-0.61438000	C	4.88994400	-0.78501100	-2.68572400
C	-1.42165800	1.17321200	-1.04970200	C	6.05711700	-2.52842200	2.87735100
C	-1.17470600	3.03303400	3.41377300	C	5.82108000	-3.25944800	1.65266400
C	-2.60233400	0.72675500	4.29446200	C	6.09125400	2.65729800	0.41088500
C	-2.58319900	0.72279400	-0.30917700	C	5.61327000	1.45053900	-1.64776100
C	-1.17271300	3.02768200	0.56085500	C	5.47519300	2.84954400	-0.99087800
C	-3.01791900	1.41708900	0.81931000	C	6.09125400	-2.65729800	0.41088500
C	-2.30150100	2.59627200	1.26304200	C	5.61327000	-1.45053900	-1.64776100
C	-3.47559900	-0.69781900	1.98833200	C	5.47519300	-2.84954400	-0.99087800
C	-3.47559900	0.69781900	1.98833200	C	6.56505700	1.21661300	2.82718400
C	-0.72373000	-2.30192400	-0.61438000	C	6.56505700	-1.21661300	2.82718400
C	-2.30624900	2.60009100	2.71480200	C	6.45808800	0.00000000	3.79003600
C	-3.03219900	1.42500800	3.16214000	H	5.93569700	3.65325600	-1.58431300
C	3.43485600	-0.69364200	-4.31742600	H	4.41956400	3.09185900	-0.86544200
C	2.37830400	-1.37291700	-4.99912800	H	4.41956400	-3.09185900	-0.86544200
C	1.25595900	-0.72465400	-5.54622300	H	5.93569700	-3.65325600	-1.58431300
C	1.25595900	0.72465400	-5.54622300	H	7.24332100	0.00000000	4.56176400
C	2.37830400	1.37291700	-4.99912800	H	5.49306200	0.00000000	4.31390500
C	3.43485600	0.69364200	-4.31742600	C	-6.41274500	-0.70158400	-0.80607500
C	0.00000000	-1.44922900	-5.57934700	C	-6.70701300	-1.40758600	0.40706000
C	0.00000000	1.44922900	-5.57934700	C	-6.41274500	0.70158400	-0.80607500
C	-1.25595900	0.72465400	-5.54622300	C	-6.95002000	-0.71503600	1.58331400
C	-1.25595900	-0.72465400	-5.54622300	C	-6.95002000	0.71503600	1.58331400
C	-2.37830400	1.37291700	-4.99912800	C	-6.70701300	1.40758600	0.40706000
C	-2.32086500	2.66506700	-4.41949100	C	-6.05711700	-2.52842200	2.87735100
C	-1.13711800	3.37407400	-4.48514500	C	-5.82108000	-3.25944800	1.65266400
C	0.00000000	2.77190000	-5.09918500	C	-4.88994400	-0.78501100	-2.68572400
C	1.13711800	3.37407400	-4.48514500	C	-4.88994400	0.78501100	-2.68572400
C	2.32086500	2.66506700	-4.41949100	C	-6.05711700	2.52842200	2.87735100
C	2.32086500	-2.66506700	-4.41949100	C	-5.82108000	3.25944800	1.65266400
C	1.13711800	-3.37407400	-4.48514500	C	-6.09125400	-2.65729800	0.41088500
C	0.00000000	-2.77190000	-5.09918500	C	-5.61327000	-1.45053900	-1.64776100
C	-1.13711800	-3.37407400	-4.48514500	C	-5.47519300	-2.84954400	-0.99087800
C	-2.32086500	-2.66506700	-4.41949100	C	-6.09125400	2.65729800	0.41088500
C	-2.37830400	-1.37291700	-4.99912800	C	-5.61327000	1.45053900	-1.64776100
C	-3.43485600	0.69364200	-4.31742600	C	-5.47519300	2.84954400	-0.99087800
C	-3.43485600	-0.69364200	-4.31742600	C	-6.56505700	-1.21661300	2.82718400
C	-3.26773200	2.81325900	-3.35308900	C	-6.56505700	1.21661300	2.82718400
C	-2.99095900	3.90267000	-2.50624500	C	-6.45808800	0.00000000	3.79003600
C	-1.74714600	4.61783700	-2.54833800	H	-5.93569700	-3.65325600	-1.58431300
C	-0.75175900	4.31025300	-3.47860300	H	-4.41956400	-3.09185900	-0.86544200
C	0.75175900	4.31025300	-3.47860300	H	-4.41956400	3.09185900	-0.86544200
C	1.74714600	4.61783700	-2.54833800	H	-5.93569700	3.65325600	-1.58431300
C	2.99095900	3.90267000	-2.50624500	H	-7.24332100	0.00000000	4.56176400
C	3.26773200	2.81325900	-3.35308900	H	-5.49306200	0.00000000	4.31390500
C	-4.01582800	-1.48360000	-3.29561700	C	2.30341800	-2.59619400	2.30937200

C	2.29913700	-2.59232600	0.85776800	C	1.13301500	-3.36186500	-4.72410900
C	3.01575400	-1.41586000	0.41370600	C	0.00000000	-2.76139400	-5.33783700
C	3.47344200	-0.69684100	1.58241900	C	-1.13301500	-3.36186500	-4.72410900
C	3.02957100	-1.42257800	2.75588400	C	-2.32030600	-2.65800500	-4.69366100
C	1.17433900	-3.03216400	3.01013200	C	-2.37783500	-1.37150100	-5.28289200
C	1.17126000	-3.02268100	0.15637000	C	-3.44703900	0.69393600	-4.62015700
C	2.57981700	-0.72285500	-0.71454800	C	-3.44703900	-0.69393600	-4.62015700
C	3.47344200	0.69684100	1.58241900	C	-3.28815000	2.81532700	-3.65450200
C	2.60162900	-0.72666300	3.89025500	C	-3.03866100	3.93804200	-2.84463300
C	2.60162900	0.72666300	3.89025500	C	-1.80204700	4.68442300	-2.85571900
C	3.02957100	1.42257800	2.75588400	C	-0.76019800	4.31913700	-3.73205000
