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

Supplementary materials

Magnetically-induced current density investigation in carbohelicenes and azahelicenes

Emna CHERNI,[a,b,c] Benoît CHAMPAGNE,[c] Sameh AYADI,[b] and Vincent LIÉGEOIS[c,*]

[a] *Chemistry Department, Faculty of Sciences of Tunis, University of Tunis El Manar, B.P 248 El Manar II, 2092 Tunis, Tunisia*

[b] *Laboratory of Materials Molecules and Applications, Preparatory Institute for Scientific and Technical Studies, Carthage University, B.P:51, La Marsa, 2075 Tunis, Tunisia*

[c] *Laboratory of Theoretical Chemistry, Unit of Theoretical and Structural Physical Chemistry, Namur Institute of Structured Matter, University of Namur, Rue de Bruxelles, 61, 5000 Namur, Belgium.*

E-mail : vincent.liegeois@unamur.be

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I- Current density, NICS and BLA analysis in carbohelicenes

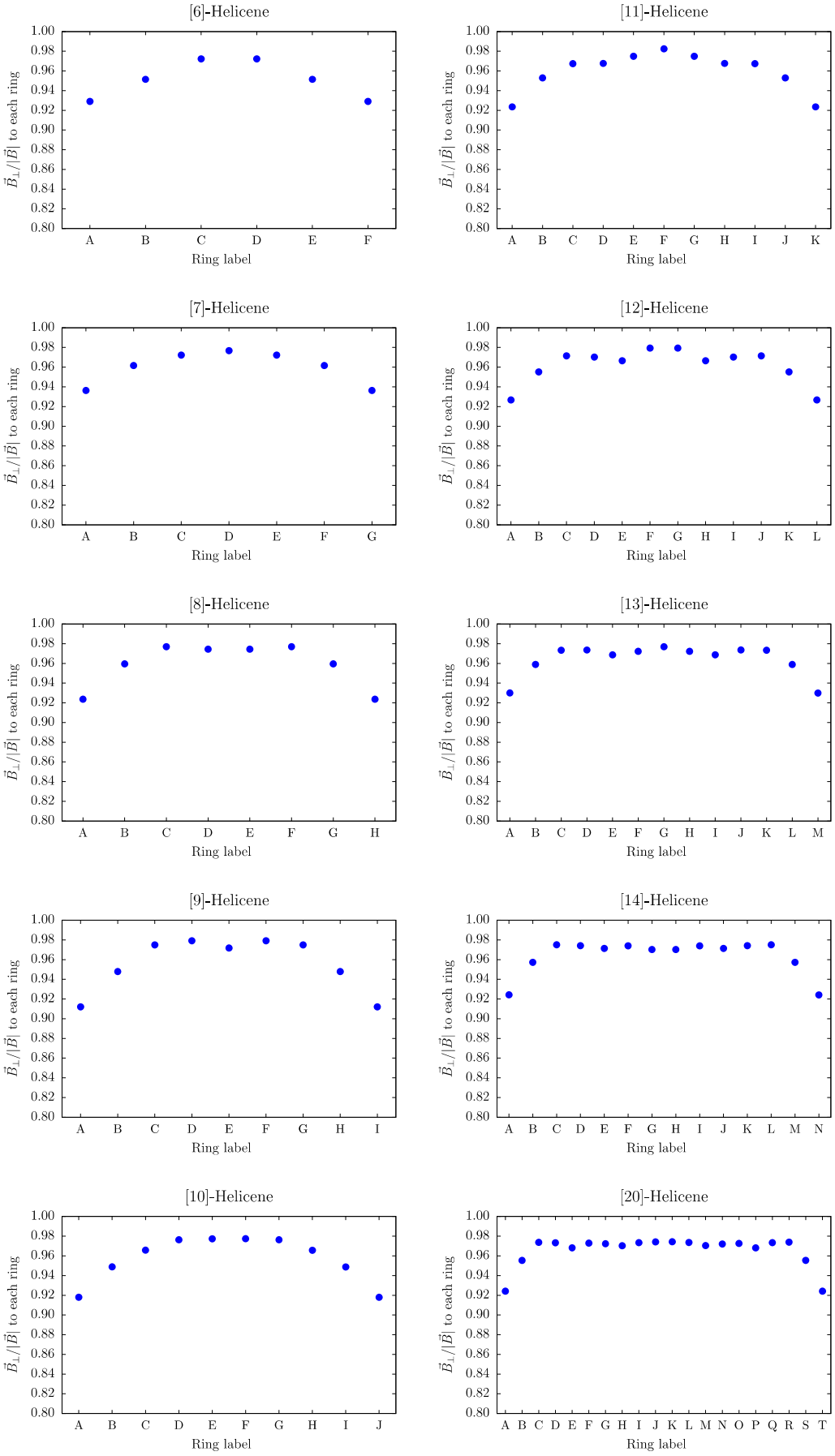
Table S1: Induced current (in nA/T), BLA, NICS(0), and $NICS_{zz}(0)$ of [n]-helicenes

Helicene	Ring	J_{middle} (nA/T)	$\bar{J}$ (nA/T)	BLA (Å)	NICS(0) (ppm)	$NICS_{zz}(0)$ (ppm)
[20]- -helicene	A	12.07	12.29	0.0195	-10.27	-21.46
	B	11.14	11.45	0.0389	-7.34	-12.05
	C	12.01	12.08	0.0334	-7.29	-12.53
	D	11.65	11.74	0.0347	-6.37	-10.81
	E	10.86	11.03	0.0356	-5.75	-8.95
	F	11.61	11.57	0.0351	-6.72	-11.39
	G	11.35	11.56	0.0356	-7.51	-13.95
	H	11.85	12.03	0.0356	-7.65	-14.68
	I	12.21	12.31	0.0359	-7.26	-14.24
	J	11.79	12.07	0.0358	-7.11	-13.54
	K	11.80	12.08	0.0358	-7.13	-13.60
	L	12.26	12.33	0.0359	-7.23	-14.21
	M	11.90	12.06	0.0357	-7.59	-14.57
	N	11.29	11.54	0.0356	-7.41	-13.91
	O	11.59	11.53	0.0351	-6.73	-11.41
	P	10.77	11.03	0.0356	-5.78	-8.85
	Q	11.61	11.71	0.0347	-6.36	-10.87
	R	11.98	12.09	0.0334	-7.30	-12.46
	S	11.25	11.50	0.0389	-7.40	-12.18
	T	12.18	12.30	0.0195	-10.33	-21.46
[14]-helicene	A	12.16	12.27	0.0199	-9.94	-20.47
	B	11.16	11.39	0.0389	-7.10	-10.91
	C	11.92	12.09	0.0335	-6.92	-10.68
	D	11.44	11.72	0.0347	-6.03	-8.85
	E	10.54	10.92	0.0362	-5.23	-6.67
	F	11.57	11.61	0.0354	-6.36	-9.32
	G	11.17	11.44	0.0359	-7.10	-11.86
	H	11.16	11.42	0.0359	-7.07	-11.82
	I	11.54	11.57	0.0354	-6.33	-9.32
	J	10.63	10.94	0.0362	-5.22	-6.62
	K	11.42	11.72	0.0347	-6.05	-8.86
	L	11.95	12.11	0.0335	-6.93	-10.68
	M	11.12	11.39	0.0389	-7.11	-10.91
	N	12.17	12.28	0.0199	-9.94	-20.44
[13]-helicene	A	12.14	12.25	0.0197	-9.89	-20.18
	B	11.13	11.53	0.0390	-6.93	-10.41
	C	11.94	12.11	0.0333	-6.84	-10.33
	D	11.45	11.70	0.0350	-5.94	-8.62
	E	10.62	10.98	0.0359	-5.25	-6.57
	F	11.32	11.42	0.0350	-6.42	-9.14
	G	10.65	10.85	0.0360	-6.69	-10.61
	H	11.32	11.42	0.0350	-6.42	-9.14
	I	10.62	10.98	0.0359	-5.25	-6.57
	J	11.44	11.70	0.0351	-5.94	-8.61

	K	11.95	12.11	0.0333	-6.84	-10.33
	L	11.14	11.53	0.0389	-6.93	-10.41
	M	12.15	12.25	0.0197	-9.89	-20.18
[12]-helicene	A	12.15	12.22	0.0200	-9.73	-19.62
	B	11.21	11.61	0.0388	-6.91	-10.25
	C	11.69	11.98	0.0336	-6.60	-9.86
	D	11.49	11.78	0.0349	-6.03	-8.82
	E	10.80	10.98	0.0359	-5.41	-6.58
	F	10.74	10.80	0.0353	-6.06	-8.07
	G	10.74	10.80	0.0353	-6.06	-8.08
	H	10.80	10.98	0.0359	-5.41	-6.58
	I	11.49	11.78	0.0349	-6.03	-8.82
	J	11.69	11.98	0.0336	-6.60	-9.86
	K	11.21	11.61	0.0388	-6.91	-10.25
	L	12.15	12.22	0.0200	-9.73	-19.62
[11]-helicene	A	12.08	12.13	0.0200	-9.52	-19.10
	B	10.99	11.39	0.0390	-6.73	-9.82
	C	11.85	12.09	0.0335	-6.69	-9.83
	D	11.42	11.67	0.0349	-6.02	-8.25
	E	10.26	10.46	0.0360	-5.05	-5.46
	F	10.85	10.79	0.0346	-5.35	-5.22
	G	10.26	10.46	0.0360	-5.06	-5.46
	H	11.43	11.68	0.0349	-6.02	-8.25
	I	11.85	12.09	0.0335	-6.69	-9.83
	J	10.98	11.39	0.0390	-6.73	-9.82
	K	12.08	12.13	0.0200	-9.52	-19.10
[10]-helicene	A	12.02	12.12	0.0200	-9.50	-18.86
	B	11.09	11.44	0.0389	-6.78	-9.82
	C	11.90	11.94	0.0333	-6.82	-9.61
	D	11.08	11.16	0.0348	-5.76	-7.06
	E	10.24	10.28	0.0353	-4.28	-2.50
	F	10.24	10.28	0.0353	-4.28	-2.50
	G	11.08	11.16	0.0348	-5.76	-7.06
	H	11.90	11.95	0.0333	-6.82	-9.61
	I	11.09	11.44	0.0389	-6.78	-9.82
	J	12.02	12.12	0.0200	-9.50	-18.86
[9]-helicene	A	12.03	12.08	0.0198	-9.57	-18.63
	B	11.14	11.39	0.0389	-6.87	-9.55
	C	11.29	11.40	0.0333	-6.41	-8.08
	D	11.09	11.11	0.0341	-5.09	-4.70
	E	9.86	9.91	0.0360	-3.43	-0.14
	F	11.09	11.13	0.0341	-5.10	-4.73
	G	11.33	11.42	0.0333	-6.42	-8.06
	H	11.11	11.41	0.0389	-6.85	-9.52
	I	12.01	12.08	0.0198	-9.56	-18.61
[8]-helicene	A	12.08	12.07	0.0208	-9.39	-18.46
	B	10.81	10.97	0.0385	-6.62	-8.49
	C	11.36	11.45	0.0323	-5.81	-5.67
	D	10.70	10.85	0.0345	-4.16	-2.17

