

Electronic Supplementary Information

Magnetically induced current density: A semiempirical approach

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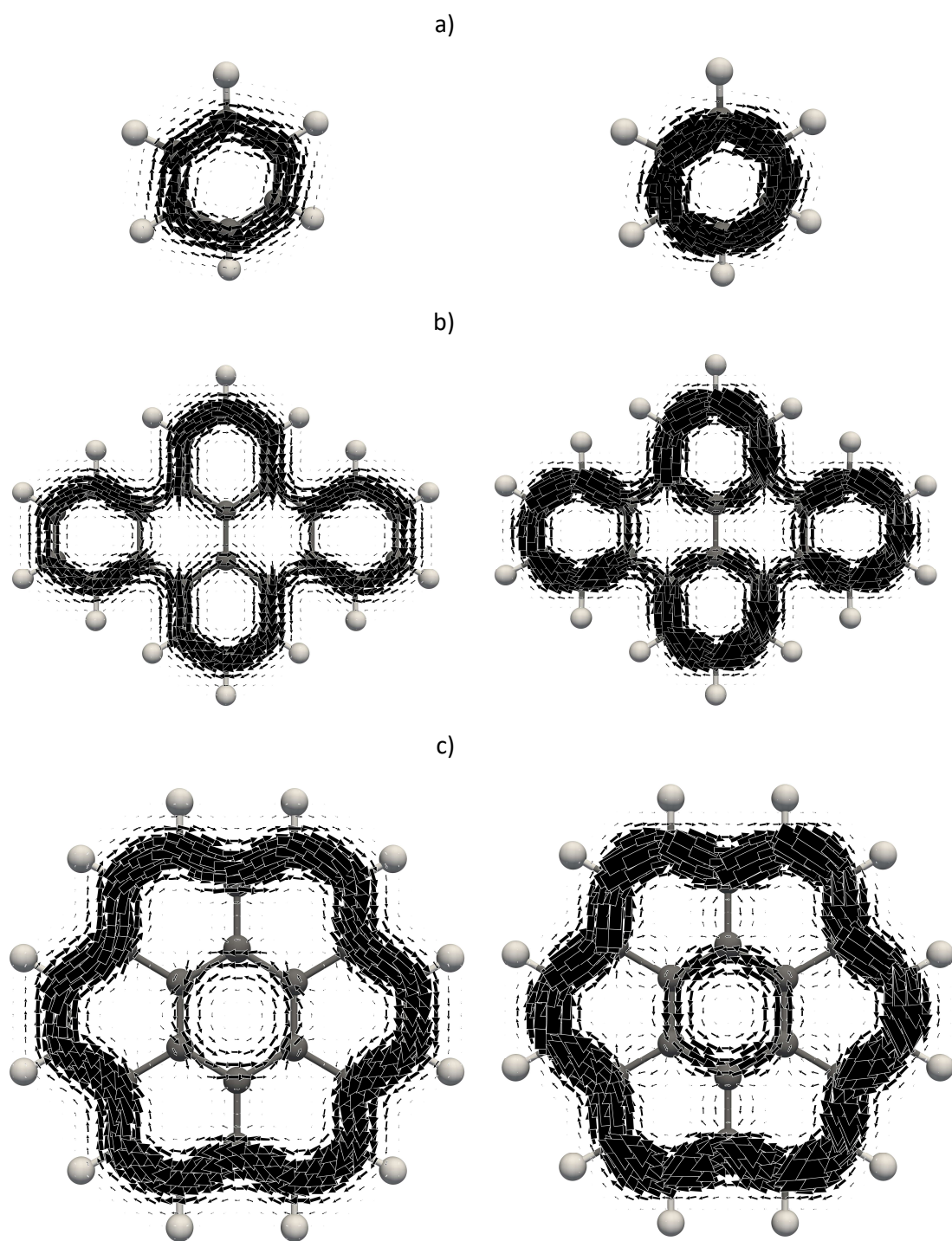


Figure S1. π -electron current density maps plotted 1 Bohr above the molecular plane of benzene (a), dibenzo[e,h]pyrene (b) and coronene (c) obtained using the B3LYP/def2-SVP (left) and MNDO (right) methods.

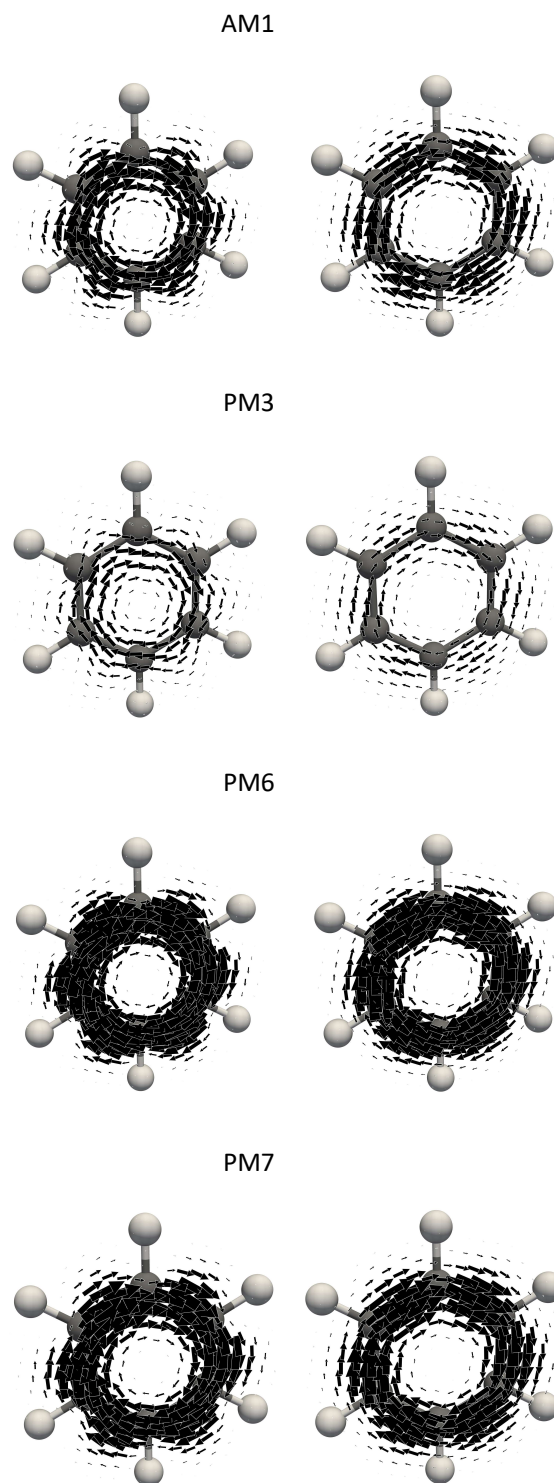
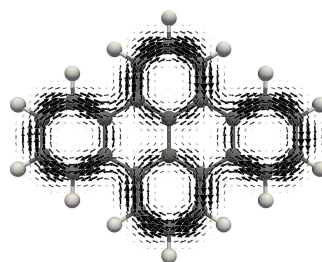
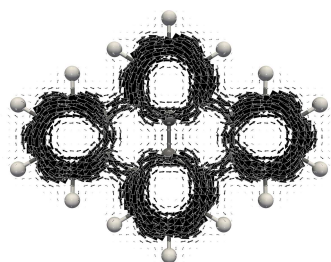
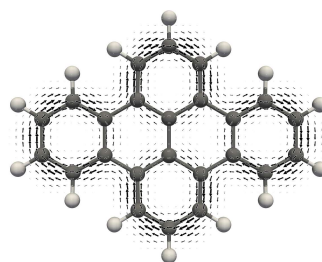
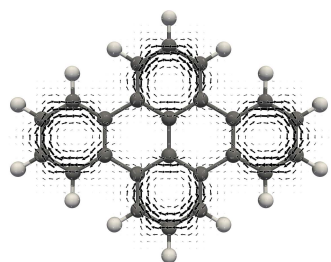


Figure S2. Total (left) and π -electron (right) current density maps plotted 1 Bohr above the molecular plane of benzene, obtained using different NDDO-based methods.

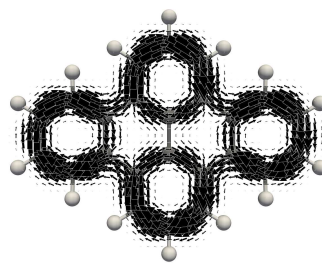
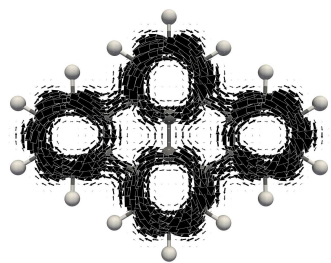
AM1



PM3



PM6



PM7

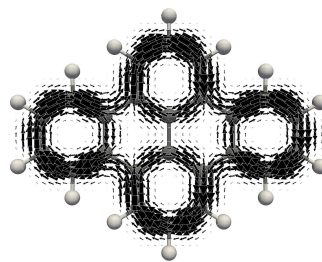
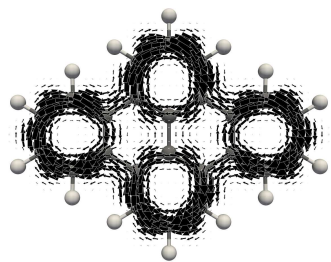


Figure S3. Total (left) and π -electron (right) current density maps plotted 1 Bohr above the molecular plane of dibenzo[e,h]pyrene, obtained using different NDDO-based methods.