C	3.01575400	1.41586000	0.41370600	C	0.76019800	4.31913700	-3.73205000
C	2.57981700	0.72285500	-0.71454800	C	1.80204700	4.68442300	-2.85571900
C	0.72391300	-2.30388400	-1.02245100	C	3.03866100	3.93804200	-2.84463300
C	1.42119500	-1.17379400	-1.45638000	C	3.28815000	2.81532700	-3.65450200
C	0.00000000	-3.47307500	0.88390100	C	-4.04249800	-1.48575200	-3.60733700
C	0.00000000	-3.48106000	2.28294100	C	-4.04249800	1.48575200	-3.60733700
C	0.72619100	-2.30796900	4.18586700	C	4.04249800	1.48575200	-3.60733700
C	1.42685100	-1.17518300	4.61588300	C	4.04249800	-1.48575200	-3.60733700
C	2.29913700	2.59232600	0.85776800	C	0.76019800	-4.31913700	-3.73205000
C	2.30341800	2.59619400	2.30937200	C	1.80204700	-4.68442300	-2.85571900
C	0.69958100	0.00000000	-1.91513400	C	3.03866100	-3.93804200	-2.84463300
C	1.42119500	1.17379400	-1.45638000	C	3.28815000	-2.81532700	-3.65450200
C	-1.17126000	-3.02268100	0.15637000	C	-0.76019800	-4.31913700	-3.73205000
C	-0.72619100	-2.30796900	4.18586700	C	-1.80204700	-4.68442300	-2.85571900
C	-1.17433900	-3.03216400	3.01013200	C	-3.03866100	-3.93804200	-2.84463300
C	1.42685100	1.17518300	4.61588300	C	-3.28815000	-2.81532700	-3.65450200
C	0.69984600	0.00000000	5.06309600	H	3.74347100	-4.26243100	-2.09142500
C	0.72391300	2.30388400	-1.02245100	H	-3.74347100	-4.26243100	-2.09142500
C	1.17126000	3.02268100	0.15637000	H	3.74347100	4.26243100	-2.09142500
C	1.17433900	3.03216400	3.01013200	H	-3.74347100	4.26243100	-2.09142500
C	0.72619100	2.30796900	4.18586700	C	-1.66006000	-5.77416800	-1.81759800
C	-0.69984600	0.00000000	5.06309600	H	-1.10847700	-6.63238800	-2.21392200
C	-1.42685100	-1.17518300	4.61588300	H	-1.12583200	-5.41223000	-0.93013100
C	-2.30341800	-2.59619400	2.30937200	H	-2.64670000	-6.12009000	-1.48608200
C	-2.29913700	-2.59232600	0.85776800	H	1.66006000	-5.77416800	-1.81759800
C	-1.42119500	-1.17379400	-1.45638000	H	1.12583200	-5.41223000	-0.93013100
C	-0.69958100	0.00000000	-1.91513400	H	1.10847700	-6.63238800	-2.21392200
C	-2.57981700	-0.72285500	-0.71454800	H	2.64670000	-6.12009000	-1.48608200
C	-3.01575400	-1.41586000	0.41370600	C	5.62073700	-3.12952700	4.19245400
C	-3.02957100	-1.42257800	2.75588400	H	5.72724300	-2.40545500	5.00710100
C	-2.60162900	-0.72666300	3.89025500	H	4.57334000	-3.45860100	4.15923500
C	-1.42685100	1.17518300	4.61588300	H	6.22564700	-4.01399600	4.44183400
C	-0.72619100	2.30796900	4.18586700	C	5.14031600	-4.60630700	1.71357100
C	0.00000000	3.48106000	2.28294100	H	4.18836600	-4.55407000	2.25962200
C	0.00000000	3.47307500	0.88390100	H	4.93638600	-4.98716900	0.70685500
C	-0.72391300	2.30388400	-1.02245100	H	5.76759800	-5.34410000	2.23515400
C	-1.42119500	1.17379400	-1.45638000	C	5.62073700	3.12952700	4.19245400
C	-1.17433900	3.03216400	3.01013200	H	5.72724300	2.40545500	5.00710100
C	-2.60162900	0.72666300	3.89025500	H	6.22564700	4.01399600	4.44183400
C	-2.57981700	0.72285500	-0.71454800	H	4.57334000	3.45860100	4.15923500
C	-1.17126000	3.02268100	0.15637000	C	5.14031600	4.60630700	1.71357100
C	-3.01575400	1.41586000	0.41370600	H	4.93638600	4.98716900	0.70685500
C	-2.29913700	2.59232600	0.85776800	H	4.18836600	4.55407000	2.25962200
C	-3.47344200	-0.69684100	1.58241900	H	5.76759800	5.34410000	2.23515400
C	-3.47344200	0.69684100	1.58241900	C	-5.14031600	4.60630700	1.71357100
C	-0.72391300	-2.30388400	-1.02245100	H	-4.18836600	4.55407000	2.25962200
C	-2.30341800	2.59619400	2.30937200	H	-4.93638600	4.98716900	0.70685500
C	-3.02957100	1.42257800	2.75588400	H	-5.76759800	5.34410000	2.23515400
C	3.44703900	-0.69393600	-4.62015700	C	-5.62073700	3.12952700	4.19245400
C	2.37783500	-1.37150100	-5.28289200	H	-4.57334000	3.45860100	4.15923500
C	1.25430300	-0.72409500	-5.82448400	H	-6.22564700	4.01399600	4.44183400
C	1.25430300	0.72409500	-5.82448400	H	-5.72724300	2.40545500	5.00710100
C	2.37783500	1.37150100	-5.28289200	C	-5.14031600	-4.60630700	1.71357100
C	3.44703900	0.69393600	-4.62015700	H	-4.93638600	-4.98716900	0.70685500
C	0.00000000	-1.44769700	-5.84200400	H	-4.18836600	-4.55407000	2.25962200
C	0.00000000	1.44769700	-5.84200400	H	-5.76759800	-5.34410000	2.23515400
C	-1.25430300	0.72409500	-5.82448400	C	-5.62073700	-3.12952700	4.19245400
C	-1.25430300	-0.72409500	-5.82448400	H	-6.22564700	-4.01399600	4.44183400