	E	10.70	10.85	0.0345	-4.16	-2.17
	F	11.36	11.45	0.0323	-5.81	-5.68
	G	10.81	10.97	0.0385	-6.62	-8.49
	H	12.08	12.07	0.0208	-9.39	-18.46
[7]-helicene	A	11.96	12.01	0.0202	-9.31	-17.55
	B	10.83	10.92	0.0381	-5.85	-5.51
	C	10.91	11.04	0.0330	-4.75	-3.10
	D	11.78	11.88	0.0337	-4.91	-4.33
	E	10.91	11.04	0.0330	-4.75	-3.10
	F	10.83	10.92	0.0381	-5.85	-5.51
	G	11.96	12.01	0.0202	-9.31	-17.55
[6]-Helicene	A	12.00	11.99	0.0200	-8.53	-14.84
	B	10.66	10.75	0.0387	-5.09	-3.55
	C	11.99	12.11	0.0316	-5.38	-5.50
	D	11.99	12.11	0.0316	-5.38	-5.50
	E	10.66	10.75	0.0387	-5.09	-3.55
	F	12.00	11.99	0.0200	-8.53	-14.84

Figure S1: Local normal magnetic field for the successive rings of [n]-helicenes where n = (6, 7, 8, 9, 10, 11, 12, 13, 14 and 20) as obtained from M06/6-311G* optimized geometries.



II- Comparison of calculated and measured ^{1}H and ^{13}C NMR chemical shifts

Table S2: Experimental and calculated ^{1}H and ^{13}C NMR chemical shifts of [6]-helicene

^{1}H NMR chemical shifts	
M06/6-311G*/*IEFPCM(chloroform)*// B3LYP/6-311+G(2d,p)/*IEFPCM(chloroform)*	H_2 (6.89), H_3 (7.46), H_1 (7.77), H_4 (8.21), H_5 (8.30), H_6 (8.36), H_7 (8.36), H_8 (8.42)
Experimental	H_2 (6.68), H_3 (7.26), H_1 (7.43), H_4 (7.94), H_5 (8.06), H_6 (8.10), H_7 (8.15), H_8 (8.18)
^{13}C NMR chemical shifts	
M06/6-311G*/*IEFPCM(chloroform)*// B3LYP/6-311+G(2d,p)/*IEFPCM(chloroform)*	C_2 (129.28), C_{1c} (129.64), C_3 (130.23), C_6 (131.60), C_7 (132.16), C_8 (132.29), C_4 (132.72), C_5 (133.07), C_{1b} (133.19), C_1 (133.83), C_{1a} (135.08), C_{6a} (137.03), C_{4a} (137.55), C_{8a} (137.62)
Experimental	C_{1c} (123.17), C_2 (124.97), C_3 (125.98), C_6 (126.47), C_1 (126.75), C_8 (127.23), C_{1b} (127.27), C_7 (127.65), C_4 (128.08), C_5 (128.24), C_{1a} (129.32), C_{8a} (130.01), C_{6a} (131.14), C_{4a} (131.63)

Table S3: Experimental and calculated ^{1}H and ^{13}C NMR chemical shifts of extended helicene

^{1}H NMR chemical shifts	
M06/6-311G*/*IEFPCM(chloroform)*// B3LYP/6-311+G(2d,p)/*IEFPCM(chloroform)*	H_b (6.34), H_c (6.97), H_d (7.34), H_e (7.60), H_a (7.72), H_h (7.91), H_k (7.94), H_f (8.38), H_g (8.58), H_l (8.78), H_i (8.88), H_j (8.90)
Experimental	H_b (6.22), H_c (6.69), H_d (7.12), H_e (7.27), H_h (7.63), H_k (7.69), H_a (7.80), H_f (7.93), H_g (8.15), H_l (8.34), H_i (8.47), H_j (8.49)
^{13}C NMR chemical shifts	
M06/6-311G*/*IEFPCM(chloroform)*// B3LYP/6-311+G(2d,p)/*IEFPCM(chloroform)*	C_f (124.97), C_g (125.92), C_l (126.64), C_i (127.19), C_j (127.31), C_b (130.51), C_e (130.62), C_c (130.84), C_k (131.46), C_h (131.48), C_d (132.28), C_w (133.86), C_t (134.68), C_x (135.53), C_q (135.62), C_a (135.63), C_s (135.88), C_p (136.05), C_n (137.02), C_r (137.14), C_o (137.18), C_v (138.80), C_m (139.31), C_u (141.94)
Experimental	C_f (119.90), C_g (121.50), C_l (122.00), C_i (122.40), C_j (122.70), C_b (125.51), C_e (125.54), C_c (125.80), C_d (126.70), C_h (126.89), C_k (126.92), C_t (127.20), C_w (128.00), C_a (128.50), C_x (129.70), C_s (130.10), C_q (130.20), C_p (130.30), C_n (131.03), C_o (131.09), C_r (131.09), C_v (131.09), C_u (133.50), C_m (134.00)

III- Current density, BLA and NICS analysis of hexa-peri-hexabenzo [7]helicene (extended helicene)

Table S4: Induced current (in nA/T), BLA, NICS(0), and $NICS_{zz}(0)$ of extended helicene

Ring	$\bar{J}$ (nA/T)	$\bar{J}_{para}$(nA/T)	$\bar{J}_{dia}$(nA/T)	BLA (Å)	NICS(0) (ppm)	$NICS_{zz}(0)$ (ppm)
A	9.06	-5.46	14.52	0.0163	-6.81	-8.21
H	9.98	-7.01	17.00	0.0216	-6.26	-5.11
B	2.47	-7.40	9.87	0.0053	5.13	29.24
I	10.85	-8.13	18.98	0.0099	-5.82	-3.57
C	6.77	-5.95	12.73	0.0330	-1.08	10.95
J	9.94	-8.42	18.36	0.0107	-4.62	-0.48
D	0.65	-7.95	8.60	0.0132	7.42	35.36
K	9.94	-8.42	18.36	0.0107	-4.62	-0.47
E	6.76	-5.96	12.72	0.0330	-1.07	10.97
L	10.87	-8.12	18.99	0.0099	-5.82	-3.58
F	2.50	-7.39	9.89	0.0053	5.12	29.21
M	9.99	-7.03	17.02	0.0216	-6.27	-5.11
G	9.05	-5.43	14.48	0.0163	-6.80	-8.24

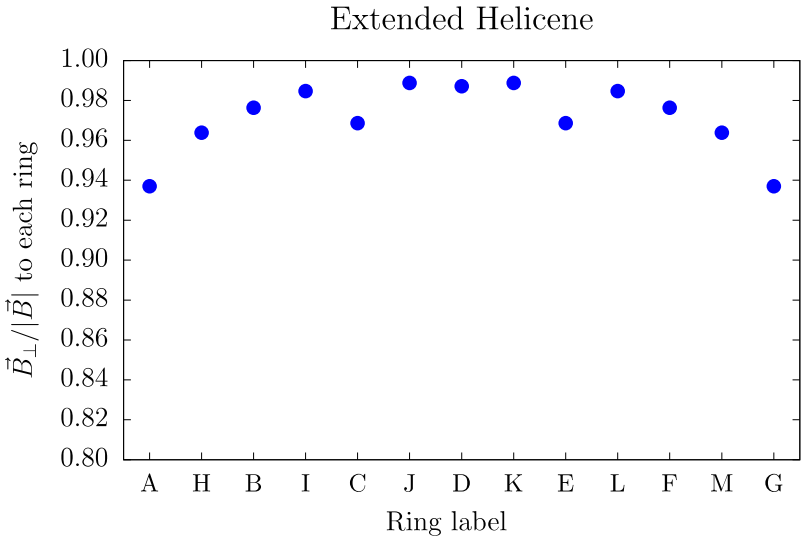


Figure S2: Local normal magnetic field for the successive rings of the extended helicene as obtained from M06/6-311G* optimized geometries.

IV- Current density and NICS analysis of azahelicenes

Table S5: Induced current (in nA/T), NICS(0), and $NICS_{zz}(0)$ of azahelicenes

Helicene	Ring	$\bar{J}$ (nA/T)	$\bar{J}_{para}$ (nA/T)	$\bar{J}_{dia}$ (nA/T)	NICS(0) (ppm)	$NICS_{zz}(0)$ (ppm)
mono-aza-[7]-helicene	A	13.15	-4.55	17.71	-9.54	-18.75
	B	11.20	-4.67	15.87	-5.51	-5.48
	C	12.28	-4.31	16.59	-8.01	-9.13
	D	11.03	-4.33	15.36	-9.20	-2.07
	E	12.28	-4.31	16.59	-8.01	-9.12
	F	11.20	-4.67	15.87	-5.51	-5.48
	G	13.15	-4.55	17.71	-9.54	-18.75
tri-aza-[7]-helicene	A	11.91	-4.38	16.29	-9.20	-14.24
	B	10.03	-4.70	14.73	-8.50	0.47
	C	12.87	-4.36	17.23	-9.81	-11.63
	D	11.05	-4.69	15.74	-9.22	1.14
	E	12.88	-4.38	17.26	-9.83	-11.61
	F	10.05	-4.70	14.74	-8.56	0.40
	G	11.95	-4.38	16.33	-9.17	-14.26
tetra-aza-[7]-helicene	A	10.91	-4.58	15.49	-12.09	-10.77
	B	11.54	-4.39	15.93	-8.97	-9.99
	C	10.77	-4.80	15.57	-9.52	0.02
	D	12.27	-4.55	16.82	-8.92	-9.26
	E	10.77	-4.80	15.57	-9.52	0.02
	F	11.54	-4.39	15.93	-8.97	-9.99
	G	10.91	-4.58	15.49	-12.09	-10.77

V- Cartesian coordinates and electronic energy of the molecules after geometry optimization at the M06/6-311G* level of approximation