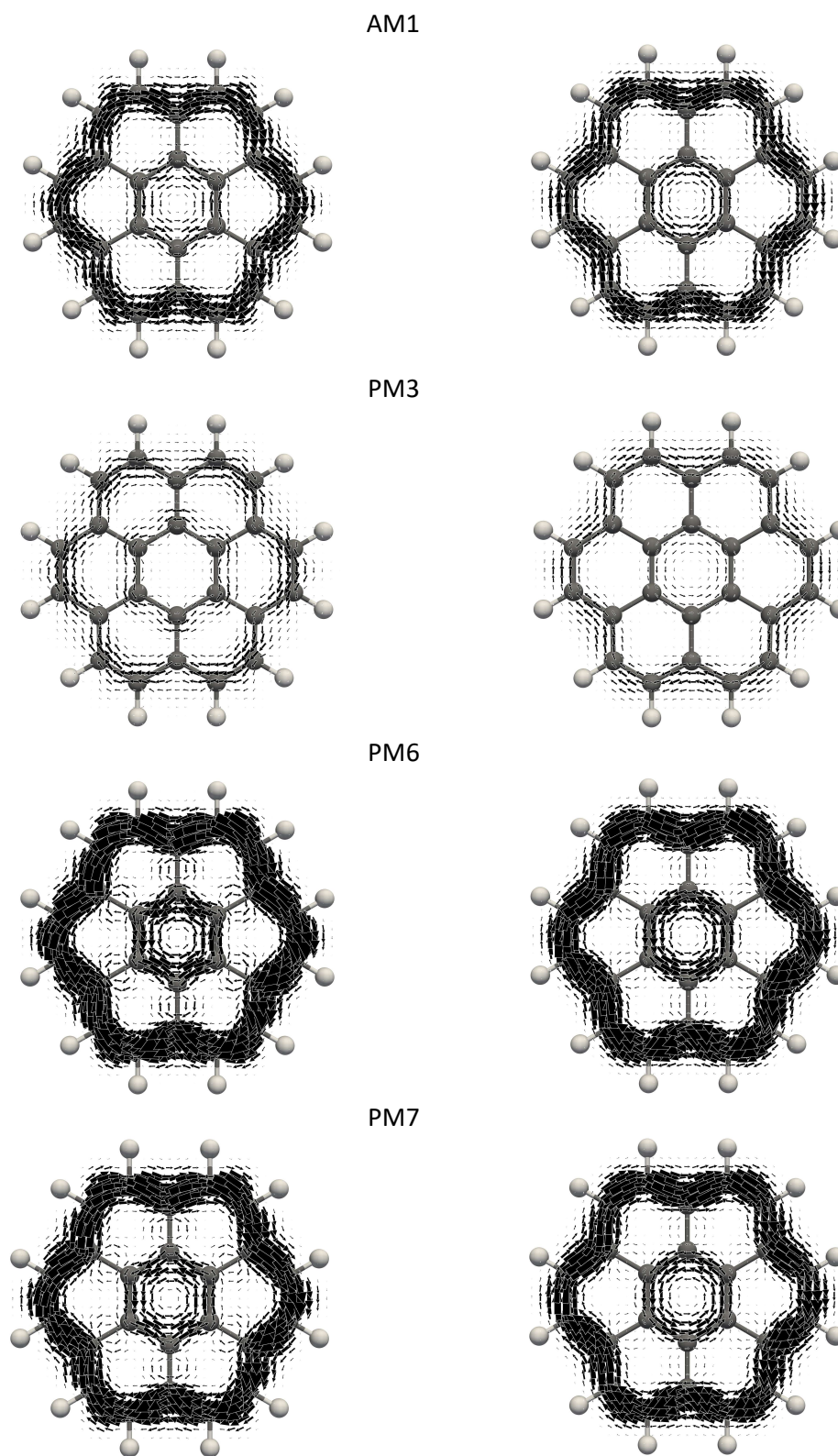


Figure S4. Total (left) and π -electron (right) current density maps plotted 1 Bohr above the molecular plane of coronene, obtained using different NDDO-based methods.

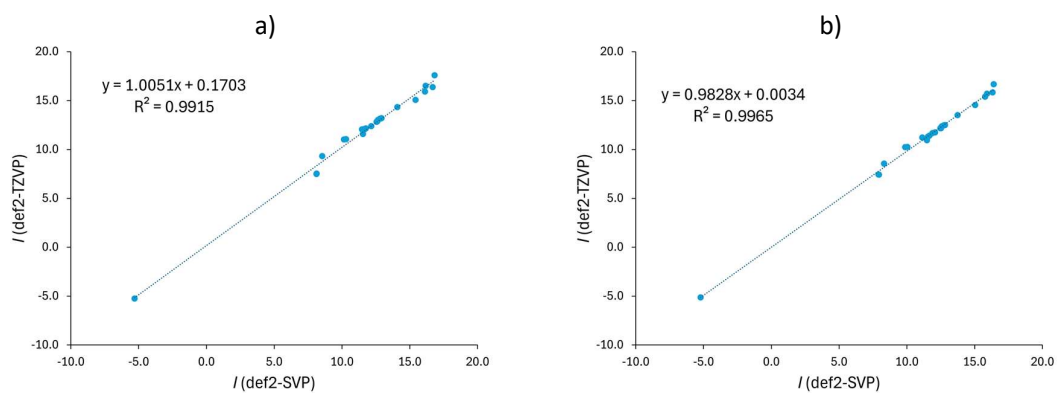


Figure S5. Correlation between the total (a) and π -only (b) current density strengths (I , in nA/T) for the selected C-C bonds in molecules 1-11, obtained using the B3LYP/def2-TZVP and B3LYP/def2-SVP methods.

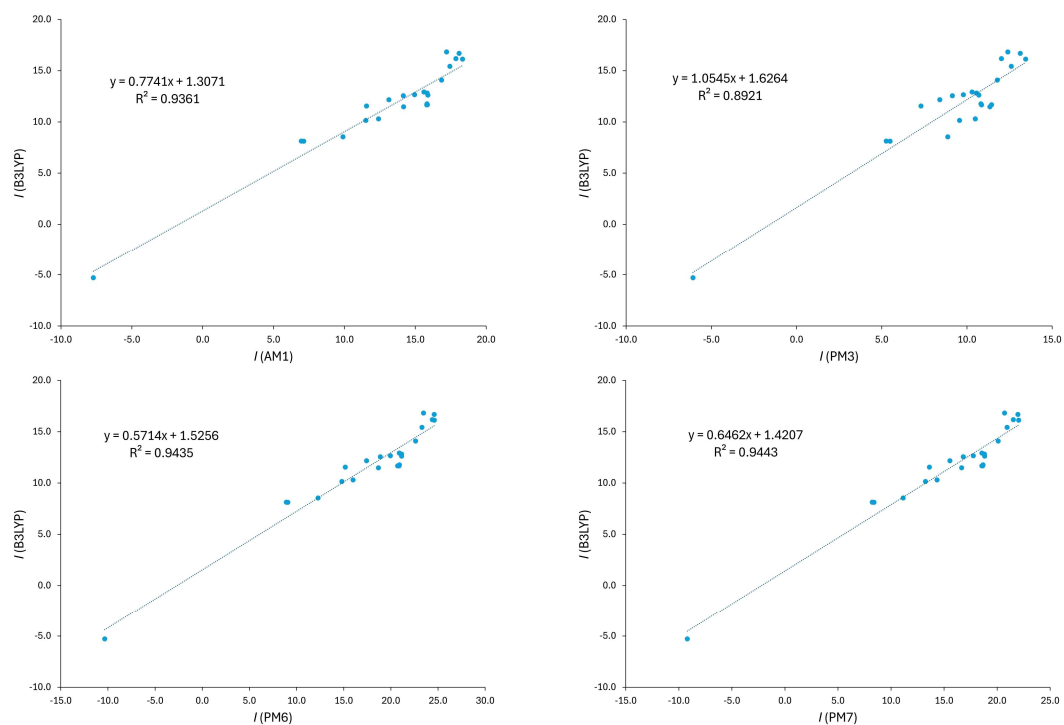


Figure S6. Correlation between the total current density strengths (I , in nA/T) for the selected C-C bonds in molecules **1-11**, obtained using the B3LYP/def2-SVP and NDDO-based methods.

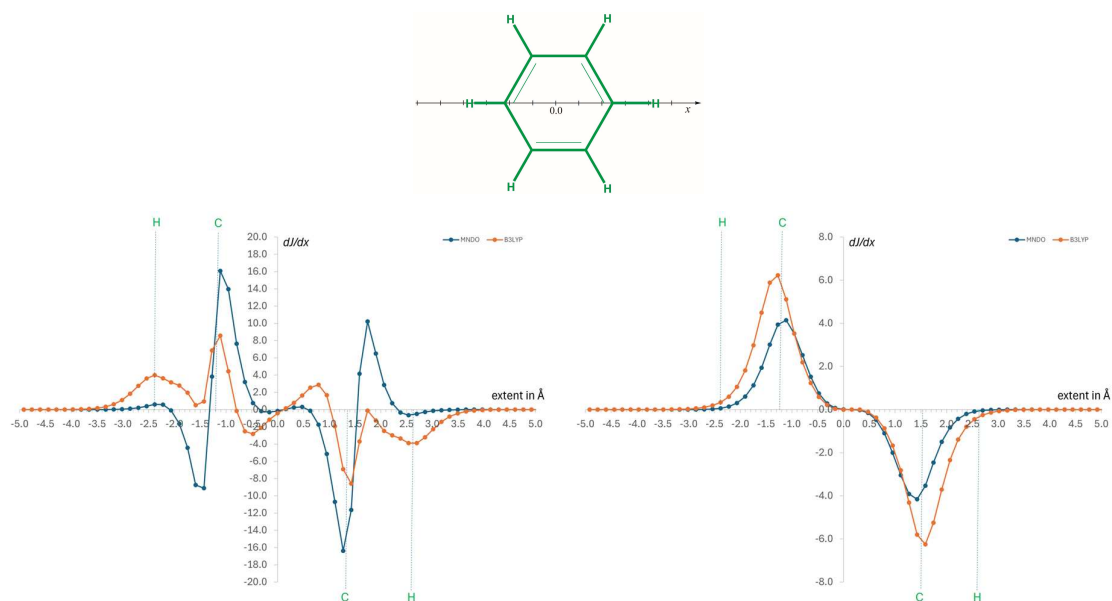


Figure S7. Profiles of total (left) and π (right) current strengths for benzene calculated using the B3LYP/def2-SVP (orange line) and MNDO (blue line) methods.