C	-2.37783500	1.37150100	-5.28289200	H	-4.57334000	-3.45860100	4.15923500
C	-2.32030600	2.65800500	-4.69366100	H	-5.72724300	-2.40545500	5.00710100
C	-1.13301500	3.36186500	-4.72410900	C	1.66006000	5.77416800	-1.81759800
C	0.00000000	2.76139400	-5.33783700	H	1.10847700	6.63238800	-2.21392200
C	1.13301500	3.36186500	-4.72410900	H	1.12583200	5.41223000	-0.93013100
C	2.32030600	2.65800500	-4.69366100	H	2.64670000	6.12009000	-1.48608200
C	2.32030600	-2.65800500	-4.69366100	C	-1.66006000	5.77416800	-1.81759800

H	-1.12583200	5.41223000	-0.93013100	C	-2.59651900	-0.72488800	-3.79787800
H	-1.10847700	6.63238800	-2.21392200	C	-2.59651900	0.72488800	-3.79787800
H	-2.64670000	6.12009000	-1.48608200	C	-3.02366500	1.42230300	-2.66626800
				C	-3.01372800	1.41974700	-0.32647300
5a...C₆₀:				C	-2.57676000	0.72313600	0.79863700
C	-6.91396600	0.70272200	-1.57142000	C	-0.72358400	-2.30315300	1.10482600
C	-6.73359100	1.41320100	-2.80401000	C	-1.42014000	-1.17401800	1.54197200
C	-6.91396600	-0.70272200	-1.57142000	C	0.00000000	-3.48177700	-0.79375100
C	-6.55417800	0.71617100	-3.99215500	C	0.00000000	-3.48488200	-2.19415300
C	-6.55417800	-0.71617100	-3.99215500	C	-0.72612100	-2.30924100	-4.09758100
C	-6.73359100	-1.41320100	-2.80401000	C	-1.42544800	-1.17524300	-4.52703700
C	-5.29593200	2.52604300	-4.89171200	C	-2.30080200	2.59956500	-0.76885500
C	-5.47949200	3.24500300	-3.66828500	C	-2.30315100	2.59979400	-2.22130900
C	-6.07179200	0.73510600	0.67217900	C	-0.69906200	0.00000000	2.00364400
C	-6.07179200	-0.73510600	0.67217900	C	-1.42014000	1.17401800	1.54197200
C	-5.29593200	-2.52604300	-4.89171200	C	1.17193200	-3.03013800	-0.06792800
C	-5.47949200	-3.24500300	-3.66828500	C	0.72612100	-2.30924100	-4.09758100
C	-6.14140300	2.66047500	-2.57843700	C	1.17458100	-3.03603800	-2.92180800
C	-6.45112300	1.45023400	-0.50124000	C	-1.42544800	1.17524300	-4.52703700
C	-6.08051700	2.85691500	-1.03954500	C	-0.69964400	0.00000000	-4.97706200
C	-6.14140300	-2.66047500	-2.57843700	C	-0.72358400	2.30315300	1.10482600
C	-6.45112300	-1.45023400	-0.50124000	C	-1.17193200	3.03013800	-0.06792800
C	-6.08051700	-2.85691500	-1.03954500	C	-1.17458100	3.03603800	-2.92180800
C	-5.77323200	1.21511600	-5.03993500	C	-0.72612100	2.30924100	-4.09758100
C	-5.77323200	-1.21511600	-5.03993500	C	0.69964400	0.00000000	-4.97706200
C	-5.36030000	0.00000000	-5.91742800	C	1.42544800	-1.17524300	-4.52703700
H	-4.64784300	2.97205600	-5.64477000	C	2.30315100	-2.59979400	-2.22130900
H	-4.95996600	4.19566900	-3.56049700	C	2.30080200	-2.59956500	-0.76885500
H	-4.64784300	-2.97205600	-5.64477000	C	1.42014000	-1.17401800	1.54197200
H	-4.95996600	-4.19566900	-3.56049700	C	0.69906200	0.00000000	2.00364400
H	-6.78047100	3.63203200	-0.68999800	C	2.57676000	-0.72313600	0.79863700
H	-5.07807900	3.15684800	-0.71141400	C	3.01372800	-1.41974700	-0.32647300
H	-5.07807900	-3.15684800	-0.71141400	C	3.02366500	-1.42230300	-2.66626800
H	-6.78047100	-3.63203200	-0.68999800	C	2.59651900	-0.72488800	-3.79787800
H	-5.86697900	0.00000000	-6.89455800	C	1.42544800	1.17524300	-4.52703700
H	-4.28002900	0.00000000	-6.10762400	C	0.72612100	2.30924100	-4.09758100
C	6.91396600	-0.70272200	-1.57142000	C	0.00000000	3.48488200	-2.19415300
C	6.73359100	-1.41320100	-2.80401000	C	0.00000000	3.48177700	-0.79375100
C	6.91396600	0.70272200	-1.57142000	C	0.72358400	2.30315300	1.10482600
C	6.55417800	-0.71617100	-3.99215500	C	1.42014000	1.17401800	1.54197200
C	6.55417800	0.71617100	-3.99215500	C	1.17458100	3.03603800	-2.92180800
C	6.73359100	1.41320100	-2.80401000	C	2.59651900	0.72488800	-3.79787800
C	5.29593200	-2.52604300	-4.89171200	C	2.57676000	0.72313600	0.79863700
C	5.47949200	-3.24500300	-3.66828500	C	1.17193200	3.03013800	-0.06792800
C	6.07179200	-0.73510600	0.67217900	C	3.01372800	1.41974700	-0.32647300
C	6.07179200	0.73510600	0.67217900	C	2.30080200	2.59956500	-0.76885500
C	5.29593200	2.52604300	-4.89171200	C	3.47049900	-0.69871700	-1.49537700
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C	6.14140300	-2.66047500	-2.57843700	C	0.72358400	-2.30315300	1.10482600
C	6.45112300	-1.45023400	-0.50124000	C	2.30315100	2.59979400	-2.22130900
C	6.08051700	-2.85691500	-1.03954500	C	3.02366500	1.42230300	-2.66626800