1) [6]-helicene E = -999.849817 hartree

C	-2.9456001349	-2.5045962091	0.6654056337
C	-2.0172517269	-3.1433857002	1.4454714274
C	-1.1764629700	3.5872766528	-0.3549648941
H	-1.1346982248	4.6744922404	-0.3972797147
H	-3.8761495496	-3.0016077481	0.3937125227
C	2.0172558386	-3.1433945268	-1.4454470588
C	2.9456034211	-2.5045981247	-0.6653862446
C	2.7390006574	-1.1823159821	-0.2254627532
C	3.7670755852	-0.4785319374	0.4645163557
C	1.2824563927	0.8018007740	0.0044305686
C	2.3971920740	1.5169823507	0.4873067238
C	3.6240837642	0.8379619135	0.7434448098
C	2.3099069178	2.9183905730	0.6866096693
H	3.1924056448	3.4510853092	1.0372826906
C	0.0000000000	1.4625001543	0.0000000000
H	4.6933639328	-1.0020745570	0.6963661995
H	3.8761534761	-3.0016062664	-0.3936891595
H	4.4418108672	1.4060075871	1.1846999678
C	1.1764610491	3.5872803782	0.3549304515
C	0.0000000000	2.8796421697	0.0000000000
C	-1.2824563239	0.8017995304	-0.0044359317
H	1.1346945788	4.6744963786	0.3972337784
C	-2.3099108549	2.9183823125	-0.6866328208
C	-2.3971943071	1.5169773129	-0.4873157272
C	-3.6240858968	0.8379531979	-0.7434473340
C	-3.7670759292	-0.4785388892	-0.4645106686
C	-2.7389993345	-1.1823172522	0.2254723800
C	-1.5215122346	-0.5218096298	0.5312137968
H	-4.4418140105	1.4059952150	-1.1847053178
H	-4.6933636629	-1.0020843785	-0.6963563991
H	-3.1924113811	3.4510729106	-1.0373074720
C	1.5215126368	-0.5218119571	-0.5312092670
C	0.6275910906	-1.1779941284	-1.4022775599
C	0.8640065711	-2.4542120774	-1.8465907800
H	2.1900011352	-4.1628007911	-1.7826306387
H	-0.2642092075	-0.6597290333	-1.7418666259
H	0.1529844707	-2.9291557625	-2.5187050260
C	-0.6275900799	-1.1779837829	1.4022873443
C	-0.8640036236	-2.4541988691	1.8466103066
H	-2.1899959863	-4.1627896995	1.7826624158
H	0.2642092117	-0.6597145762	1.7418725580
H	-0.1529810681	-2.9291363894	2.5187284262

2) [7]-helicene E = -1153.400930 hartree

C	-0.6618651312	0.0507405776	-1.9116005813
C	-1.7910137106	0.4775010579	-2.5644224762
C	-0.6816426320	-1.0792194448	-1.0677407868
C	-1.8787385284	-1.8374690402	-1.0174849276
C	-3.0347973194	-1.3598978050	-1.6656171853
C	-3.0032811017	-0.2101267917	-2.4108718182
H	0.2710641093	0.5836107916	-2.0701140484
H	-1.7395617152	1.3515505742	-3.2099260937
H	-3.9516404252	-1.9427612978	-1.5859920438
H	-3.9004423819	0.1449985558	-2.9126618751
C	0.4733413382	-1.5365960341	-0.3280280146
C	0.4806962606	-2.8757306928	0.1086458705
C	-0.7247552392	-3.6355636340	0.0970775053
C	-1.8784808297	-3.1090550693	-0.3770377884
H	-0.6981647352	-4.6467226185	0.5009904638
H	-2.8071458867	-3.6768926652	-0.3443303626
C	1.6253450109	-0.7224953561	-0.0341151248
C	2.8505434451	-1.3847858506	0.2120907859
C	2.8541443161	-2.7717800899	0.5115504331
C	1.6905731031	-3.4695466828	0.5538350959
H	3.8035017896	-3.2495324096	0.7484788779
H	1.6756232119	-4.5138039397	0.8621401525
C	4.0703339846	-0.6605070879	0.1542228364
C	4.0703430917	0.6604527943	-0.1542263845
C	2.8505626225	1.3847486071	-0.2120931174
C	1.6253550494	0.7224748876	0.0341120929
H	5.0031859393	-1.2021142055	0.3025749564
H	5.0032025449	1.2020471165	-0.3025778425
C	2.8541829037	2.7717435026	-0.5115494896
C	1.6906218245	3.4695269762	-0.5538301587
C	0.4807369855	2.8757270256	-0.1086414445
C	0.4733630937	1.5365910652	0.3280276553
H	3.8035470025	3.2494829421	-0.7484771317
H	1.6756866656	4.5137854238	-0.8621316116
C	-0.7247033957	3.6355773503	-0.0970687718
C	-1.8784358496	3.1090841952	0.3770465013
C	-1.8787115615	1.8374954144	1.0174880074
C	-0.6816268837	1.0792279487	1.0677390193
H	-0.6980987098	4.6467373402	-0.5009780720
H	-2.8070925509	3.6769355498	0.3443426914
C	-3.0347767186	1.3599379484	1.6656189580
C	-3.0032769265	0.2101624498	2.4108674260
C	-1.7910196586	-0.4774846835	2.5644128187
C	-0.6618653270	-0.0507374086	1.9115920563
H	-3.9516112887	1.9428154379	1.5859981029
H	-3.9004430275	-0.1449522628	2.9126565780
H	-1.7395801094	-1.3515385672	3.2099117318
H	0.2710562955	-0.5836225340	2.0701016075

3) [8]-helicene E = -1306.951634 hartree

C	0.0274740737	1.1672436975	2.0753660052
C	0.6879757614	2.2549597545	2.5877033154
C	0.7234409270	0.0205065559	1.6370448492
C	2.1247550351	-0.0163795018	1.8526222043
C	2.7856891743	1.1267695098	2.3441951404
C	2.0867814901	2.2533081184	2.6910590596
H	-1.0578332082	1.1829328546	2.0304401407
H	0.1189448688	3.1207050432	2.9195597688
H	3.8666191791	1.0844478691	2.4734057211
H	2.6070887065	3.1255103110	3.0804591425
C	0.0640911068	-1.1430332686	1.0859924475
C	0.7644033548	-2.3644474772	1.1169776411
C	2.1677296169	-2.3745557462	1.3637169774
C	2.8360873133	-1.2329976914	1.6493027154
H	2.6924734074	-3.3268132696	1.3003389099
H	3.9142761432	-1.2393087805	1.8027574864
C	-1.2784096105	-1.1470070349	0.5664677995
C	-1.9821744853	-2.3731158974	0.5700985849
C	-1.2777578229	-3.5904086569	0.7549373800
C	0.0696253728	-3.5856729601	0.9214282993
H	-1.8345928298	-4.5252125558	0.7113747605
H	0.6297495939	-4.5177860246	0.9781970705
C	-3.3894047893	-2.3801756876	0.3741387863
C	-4.0661201782	-1.2172937385	0.1991463514
C	-3.3615561347	0.0000000000	0.0000000000
C	-1.9495715968	0.0000000000	0.0000000000
H	-3.9155493277	-3.3321474605	0.4256723142
H	-5.1537155140	-1.2026676349	0.1485135688
C	-4.0661005299	1.2173557898	-0.1991508653
C	-3.3893664557	2.3802272771	-0.3741406188
C	-1.9821358394	2.3731455101	-0.5700973784
C	-1.2783904543	1.1470253815	-0.5664670375
H	-5.1536961620	1.2027470221	-0.1485193930
H	-3.9154957538	3.3322075221	-0.4256735805
C	-1.2776992271	3.5904274109	-0.7549322258
C	0.0696843189	3.5856705523	-0.9214202717
C	0.7644432812	2.3644342478	-1.1169696823
C	0.0641114606	1.1430313054	-1.0859878595
H	-1.8345194382	4.5252401101	-0.7113691671
H	0.6298234829	4.5177747638	-0.9781866934
C	2.1677701572	2.3745200479	-1.3637068384
C	2.8361087820	1.2329523091	-1.6492990217
C	2.1247562363	0.0163466535	-1.8526234955
C	0.7234419272	-0.0205174831	-1.6370437167
H	2.6925292779	3.3267689721	-1.3003267812
H	3.9142973843	1.2392466710	-1.8027560259
C	2.7856700339	-1.1268106004	-2.3442046709
C	2.0867428549	-2.2533362600	-2.6910716751
C	0.6879375019	-2.2549664169	-2.5877101206
C	0.0274550023	-1.1672416919	-2.0753664921
H	3.8666003404	-1.0845060945	-2.4734181620
H	2.6070347198	-3.1255451784	-3.0804771980
H	0.1188916447	-3.1207010797	-2.9195684897
H	-1.0578525126	-1.1829131745	-2.0304365740

4) [9]-helicene E = -1460.502978 hartree

C	2.1713033993	0.6241165712	1.6380665845
C	3.5438386387	0.6135447483	1.6382762392
C	1.4225802267	-0.5637279157	1.4966283378
C	2.1414363783	-1.7868266065	1.4694255864
C	3.5494901455	-1.7704511701	1.4331735025
C	4.2457483399	-0.5916779659	1.4981635550
H	1.6542654292	1.5684966409	1.7799793603
H	4.0865881918	1.5490251844	1.7555694740
H	4.0768282114	-2.7226116106	1.3841145681
H	5.3333359603	-0.5928602801	1.4814562451
C	-0.0251315282	-0.5958905393	1.4932796197
C	-0.6513830567	-1.8196108704	1.7998851284
C	0.1020400609	-3.0289180019	1.7874303236
C	1.4359300501	-3.0203992648	1.5611043634
H	-0.4301470139	-3.9654459919	1.9494953583
H	2.0027947907	-3.9497586235	1.5220714744
C	-0.8629452745	0.5569312007	1.2858647490
C	-2.1591728690	0.5413394704	1.8468253378
C	-2.7278917355	-0.6889172841	2.2664455247
C	-2.0269025434	-1.8452475007	2.1485079215
H	-3.7517426385	-0.6885126699	2.6371536610
H	-2.4843721409	-2.8036834061	2.3899797379
C	-2.8844654771	1.7556255138	1.9782589814
C	-2.3379922998	2.9330156129	1.5803117234
C	-1.1311355393	2.9445632862	0.8315002311
C	-0.4850378706	1.7270782819	0.5333519902
H	-3.8622029413	1.7256215946	2.4567352472
H	-2.8438070933	3.8788631121	1.7683674396
C	-0.5752970207	4.1659292391	0.3605142829
C	0.5748963489	4.1659785849	-0.3605529155
C	1.1308474287	2.9446468486	-0.8314970031
C	0.4848598919	1.7271037882	-0.5333038245
H	-1.0612698438	5.0996540558	0.6395601583
H	1.0607790584	5.0997470798	-0.6396047574
C	2.3377329447	2.9331717783	-1.5802605784
C	2.8843245360	1.7558278871	-1.9781801551
C	2.1591554697	0.5414690395	-1.8467310437
C	0.8629525083	0.5569200192	-1.2856994023
H	2.8434524864	3.8790624955	-1.7683653282
H	3.8620536922	1.7259347829	-2.4566812288
C	2.7279536281	-0.6887315852	-2.2663770069
C	2.0270444793	-1.8451116556	-2.1484684766
C	0.6515269665	-1.8195986676	-1.7998528274
C	0.0251970917	-0.5959310108	-1.4932063657
H	3.7517983873	-0.6882628771	-2.6371066330
H	2.4845968401	-2.8035046130	-2.3899644500
C	-0.1018115109	-3.0289522238	-1.7873960329
C	-1.4356928094	-3.0205134824	-1.5610190812
C	-2.1412847425	-1.7869903234	-1.4694158284
C	-1.4225264835	-0.5638478590	-1.4966845629
H	0.4304208171	-3.9654505693	-1.9494878916
H	-2.0024966311	-3.9499078620	-1.5219259771
C	-3.5493459447	-1.7707094298	-1.4332174613
C	-4.2456737524	-0.5919927840	-1.4983564612
C	-3.5438468357	0.6132794823	-1.6385147182
C	-2.1713186978	0.6239536376	-1.6382108911
H	-4.0766342838	-2.7228920163	-1.3840474737
H	-5.3332621401	-0.5932477860	-1.4816799336
H	-4.0866877353	1.5486824311	-1.7559889898
H	-1.6543066098	1.5683577901	-1.7800461795