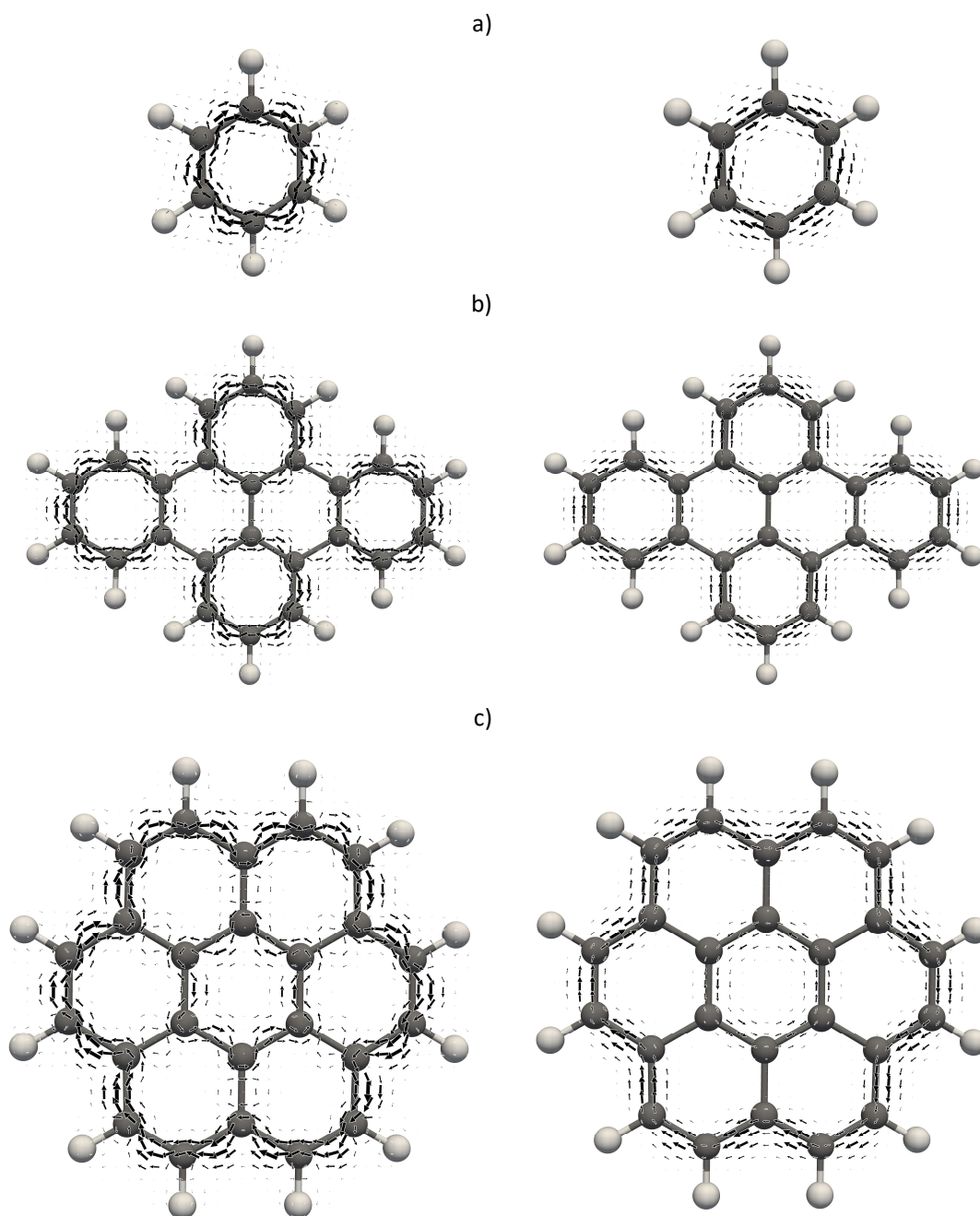


Figure S8. Total (left) and π -electron (right) current density maps plotted 1 Bohr above the molecular plane of benzene (a), dibenzo[*e,h*]pyrene (b) and coronene (c) obtained using the modified MNDO ($\xi = 0$; $\alpha = 1.0$) method.

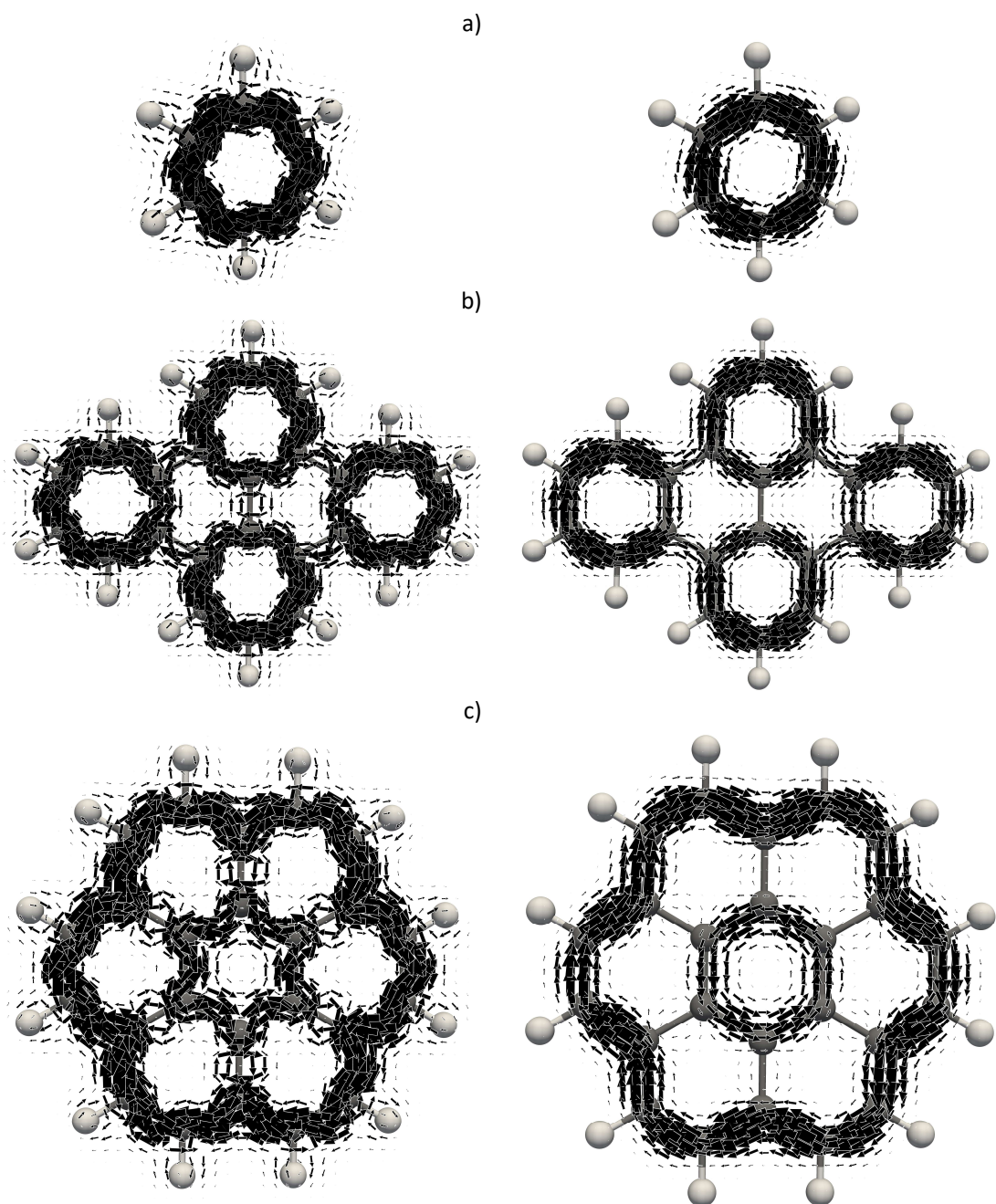


Figure S9. Total (left) and π -electron (right) current density maps plotted 1 Bohr above the molecular plane of benzene (a), dibenzo[e,/]pyrene (b) and coronene (c) obtained using the α -MNDO method.