C	6.14140300	2.66047500	-2.57843700	C	-3.44950800	-0.68725300	4.84873100
C	6.45112300	1.45023400	-0.50124000	C	-2.38704300	-1.37372800	5.50067100
C	6.08051700	2.85691500	-1.03954500	C	-1.25325300	-0.72205100	6.03638300
C	5.77323200	-1.21511600	-5.03993500	C	-1.25325300	0.72205100	6.03638300
C	5.77323200	1.21511600	-5.03993500	C	-2.38704300	1.37372800	5.50067100
C	5.36030000	0.00000000	-5.91742800	C	-3.44950800	0.68725300	4.84873100
H	4.64784300	-2.97205600	-5.64477000	C	0.00000000	-1.44310600	6.02828900
H	4.95996600	-4.19566900	-3.56049700	C	0.00000000	1.44310600	6.02828900
H	4.64784300	2.97205600	-5.64477000	C	1.25325300	0.72205100	6.03638300
H	4.95996600	4.19566900	-3.56049700	C	1.25325300	-0.72205100	6.03638300
H	6.78047100	-3.63203200	-0.68999800	C	2.38704300	1.37372800	5.50067100
H	5.07807900	-3.15684800	-0.71141400	C	2.31872000	2.63276300	4.84148600
H	5.07807900	3.15684800	-0.71141400	C	1.12353000	3.30886100	4.81403800
H	6.78047100	3.63203200	-0.68999800	C	0.00000000	2.74034900	5.47110900
H	5.86697900	0.00000000	-6.89455800	C	-1.12353000	3.30886100	4.81403800
H	4.28002900	0.00000000	-6.10762400	C	-2.31872000	2.63276300	4.84148600
C	-2.30315100	-2.59979400	-2.22130900	C	-2.31872000	-2.63276300	4.84148600
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C	-3.01372800	-1.41974700	-0.32647300	C	0.00000000	-2.74034900	5.47110900
C	-3.47049900	-0.69871700	-1.49537700	C	1.12353000	-3.30886100	4.81403800
C	-3.02366500	-1.42230300	-2.66626800	C	2.31872000	-2.63276300	4.84148600
C	-1.17458100	-3.03603800	-2.92180800	C	2.38704300	-1.37372800	5.50067100
C	-1.17193200	-3.03013800	-0.06792800	C	3.44950800	0.68725300	4.84873100
C	-2.57676000	-0.72313600	0.79863700	C	3.44950800	-0.68725300	4.84873100
C	-3.47049900	0.69871700	-1.49537700	C	3.30818400	2.74291900	3.79892700

C	3.13528500	3.91989400	2.94653800	C	-5.46456900	-3.25041300	-3.10846100
C	1.83883700	4.61674500	2.88544300	C	-6.16561000	2.65363900	-2.04948500
C	0.72249500	4.19246300	3.73972500	C	-6.49655600	1.44880600	0.02372300
C	-0.72249500	4.19246300	3.73972500	C	-6.12020700	2.85337200	-0.51041600
C	-1.83883700	4.61674500	2.88544300	C	-6.16561000	-2.65363900	-2.04948500
C	-3.13528500	3.91989400	2.94653800	C	-6.49655600	-1.44880600	0.02372300
C	-3.30818400	2.74291900	3.79892700	C	-6.12020700	-2.85337200	-0.51041600
C	4.02136300	-1.49049200	3.78440400	C	-5.75654700	1.21522700	-4.48317800
C	4.82983600	-0.74420700	2.82496700	C	-5.75654700	-1.21522700	-4.48317800
C	4.82983600	0.74420700	2.82496700	C	-5.32329100	0.00000000	-5.35167900
C	4.02136300	1.49049200	3.78440400	H	-6.82106600	3.62976000	-0.16434000
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C	-4.82983600	0.74420700	2.82496700	H	-5.12057200	-3.15120400	-0.17212600
C	-4.82983600	-0.74420700	2.82496700	H	-6.82106600	-3.62976000	-0.16434000
C	-4.02136300	-1.49049200	3.78440400	H	-5.80074500	0.00000000	-6.34389900
C	-0.72249500	-4.19246300	3.73972500	H	-4.23850000	0.00000000	-5.51360200
C	-1.83883700	-4.61674500	2.88544300	C	6.95955600	-0.70314300	-1.04862900
C	-3.13528500	-3.91989400	2.94653800	C	6.76850200	-1.41307300	-2.27939100
C	-3.30818400	-2.74291900	3.79892700	C	6.95955600	0.70314300	-1.04862900
C	0.72249500	-4.19246300	3.73972500	C	6.57014400	-0.71591100	-3.46165900
C	1.83883700	-4.61674500	2.88544300	C	6.57014400	0.71591100	-3.46165900
C	3.13528500	-3.91989400	2.94653800	C	6.76850200	1.41307300	-2.27939100
C	3.30818400	-2.74291900	3.79892700	C	5.25131200	-2.51753700	-4.33944700
C	-1.74906200	-5.72405600	2.02081800	C	5.46456900	-3.25041300	-3.10846100
C	-4.20509400	-4.46599700	2.21098900	C	6.10800700	-0.73451900	1.19281500
C	-4.05991200	-5.55609900	1.35924100	C	6.10800700	0.73451900	1.19281500
C	-5.48105500	-1.38313300	1.77428900	C	5.25131200	2.51753700	-4.33944700
C	-5.48105500	1.38313300	1.77428900	C	5.46456900	3.25041300	-3.10846100
C	-4.20509400	4.46599700	2.21098900	C	6.16561000	-2.65363900	-2.04948500
C	-1.74906200	5.72405600	2.02081800	C	6.49655600	-1.44880600	0.02372300
C	-4.05991200	5.55609900	1.35924100	C	6.12020700	-2.85337200	-0.51041600
C	4.20509400	4.46599700	2.21098900	C	6.16561000	2.65363900	-2.04948500