5) [10]-helicene E =-1614.053054 hartree

C	-0.3349571853	-0.2944811825	1.5312454281
C	-1.3563760830	-1.0216358201	2.1832347949
C	-0.6584258339	1.0392227390	1.0864892179
C	-1.6916521854	1.7290947064	1.7520532766
C	-2.6163619762	1.0036291950	2.5494955301
C	-2.5075660098	-0.3437848693	2.6676619919
H	-3.4442020631	1.5427821422	3.0073927981
C	0.0000000000	1.7152168329	0.0000000000
C	0.0000000000	3.1241560565	0.0000000000
C	-0.9125226649	3.8225035642	0.8368922399
C	-1.7995532973	3.1390278465	1.6054198379
H	-0.9263267499	4.9108077911	0.7986000139
H	-2.5726571245	3.6611210041	2.1672334604
C	0.6584198754	1.0390692829	-1.0863494569
C	1.6917454106	1.7288370923	-1.7518709168
C	1.7996228259	3.1388001098	-1.6054489215
C	0.9125282266	3.8223886957	-0.8371021328
H	2.5727896305	3.6607998835	-2.1672633007
H	0.9263292106	4.9106980557	-0.7989625691
C	2.6165851090	1.0032407154	-2.5490307908
C	2.5077702881	-0.3441848082	-2.6670445585
C	1.3564757006	-1.0219350593	-2.1827491849
C	0.3349811750	-0.2946831340	-1.5309760081
H	3.4445179819	1.5423092800	-3.0068605357
H	3.2679968525	-0.9235492099	-3.1890556726
H	-3.2677114936	-0.9230633670	3.1898848456
C	1.2238695274	-2.4236261479	-2.3543201102
C	-0.9492691167	-0.9300605079	-1.3720455018
C	0.1170765303	-3.0694641313	-1.9078827198
C	-1.0039817910	-2.3362101897	-1.4396024817
H	2.0487778297	-2.9714597604	-2.8075761289
H	0.0414583277	-4.1546923463	-1.9648932456
C	-2.1917884947	-3.0244032207	-1.0577617640
C	-3.3066363140	-2.3492484176	-0.6947888651
C	-3.3633638147	-0.9331798329	-0.8324651275
C	-2.2058267089	-0.2208588030	-1.2405709581
H	-2.1710848491	-4.1135811350	-1.0472352016
H	-4.2016004293	-2.8786736537	-0.3703229910
C	0.9492461028	-0.9299011991	1.3722063240
C	1.0039363400	-2.3360478699	1.4398759288
C	-0.1170812204	-3.0692313145	1.9083587730
C	-1.2237966279	-2.4233163252	2.3548975114
H	-0.0414952236	-4.1544570847	1.9654448017
H	-2.0486589606	-2.9710833831	2.8083165113
C	2.2057911270	-0.2207391385	1.2404253656
C	3.3632078609	-0.9331020597	0.8320636672
C	3.3064217380	-2.3491835617	0.6945338175
C	2.1916633814	-3.0242916489	1.0578750132
H	4.2013014759	-2.8786556405	0.3699115944
H	2.1709472578	-4.1134705370	1.0474605782
C	2.3772667528	1.1299644384	1.6121742399
C	4.6923068060	1.0863838904	0.9483039610
C	4.5809771921	-0.2475571056	0.6540647469
H	5.4467658892	-0.8122997874	0.3096251875
C	-4.5811776285	-0.2476153807	-0.6548497813
C	-4.6924129801	1.0863091653	-0.9491883749
C	-3.5839381743	1.7681487095	-1.4708467870
C	-2.3771898898	1.1298325039	-1.6124244455

H	-5.4470634984	-0.8123281090	-0.3106065292
H	-5.6415971375	1.6016902022	-0.8205204178
H	-3.6778812476	2.8087298834	-1.7739928209
H	-1.5457932346	1.6727754924	-2.0514167041
C	3.5839863241	1.7682584344	1.4702463667
H	5.6414566938	1.6017532854	0.8193374580
H	3.6780224162	2.8088571611	1.7733034247
H	1.5459819974	1.6729362882	2.0513475830

6) [11]-helicene E = -1767.603381 hartree

C	-0.4911246865	0.1026134361	1.4704901586
C	-1.5838783248	0.0740606488	2.3609639672
C	-0.3514823461	1.2602812905	0.6262551669
C	-0.9123874443	2.4742622314	1.0665438567
C	-1.8924621414	2.4542742557	2.0963440345
C	-2.2874389372	1.2769856475	2.6455251757
H	-2.3612601212	3.3932914159	2.3868928567
C	0.3514665940	1.2602634307	-0.6263453122
C	0.9123368496	2.4742432393	-1.0666858667
C	0.4821975628	3.6945486470	-0.4787977357
C	-0.4822969497	3.6945551294	0.4785943904
H	0.8950917317	4.6282869788	-0.8580694833
H	-0.8952458069	4.6282961442	0.8577990949
C	0.4911221687	0.1025688989	-1.4705444787
C	1.5838586871	0.0740119720	-2.3610373111
C	2.2874047100	1.2769376035	-2.6456339798
C	1.8924139280	2.4542365836	-2.0964853460
H	3.1089727399	1.2403570170	-3.3597131798
H	2.3611978370	3.3932522568	-2.3870619235
C	1.9658984971	-1.1545149007	-2.9620462217
C	1.2897532860	-2.2960991445	-2.6775312210
C	0.0727693183	-2.2532546926	-1.9453214942
C	-0.4229476760	-1.0149559950	-1.4781880995
H	2.8463142873	-1.1683648177	-3.6029774782
H	1.6336070388	-3.2587979692	-3.0538841011
H	-3.1090018606	1.2404172215	3.3596110116
C	-0.6453470657	-3.4469711945	-1.6774186520
C	-1.8036435196	-0.9599401287	-1.0649148006
C	-1.8110266159	-3.4078247653	-0.9835720928
C	-2.4315942073	-2.1651512856	-0.6936460593
H	-0.2140550081	-4.3946563780	-1.9970553136
H	-2.3272441550	-4.3252283121	-0.7032746503
C	-3.7050005637	-2.1389910504	-0.0542631970
C	-4.3724622995	-0.9767292123	0.1314265515
C	-3.8822245674	0.2300197299	-0.4445430217
C	-2.6268489720	0.2312773963	-1.1061364723
H	-4.1213777145	-3.0831294977	0.2952215511
H	-5.3311848020	-0.9573577280	0.6481549488
C	0.4229472188	-1.0149107715	1.4781663662
C	-0.0727779429	-2.2532060877	1.9453001895
C	-1.2897755221	-2.2960469941	2.6774871299
C	-1.9659273690	-1.1544607076	2.9619773281
H	-1.6336420651	-3.2587436386	3.0538338240
H	-2.8463605639	-1.1683059732	3.6028850362
C	1.8036566644	-0.9598941643	1.0649312844
C	2.4316259367	-2.1651089991	0.6937038084
C	1.8110482646	-3.4077808436	0.9836146757
C	0.6453468540	-3.4469229230	1.6774233511
H	2.3272714605	-4.3251864807	0.7033347436
H	0.2140441382	-4.3946067359	1.9970501541

C	2.6268609896	0.2313252339	1.1061832939
C	3.8822750774	0.2300556790	0.4446606869
C	4.3725348497	-0.9766964457	-0.1312820195
C	3.7050603660	-2.1389556220	0.0543789545
H	5.3312859278	-0.9573315813	-0.6479583700
H	4.1214545510	-3.0830965141	-0.2950792565
C	2.3031788265	1.3684755347	1.8765063266
C	3.1075839990	2.4801011940	1.8915462309
C	4.2886678079	2.5134079516	1.1367888770
C	4.6733994842	1.3957155190	0.4429884345
H	4.9141275473	3.4033741521	1.1378014946
H	5.6194629777	1.3780455987	-0.0972163307
C	-4.6733387294	1.3956863243	-0.4428338010
C	-4.2886262569	2.5133795982	-1.1366447662
C	-3.1075875022	2.4800588069	-1.8914713523
C	-2.3031984113	1.3684209713	-1.8764814500
H	-5.6193723296	1.3780269347	0.0974237110
H	-4.9140723383	3.4033552341	-1.1376164308
H	-2.8262947620	3.3363047878	-2.5007432328
H	-1.4119143796	1.3576402133	-2.4964776781
H	2.8262718910	3.3363482968	2.5008073637
H	1.4118644782	1.3577032277	2.4964586966

7) [12]-helicene E = -1921.153769 hartree

C	-0.3955971455	-0.5047997062	-1.2057755774
C	-1.2440142242	-1.1912758360	-2.0965565045
C	0.0000000000	-1.1789732861	0.0000000000
C	0.0000000000	-2.5860685547	0.0000000000
C	-0.7258654212	-3.2807791703	-1.0053623668
C	-1.4145144230	-2.5957734160	-1.9552225004
H	-0.7679822650	-4.3679655315	-0.9580024775
C	0.3956016816	-0.5047975604	1.2058035761
C	1.2440470650	-1.1912439796	2.0965807620
C	1.4146277622	-2.5957289016	1.9552209710
C	0.7260251216	-3.2807561194	1.0053424432
H	2.0561490248	-3.1156224178	2.6656408048
H	0.7682021857	-4.3679393849	0.9579644932
C	-0.0695501392	0.8049346778	1.5855055553
C	0.7152105915	1.5383729953	2.4990651959
C	1.7128286615	0.8695011345	3.2602820255
C	1.8963285429	-0.4698346533	3.1331349925
H	2.2840215743	1.4461702483	3.9868859982
H	2.5914954998	-1.0036090862	3.7797492471
C	0.5034433462	2.9354667088	2.6422457057
C	-0.4408412668	3.5652697495	1.8985067474
C	-1.3745680313	2.8162204662	1.1333309579
C	-1.2966990227	1.4050595820	1.1167539738
H	1.1574722710	3.4945121947	3.3100766962
H	-0.5430270589	4.6494984123	1.9236268531
H	-2.0560119309	-3.1156897503	-2.6656470915
C	-2.3884705404	3.4747703816	0.3909206805
C	-2.4577676984	0.6780791686	0.6651275087
C	-3.2987662847	2.7588748495	-0.3165630389
C	-3.3790957981	1.3503918137	-0.1621912043
H	-2.3894514920	4.5637215064	0.3671222209
H	-4.0324405623	3.2557517606	-0.9502127085
C	-4.4145677078	0.6224821598	-0.8166113328
C	-4.5894514677	-0.7006459149	-0.5940924163
C	-3.8313935509	-1.3639849104	0.4124048520
C	-2.8040195606	-0.6615173189	1.0942894434