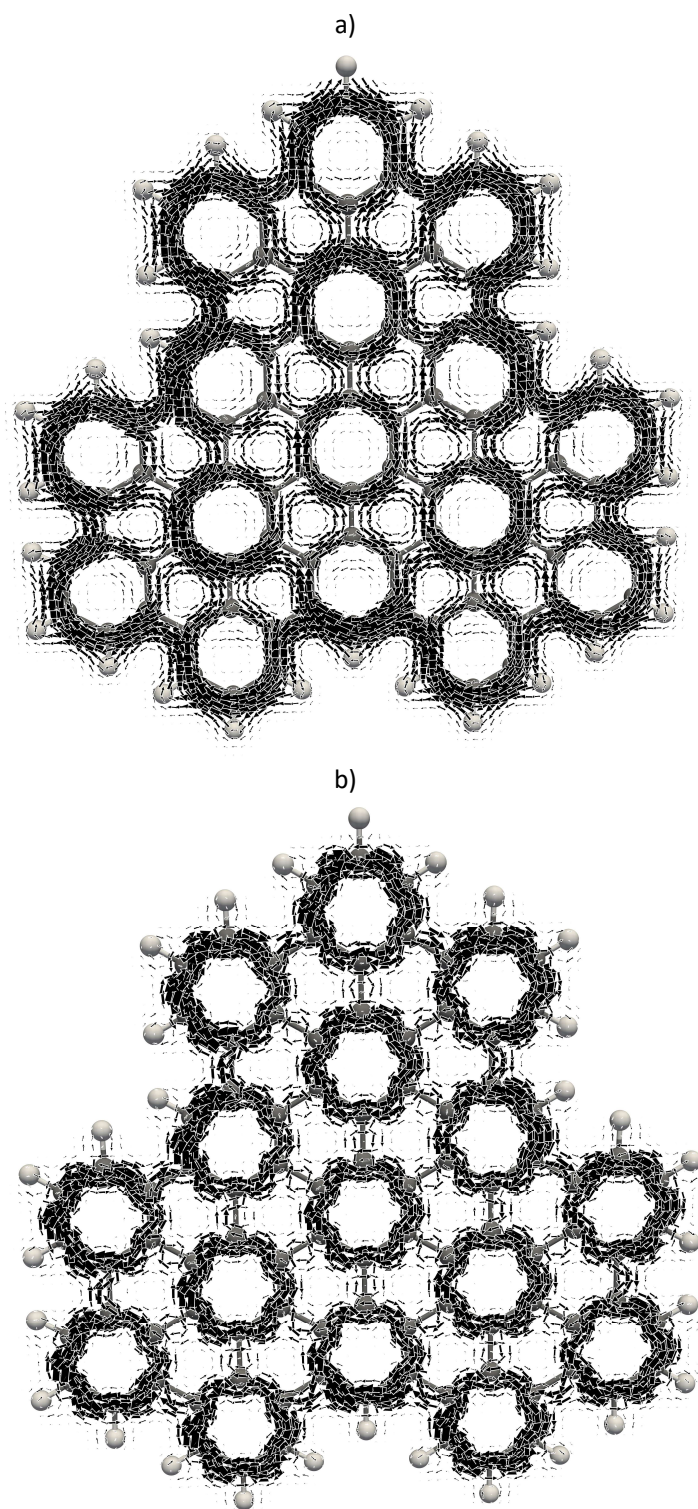


Figure S10. Total current density maps plotted 1 Bohr above molecular plane of **17** obtained using the B3LYP/def2-SVP (a) and α -MNDO (b) methods.

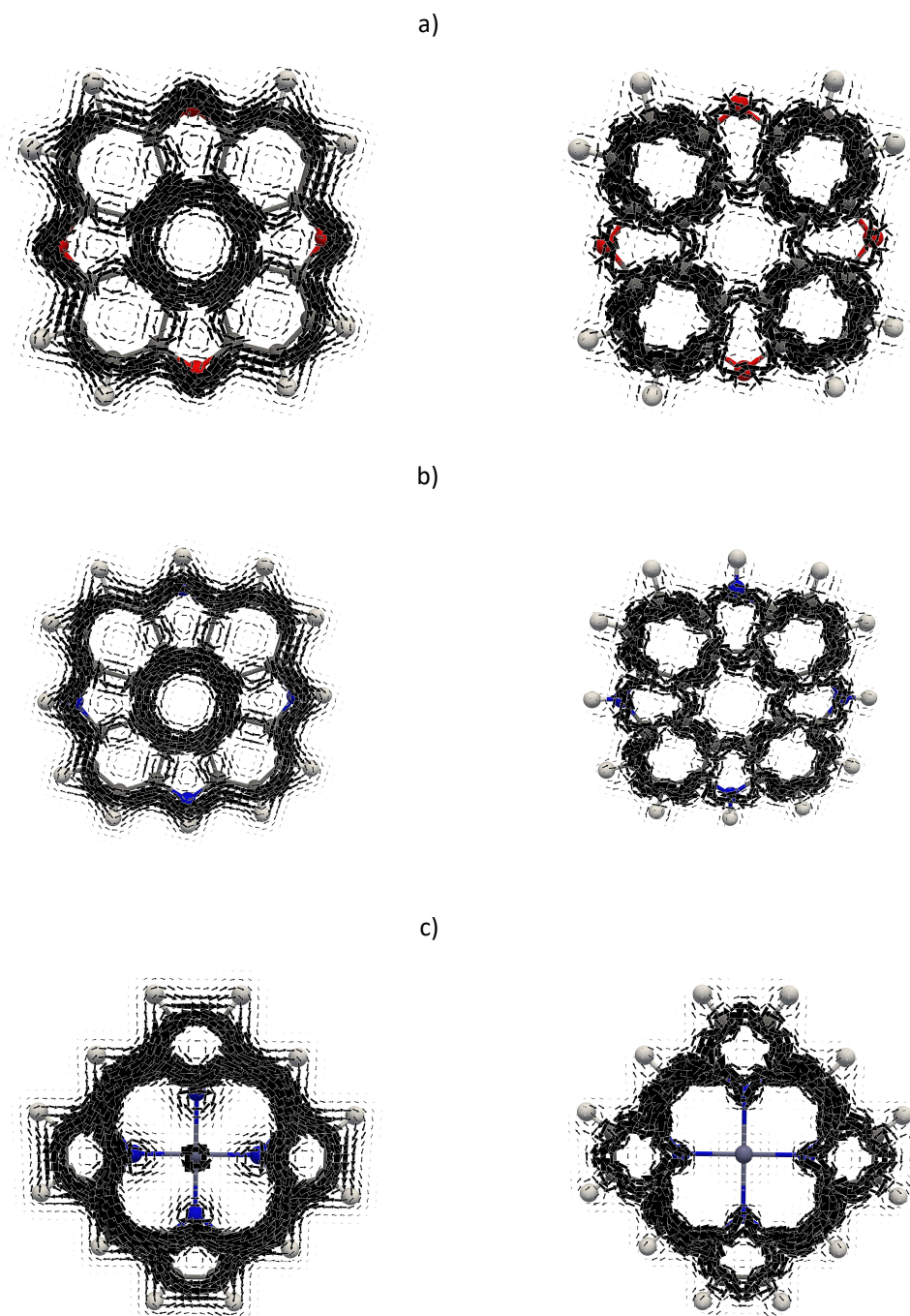


Figure S11. Total current density maps plotted 1 Bohr above the molecular plane of **19** (a), **21** (b) and **22** (c) obtained using the B3LYP/def2-SVP (left) and α -MNDO (right) methods.

Table S1. Total and π -electron current density strengths (in nA/T) for the selected C-C bonds in molecules **1-11**, obtained with different methods. The Average Absolute Error (AAE, in nA/T) calculated relative to the corresponding B3LYP/def2-SVP values.

Comp.	bond	B3LYP/def2-TZVP		B3LYP/def2-SVP		MNDO		AM1	PM3	PM6	PM7	α -MNDO
		total	π	total	π	total	π	total	total	total	total	total
1	<i>a</i>	12.1	11.7	11.7	11.9	17.5	16.3	15.9	11.4	20.7	18.6	14.8
2	<i>a</i>	13.0	12.4	12.7	12.6	16.6	15.3	14.9	9.8	19.9	17.8	14.2
3	<i>a</i>	12.4	11.7	12.2	12.1	14.3	13.1	13.1	8.4	17.4	15.6	12.3
	<i>b</i>	15.9	15.4	16.1	15.8	21.7	20.9	18.3	13.4	24.6	22.0	15.7
4	<i>a</i>	11.6	10.9	11.5	11.5	12.4	11.3	11.6	7.3	15.2	13.6	10.7
	<i>b</i>	16.4	15.8	16.7	16.3	22.3	21.5	18.1	13.1	24.6	22.0	14.6
5	<i>a</i>	11.1	10.3	10.3	10.0	15.2	14.4	12.4	10.5	16.0	14.3	8.6
	<i>b</i>	13.1	12.5	12.8	12.7	17.8	16.6	15.8	10.6	21.1	18.8	14.8
6	<i>a</i>	11.0	10.2	10.1	9.9	14.6	13.8	11.5	9.6	14.8	13.2	7.8
	<i>b</i>	16.5	15.7	16.2	15.9	21.8	20.6	17.9	12.0	24.4	21.5	15.7
7	<i>a</i>	13.2	12.5	12.9	12.8	17.6	16.4	15.6	10.3	20.9	18.6	14.6
	<i>b</i>	12.0	11.2	11.5	11.1	17.6	16.7	14.2	11.4	18.7	16.7	10.3
8	<i>a</i>	12.8	12.2	12.6	12.5	15.6	14.3	14.2	9.1	18.9	16.8	13.3
	<i>b</i>	15.1	14.5	15.4	15.0	20.2	19.4	17.4	12.6	23.3	20.9	15.4
	<i>c</i>	9.3	8.6	8.5	8.3	11.6	11.0	9.9	8.9	12.3	11.1	6.4
	<i>d</i>	12.9	12.2	12.6	12.5	17.8	16.6	15.9	10.7	21.1	18.8	14.7
9	<i>a</i>	12.1	11.4	11.8	11.7	17.6	16.5	15.8	10.8	20.9	18.7	14.6
	<i>b</i>	7.5	7.4	8.1	7.9	8.4	8.3	7.1	5.5	9.1	8.4	6.1
10	<i>a</i>	14.3	13.5	14.1	13.7	20.0	18.8	16.9	11.8	22.6	20.1	14.9
	<i>b</i>	7.5	7.4	8.1	7.9	8.4	8.3	7.0	5.3	8.9	8.2	5.7
	<i>c</i>	12.0	11.3	11.7	11.6	17.5	16.4	15.8	10.9	20.9	18.6	14.6
11	<i>a</i>	17.6	16.7	16.8	16.4	23.0	22.0	17.2	12.4	23.5	20.7	12.9
	<i>b</i>	-5.2	-5.1	-5.3	-5.2	-8.1	-7.8	-7.7	-6.1	-10.3	-9.2	-8.7
AAE						4.2	3.5	2.0	2.3	6.4	4.4	1.8

Table S2. Total current density strengths (in nA/T) for the selected C-C bonds in molecules **12-18**, obtained with the B3LYP/def2-SVP and α -MNDO methods. The Average Absolute Error (AAE) for molecules from the test set (**16-18**) calculated relative to the corresponding B3LYP/def2-SVP was found to be 1.6 nA/T.