C	1.74906200	5.72405600	2.02081800	C	6.49655600	1.44880600	0.02372300
C	2.81320500	6.17709200	1.24865500	C	6.12020700	2.85337200	-0.51041600
C	5.48105500	-1.38313300	1.77428900	C	5.75654700	-1.21522700	-4.48317800
C	5.48105500	1.38313300	1.77428900	C	5.75654700	1.21522700	-4.48317800
C	1.74906200	-5.72405600	2.02081800	C	5.32329100	0.00000000	-5.35167900
C	4.20509400	-4.46599700	2.21098900	H	6.82106600	-3.62976000	-0.16434000
C	4.05991200	-5.55609900	1.35924100	H	5.12057200	-3.15120400	-0.17212600
C	-2.81320500	6.17709200	1.24865500	H	5.12057200	3.15120400	-0.17212600
C	-2.81320500	-6.17709200	1.24865500	H	6.82106600	3.62976000	-0.16434000
C	2.81320500	-6.17709200	1.24865500	H	5.80074500	0.00000000	-6.34389900
C	4.05991200	5.55609900	1.35924100	H	4.23850000	0.00000000	-5.51360200
H	-0.82644000	-6.28328400	1.98903500	C	-2.30184500	-2.59605200	-1.73718400
H	-5.19847500	-4.06475400	2.37458700	C	-2.30237300	-2.59779700	-0.28555200
H	-4.92124300	-5.93974600	0.81642000	C	-3.01979900	-1.42000300	0.15790700
H	-5.46795100	-2.46004700	1.74084900	C	-3.47640100	-0.69887400	-1.01144300
H	-5.46795100	2.46004700	1.74084900	C	-3.02627000	-1.42219300	-2.18328500
H	-5.19847500	4.06475400	2.37458700	C	-1.17413900	-3.03426000	-2.43813500
H	-0.82644000	6.28328400	1.98903500	C	-1.17209800	-3.02690300	0.41353900
H	-4.92124300	5.93974600	0.81642000	C	-2.58257900	-0.72324900	1.28381000
H	5.19847500	4.06475400	2.37458700	C	-3.47640100	0.69887400	-1.01144300
H	0.82644000	6.28328400	1.98903500	C	-2.59550700	-0.72485200	-3.31386500
H	2.67973400	7.04104500	0.60117200	C	-2.59550700	0.72485200	-3.31386500
H	5.46795100	-2.46004700	1.74084900	C	-3.02627000	1.42219300	-2.18328500
H	5.46795100	2.46004700	1.74084900	C	-3.01979900	1.42000300	0.15790700
H	0.82644000	-6.28328400	1.98903500	C	-2.58257900	0.72324900	1.28381000
H	5.19847500	-4.06475400	2.37458700	C	-0.72331400	-2.29916800	1.58500100
H	4.92124300	-5.93974600	0.81642000	C	-1.42175500	-1.17263500	2.02352500
H	-2.67973400	7.04104500	0.60117200	C	0.00000000	-3.48006800	-0.31132400
H	-2.67973400	-7.04104500	0.60117200	C	0.00000000	-3.48480800	-1.71124500
H	2.67973400	-7.04104500	0.60117200	C	-0.72558300	-2.30850100	-3.61302100
H	4.92124300	5.93974600	0.81642000	C	-1.42540300	-1.17449100	-4.04214000
				C	-2.30237300	2.59779700	-0.28555200
				C	-2.30184500	2.59605200	-1.73718400
				C	-0.69958800	0.00000000	2.48434600
				C	-1.42175500	1.17263500	2.02352500
				C	1.17209800	-3.02690300	0.41353900
				C	0.72558300	-2.30850100	-3.61302100
				C	1.17413900	-3.03426000	-2.43813500
				C	-1.42540300	1.17449100	-4.04214000
				C	-0.69960700	0.00000000	-4.49284900
				C	-0.72331400	2.29916800	1.58500100
				C	-1.17209800	3.02690300	0.41353900
				C	-1.17413900	3.03426000	-2.43813500
				C	-0.72558300	2.30850100	-3.61302100

5b...C₆₀:

C	-6.95955600	0.70314300	-1.04862900
C	-6.76850200	1.41307300	-2.27939100
C	-6.95955600	-0.70314300	-1.04862900
C	-6.57014400	0.71591100	-3.46165900
C	-6.57014400	-0.71591100	-3.46165900
C	-6.76850200	-1.41307300	-2.27939100
C	-5.25131200	2.51753700	-4.33944700
C	-5.46456900	3.25041300	-3.10846100
C	-6.10800700	0.73451900	1.19281500
C	-6.10800700	-0.73451900	1.19281500
C	-5.25131200	-2.51753700	-4.33944700

C	0.69960700	0.00000000	-4.49284900	C	-4.19291700	-4.42160500	2.64885500
C	1.42540300	-1.17449100	-4.04214000	C	-4.02292900	-5.44648500	1.72709100
C	2.30184500	-2.59605200	-1.73718400	C	-5.50973400	-1.38222600	2.29017100
C	2.30237300	-2.59779700	-0.28555200	C	-5.50973400	1.38222600	2.29017100
C	1.42175500	-1.17263500	2.02352500	C	-4.19291700	4.42160500	2.64885500
C	0.69958800	0.00000000	2.48434600	C	-1.73214800	5.62920000	2.40201300
C	2.58257900	-0.72324900	1.28381000	C	-4.02292900	5.44648500	1.72709100
C	3.01979900	-1.42000300	0.15790700	C	4.19291700	4.42160500	2.64885500
C	3.02627000	-1.42219300	-2.18328500	C	1.73214800	5.62920000	2.40201300
C	2.59550700	-0.72485200	-3.31386500	C	2.76606200	6.04370100	1.56364900
C	1.42540300	1.17449100	-4.04214000	C	5.50973400	-1.38222600	2.29017100
C	0.72558300	2.30850100	-3.61302100	C	5.50973400	1.38222600	2.29017100
C	0.00000000	3.48480800	-1.71124500	C	1.73214800	-5.62920000	2.40201300
C	0.00000000	3.48006800	-0.31132400	C	4.19291700	-4.42160500	2.64885500