H	-5.0563119022	1.1604422834	-1.5135353697
H	-5.3641732331	-1.2593312904	-1.1178400518
C	0.0695061349	0.8049482777	-1.5854795040
C	-0.7152965405	1.5383650365	-2.4990199143
C	-1.7129027939	0.8694625840	-3.2602246257
C	-1.8963417088	-0.4698833408	-3.1330929282
H	-2.2841281400	1.4461149175	-3.9868166019
H	-2.5914913193	-1.0036805939	-3.7797068759
C	1.2966580591	1.4051018368	-1.1167691718
C	1.3744864851	2.8162647266	-1.1333420389
C	0.4407134604	3.5652921126	-1.8984845590
C	-0.5035753129	2.9354659785	-2.6421987518
H	0.5428674061	4.6495235800	-1.9236016908
H	-1.1576375807	3.4944948906	-3.3100113110
C	2.4577561412	0.6781509673	-0.6651646358
C	3.3790651216	1.3504854622	0.1621580476
C	3.2987086732	2.7589675931	0.3165212090
C	2.3883896080	3.4748402647	-0.3909550919
H	4.0323712242	3.2558627714	0.9501707395
H	2.3893402590	4.5637911779	-0.3671516484
C	2.8040475223	-0.6614395669	-1.0943220725
C	3.8314095797	-1.3638901666	-0.4124012128
C	4.5894368730	-0.7005316496	0.5941052488
C	4.4145373277	0.6225982348	0.8166005905
H	5.3641555056	-1.2592009911	1.1178746283
H	5.0562610906	1.1605731489	1.5135321523
C	-4.1526708523	-2.6810339349	0.7954023442
C	-3.5420404681	-3.2750884515	1.8690111982
C	-2.6106658968	-2.5440253935	2.6194188265
C	-2.2555107709	-1.2733907033	2.2417854328
H	-4.9252384325	-3.2082420825	0.2364412271
H	-3.8070731325	-4.2884726421	2.1623270616
H	-2.1680382913	-2.9801262014	3.5124144555
H	-1.5570441295	-0.7190944294	2.8613397768
C	2.2556064038	-1.2733204921	-2.2418478704
C	2.6107925501	-2.5439519173	-2.6194622508
C	3.5421365085	-3.2750053231	-1.8690082613
C	4.1527161075	-2.6809386407	-0.7953778433
H	1.5571732964	-0.7190322511	-2.8614447814
H	2.1682152640	-2.9800573661	-3.5124803963
H	3.8071953724	-4.2883865661	-2.1623104454
H	4.9252716119	-3.2081333471	-0.2363870674

8) [13]-helicene E =-2074.703948 hartree

C	0.1130836660	-0.8057215802	0.7096988087
C	0.4802032267	-2.0197619637	1.3203790996
C	-0.1126214324	-0.8058795873	-0.7099921052
C	-0.4789292595	-2.0201801724	-1.3206056139
C	-0.2802929789	-3.2402593410	-0.6179617376
C	0.2822487702	-3.2400209890	0.6178567858
H	-0.5290475326	-4.1746139632	-1.1194142164
C	0.0413671781	0.3515500421	-1.5492450734
C	-0.6554701887	0.3773807852	-2.7735941994
C	-1.2063477608	-0.8274723670	-3.2886572907
C	-1.0269115529	-2.0028121160	-2.6314286197
H	-1.7182094835	-0.7957950042	-4.2499461334
H	-1.3573772016	-2.9444470736	-3.0679179972
C	0.9152265435	1.4577676272	-1.2487278861
C	0.6300335292	2.6987158093	-1.8553262628

C	-0.2436026114	2.7458568097	-2.9761194886
C	-0.7794382213	1.6046265960	-3.4801579612
H	-0.4200014316	3.7076514028	-3.4562667902
H	-1.3671622968	1.6189574186	-4.3971609473
C	1.2224220001	3.8830793104	-1.3417533715
C	2.0609843234	3.8238837378	-0.2767376574
C	2.5309947804	2.5712261446	0.2018643278
C	2.0844729651	1.3747345846	-0.4042586625
H	0.9413665007	4.8382564208	-1.7833451708
H	2.4439040493	4.7322599130	0.1867708057
H	0.5314246422	-4.1741852080	1.1194470572
C	3.4546277961	2.5153635365	1.2768919356
C	2.8511600689	0.1769735506	-0.1634155161
C	3.9307655008	1.3221795510	1.7142596466
C	3.6714230049	0.1350544185	0.9815606426
H	3.7362822395	3.4462008183	1.7674451843
H	4.5814189915	1.2639293111	2.5860261676
C	4.2697015728	-1.0927259946	1.3879853512
C	4.1326033412	-2.2174884728	0.6489041737
C	3.5108254581	-2.1615563784	-0.6310553862
C	2.9272094752	-0.9464617523	-1.0753658070
H	4.8297722919	-1.1039515207	2.3224140477
H	4.5650741098	-3.1613199286	0.9786363723
C	-0.0415402465	0.3516881457	1.5488842275
C	0.6554021206	0.3779894522	2.7731631422
C	1.2070527360	-0.8264751061	3.2882795270
C	1.0282737714	-2.0019628289	2.6311638512
H	1.7190745083	-0.7943920708	4.2494717472
H	1.3595041977	-2.9433306314	3.0676399463
C	-0.9160871550	1.4574480412	1.2484714574
C	-0.6314888035	2.6985881241	1.8550088570
C	0.2422212620	2.7462362826	2.9757279556
C	0.7787098988	1.6053146692	3.4797198395
H	0.4181493770	3.7081269056	3.4558556248
H	1.3664657197	1.6199636491	4.3966989597
C	-2.0854278178	1.3738090377	0.4041850116
C	-2.5328002273	2.5700450211	-0.2018437729
C	-2.0633439245	3.8229299329	0.2766270630
C	-1.2246149475	3.8825776398	1.3414909895
H	-2.4468305051	4.7311251295	-0.1867712634
H	-0.9439855416	4.8379357606	1.7829685766
C	-2.8514850260	0.1755467502	0.1635345571
C	-3.6721670228	0.1331823927	-0.9811131439
C	-3.9324624663	1.3201855954	-1.7136680794
C	-3.4567759486	2.5136155478	-1.2765571833
H	-4.5834561492	1.2615821668	-2.5851646459
H	-3.7392203583	3.4442742323	-1.7669934627
C	3.5521016509	-3.2748611487	-1.4929435393
C	3.1096779479	-3.1852845441	-2.7870761901
C	2.6463044367	-1.9534345852	-3.2695863420
C	2.5613870628	-0.8664037492	-2.4360354699
H	3.9775107561	-4.2046682654	-1.1165085996
H	3.1577788335	-4.0488053623	-3.4468050488
C	-2.9265097071	-0.9479634990	1.0755262853
C	-3.5096192674	-2.1633785737	0.6314045268
C	-4.1317685112	-2.2196429755	-0.6483631641
C	-4.2697961950	-1.0949646682	-1.3873718814
H	-4.5636871999	-3.1637477725	-0.9780435615
H	-4.8301474044	-1.1065407160	-2.3216372526
C	-3.5500414899	-3.2767001295	1.4933096929
C	-3.1070428042	-3.1869260571	2.7872270744
C	-2.6441169504	-1.9548473296	3.2695756103

C	-2.5601889262	-0.8677161457	2.4360568804
H	-3.9750247768	-4.2067680829	1.1170286485
H	-3.1544834353	-4.0504661638	3.4469795079
H	-2.3547669263	-1.8522003918	4.3132558577
H	-2.2313811738	0.0824092057	2.8458607189
H	2.2322194064	0.0835662316	-2.8459328352
H	2.3572799201	-1.8508889214	-4.3133668367

9) [14]-helicene E = -2228.253978 hartree

C	-0.4718782658	0.2298597263	-1.1793756196
C	-0.4131008708	0.9180652935	-2.4059509094
C	0.0000000000	0.9051890149	-0.0002819879
C	0.0000000000	2.3134233269	-0.0005534057
C	-0.1331536007	3.0091581861	-1.2331720394
C	-0.2295192558	2.3278722407	-2.4041740805
H	-0.0918442846	4.0976996432	-1.2213031290
C	0.4717703798	0.2303174429	1.1790883345
C	0.4129187889	0.9189908139	2.4053968397
C	0.2293588638	2.3287998354	2.4030688092
C	0.1330519490	3.0096343768	1.2317992426
H	0.2328502544	2.8544290823	3.3573150122
H	0.0917405997	4.0981711189	1.2195090383
C	1.0346546537	-1.0934640063	1.1811132206
C	0.9865535989	-1.8300641365	2.3812903359
C	0.7133911480	-1.1557307594	3.6023867947
C	0.5450872728	0.1921503630	3.6196146986
H	0.7107884481	-1.7330592491	4.5263521760
H	0.4413364036	0.7314613273	4.5604218907
C	1.2383057463	-3.2290639304	2.3510542878
C	1.5240959635	-3.8522298930	1.1791080305
C	1.7914407513	-3.0937800411	0.0061747173
C	1.7162428864	-1.6863122212	0.0574432128
H	1.1372814934	-3.7949116930	3.2763844330
H	1.6212618954	-4.9361271109	1.1296014651
H	-0.2330565880	2.8531349159	-3.3586217095
C	2.1415777956	-3.7333485604	-1.2125451721
C	2.3682746562	-0.9384245400	-0.9919705902
C	2.4060985128	-2.9980257423	-2.3220295845
C	2.5483733146	-1.5871105287	-2.2349197818
H	2.1353601644	-4.8219684574	-1.2485351651
H	2.5812813054	-3.4780129202	-3.2841343126
C	2.8781101487	-0.8262196511	-3.3859857330
C	3.0402406426	0.5184368390	-3.2994910247
C	3.0864325160	1.1542666848	-2.0318546366
C	2.8856877124	0.4015607123	-0.8579266107
H	2.9512630137	-1.3399801569	-4.3436758319
H	3.2166109354	1.1200792017	-4.1903575409
C	-1.0347566897	-1.0939255811	-1.1808561568
C	-0.9867698366	-1.8309749140	-2.3807627568
C	-0.7137073155	-1.1571026460	-3.6021357372
C	-0.5453738699	0.1907675960	-3.6198835312
H	-0.7111857279	-1.7347783924	-4.5258842458
H	-0.4416873767	0.7297213450	-4.5609022302
C	-1.7162018434	-1.6863682504	-0.0568853817
C	-1.7913701908	-3.0938184487	-0.0050853521
C	-1.5241670797	-3.8526985905	-1.1777717998
C	-1.2385169991	-3.2299637116	-2.3499808994
H	-1.6213132045	-4.9365786842	-1.1278520053
H	-1.1375865429	-3.7961545344	-3.2751113860