Comp.	bond	B3LYP	α -MNDO	Comp.	bond	B3LYP	α -MNDO
12	<i>a</i>	13.9	15.0	15	<i>a</i>	14.6	15.2
	<i>b</i>	7.6	5.3		<i>b</i>	9.9	7.2
	<i>c</i>	8.3	6.4		<i>c</i>	15.7	15.1
	<i>d</i>	15.3	14.7		<i>d</i>	-0.3	-0.3
	<i>e</i>	11.6	14.6		<i>e</i>	11.9	10.2
13	<i>a</i>	15.3	13.1		<i>f</i>	10.0	7.3
	<i>b</i>	8.1	5.8		<i>g</i>	7.8	6.0
	<i>c</i>	13.8	14.8		<i>h</i>	13.8	15.1
	<i>d</i>	7.2	5.0		<i>i</i>	13.1	12.0
	<i>e</i>	6.7	8.2		<i>j</i>	7.7	6.1
	<i>f</i>	7.2	5.3		<i>k</i>	13.8	15.1
14	<i>g</i>	11.5	14.5		<i>l</i>	7.9	6.0
	<i>a</i>	13.8	15.1		<i>m</i>	14.5	15.2
	<i>b</i>	7.8	6.0		<i>n</i>	9.3	6.5
	<i>c</i>	12.6	11.7				
16	<i>a</i>	14.6	15.2	17	<i>a</i>	16.4	15.5
	<i>b</i>	15.7	15.2		<i>b</i>	8.1	6.2
	<i>c</i>	9.9	7.1		<i>c</i>	15.2	15.2
	<i>d</i>	9.5	9.3		<i>d</i>	10.6	7.1
	<i>e</i>	7.8	5.9		<i>e</i>	14.6	10.9
	<i>f</i>	13.8	15.2		<i>f</i>	15.8	12.7
	<i>g</i>	10.0	7.4		<i>g</i>	4.7	2.2
	<i>h</i>	8.6	10.2		<i>h</i>	10.0	10.9
	<i>i</i>	7.7	6.2	18	<i>a</i>	16.3	15.8
	<i>j</i>	12.0	10.2		<i>b</i>	10.9	7.8
	<i>k</i>	9.3	6.5		<i>c</i>	17.8	15.8
	<i>l</i>	7.9	5.9		<i>d</i>	1.9	0.6
	<i>m</i>	13.8	15.2		<i>e</i>	14.8	12.4
	<i>n</i>	14.5	15.2		<i>f</i>	5.0	2.2
	<i>o</i>	15.4	15.2		<i>g</i>	11.7	11.2
	<i>p</i>	12.1	11.8				
	<i>q</i>	12.0	10.2				
	<i>r</i>	-0.5	-0.3				
	<i>s</i>	10.0	7.4				
	<i>t</i>	10.1	7.4				
	<i>u</i>	15.7	15.2				

Table S3. Total current density strengths (in nA/T) for the selected C-C bonds in molecules from the test set (**19-22**), obtained with the B3LYP/def2-SVP and α -MNDO methods.

Comp.	bond	B3LYP	α -MNDO
19	<i>a</i>	11.0	11.4
	<i>b</i>	8.5	3.2
	<i>c</i>	-11.4	-7.0
	<i>d</i>	-14.3	-12.9
20	<i>a</i>	4.9	12.0
	<i>b</i>	-13.0	-7.9
21	<i>a</i>	12.1	11.2
	<i>b</i>	10.9	6.6
	<i>c</i>	-12.9	-9.1
	<i>d</i>	-14.5	-12.7
22	<i>a</i>	13.8	8.0
	<i>b</i>	10.8	7.9
	<i>c</i>	25.0	19.3

Table S4. Cartesian coordinates of the optimized geometries for studied molecules at the B3LYP/def2svp level of theory.

1			
C	-1.03032800	-0.93461600	0.00000100
C	0.29436000	-1.35951100	0.00000600
C	1.32462200	-0.42492800	0.00000100
C	1.03028700	0.93466000	0.00000100
C	-0.29430200	1.35952400	0.00000200
C	-1.32464000	0.42487100	-0.00000500
H	-1.83222500	-1.66239800	-0.00000900
H	0.52345600	-2.41792700	-0.00000500
H	2.35583600	-0.75553600	-0.00002400
H	1.83228000	1.66233600	-0.00000200
H	-0.52353300	2.41791000	0.00000300
H	-2.35581100	0.75561500	0.00000300
2			
C	2.43821900	-0.70930300	-0.00000200
C	1.24722400	-1.40455400	0.00000500
C	0.00001200	-0.71815100	-0.00000100
C	-0.00001400	0.71814700	0.00000100
C	1.24720900	1.40455500	0.00000500
C	2.43820700	0.70931800	-0.00000300
H	-1.24536000	-2.49822200	0.00000700
H	3.38835500	-1.24966500	-0.00000600
H	1.24538500	-2.49821300	0.00000300
C	-1.24721500	-1.40456200	0.00000000
C	-1.24722500	1.40456200	-0.00000100
H	1.24536600	2.49821600	0.00000100
H	3.38834100	1.24968300	-0.00000700
C	-2.43821500	0.70930400	0.00000100
C	-2.43820400	-0.70931500	-0.00000400
H	-1.24537000	2.49821800	0.00000400
H	-3.38836300	1.24964700	0.00000000
H	-3.38834200	-1.24967400	-0.00000200
3			
C	3.66769700	0.71389200	-0.00002000
C	2.48423500	1.40900600	0.00005400
C	1.22639600	0.72369900	0.00001900
C	1.22639600	-0.72369900	0.00002600
C	2.48423600	-1.40900600	-0.00002300
C	3.66769800	-0.71388900	-0.00006400
C	0.00000000	1.40554300	0.00002300
C	0.00000100	-1.40554500	0.00003100
C	-1.22639500	-0.72370100	0.00002400
C	-1.22639600	0.72369800	0.00000300
C	-2.48423500	1.40900700	-0.00002400
H	-2.48304600	2.50252800	-0.00006000
C	-3.66769700	0.71389100	-0.00006200

C	-3.66769700	-0.71388900	-0.00000500
C	-2.48423600	-1.40900700	0.00003000
H	-0.00000600	2.49958600	0.00005900
H	4.61967200	1.25091100	-0.00005000
H	2.48304400	2.50252700	0.00011800
H	2.48304600	-2.50252700	-0.00003000
H	4.61966700	-1.25091800	-0.00013300
H	-0.00000600	-2.49958700	0.00005500
H	-4.61966900	1.25091700	-0.00009900
H	-4.61966900	-1.25091500	-0.00001900
H	-2.48305100	-2.50252800	0.00007600
4			
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C	0.00000000	-0.72694100	0.00000000
C	1.23759800	1.40843400	0.00000000
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C	-1.23759800	-1.40843400	0.00000000
C	2.45526200	0.72683100	0.00000000
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5			
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C	-1.42595100	0.86882900	0.00000000
C	-2.84303900	0.87948000	0.00000000
C	3.56676500	-0.29915300	0.00000000

C	0.72980300	-0.37943200	0.00000000
C	-0.72980300	-0.37943200	0.00000000
C	-3.56676500	-0.29915300	0.00000000
C	2.88572900	-1.53315100	0.00000000
C	1.50082400	-1.56831600	0.00000000
C	-1.50082400	-1.56831600	0.00000000
C	-2.88572900	-1.53315100	0.00000000
H	1.23573600	3.04050700	0.00000000
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H	3.35902700	1.84364900	0.00000000
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H	4.65936600	-0.27597800	0.00000000
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H	3.45163100	-2.46818800	0.00000000
H	1.00256100	-2.53850300	0.00000000
H	-1.00256100	-2.53850300	0.00000000
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6

C	0.71463500	0.00000000	0.00000000
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C	1.43172200	1.23827300	0.00000000
C	1.43172200	-1.23827300	0.00000000
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C	0.68208200	2.46760100	0.00000000
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C	-0.68208200	-2.46760100	0.00000000
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C	3.53029800	0.00000000	0.00000000
C	-3.53029800	0.00000000	0.00000000
H	1.23400400	3.41160100	0.00000000
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H	-3.38804500	2.15769100	0.00000000
H	4.62331500	0.00000000	0.00000000
H	-4.62331500	0.00000000	0.00000000

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C	0.43077600	0.56451300	-0.00000600
C	-0.43077500	-0.56451300	-0.00000800
C	1.87368100	0.37677500	0.00001100
C	-1.87368100	-0.37677500	-0.00000900
C	2.40688800	-0.95034400	0.00000500

C	-2.40688900	0.95034500	-0.00002300
C	-0.15185000	1.87383000	-0.00002300
C	0.15184900	-1.87382800	-0.00001600
C	-1.50571200	2.05957200	-0.00003400
C	1.50571200	-2.05957200	-0.00001300
C	2.79670300	1.45647000	0.00003500
C	-2.79670200	-1.45647000	0.00000500
C	3.81204100	-1.14654800	0.00001800
C	-3.81204100	1.14654700	-0.00002400
C	4.16341300	1.24036900	0.00004800
C	-4.16341300	-1.24036900	0.00000400
C	4.68086300	-0.07290800	0.00003800
C	-4.68086300	0.07290600	-0.00001200
H	0.49537800	2.75054200	-0.00003500
H	-0.49537800	-2.75054100	-0.00003100
H	-1.92087000	3.07104900	-0.00005200
H	1.92086900	-3.07104900	-0.00002300
H	2.43386100	2.48433200	0.00004800
H	-2.43386100	-2.48433100	0.00002100
H	4.19659600	-2.17023200	0.00001200
H	-4.19659700	2.17023000	-0.00003400
H	4.84593100	2.09402900	0.00006600
H	-4.84592900	-2.09403100	0.00001600
H	5.76144600	-0.23599800	0.00004700
H	-5.76144600	0.23599800	-0.00001300