C	0.72331400	2.29916800	1.58500100	C	4.02292900	-5.44648500	1.72709100
C	1.42175500	1.17263500	2.02352500	C	-2.76606200	6.04370100	1.56364900
C	1.17413900	3.03426000	-2.43813500	C	-2.76606200	-6.04370100	1.56364900
C	2.59550700	0.72485200	-3.31386500	C	2.76606200	-6.04370100	1.56364900
C	2.58257900	0.72324900	1.28381000	C	4.02292900	5.44648500	1.72709100
C	1.17209800	3.02690300	0.41353900	H	-0.80500900	-6.17820200	2.34620800
C	3.01979900	1.42000300	0.15790700	H	-5.19542100	-4.05535000	2.83541000
C	2.30237300	2.59779700	-0.28555200	H	-4.87634200	-5.80735000	1.15493600
C	3.47640100	-0.69887400	-1.01144300	H	-5.50811000	-2.45857700	2.26196600
C	3.47640100	0.69887400	-1.01144300	H	-5.50811000	2.45857700	2.26196600
C	0.72331400	-2.29916800	1.58500100	H	-5.19542100	4.05535000	2.83541000
C	2.30184500	2.59605200	-1.73718400	H	-0.80500900	6.17820200	2.34620800
C	3.02627000	1.42219300	-2.18328500	H	-4.87634200	5.80735000	1.15493600
C	-3.45636100	-0.68739600	5.35041500	H	5.19542100	4.05535000	2.83541000
C	-2.38845600	-1.37504000	5.99327000	H	0.80500900	6.17820200	2.34620800
C	-1.25276700	-0.72271300	6.52355800	H	5.50811000	-2.45857700	2.26196600
C	-1.25276700	0.72271300	6.52355800	H	5.50811000	2.45857700	2.26196600
C	-2.38845600	1.37504000	5.99327000	H	0.80500900	-6.17820200	2.34620800
C	-3.45636100	0.68739600	5.35041500	H	5.19542100	-4.05535000	2.83541000
C	0.00000000	-1.44409700	6.51031300	H	4.87634200	-5.80735000	1.15493600
C	0.00000000	1.44409700	6.51031300	H	4.87634200	5.80735000	1.15493600
C	1.25276700	0.72271300	6.52355800	C	4.78342400	4.58428200	-2.91518700
C	1.25276700	-0.72271300	6.52355800	H	3.70614500	4.52026900	-3.11690700
C	2.38845600	1.37504000	5.99327000	H	4.91759500	4.94564800	-1.88978200
C	2.32149000	2.63208200	5.32844300	H	5.19487800	5.34071900	-3.59983000
C	1.12423700	3.30519100	5.28754600	C	4.32049200	3.09339900	-5.37913000
C	0.00000000	2.73970800	5.94616900	H	3.31569300	3.25848600	-4.96502100
C	-1.12423700	3.30519100	5.28754600	H	4.67981700	4.06701600	-5.74161000
C	-2.32149000	2.63208200	5.32844300	H	4.22806000	2.42107100	-6.23832600
C	-2.32149000	-2.63208200	5.32844300	C	4.32049200	-3.09339900	-5.37913000
C	-1.12423700	-3.30519100	5.28754600	H	4.67981700	-4.06701600	-5.74161000
C	0.00000000	-2.73970800	5.94616900	H	3.31569300	-3.25848600	-4.96502100
C	1.12423700	-3.30519100	5.28754600	H	4.22806000	-2.42107100	-6.23832600
C	2.32149000	-2.63208200	5.32844300	C	4.78342400	-4.58428200	-2.91518700
C	2.38845600	-1.37504000	5.99327000	H	4.91759500	-4.94564800	-1.88978200
C	3.45636100	0.68739600	5.35041500	H	3.70614500	-4.52026900	-3.11690700
C	3.45636100	-0.68739600	5.35041500	H	5.19487800	-5.34071900	-3.59983000
C	3.31721700	2.73935200	4.29234900	C	-4.78342400	-4.58428200	-2.91518700
C	3.13618400	3.89291400	3.41485000	H	-3.70614500	-4.52026900	-3.11690700
C	1.83674900	4.57880700	3.33207600	H	-4.91759500	-4.94564800	-1.88978200
C	0.72389500	4.17639600	4.20190500	H	-5.19487800	-5.34071900	-3.59983000
C	-0.72389500	4.17639600	4.20190500	C	-4.32049200	3.09339900	-5.37913000
C	-1.83674900	4.57880700	3.33207600	H	-3.31569300	-3.25848600	-4.96502100
C	-3.13618400	3.89291400	3.41485000	H	-4.67981700	-4.06701600	-5.74161000
C	-3.31721700	2.73935200	4.29234900	H	-4.22806000	-2.42107100	-6.23832600
C	4.03321100	-1.48855100	4.28767000	C	-4.32049200	3.09339900	-5.37913000
C	4.84533000	-0.74385700	3.33252300	H	-4.67981700	4.06701600	-5.74161000
C	4.84533000	0.74385700	3.33252300	H	-3.31569300	3.25848600	-4.96502100
C	4.03321100	1.48855100	4.28767000	H	-4.22806000	2.42107100	-6.23832600
C	-4.03321100	1.48855100	4.28767000	C	-4.78342400	4.58428200	-2.91518700
C	-4.84533000	0.74385700	3.33252300	H	-4.91759500	4.94564800	-1.88978200
C	-4.84533000	-0.74385700	3.33252300	H	-3.70614500	4.52026900	-3.11690700
C	-4.03321100	-1.48855100	4.28767000	H	-5.19487800	5.34071900	-3.59983000
C	-0.72389500	-4.17639600	4.20190500	C	-2.53189300	-7.10397400	0.51664300
C	-1.83674900	-4.57880700	3.33207600	H	-2.26526100	-6.63807500	-0.44449200
C	-3.13618400	-3.89291400	3.41485000	H	-1.70788400	-7.77036200	0.80062700
C	-3.31721700	-2.73935200	4.29234900	H	-3.43180000	-7.70990100	0.35173400