C	-2.3680997684	-0.9381028320	0.9923429299
C	-2.5480183266	-1.5863329715	2.2355566043
C	-2.4057061014	-2.9972132436	2.3231686755
C	-2.1413282091	-3.7329415755	1.2139195194
H	-2.5807500380	-3.4768480371	3.2854743269
H	-2.1350873154	-4.8215480314	1.2503112425
C	-2.8855510206	0.4018249379	0.8578728093
C	-3.0861704781	1.1549570229	2.0315495766
C	-3.0397983351	0.5195959757	3.2994144051
C	-2.8776201148	-0.8250240757	3.3863850977
H	-3.2160687139	1.1215624907	4.1900818766
H	-2.9506366107	-1.3384321283	4.3442746012
C	3.3737845152	2.5474418516	-1.9466492474
C	3.5469885449	3.1554107760	-0.7504534022
C	3.5924099998	2.3828152711	0.4449153836
C	3.3272904286	0.9897137817	0.3901439352
H	3.4374890639	3.1142353755	-2.8748932540
H	3.7373625918	4.2261355613	-0.6881327894
C	-3.3273100823	0.9895109851	-0.3903623340
C	-3.5924808461	2.3825840472	-0.4456117596
C	-3.5469454646	3.1556172874	0.7494697146
C	-3.3735761358	2.5480920516	1.9458671394
H	-3.7373596443	4.2263132749	0.6867799373
H	-3.4371838503	3.1152243337	2.8739110746
C	3.9874590865	2.9732534119	1.6612964216
C	4.1973049127	2.2129934405	2.7822292443
C	4.0547079795	0.8207384441	2.7030489134
C	3.6351306718	0.2288704475	1.5381626580
H	4.1557028684	4.0495717114	1.6829784206
H	4.5137342470	2.6790671314	3.7127913487
H	4.2844525569	0.1993935951	3.5660274890
H	3.5704692755	-0.8539452719	1.4950581685
C	-3.9876830502	2.9725652010	-1.6621642087
C	-4.1976231704	2.2118902489	-2.7827978188
C	-4.0549642865	0.8196697707	-2.7031289673
C	-3.6352401321	0.2282392650	-1.5380731688
H	-4.1559650545	4.0488697949	-1.6842200397
H	-4.5141686327	2.6776149738	-3.7134948633
H	-4.2847762704	0.1980033921	-3.5658579035
H	-3.5705275061	-0.8545586042	-1.4945832954

10) [20]-helicene E = -3149.553138 hartree

C	-0.5975818267	0.9206042963	-1.1266160484
C	-0.6325382995	1.6084615644	-2.3561028130
C	0.0000000000	1.5909059093	0.0005519391
C	0.0000000000	3.0003242658	0.0011764184
C	-0.2340265846	3.6974338799	-1.2153841073
C	-0.4325945776	3.0157391292	-2.3729301615
H	-0.1821106643	4.7859638750	-1.2075076326
C	0.5974316727	0.9196158462	1.1271415425
C	0.6323390696	1.6063812471	2.3572387766
C	0.4323829051	3.0136450480	2.3753040716
C	0.2338274700	3.6963587559	1.2183608402
H	0.5099630656	3.5361459420	3.3285827852
H	0.1818897264	4.7848947042	1.2114455789
C	1.1682620991	-0.4028470765	1.0830257953
C	1.2123585577	-1.1412199794	2.2824059222
C	1.0396969823	-0.4676941177	3.5221345889
C	0.8670705230	0.8786277586	3.5553861904

H	1.1217210481	-1.0456532369	4.4424074457
H	0.8401532839	1.4171794335	4.5024714880
C	1.4417319120	-2.5430080133	2.2301787033
C	1.6053892197	-3.1730360655	1.0384613905
C	1.7688565369	-2.4211578484	-0.1564073831
C	1.7210842122	-1.0140618496	-0.0984391942
H	1.4238200254	-3.1056712509	3.1633371468
H	1.6890223758	-4.2581148779	0.9847328747
H	-0.5101987817	3.5390836375	-3.3257437230
C	1.9910611645	-3.0609218934	-1.4063962202
C	2.2625093300	-0.2829103629	-1.2137585172
C	2.1401928330	-2.3295748208	-2.5407446589
C	2.2982833552	-0.9187967540	-2.4700784135
H	1.9794470371	-4.1499041974	-1.4398844115
H	2.2159833235	-2.8131544399	-3.5140987472
C	2.5138989275	-0.1410362615	-3.6395764695
C	2.6866695081	1.2033709220	-3.5533292415
C	2.8813786012	1.8209254789	-2.2882685548
C	2.8343708635	1.0346878649	-1.1192354392
H	2.4764309055	-0.6401222662	-4.6072561324
H	2.7531184387	1.8197737141	-4.4493296710
C	-1.1684067867	-0.4019010209	-1.0836519707
C	-1.2125660958	-1.1392050631	-2.2836878116
C	-1.0399293123	-0.4645816667	-3.5228260806
C	-0.8672944603	0.8817663933	-3.5548897957
H	-0.8403995471	1.4211598886	-4.5014962091
C	-1.7211564873	-1.0141620916	0.0973012033
C	-1.7689729347	-2.4213098916	0.1540041523
C	-1.6056087595	-3.1721203667	-1.0415471710
C	-1.4419788102	-2.5410285730	-2.2327075089
H	-1.6892686549	-4.2572445666	-0.9887923995
H	-1.4241275091	-3.1028577427	-3.1663694275
C	-2.2624213702	-0.2839999700	1.2133506539
C	-2.2980631751	-0.9210251827	2.4690977476
C	-2.1400467801	-2.3318761066	2.5384633653
C	-1.9910831889	-3.0621968613	1.4034343783
H	-2.2157496547	-2.8163369328	3.5113856186
H	-1.9795125440	-4.1512098946	1.4359309285
C	-2.8342562808	1.0337025211	1.1200978446
C	-2.8810813623	1.8188775684	2.2898539432
C	-2.6862045466	1.2001726808	3.5543265924
C	-2.5134793270	-0.1443189472	3.6393320531
H	-2.7525096626	1.8157653925	4.4508944427
H	-2.4759017706	-0.6442857373	4.6065526812
C	3.1604774573	3.2107293212	-2.1846207894
C	3.3853727288	3.7799261934	-0.9727523186
C	3.5614901595	2.9685369506	0.1812415791
C	3.4572766350	1.5659470333	0.0680597385
H	3.1321105478	3.8144952186	-3.0909218650
H	3.5045207773	4.8581371270	-0.8724335383
C	-3.4573708232	1.5660309185	-0.0666074773
C	-3.5616529344	2.9687215224	-0.1784860740
C	-3.3853254733	3.7790666456	0.9762075282
C	-3.1601948291	3.2087732917	2.1875175319
H	-3.5045165438	4.8573657242	0.8768913747
H	-3.1316766701	3.8117158211	3.0943618238
C	3.8548733924	3.5517534206	1.4423417570
C	4.0436910550	2.7678393655	2.5333992717
C	4.1702316774	1.3597354111	2.3941706521
C	4.0451513989	0.7646410401	1.1173626493
H	3.8665751304	4.6380489013	1.5217693407
H	4.1740725673	3.2046670829	3.5228047124

C	-3.8553208170	3.5530831476	-1.4389899221
C	-4.0443469967	2.7701642844	-2.5307240587
C	-4.1707868055	1.3619260301	-2.3927654431
C	-4.0454116324	0.7656593464	-1.1165336509
H	-3.8670837173	4.6394506494	-1.5174154876
H	-4.1749591296	3.2078934605	-3.5197006489
C	-4.4401393445	0.5535775877	-3.5266933288
C	-4.6088779176	-0.7860157988	-3.3932632902
C	-4.7222385508	-1.3671641807	-2.1040209830
C	-4.5717034461	-0.5684708517	-0.9526378059
H	-4.4657135583	1.0280705356	-4.5068701571
H	-4.7428547816	-1.4243213415	-4.2658413838
C	4.4394095033	0.5503506439	3.5274013785
C	4.6083010986	-0.7891016375	3.3927547244
C	4.7220013682	-1.3690325784	2.1029937812
C	4.5716086758	-0.5692805087	0.9523286077
H	4.4647425552	1.0239329414	4.5080249012
H	4.7421724869	-1.4282068939	4.2647640319
H	-1.1219893568	-1.0417261441	-4.4436067729
C	-5.0327576054	-2.7522942981	-1.9787796970
C	-5.2796765021	-3.3092592179	-0.7710443701
C	-5.3775834832	-2.4878276522	0.3878580664
C	-5.0872076702	-1.1014172064	0.2927339282
H	-5.0554528941	-3.3548795852	-2.8862406655
H	-5.4905701732	-4.3738099975	-0.6766443892
C	5.0327473129	-2.7539992171	1.9765174909
C	5.2800402585	-3.3097875326	0.7683163081
C	5.3780917050	-2.4872504680	-0.3897904718
C	5.0874580292	-1.1009809527	-0.2934317971
C	5.8510434666	-3.0215722231	-1.6041116748
C	6.1125694588	-2.2133249859	-2.6797786895
C	5.9436796416	-0.8278135275	-2.5524258278
C	5.4484776716	-0.2902609641	-1.3906936114
H	6.0377801557	-4.0937063820	-1.6589685816
H	6.4893649587	-2.6364437433	-3.6084199388
H	6.2121331456	-0.1677682727	-3.3745575161
H	5.3660575273	0.7888953378	-1.3080353638
C	-5.8501633920	-3.0233733995	1.6017847873
C	-6.1115926506	-2.2161823788	2.6782682643
C	-5.9429859961	-0.8305223222	2.5521711136
C	-5.4481378340	-0.2917915885	1.3908335841
H	-6.0367033330	-4.0955906550	1.6556739137
H	-6.4881032943	-2.6402371343	3.6065978706
H	-6.2113730354	-0.1712932433	3.3749794926
H	-5.3659405262	0.7874570923	1.3091713274
H	5.4911158608	-4.3742175327	0.6729663801
H	5.0553385495	-3.3574345587	2.8834163832