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C	0.34451400	-0.05922100	0.00000400
C	-0.06187300	1.32750700	0.00002400
C	1.77693900	-0.37818700	0.00000400
C	-2.02647900	-0.71740800	-0.00002100
C	-2.42481900	0.66679000	0.00000300
C	2.72758000	0.68620200	0.00001400
C	-0.65257500	-1.03608100	-0.00001900
C	-1.42019600	1.65260500	0.00002500
C	0.94588000	2.35966300	0.00003900
C	2.27002700	2.05513900	0.00003100
C	2.26751800	-1.70390500	-0.00000400
C	4.11003300	0.38869800	0.00001300
C	-3.04134600	-1.72279700	-0.00004600
C	-3.81795900	0.98285500	0.00000000
C	3.62909100	-1.97467300	-0.00000200
C	4.56130800	-0.92166700	0.00000400
C	-4.37386700	-1.38173900	-0.00004500
C	-4.76667700	-0.01283700	-0.00002100
H	-0.38387800	-2.09375700	-0.00004100
H	-1.71204700	2.70696200	0.00004000
H	0.61605100	3.40208000	0.00005500
H	3.02109600	2.84973100	0.00004000
H	1.56926800	-2.54184300	-0.00000700
H	4.82409600	1.21697300	0.00002100
H	-2.73874400	-2.77375100	-0.00006500

H	-4.11758100	2.03457600	0.00001800
H	3.97506700	-3.01135200	-0.00000600
H	5.63292000	-1.13582600	0.00000500
H	-5.13939700	-2.16175800	-0.00006100
H	-5.82944900	0.24229600	-0.00002100
9			
C	-3.56308500	1.24445900	0.00000000
C	-2.86119500	0.04973500	0.00000100
C	-1.44616700	0.01235000	0.00000000
C	-0.73505100	1.24548000	0.00000000
C	-1.47647700	2.45132400	-0.00000100
C	-2.86207400	2.46007000	-0.00000100
C	-0.71111500	-1.25923900	0.00000000
C	0.73369100	1.24628200	0.00000000
C	1.44615200	0.01392900	0.00000000
C	0.71249000	-1.25846200	0.00000000
C	2.86113900	0.05286000	0.00000000
H	3.42918200	-0.87669700	0.00000100
C	3.56172400	1.24834900	0.00000100
C	2.85938500	2.46319400	0.00000000
C	1.47379900	2.45293500	0.00000000
H	-4.65580800	1.23563800	0.00000000
H	-3.42822300	-0.88044000	0.00000100
H	-0.95577500	3.40819800	-0.00000100
H	-3.40181700	3.41023900	-0.00000100
H	4.65445500	1.24072100	0.00000100
H	3.39809100	3.41395200	0.00000100
H	0.95205300	3.40923900	0.00000000
C	1.38749800	-2.50269400	-0.00000100
H	2.47655800	-2.52841000	-0.00000200
C	0.70367500	-3.70782200	-0.00000100
H	1.25751900	-4.64983200	-0.00000100
C	-0.69962500	-3.70858900	0.00000000
H	-1.25244000	-4.65120300	0.00000100
C	-1.38476400	-2.50420800	0.00000100
H	-2.47379500	-2.53111400	0.00000100
10			
C	0.00020400	-3.54041700	-0.00000200
C	-1.20503400	-2.84707500	-0.00000200
C	-1.23690400	-1.44225400	-0.00000100
C	0.00002700	-0.72455700	0.00000000
C	1.23701800	-1.44213100	-0.00000100
C	1.20535300	-2.84694000	-0.00000200
C	-2.50986400	-0.71030500	0.00000000
C	-0.00002500	0.72455900	0.00000000
C	-1.23701600	1.44213400	-0.00000100
C	-2.50989300	0.71012300	0.00000000
C	-1.20535600	2.84693800	-0.00000100
H	-2.13241100	3.41816500	-0.00000200
C	-0.00020500	3.54041900	-0.00000200

C	1.20503000	2.84708100	-0.00000100
C	1.23690500	1.44225600	-0.00000100
C	2.50986300	0.71030300	0.00000000
C	2.50988800	-0.71011800	0.00000000
H	0.00027100	-4.63316500	-0.00000300
H	-2.13198400	-3.41845100	-0.00000200
H	2.13240800	-3.41816800	-0.00000200
H	-0.00027900	4.63316700	-0.00000200
H	2.13198000	3.41845700	-0.00000200
C	-3.75406500	1.38590500	0.00000100
C	-4.95861100	0.70161700	0.00000200
H	-5.90085000	1.25513600	0.00000300
C	-4.95861200	-0.70174700	0.00000200
H	-5.90085900	-1.25525300	0.00000300
C	-3.75407200	-1.38605600	0.00000100
C	3.75408100	1.38605500	0.00000100
C	4.95861200	0.70174700	0.00000200
H	5.90086800	1.25523800	0.00000300
C	4.95860800	-0.70162600	0.00000200
H	5.90085300	-1.25513400	0.00000200
C	3.75406900	-1.38590800	0.00000100
H	3.78096600	-2.47480400	0.00000100
H	3.78103800	2.47493800	0.00000100
H	-3.78097700	2.47480200	0.00000100
H	-3.78103600	-2.47494000	0.00000200

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C	0.00000000	1.42999200	0.00000000
C	1.23841000	0.71499600	0.00000000
C	1.23841000	-0.71499600	0.00000000
C	0.00000000	-1.42999200	0.00000000
C	-1.23841000	-0.71499600	0.00000000
C	-1.23841000	0.71499600	0.00000000
C	0.00000000	2.85399400	0.00000000
C	2.47163100	1.42699700	0.00000000
C	2.47163100	-1.42699700	0.00000000
C	0.00000000	-2.85399400	0.00000000
C	-2.47163100	-1.42699700	0.00000000
C	-2.47163100	1.42699700	0.00000000
C	1.25033900	3.54044300	0.00000000
C	2.44094400	2.85304700	0.00000000
C	3.69128400	0.68739600	0.00000000
C	3.69128400	-0.68739600	0.00000000
C	2.44094400	-2.85304700	0.00000000
C	1.25033900	-3.54044300	0.00000000
C	-1.25033900	-3.54044300	0.00000000
C	-2.44094400	-2.85304700	0.00000000
C	-3.69128400	-0.68739600	0.00000000
C	-3.69128400	0.68739600	0.00000000
C	-2.44094400	2.85304700	0.00000000
C	-1.25033900	3.54044300	0.00000000
H	1.24767100	4.63386400	0.00000000

H	3.38920800	3.39744700	0.00000000
H	4.63687900	1.23641700	0.00000000
H	4.63687900	-1.23641700	0.00000000
H	3.38920800	-3.39744700	0.00000000
H	1.24767100	-4.63386400	0.00000000
H	-1.24767100	-4.63386400	0.00000000
H	-3.38920800	-3.39744700	0.00000000
H	-4.63687900	-1.23641700	0.00000000
H	-4.63687900	1.23641700	0.00000000
H	-3.38920800	3.39744700	0.00000000
H	-1.24767100	4.63386400	0.00000000

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C	3.55118600	2.24704900	0.00000500
C	2.87594800	1.01456500	0.00000200
C	1.44494000	1.01221100	0.00000100
C	0.73394900	2.25040700	0.00000100
C	1.46354600	3.45130900	0.00000400
C	2.85405600	3.44965300	0.00000600
C	0.71849100	-0.24006000	0.00000000
C	-0.73411700	2.25029300	-0.00000100
C	-1.44501000	1.01197400	-0.00000100
C	-0.71827500	-0.24013200	0.00000000
C	-2.87596000	1.01441400	-0.00000200
C	-3.55140700	2.24671500	-0.00000500
C	-2.85429500	3.44941000	-0.00000600
C	-1.46384600	3.45113200	-0.00000400
H	4.63966200	2.27722400	0.00000600
H	0.94727300	4.40981600	0.00000500
H	3.40002400	4.39614000	0.00000800
H	-4.63983500	2.27686200	-0.00000600
H	-3.40020300	4.39594300	-0.00000900
H	-0.94769500	4.40970600	-0.00000600
C	-1.43124700	-1.46942000	0.00000000
C	-0.68914300	-2.66837700	0.00000000
H	-1.20024500	-3.62987500	0.00000000
C	0.68935900	-2.66839200	-0.00000100
H	1.20023200	-3.62994300	-0.00000100
C	1.43139000	-1.46936700	-0.00000100
C	3.61129400	-0.25428700	0.00000000
C	2.89575200	-1.48166100	-0.00000100
C	5.02641800	-0.29644700	0.00000000
C	5.72190800	-1.49451400	-0.00000200
H	6.81459500	-1.49113800	-0.00000200
C	3.62993700	-2.69298800	-0.00000300
C	5.01492100	-2.70748600	-0.00000400
H	5.55060500	-3.65987800	-0.00000600
H	3.10498900	-3.64731500	-0.00000500
H	5.59801200	0.63086700	0.00000100
C	-3.61138800	-0.25454400	0.00000000
C	-2.89546300	-1.48167700	0.00000100
C	-3.62985100	-2.69303200	0.00000300

H	-3.10486900	-3.64740500	0.00000400
C	-5.01480200	-2.70749000	0.00000400
H	-5.55042500	-3.65992100	0.00000500
C	-5.72188800	-1.49456100	0.00000300
H	-6.81457100	-1.49125800	0.00000400
C	-5.02635400	-0.29647900	0.00000100
H	-5.59784500	0.63085500	0.00000100