C	0.72389500	-4.17639600	4.20190500	C	2.53189300	-7.10397400	0.51664300
C	1.83674900	-4.57880700	3.33207600	H	1.70788400	-7.77036200	0.80062700
C	3.13618400	-3.89291400	3.41485000	H	2.26526100	-6.63807500	-0.44449200
C	3.31721700	-2.73935200	4.29234900	H	3.43180000	-7.70990100	0.35173400
C	-1.73214800	-5.62920000	2.40201300	C	-2.53189300	7.10397400	0.51664300

H	-1.70788400	7.77036200	0.80062700	C	-4.81847800	-0.70490800	4.99365900
H	-2.26526100	6.63807500	-0.44449200	C	-5.81976000	-1.41129800	-2.86231400
H	-3.43180000	7.70990100	0.35173400	C	-6.36063500	-0.73013300	-1.79662200
C	2.53189300	7.10397400	0.51664300	C	-6.36063500	0.73013300	-1.79662200
H	2.26526100	6.63807500	-0.44449200	C	-5.81976000	1.41129800	-2.86231400
H	1.70788400	7.77036200	0.80062700	C	-5.61767300	-4.36507900	-1.04284900
H	3.43180000	7.70990100	0.35173400	C	-4.81866400	-5.51338700	-0.96289200
6a...C₆₀:				C	-4.24355200	-5.88722500	0.25274200
C	-1.29927800	3.47811300	-5.43838700	C	-4.48861100	-5.14272800	1.41563400
C	0.00000000	1.51062000	-6.29026500	C	-5.27868800	-3.99604500	1.35655000
C	-1.20043300	0.73279100	-6.41906700	C	-5.81770100	-3.57810600	0.08747900
C	-2.39390800	1.36329600	-6.11114600	C	-1.91909800	-2.89901800	6.24748800
C	-2.43593900	2.65147300	-5.54839600	C	-2.73917300	-1.76665500	6.17278100
C	1.20043300	0.73279100	-6.41906700	C	-3.80955700	-1.74257800	5.28110800
C	-1.20043300	-0.73279100	-6.41906700	C	-4.08156200	-2.89674500	4.46159700
C	0.00000000	-1.51062000	-6.29026500	C	-3.24685400	-4.00928500	4.54572800
C	1.20043300	-0.73279100	-6.41906700	C	-2.16279000	-4.00592900	5.43377800
C	0.00000000	-2.88907700	-5.81475400	C	-4.08156200	2.89674500	4.46159700
C	-1.29927800	-3.47811300	-5.43838700	C	-3.80955700	1.74257800	5.28110800
C	-2.43593900	-2.65147300	-5.54839600	C	-2.73917300	1.76665500	6.17278100
C	-2.39390800	-1.36329600	-6.11114600	C	-1.91909800	2.89901800	6.24748800
C	-3.58898400	-0.68939800	-5.74084900	C	-2.16279000	4.00592900	5.43377800
C	-3.58898400	0.68939800	-5.74084900	C	-3.24685400	4.00928500	4.54572800
C	1.29927800	3.47811300	-5.43838700	C	-5.61767300	4.36507900	-1.04284900
C	2.43593900	2.65147300	-5.54839600	C	-5.81770100	3.57810600	0.08747900
C	2.39390800	1.36329600	-6.11114600	C	-5.27868800	3.99604500	1.35655000
C	3.58898400	0.68939800	-5.74084900	C	-4.48861100	5.14272800	1.41563400
C	3.58898400	-0.68939800	-5.74084900	C	-4.24355200	5.88722500	0.25274200
C	2.39390800	-1.36329600	-6.11114600	C	-4.81866400	5.51338700	-0.96289200
C	1.29927800	-3.47811300	-5.43838700	C	7.33319100	1.15268000	2.31627900
C	2.43593900	-2.65147300	-5.54839600	C	6.85117600	0.71306600	3.58335200
C	-3.66704100	-2.79609800	-4.81173700	C	6.85117600	-0.71306600	3.58335200
C	-4.35823100	-1.46600600	-4.85886600	C	7.33319100	-1.15268000	2.31627900
C	-5.18352400	-0.74332900	-3.94630300	C	7.63244500	0.00000000	1.52724400
C	-5.18352400	0.74332900	-3.94630300	C	6.74340400	2.24591600	1.71840500
C	-4.35823100	1.46600600	-4.85886600	C	5.80615300	1.38678300	4.18154000
C	3.66704100	-2.79609800	-4.81173700	C	5.80615300	-1.38678300	4.18154000
C	-3.66704100	2.79609800	-4.81173700	C	6.74340400	-2.24591600	1.71840500
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C	4.35823100	1.46600600	-4.85886600	C	6.86140700	-1.20277800	-0.49667700
C	5.18352400	0.74332900	-3.94630300	C	6.60639300	-2.35155100	0.28197500
C	5.18352400	-0.74332900	-3.94630300	C	5.76508600	-3.07446700	2.40349700
C	4.35823100	-1.46600600	-4.85886600	C	5.28876000	-2.63631000	3.65389900
C	-1.57981600	4.71518000	-4.77384500	C	4.81847800	0.70490800	4.99365900
C	-3.84412800	3.97897900	-4.11826000	C	4.81847800	-0.70490800	4.99365900
C	-2.80824200	4.94542100	-4.16839700	C	5.28876000	2.63631000	3.65389900
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C	2.80824200	4.94542100	-4.16839700	C	6.86140700	1.20277800	-0.49667700
C	1.57981600	-4.71518000	-4.77384500	C	2.16279000	-4.00592900	5.43377800
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C	6.79814400	2.24423300	1.85507700	H	6.30724600	4.18572500	-1.81328500
C	5.83664500	1.38680000	4.30684100	H	5.03358100	6.29394000	-1.63799400
C	5.83664500	-1.38680000	4.30684100	H	4.28093600	5.57725300	2.51168700
C	6.79814400	-2.24423300	1.85507700	H	2.55951100	0.93739700	6.93583900