11) Benzene E = -232.099491 hartree

C	-1.2021762035	0.6940733130	0.0001951594
C	0.0000000000	1.3881572762	0.0000000000
C	1.2020872301	0.6941039058	0.0000000000
C	1.2020892934	-0.6941235430	-0.0001175045
C	0.0000000000	-1.3881572762	0.0000000000
C	-1.2021738776	-0.6940563228	0.0002248331
H	-2.1441044594	1.2381243881	0.0003324018
H	0.0000000000	2.4759209569	0.0000000000
H	2.1442356750	1.2377717148	0.0000000000
H	2.1440892236	-1.2380483174	-0.0001872443
H	-0.0002321271	-2.4759196496	0.0000000000
H	-2.1442514268	-1.2378491300	0.0003391703

12) Phenanthrene E = -692.753348 hartree

C	-0.1213206067	1.2750416674	-0.2772172115
C	0.0623013861	2.4719226226	0.4699632148
C	0.0000000000	0.0000000000	0.3955589331
C	0.0000000000	0.0000000000	1.8029387243
C	0.1310607065	1.2198396471	2.5240390371
C	0.2278741090	2.4060066423	1.8802491812
C	0.1213206067	-1.2750416674	-0.2772172115
C	-0.0623013861	-2.4719226226	0.4699632148
C	-0.2278741090	-2.4060066423	1.8802491812
C	-0.1310607065	-1.2198396471	2.5240390371
C	0.5217650731	-1.4207961904	-1.6249661677
C	0.6125903560	-2.6530628552	-2.2241440140
C	0.3106750497	-3.8183553653	-1.5073731752
C	0.0000000000	-3.7216918554	-0.1765531627
C	-0.5217650731	1.4207961904	-1.6249661677
C	-0.6125903560	2.6530628552	-2.2241440140
C	-0.3106750497	3.8183553653	-1.5073731752
C	0.0000000000	3.7216918554	-0.1765531627
H	0.3702253409	3.3333788665	2.4328612745
H	0.1783435565	1.1713781908	3.6109126122
H	-0.3702253409	-3.3333788665	2.4328612745
H	-0.1783435565	-1.1713781908	3.6109126122
H	0.8292570171	-0.5476723299	-2.1896345530
H	0.9422357272	-2.7225902371	-3.2583588156
H	0.3662376625	-4.7902399814	-1.9919384398
H	-0.1736886132	-4.6186027977	0.4166787353
H	-0.8292570171	0.5476723299	-2.1896345530
H	-0.9422357272	2.7225902371	-3.2583588156
H	-0.3662376625	4.7902399814	-1.9919384398
H	0.1736886132	4.6186027977	0.4166787353

13) [6]-helicene IEFPCM(chloroform) E = -999.855656 hartree

C	2.9490605093	-2.5051347157	0.6642446930
C	2.0211258015	-3.1448680102	1.4452962645
C	1.1771968118	3.5882955729	-0.3547965522
H	1.1353224793	4.6753173706	-0.3963226877
H	3.8795901010	-3.0014240231	0.3919567174
C	-2.0222453553	-3.1442481161	-1.4453135633
C	-2.9498626626	-2.5042434437	-0.6641096258
C	-2.7411047136	-1.1815848074	-0.2240868453
C	-3.7695857585	-0.4770717555	0.4658126430
C	-1.2826151458	0.8017707008	0.0050030679
C	-2.3974202499	1.5179014151	0.4874254632
C	-3.6255706516	0.8400364733	0.7440600366
C	-2.3102741933	2.9199801472	0.6865184021
H	-3.1922584277	3.4529132619	1.0373556536
C	0.0002528603	1.4621882784	0.0000000000
H	-4.6959017502	-0.9998916587	0.6981825103
H	-3.8805064719	-3.0002495513	-0.3916956235
H	-4.4428755029	1.4089338842	1.1845261648
C	-1.1760192866	3.5886568157	0.3547305406
C	0.0004739427	2.8797549532	0.0000000000
C	1.2829174383	0.8013869045	-0.0050540520
H	-1.1338052595	4.6756650136	0.3962701589
C	2.3112693798	2.9192721875	-0.6865130944
C	2.3979812836	1.5171715792	-0.4873870650
C	3.6259555063	0.8389296145	-0.7438819790
C	3.7695463983	-0.4782151074	-0.4655860742
C	2.7407725385	-1.1824081331	0.2242057308
C	1.5223892982	-0.5226855261	0.5300468764
H	4.4434785109	1.4075715810	-1.1842730118
H	4.6957268042	-1.0013214955	-0.6978522031
H	3.1934407736	3.4519355912	-1.0372891096
C	-1.5225541846	-0.5222344051	-0.5300765262
C	-0.6294805496	-1.1796829551	-1.4018720355
C	-0.8678350518	-2.4558887542	-1.8471493795
H	-2.1963199715	-4.1631478784	-1.7828381926
H	0.2630872322	-0.6630415451	-1.7422201057
H	-0.1589659808	-2.9312062290	-2.5212529296
C	0.6289466733	-1.1798904190	1.4016435844
C	0.8668451412	-2.4561763620	1.8469379255
H	2.1948339943	-4.1638286173	1.7828256511
H	-0.2635498823	-0.6629960676	1.7418058128
H	0.1577087182	-2.9313024016	2.5208947349

14) Hexa-peri-hexabenzo [7] helicene E =-1842.622090 hartree

C	-2.7052089195	2.8489983218	0.1137772438
C	-1.4304807737	3.5323120002	0.0284857082
C	-2.7213979268	1.4372427906	0.0462487316
C	-1.5002292035	0.7129288217	-0.1588089469
C	-0.3906581684	1.3933428313	-0.6406343881
C	-0.2873472694	2.7992271360	-0.3764967401
C	-1.2903621309	4.8916347112	0.3306802412
C	-0.0624289813	5.5096037250	0.2486007187
C	1.0677281183	4.7809506988	-0.1011397273
C	0.9892123175	3.4269103458	-0.3948463415
H	-2.1516673317	5.4699203555	0.6530003493
H	0.0285850779	6.5688593880	0.4775351533

H	2.0261186626	5.2913462355	-0.1417893717
C	-5.1035456514	2.8337634527	0.3861306282
C	-3.9187660160	3.5273457038	0.2822027906
C	-5.1193874708	1.4464843837	0.2913018816
C	-3.9484517251	0.7274100154	0.0999817891
H	-6.0727731629	0.9306731893	0.3652636288
H	-6.0370934424	3.3735764215	0.5264561100
H	-3.9381499519	4.6130044468	0.3170975534
C	-3.9484625097	-0.7273526367	-0.0999948032
C	-2.7214199406	-1.4372050073	-0.0462549385
C	-1.5002410994	-0.7129092845	0.1588060920
C	-5.1194089607	-1.4464082775	-0.2913179331
C	-5.1035889752	-2.8336879286	-0.3861418246
C	-3.9188209552	-3.5272890766	-0.2822062260
C	-2.7052529894	-2.8489613058	-0.1137787302
H	-6.0727861278	-0.9305819697	-0.3652839624
H	-6.0371450901	-3.3734860381	-0.5264689008
H	-3.9382227190	-4.6129475444	-0.3170968083
C	-0.3906821275	-1.3933385926	0.6406352030
C	-0.2873920393	-2.7992252786	0.3765030167
C	-1.4305358663	-3.5322954581	-0.0284770500
C	-1.2904368189	-4.8916239372	-0.3306571077
C	-0.0625142884	-5.5096122447	-0.2485638679
C	1.0676538853	-4.7809723792	0.1011696973
C	0.9891583626	-3.4269267820	0.3948563329
H	-2.1517499310	-5.4698998764	-0.6529731602
H	0.0284830562	-6.5688727233	-0.4774828150
H	2.0260366401	-5.2913817327	0.1418323599
C	0.7326519972	-0.7409511152	1.3087186215
C	2.1876569701	-2.6289188222	0.6734323947
C	2.0233355027	-1.3228837112	1.2079937559
C	0.5862221065	0.4207313374	2.0474118116
C	1.6964526324	1.1089476786	2.5456827289
C	2.9644667841	0.6429730338	2.3073453350
C	3.1574773982	-0.5904519364	1.6534227886
H	-0.4084304961	0.8312155972	2.2094487681
H	1.5462799454	2.0370699056	3.0928237543
H	3.8369450643	1.2040347061	2.6388798529
C	4.4467716971	-1.1223989082	1.4318646832
C	4.5955040590	-2.3426057937	0.8312758705
C	3.4705473252	-3.1007761342	0.4719188119
H	3.6300978579	-4.0806146913	0.0290776505
H	5.3139017685	-0.5442667200	1.7480016630
H	5.5890914338	-2.7475323011	0.6517002773
C	2.1876989286	2.6288886379	-0.6734338976
C	2.0233584954	1.3228567920	-1.2079974549
C	0.7326668830	0.7409418122	-1.3087218389
C	0.5862208206	-0.4207340811	-2.0474237816
C	1.6964415355	-1.1089669089	-2.5456934554
C	2.9644616670	-0.6430114733	-2.3073532303
C	3.1574894741	0.5904097345	-1.6534284772
H	-0.4084375633	-0.8312004628	-2.2094685488
H	1.5462557672	-2.0370838865	-3.0928398731
H	3.8369326551	-1.2040829194	-2.6388903783
C	3.4705964222	3.1007288416	-0.4719250224
C	4.5955419428	2.3425427211	-0.8312831203
C	4.4467916418	1.1223378200	-1.4318715625
H	3.6301627773	4.0805644723	-0.0290831855
H	5.5891350380	2.7474562954	-0.6517100988
H	5.3139129870	0.5441925082	-1.7480085106