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C	-2.50981600	3.54210900	0.00019100
C	-3.71357100	2.84757200	0.00008400
C	-3.74367800	1.44197100	-0.00003800
C	-2.50663600	0.72559300	0.00004800
C	-1.27073900	1.44512100	0.00008700
C	-1.30391500	2.84898300	0.00015900
C	-5.01660800	0.71018800	-0.00020700
C	-2.50664000	-0.72557600	0.00015700
C	-3.74368500	-1.44194700	0.00025400
C	-5.01660400	-0.71017200	0.00009300
C	-3.71359800	-2.84754600	0.00045200
H	-4.64133600	-3.41752500	0.00049900
C	-2.50985000	-3.54209400	0.00056300
C	-1.30394200	-2.84897900	0.00045800
C	-1.27074900	-1.44511500	0.00023800
C	0.00241800	-0.71142700	0.00009000
C	0.00242100	0.71142500	0.00004000
H	-2.51053700	4.63479200	0.00031100
H	-4.64129800	3.41756500	0.00016900
H	-0.37782200	3.42201900	0.00022500
H	-2.51058300	-4.63477700	0.00072700
H	-0.37785800	-3.42202800	0.00056200
C	-6.26080700	-1.38599500	0.00018100
C	-7.46531100	-0.70171400	-0.00015000
H	-8.40751600	-1.25523100	-0.00005300
C	-7.46532000	0.70168900	-0.00063100
H	-8.40753300	1.25519200	-0.00100300
C	-6.26082600	1.38598900	-0.00065000
C	1.23907100	-1.37188300	0.00001200
C	2.47586800	-0.71300800	-0.00012000
C	2.47587100	0.71300200	-0.00012900
C	1.23907500	1.37187800	-0.00004800
H	1.23956900	2.45701100	-0.00002600
H	1.23956100	-2.45701700	0.00007100
H	-6.28795700	-2.47484400	0.00052700
H	-6.28799900	2.47483500	-0.00108500
C	3.74809000	-1.44935900	-0.00021700
C	3.74809400	1.44935300	-0.00010900
C	4.97939700	-0.73560100	0.00001600
C	4.97939900	0.73559200	0.00017800
C	3.78805600	-2.86338400	-0.00056000
C	4.98420800	-3.56385300	-0.00060500
H	4.97699200	-4.65656600	-0.00087800

C	6.19778000	-2.86075500	-0.00033100
H	7.14919600	-3.39825700	-0.00037800
C	6.18591400	-1.47447100	-0.00004500
H	7.14200200	-0.95244400	0.00009300
H	2.85939100	-3.43323100	-0.00083700
C	3.78806400	2.86337800	-0.00029300
C	4.98421700	3.56384400	-0.00004600
H	4.97700600	4.65655700	-0.00020600
C	6.19778700	2.86074400	0.00042300
H	7.14920400	3.39824400	0.00069900
C	6.18591800	1.47446000	0.00051600
H	7.14200700	0.95243200	0.00086800
H	2.85940000	3.43322500	-0.00065900

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C	1.47063000	-3.50527600	0.00979100
C	0.19341200	-2.86877900	-0.00067600
C	0.09594000	-1.42258500	0.00007100
C	1.28000600	-0.62817600	0.00194000
C	2.58128800	-1.26680300	0.01069800
C	2.68589100	-2.68988600	0.02166600
C	-1.18410300	-0.79438200	-0.00153700
C	1.18410300	0.79438200	-0.00153700
C	-0.09594000	1.42258500	0.00007200
C	-1.28000600	0.62817600	0.00194000
C	-0.19341200	2.86877900	-0.00067600
C	0.98671900	3.67107100	-0.01226600
C	2.30051100	3.02624300	-0.02152200
C	2.38780000	1.60195500	-0.00969700
C	3.67270500	0.98099600	-0.00938300
C	3.77119000	-0.47901700	0.01189800
C	-0.98671900	-3.67107100	-0.01226500
C	-2.30051100	-3.02624300	-0.02152200
C	-2.38780000	-1.60195500	-0.00969700
C	-3.67270500	-0.98099600	-0.00938300
C	-3.77119000	0.47901700	0.01189900
C	-2.58128800	1.26680300	0.01069800
C	-1.47063000	3.50527600	0.00979000
C	-2.68589100	2.68988600	0.02166700
C	3.48310000	3.78497700	-0.04129400
C	4.73071000	3.17345100	-0.04733100
H	5.63792600	3.78210600	-0.06525600
C	4.82341100	1.78726800	-0.03054200
C	0.86353500	5.07085000	-0.01294900
C	-1.53673700	4.90893400	0.00702500
C	-0.38345300	5.68371800	-0.00394600
H	-0.45694500	6.77388600	-0.00554800
C	-3.95958500	3.28307900	0.04304100
C	-5.01973000	1.12356100	0.03429400
C	-5.11384000	2.50966000	0.05098800
H	-6.09453300	2.99100500	0.07017200
C	-4.82341100	-1.78726800	-0.03054400

C	-3.48310000	-3.78497700	-0.04129600
C	-4.73071000	-3.17345100	-0.04733300
H	-5.63792600	-3.78210600	-0.06526000
C	-0.86353500	-5.07085000	-0.01294800
C	1.53673700	-4.90893400	0.00702600
C	0.38345300	-5.68371800	-0.00394300
H	0.45694400	-6.77388600	-0.00554400
C	3.95958500	-3.28307900	0.04303800
C	5.01973000	-1.12356100	0.03429200
C	5.11384000	-2.50966000	0.05098500
H	6.09453300	-2.99100500	0.07016700
H	5.81297900	1.33390300	-0.03660700
H	5.93966100	-0.54160000	0.04152800
H	3.43935900	4.87254600	-0.05389600
H	1.75062600	5.70167100	-0.02002600
H	-2.50074900	5.41455000	0.01236600
H	-4.06194100	4.36672900	0.05567300
H	-5.93966100	0.54160000	0.04153100
H	-5.81297900	-1.33390300	-0.03660900
H	-3.43935900	-4.87254600	-0.05389900
H	-1.75062600	-5.70167100	-0.02002400
H	2.50074900	-5.41455000	0.01236800
H	4.06194100	-4.36673000	0.05566900

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C	2.17309600	1.41407800	0.00012400
C	3.52894700	1.88015300	0.00018500
C	4.62383500	0.93635600	0.00011700
C	4.35210000	-0.46031900	0.00002700
C	2.98352800	-0.92502200	0.00002300
C	1.90089500	-0.00069500	0.00007900
C	5.97226100	1.40175900	0.00015100
C	5.42788900	-1.39670500	-0.00007500
C	6.77559600	-0.93282600	-0.00008200
C	7.04829000	0.46654700	0.00002700
C	7.86904400	-1.88381700	-0.00027000
C	7.60395700	-3.28610500	-0.00038500
C	6.21966100	-3.76176000	-0.00020100
C	5.14935700	-2.81778700	-0.00012700
C	3.80123300	-3.28649900	-0.00009300
C	2.70170100	-2.32047700	-0.00002700
C	3.79414200	3.27399900	0.00029500
C	5.16922700	3.75939600	0.00043900
C	6.24589800	2.82164100	0.00032500
C	7.59112300	3.29849500	0.00042900
C	8.69692000	2.33948700	0.00018000
C	8.41755100	0.93955300	0.00001600
C	9.22107000	-1.42713600	-0.00038000
C	9.50047300	0.00998000	-0.00018700
C	5.92102800	-5.13471700	-0.00010000
C	4.60623500	-5.58479400	-0.00006500
H	4.39564400	-6.65689300	-0.00001100

C	3.55968600	-4.67101900	-0.00009800
C	8.68267400	-4.18661300	-0.00071400
C	10.26200200	-2.37110100	-0.00069000
C	9.99677300	-3.73517200	-0.00087000
H	10.82118300	-4.45220900	-0.00114300
C	10.81897800	0.49569900	-0.00019800
C	10.03423400	2.77068500	0.00008100
C	11.08374400	1.85997700	-0.00008700
H	12.11664200	2.21626200	-0.00013700
C	7.82466200	4.68352100	0.00076400
C	5.45987000	5.13593300	0.00070800
C	6.77154600	5.59209500	0.00089800
H	6.97674400	6.66528700	0.00115700
C	2.70078500	4.16523500	0.00027300
C	1.09469800	2.33837300	0.00011900
C	1.39927400	3.71506300	0.00017900
H	0.60189400	4.45660700	0.00016500
C	0.54881300	-0.46342700	0.00008600
C	1.36970300	-2.74155900	0.00000000
C	0.28510300	-1.85982700	0.00008200
H	2.54076800	-5.05403300	-0.00011300
H	1.16640100	-3.80637800	-0.00005600
H	6.72131300	-5.87261400	-0.00002100
H	8.50346900	-5.26028400	-0.00089300
H	11.30067900	-2.04539500	-0.00082600
H	11.66023100	-0.19515400	-0.00029600
H	10.26938300	3.83360100	0.00011400
H	8.84229900	5.07015700	0.00095100
H	4.65508500	5.86904900	0.00079700
H	2.86989500	5.24057400	0.00032400
C	-9.22107200	1.42713100	-0.00021300
C	-7.86904700	1.88381500	-0.00025500
C	-6.77559700	0.93282500	-0.00014500
C	-7.04828900	-0.46654900	-0.00002100
C	-8.41755000	-0.93955700	0.00002100
C	-9.50047300	-0.00998600	-0.00006800
C	-5.42789100	1.39670500	-0.00014800
C	-5.97226000	-1.40176000	0.00009500
C	-4.62383400	-0.93635400	0.00007500
C	-4.35210100	0.46032200	-0.00003100
C	-3.52894500	-1.88015000	0.00016000
C	-3.79413700	-3.27399700	0.00027500
C	-5.16922200	-3.75939500	0.00033900
C	-6.24589400	-2.82164200	0.00022000
C	-7.59111800	-3.29849800	0.00023000
C	-8.69691600	-2.33949100	0.00017300
C	-7.60396100	3.28610300	-0.00038400
C	-6.21966600	3.76176000	-0.00044700
C	-5.14936100	2.81778800	-0.00027600
C	-3.80123800	3.28650200	-0.00025100
C	-2.70170300	2.32048100	-0.00009700