C	7.36288800	0.00000000	0.32043600	H	3.42734100	4.86411200	3.99680200
C	6.91190200	-1.20169800	-0.35839700	H	1.50041800	4.85586500	5.53200400
C	6.66821400	-2.35205000	0.41857200	H	1.09055900	2.91325100	7.02284500
C	5.82215300	-3.07963000	2.53350300	C	0.72581700	-2.30473200	2.87220500
C	5.32421000	-2.63590400	3.77288900	C	1.17636200	-3.03315800	1.70023100
C	4.84257900	0.70525100	5.11094300	C	2.30969200	-2.60292800	1.00211100
C	4.84257900	-0.70525100	5.11094300	C	3.03561600	-1.42648100	1.44887900
C	5.32421000	2.63590400	3.77288900	C	2.59445800	-0.72439500	2.57276000
C	5.82215300	3.07963000	2.53350300	C	1.42232400	-1.17206400	3.29716800
C	6.66821400	2.35205000	0.41857200	C	-0.72581700	-2.30473200	2.87220500
C	6.91190200	1.20169800	-0.35839700	C	-1.17636200	-3.03315800	1.70023100
C	2.15709500	-3.98965600	5.49080900	C	0.00000000	-3.48343700	0.97505900

C	0.00000000	-3.48705800	-0.42491200	H	3.93316800	-6.73742000	-3.56407700
C	2.30900200	-2.60323600	-0.44922300	H	2.87129600	-6.18356600	-2.26044000
C	3.48652100	-0.70019400	0.27759400	H	2.18172300	-7.02332600	-3.66656100
C	3.48652100	0.70019400	0.27759400	C	-2.94689900	-6.30506400	-3.34886900
C	3.03561600	1.42648100	1.44887900	H	-2.87129600	-6.18356600	-2.26044000
C	2.59445800	0.72439500	2.57276000	H	-3.93316800	-6.73742000	-3.56407700
C	1.42232400	1.17206400	3.29716800	H	-2.18172300	-7.02332600	-3.66656100
C	0.69869700	0.00000000	3.74789800				
C	-0.69869700	0.00000000	3.74789800				
C	-1.42232400	-1.17206400	3.29716800				
C	-2.30969200	-2.60292800	1.00211100				
C	-3.03561600	-1.42648100	1.44887900				
C	-2.59445800	-0.72439500	2.57276000				
C	-2.59445800	0.72439500	2.57276000				
C	-1.42232400	1.17206400	3.29716800				
C	-0.72581700	2.30473200	2.87220500				
C	0.72581700	2.30473200	2.87220500				
C	1.17636200	3.03315800	1.70023100				
C	2.30969200	2.60292800	1.00211100				
C	3.03033800	-1.42562400	-0.89393700				
C	0.72516600	2.30729800	-2.31905500				
C	1.42037000	1.17325900	-2.74469200				
C	0.69756500	0.00000000	-3.19415900				
C	-0.69756500	0.00000000	-3.19415900				
C	-1.42037000	1.17325900	-2.74469200				
C	-1.17638200	3.03619100	-1.14960500				
C	0.00000000	3.48705800	-0.42491200				
C	1.17638200	3.03619100	-1.14960500				
C	2.30900200	2.60323600	-0.44922300				
C	3.03033800	1.42562400	-0.89393700				
C	2.58834000	0.72486000	-2.01721900				
C	1.42037000	-1.17325900	-2.74469200				
C	0.72516600	-2.30729800	-2.31905500				
C	-0.72516600	-2.30729800	-2.31905500				
C	-1.42037000	-1.17325900	-2.74469200				
C	-2.58834000	-0.72486000	-2.01721900				
C	-2.58834000	0.72486000	-2.01721900				
C	-3.03033800	1.42562400	-0.89393700				
C	-2.30900200	2.60323600	-0.44922300				
C	0.00000000	3.48343700	0.97505900				
C	-1.17636200	3.03315800	1.70023100				
C	-2.30969200	2.60292800	1.00211100				
C	-3.03561600	1.42648100	1.44887900				
C	-3.48652100	0.70019400	0.27759400				
C	-3.48652100	-0.70019400	0.27759400				
C	-3.03033800	-1.42562400	-0.89393700				
C	-2.30900200	-2.60323600	-0.44922300				
C	-1.17638200	-3.03619100	-1.14960500				
C	2.58834000	-0.72486000	-2.01721900				
C	1.17638200	-3.03619100	-1.14960500				
C	-0.72516600	2.30729800	-2.31905500				
C	2.94689900	6.30506400	-3.34886900				
H	2.87129600	6.18356600	-2.26044000				
H	3.93316800	6.73742000	-3.56407700				
H	2.18172300	7.02332600	-3.66656100				
C	-2.94689900	6.30506400	-3.34886900				
H	-3.93316800	6.73742000	-3.56407700				
H	-2.87129600	6.18356600	-2.26044000				
H	-2.18172300	7.02332600	-3.66656100				
C	-3.68642300	7.29859700	0.50853200				
H	-2.61197900	7.08135500	0.40796100				
H	-3.96085200	7.99882300	-0.28957900				
H	-3.83012000	7.79774600	1.47552800				
C	3.68642300	7.29859700	0.50853200				
H	3.96085200	7.99882300	-0.28957900				
H	2.61197900	7.08135500	0.40796100				
H	3.83012000	7.79774600	1.47552800				
C	-3.68642300	-7.29859700	0.50853200				
H	-3.96085200	-7.99882300	-0.28957900				
H	-2.61197900	-7.08135500	0.40796100				
H	-3.83012000	-7.79774600	1.47552800				
C	3.68642300	-7.29859700	0.50853200				
H	2.61197900	-7.08135500	0.40796100				
H	3.96085200	-7.99882300	-0.28957900				
H	3.83012000	-7.79774600	1.47552800				
C	2.94689900	-6.30506400	-3.34886900				