15) Hexa-peri-hexabenzo [7] helicene IEFPCM(chloroform) E =-1842.630774 hartree

C	2.6967106669	2.8477079549	-0.1429683219
C	1.4204430017	3.5290611376	-0.0592577774
C	2.7151812958	1.4368882948	-0.0607508868
C	1.4951960085	0.7137795164	0.1532979515
C	0.3859388787	1.3941472971	0.6347035075
C	0.2807618929	2.7989658653	0.3626979845
C	1.2777475357	4.8851886025	-0.3765090515
C	0.0493660273	5.5029338167	-0.2926955983
C	-1.0770954863	4.7784190462	0.0792079471
C	-0.9947874640	3.4282318653	0.3913272289
H	2.1357616247	5.4610114455	-0.7113279972
H	-0.0451597652	6.5584259714	-0.5358722284
H	-2.0344837319	5.2901233387	0.1200365074
C	5.0954348994	2.8327342719	-0.4162432849
C	3.9093088943	3.5266315315	-0.3208026242
C	5.1139377235	1.4458972934	-0.3048263514
C	3.9431354627	0.7274045225	-0.1073623078
H	6.0690794002	0.9322221439	-0.3689473965
H	6.0281006578	3.3720673616	-0.5621965298
H	3.9282410715	4.6116363015	-0.3699878499
C	3.9434501432	-0.7257490763	0.1075645842
C	2.7158190072	-1.4357874633	0.0608109426
C	1.4955296865	-0.7132124184	-0.1532789821
C	5.1145547758	-1.4437162789	0.3051288572
C	5.0966666070	-2.8305656296	0.4165058891
C	3.9108684854	-3.5249976969	0.3208954170
C	2.6979783532	-2.8466218557	0.1429383387
H	6.0694563860	-0.9296094531	0.3693636965
H	6.0295567948	-3.3694831141	0.5625595718
H	3.9302984385	-4.6099937989	0.3700509902
C	0.3866016039	-1.3940413611	-0.6347625425
C	0.2820405020	-2.7989354800	-0.3629239400
C	1.4220315546	-3.5285594723	0.0590165874
C	1.2799382235	-4.8848086533	0.3760334397
C	0.0518538445	-5.5031128373	0.2920145325
C	-1.0749196101	-4.7790553712	-0.0798402086
C	-0.9932180726	-3.4287767538	-0.3917130853
H	2.1381881615	-5.4602912353	0.7108302002
H	-0.0421994472	-6.5586879141	0.5350135749
H	-2.0320707262	-5.2911902975	-0.1208038625
C	-0.7283073571	-0.7451880519	-1.3219924286
C	-2.1884095660	-2.6388255435	-0.7087662556
C	-2.0175303176	-1.3362319523	-1.2516523099
C	-0.5709901797	0.4114930484	-2.0674187372
C	-1.6709575041	1.0808146231	-2.6138135434
C	-2.9417802850	0.6024797587	-2.4158850261
C	-3.1438263672	-0.6214672402	-1.7452996525
H	0.4238988027	0.8296839256	-2.2066555115
H	-1.5111827960	1.9991588829	-3.1743214581
H	-3.8074334440	1.1437175794	-2.7945414306
C	-4.4351278141	-1.1659450014	-1.5661788394
C	-4.5927016212	-2.3809208008	-0.9559567366
C	-3.4730689657	-3.1225657679	-0.5476872792
H	-3.6396234340	-4.1008272869	-0.1045264165
H	-5.2961924298	-0.6036633429	-1.9240617098
H	-5.5873081595	-2.7950369045	-0.8076950567
C	-2.1896204240	2.6378054221	0.7085309993
C	-2.0181552123	1.3354130718	1.2517091859
C	-0.7286861156	0.7449045346	1.3220529136
C	-0.5708385387	-0.4115702098	2.0676923853
C	-1.6704812869	-1.0811853011	2.6143867270

C	-2.9415091293	-0.6033433494	2.4165739831
C	-3.1441145148	0.6203405743	1.7456787921
H	0.4242245017	-0.8293569311	2.2068843807
H	-1.5102895766	-1.9993210334	3.1751145572
H	-3.8068984511	-1.1447767911	2.7955552177
C	-3.4744946273	3.1209286259	0.5473295977
C	-4.5937909536	2.3789345818	0.9558885045
C	-4.4356573405	1.1642337852	1.5665124698
H	-3.6414811423	4.0989695150	0.1038434752
H	-5.5885840058	2.7925749075	0.8075499563
H	-5.2964567009	0.6017140128	1.9246573411

16) mono-aza-[7]-helicene E =-1131.373207 hartree

C	-1.7823386546	0.6051558025	0.0618138382
C	-3.0778189610	1.0164986366	-0.3453275447
C	-0.7285472066	1.5670724663	-0.0348436650
C	-1.1069848227	2.9207535556	-0.1547810596
C	-2.4089806976	3.3438352547	-0.4361762823
C	-3.3622547227	2.3783573818	-0.5967117376
H	-2.6369725289	4.4004927158	-0.5602742565
H	-4.3778535728	2.6508306693	-0.8785747192
C	0.7285794494	1.5670432504	0.0348363296
C	1.1070292524	2.9206940073	0.1550076347
N	0.0000000000	3.7126442268	0.0005213887
H	0.0002616419	4.7204889268	-0.0009476100
C	3.0778664282	1.0164402471	0.3450812762
C	3.3623922347	2.3782873240	0.5964292205
C	2.4090638208	3.3437819983	0.4362199633
H	4.3780366046	2.6507247175	0.8781546319
H	2.6370344162	4.4004232984	0.5604881076
C	-1.6488420983	-0.7253767102	0.6082656870
C	-2.6914356803	-1.6688738318	0.4176577862
C	-3.9154688716	-1.2539119389	-0.1811770057
C	-4.1166165219	0.0483363923	-0.4858237411
H	-4.7050349414	-1.9905347232	-0.3218721749
H	-5.0812136958	0.3867476811	-0.8622197884
C	-0.5512302687	-1.1142148281	1.4000786804
C	-0.4298201025	-2.3943897685	1.8810298181
C	-1.4104275610	-3.3522061026	1.5933201216
C	-2.5297018365	-2.9848141665	0.8894038281
H	0.2071521025	-0.3796820440	1.6521150594
H	0.4339801678	-2.6622956058	2.4853596279
H	-1.3011773806	-4.3715012555	1.9569875551
H	-3.3288623760	-3.7027589690	0.7082282041
C	1.7823357494	0.6051116162	-0.0619031623
C	1.6488051194	-0.7254322050	-0.6082687033
C	2.6913303793	-1.6689808261	-0.4175413915
C	3.9154416930	-1.2540239340	0.1811495710
C	4.1166781023	0.0482766176	0.4855536258
H	4.7049867863	-1.9906634614	0.3218581247
H	5.0813275218	0.3867264659	0.8617791584
C	2.5295097875	-2.9849596373	-0.8891452456
C	1.4102485773	-3.3523357828	-1.5931173885
C	0.5513310823	-1.1142056204	-1.4002790533
H	3.3285973217	-3.7029469010	-0.7078342581
C	0.4298179229	-2.3944259642	-1.8810937744
H	1.3009173482	-4.3716633425	-1.9566680590
H	-0.2068604359	-0.3795811977	-1.6526518726
H	-0.4339288884	-2.6622759310	-2.4855232654

17) tri-aza-[7]-helicene E =-1087.298895 hartree

C	1.0990025073	-1.7488592847	-1.0317761890
C	1.6003102298	-2.9862183752	-1.3896872222
C	1.9111750647	-0.8546079605	-0.3298745599
C	3.2544005225	-1.2182670541	-0.0784857964
C	3.7597477297	-2.4669757682	-0.4229022324
C	2.9138751620	-3.3473410749	-1.0722278391
H	0.0854065215	-1.4706793607	-1.3067595175
H	0.9674103381	-3.6848193271	-1.9314374188
H	4.7931830798	-2.7328156977	-0.2081184700
H	3.2844235026	-4.3287505262	-1.3604117207
C	1.7545728375	0.5074592562	0.1207658321
C	3.0352385791	0.9346755682	0.5275030623
N	3.9034576231	-0.1428067472	0.4802794700
H	4.9031686207	-0.0726799943	0.5852480183
C	0.7114510203	1.4612442527	0.1165067033
C	1.0905460756	2.8160607446	0.2676825383
C	2.3747323485	3.2235839458	0.6320673212
C	3.3504325916	2.2648799063	0.8081385283
H	2.5994708513	4.2784196297	0.7761667525
H	4.3595416230	2.5463088302	1.1022667846
C	-0.7114509674	1.4612442580	-0.1165067213
C	-1.0905460068	2.8160607605	-0.2676825701
N	0.0000000000	3.6118409213	0.0000000000
H	0.0000000000	4.6188272218	0.0000000000
C	-1.7545728269	0.5074593080	-0.1207657236
C	-3.0352385474	0.9346756581	-0.5275030310
C	-3.3504324964	2.2648799804	-0.8081386659
C	-2.3747322374	3.2235840040	-0.6320674482
H	-4.3595415330	2.5463088885	-1.1022669274
H	-2.5994707031	4.2784196985	-0.7761668266
C	-1.9111750858	-0.8546079076	0.3298746049
C	-3.2544005436	-1.2182669906	0.0784858007
N	-3.9034576496	-0.1428065836	-0.4802792403
H	-4.9031686207	-0.0726799197	-0.5852481135
C	-1.0990025655	-1.7488593006	1.0317762155
C	-1.6003103144	-2.9862184017	1.3896871534
C	-2.9138752467	-3.3473410802	1.0722277227
C	-3.7597477879	-2.4669757206	0.4229021667
H	-0.0854065771	-1.4706794242	1.3067595810
H	-0.9674104281	-3.6848193853	1.9314373288
H	-3.2844236138	-4.3287505368	1.3604115725
H	-4.7931831645	-2.7328155707	0.2081184314

18) tetra-aza-[7]-helicene E =-1065.244613 hartree

C	1.9094155875	-1.0009022072	-0.3832917893
C	3.1880057109	-1.5945894484	-0.2933717238
C	1.7613097026	0.3240848246	0.0901802461
C	2.9375172281	1.0003590968	0.4735539843
C	4.1936340262	0.3882473048	0.5679599470
C	4.3178452846	-0.9321092280	0.1975313200
C	0.6998285424	1.2976110808	0.1035276850
C	1.3129313801	2.5459101852	0.3534093729
N	2.6399639042	2.3331088778	0.6645190396
C	-0.6997486367	1.2976494461	-0.1035392507
C	-1.3127848721	2.5459833016	-0.3534103202

C	-0.6573757029	3.7706956177	-0.2073392518
C	0.6575875008	3.7706587870	0.2073490480
C	-1.7612814339	0.3241793913	-0.0902017460
C	-2.9374527585	1.0005194004	-0.4735709984
N	-2.6398285195	2.3332552536	-0.6645227809
C	-1.9094576571	-1.0008037538	0.3832585882
C	-3.1880785627	-1.5944232815	0.2933295870
C	-4.3178824805	-0.9318791471	-0.1975691112
C	-4.1936015824	0.3884743821	-0.5679847971
C	-1.0754578363	-1.9268813194	1.0772476141
C	-1.8318334087	-3.0289760103	1.3488715776
N	-3.1011684133	-2.8469481358	0.8587987741
C	1.0753646270	-1.9269306493	-1.0772847729
C	1.8316861281	-3.0290561912	-1.3489342851
N	3.1010282078	-2.8471045553	-0.8588517871
H	5.0590756519	0.9552927251	0.9052133730
H	5.2829961525	-1.4333071356	0.2429077970
H	3.3323292488	3.0617132515	0.7352528450
H	-1.1873672485	4.7057955543	-0.3777787307
H	1.1876291013	4.7057289044	0.3777964227
H	-3.3321550172	3.0618971088	-0.7352507336
H	-5.2830596061	-1.4330259150	-0.2429517552
H	-5.0590130555	0.9555685269	-0.9052336457
H	-0.0363630026	-1.7933173831	1.3440292092
H	-1.5638339705	-3.9453888103	1.8579595068
H	-3.8753252344	-3.4758844636	0.9953951870
H	0.0362750777	-1.7933108213	-1.3440591553
H	1.5636397255	-3.9454469140	-1.8580372376
H	3.8751510980	-3.4760816880	-0.9954524016