C	-2.98352900	0.92502500	-0.00002700
C	-2.17309500	-1.41407200	0.00011200
C	-1.90089600	0.00070200	0.00004700
C	-5.45986300	-5.13593200	0.00050000
C	-6.77153900	-5.59209600	0.00045600
H	-6.97673400	-6.66528900	0.00054400
C	-7.82465500	-4.68352500	0.00029800
C	-2.70077900	-4.16523100	0.00031700
C	-1.09469700	-2.33836600	0.00015100
C	-1.39926800	-3.71505600	0.00026200
H	-0.60188500	-4.45659700	0.00031300
C	-0.54881300	0.46343500	0.00006700
C	-1.36970700	2.74156400	-0.00004100
C	-0.28510200	1.85983400	0.00004900
C	-3.55969200	4.67102200	-0.00039600
C	-5.92103500	5.13471700	-0.00066300
C	-4.60624300	5.58479500	-0.00062300
H	-4.39565300	6.65689500	-0.00077400
C	-8.68268000	4.18660900	-0.00042800
C	-10.26200600	2.37109500	-0.00029900
C	-9.99677800	3.73516600	-0.00039400
H	-10.82119000	4.45220200	-0.00043500
C	-10.81897700	-0.49570700	0.00000400
C	-10.03423000	-2.77069100	0.00028600
C	-11.08374100	-1.85998500	0.00019200
H	-12.11663900	-2.21627100	0.00027300
H	-8.84229200	-5.07016100	0.00022100
H	-10.26937700	-3.83360800	0.00047100
H	-4.65507700	-5.86904800	0.00066600
H	-2.86988500	-5.24057000	0.00038000
H	-1.16640700	3.80638300	-0.00008200
H	-2.54077500	5.05403700	-0.00034500
H	-6.72132100	5.87261300	-0.00088000
H	-8.50347700	5.26028000	-0.00046900
H	-11.30068200	2.04538800	-0.00027800
H	-11.66023200	0.19514500	-0.00007400

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C	7.87145500	1.41577600	-0.00007200
C	9.22756300	1.88121500	-0.00020000
C	10.32211400	0.93695100	-0.00019300
C	10.04990500	-0.45961100	-0.00014600
C	8.68119300	-0.92372400	-0.00005700
C	7.59889800	0.00104200	0.00002800
C	11.67075300	1.40173600	-0.00021600
C	11.12526300	-1.39650700	-0.00019400
C	12.47315200	-0.93323900	-0.00021100
C	12.74639800	0.46603300	-0.00020300
C	13.56617100	-1.88473500	-0.00031700
C	13.30049500	-3.28690200	-0.00043400
C	11.91602400	-3.76193600	-0.00027200
C	10.84617500	-2.81747500	-0.00020200

C	9.49791700	-3.28562700	-0.00014900
C	8.39890800	-2.31909400	-0.00003200
C	9.49341000	3.27495800	-0.00034300
C	10.86875000	3.75972800	-0.00039300
C	11.94501400	2.82148100	-0.00027100
C	13.29047200	3.29768600	-0.00019800
C	14.39586200	2.33820000	-0.00005500
C	14.11587700	0.93839900	-0.00012900
C	14.91838000	-1.42866600	-0.00035700
C	15.19837600	0.00832400	-0.00009900
C	11.61675400	-5.13475200	-0.00018100
C	10.30177500	-5.58426900	-0.00016500
H	10.09069100	-6.65626500	-0.00013400
C	9.25566700	-4.67001700	-0.00018400
C	14.37877400	-4.18791300	-0.00073900
C	15.95888900	-2.37310500	-0.00068000
C	15.69306600	-3.73706000	-0.00088300
H	16.51714500	-4.45447000	-0.00116700
C	16.51709200	0.49343600	0.00018900
C	15.73337600	2.76878500	0.00015800
C	16.78246700	1.85759200	0.00031800
H	17.81552900	2.21338800	0.00054500
C	13.52462900	4.68260200	-0.00028300
C	11.16004000	5.13613100	-0.00052400
C	12.47194000	5.59166800	-0.00046700
H	12.67767100	6.66475300	-0.00055900
C	8.40041500	4.16668900	-0.00040100
C	6.79335100	2.34061900	-0.00006000
C	7.09866000	3.71717300	-0.00027000
H	6.30165400	4.45913600	-0.00033300
C	6.24674500	-0.46128200	0.00016800
C	7.06684800	-2.73976300	0.00011100
C	5.98260600	-1.85773400	0.00023100
H	8.23659400	-5.05260700	-0.00022300
H	6.86317600	-3.80449800	0.00013800
H	12.41669500	-5.87301300	-0.00010200
H	14.19907600	-5.26150000	-0.00091700
H	16.99771500	-2.04789100	-0.00083400
H	17.35802800	-0.19780000	0.00035400
H	15.96905800	3.83158100	0.00022600
H	14.54244500	5.06876900	-0.00021600
H	10.35563700	5.86966600	-0.00067600
H	8.57006300	5.24194300	-0.00053200
C	-3.52501900	1.41170400	0.00031200
C	-2.16930700	1.87805400	0.00042800
C	-1.07531500	0.93393500	0.00043800
C	-1.34812900	-0.46233500	0.00036500
C	-2.71548800	-0.92790000	0.00027800
C	-3.79775400	-0.00321900	0.00025500
C	0.27274500	1.39875800	0.00051900
C	-0.27274600	-1.39874800	0.00039300

C	1.07531500	-0.93392500	0.00044600
C	1.34812900	0.46234500	0.00049100
C	2.16930700	-1.87804400	0.00043700
C	1.90272700	-3.27163100	0.00047100
C	0.52690200	-3.75578400	0.00043400
C	-0.54867600	-2.81664900	0.00034700
C	-1.89588800	-3.28913100	0.00019900
C	-2.99658300	-2.32398800	0.00021500
C	-1.90272700	3.27163900	0.00053500
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C	1.89588800	3.28914200	0.00079800
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C	2.71548800	0.92791000	0.00046900
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C	3.79775300	0.00323000	0.00034500
C	0.23347200	-5.13150800	0.00042500
C	-1.07965200	-5.58439300	0.00019700
H	-1.28724500	-6.65708600	0.00012400
C	-2.13116300	-4.67401400	0.00004900
C	2.99582700	-4.16323000	0.00049500
C	4.60285900	-2.33636600	0.00034200
C	4.29749800	-3.71308800	0.00044600
H	5.09467600	-4.45484300	0.00047200
C	5.14954600	0.46610800	0.00021400
C	4.32859000	2.74506600	0.00032900
C	5.41324600	1.86281300	0.00014200
C	2.13116200	4.67402400	0.00115600
C	-0.23347200	5.13151800	0.00094400
C	1.07965100	5.58440300	0.00121400
H	1.28724400	6.65709600	0.00147300
C	-2.99582900	4.16324000	0.00047600
C	-4.60286300	2.33637400	0.00024300
C	-4.29749800	3.71309900	0.00031900
H	-5.09467400	4.45485500	0.00026300
C	-5.14954500	-0.46609900	0.00017000
C	-4.32859000	-2.74505600	0.00019500
C	-5.41324500	-1.86280300	0.00016700
H	-3.14857100	-5.06140700	-0.00020400
H	-4.53155300	-3.81012000	0.00021400
H	1.03657500	-5.86651200	0.00058900
H	2.82639200	-5.23857200	0.00052600
H	4.53155200	3.81012900	0.00027200
H	3.14857000	5.06141800	0.00143100
H	-1.03657600	5.86652100	0.00094000
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C	-9.49340200	-3.27495700	-0.00015400
C	-10.86874100	-3.75973200	-0.00033600
C	-11.94500700	-2.82148700	-0.00022000
C	-13.29046500	-3.29769600	-0.00024900
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C	-13.30050200	3.28689300	-0.00050000
C	-11.91603300	3.76192900	-0.00071100
C	-10.84618100	2.81747200	-0.00050200
C	-9.49792500	3.28562700	-0.00056200
C	-8.39891200	2.31909600	-0.00026900
C	-8.68119500	0.92372500	-0.00018100
C	-7.87145200	-1.41577200	-0.00001800
C	-7.59889800	-0.00103700	-0.00004200
C	-11.16002700	-5.13613600	-0.00065000
C	-12.47192600	-5.59167600	-0.00085300
H	-12.67765400	-6.66476100	-0.00118300
C	-13.52461700	-4.68261200	-0.00064600
C	-8.40040400	-4.16668600	-0.00000800
C	-6.79334600	-2.34061100	0.00008800
C	-7.09865100	-3.71716700	0.00012100
H	-6.30164200	-4.45912600	0.00024500
C	-6.24674600	0.46129100	0.00006200
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C	-5.98260600	1.85774100	0.00007500
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C	-15.69307400	3.73704600	-0.00035800
H	-16.51715500	4.45445400	-0.00040000
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C	-15.73337000	-2.76880100	0.00058000
C	-16.78246200	-1.85761000	0.00084600
H	-17.81552400	-2.21340800	0.00124000
H	-14.54243200	-5.06878200	-0.00085700
H	-15.96905000	-3.83159700	0.00080500
H	-10.35562200	-5.86966900	-0.00078800
H	-8.57005000	-5.24194000	0.00002600
H	-6.86318500	3.80450100	-0.00005000
H	-8.23660500	5.05260700	-0.00106400
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H	-17.35802800	0.19778000	0.00083000
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18			
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