

Electronic Supplementary Information to:

On the HOMA index of some acyclic and conducting systems

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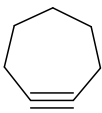
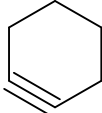
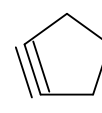
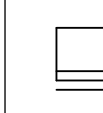
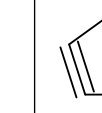
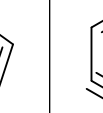
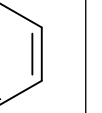
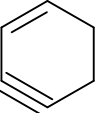
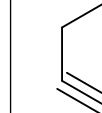
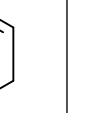
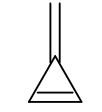
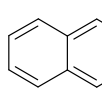
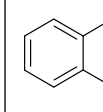
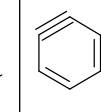
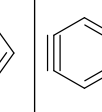
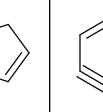
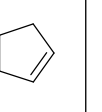
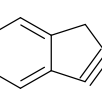
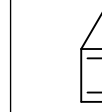
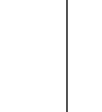
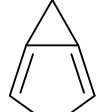
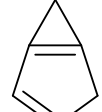
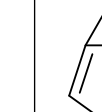
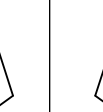
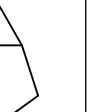
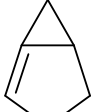
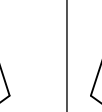
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	3	the other compounds
HOMA	4	HOMA(R) and HOMA(Rho) values used in Figures.
XYZ coordinates	5	Polycyclopentadienes
	11	Polypyrroles
	16	Polyfurans
	21	Polythiophenes
	26	Polyselenophenes
	31	Polyenes-all- <i>cis cisoid</i>
	34	Polyenes-all- <i>cis transoid</i>
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	40	Alkanes
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	45	Polyynes
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	52	Cyclic and bicyclic hydrocarbons
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R and Rho	58	All compounds

values		
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Total energies of polycyclopentadienes (C), polypyrroles (NH), polyfurans (O), polythiophenes (S) and polyselenophenes (Se) at the B3LYP/6-31G** level

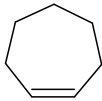
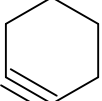
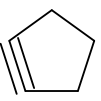
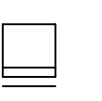
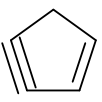
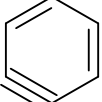
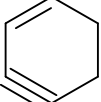
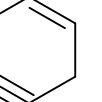
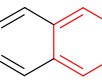
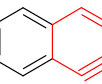
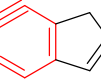
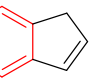
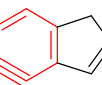
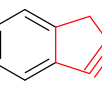
ring	C	NH	O	S	Se
1	-194.110690	-210.176337	-230.027372	-553.009299	-2554.192370
2	-387.038298	-419.165335	-458.870047	-1104.826559	-5107.199324
3	-579.967514	-628.154935	-687.713633	-1656.644944	-7660.207380
4	-772.897169	-837.144666	-916.557389	-2208.463482	-10213.215620
5	-965.826854	-1046.134342	-1145.401107	-2760.282048	-12766.223901
6	-1158.756648	-1255.124043	-1374.244865	-3312.100605	-15319.232136
7	-1351.686452	-1464.113745	-1603.088606	-3863.919192	-17872.240489
8	-1544.616273	-1673.103438	-1831.932369	-4415.737762	-20425.248783
9	-1737.546100	-1882.093142	-2060.776101	-4967.556332	-22978.257076
10	-1930.475997	-2091.082841	-2289.619825	-5519.374901	-25531.265368

Total Energy calculated at the B3LYP/6-31G** level

units	alkanes	allenes	cyclic-allene n-atoms	cyclic-polyenes	polyacetylenes	polyenes-all-cis	polyenes-all-trans	polyenes-cis-transoid	spiro-cyclopropanes		
1	-79.838739	-78.593808			-77.329567	-78.593808	-78.593808		-117.904157		
2	-158.471954	-116.664061			-153.485577	-155.996045	-156.001662		-195.283439		
3	-237.105010	-154.737026	n=6 -228.220743		-229.644035	-233.392277	-233.411275	-233.408231	-272.662751		
4	-315.738041	-192.813038		-304.354370	-305.803610	-310.792841	-310.821547	-310.815141	-350.042148		
5	-394.371071	-230.889475	n=10 -380.653499		-381.963643	-388.188153	-388.232176	-388.222222	-427.421446		
6	-473.004102	-268.967326		-456.770988	-458.123902	-465.598030	-465.642888	-465.629332	-504.800780		
7	-551.637132	-307.045047	n=14 -533.013666		-534.284277	-542.983645	-543.053782	-543.036633	-582.180111		
8	-630.270162	-345.123616		-609.141666	-610.444661	-620.381346	-620.464612	-620.443742	-659.559488		
9	-708.903193	-383.153795	n=18 -685.353963		-686.605148	-697.779107	-697.875612	-697.850957	-736.938785		
10	-787.536223	-421.280880		-761.492713	-762.765652	-775.176795	-775.286475	-775.258179	-814.318149		
20					-1524.370780	-1549.151913	1549.396225	-1549.330434			
											
	-272.673502	-233.34360362	-192.644989	-154.607706	-115.250579	-192.732475	-230.91630514	-232.101082	-232.109043	-193.967342	-195.292071
											
	-116.625633	-153.352493	-384.561353	-384.565469	-346.433050	-346.432199	-346.433311	-346.401014	-192.635396	-194.034008	-193.958530
											
	-232.097469	-232.099620	-230.89872382	-232.10480923	-232.10756102	-232.085678	-233.409974	-233.351359	-233.334059	-233.346050	-234.645303

The HOMA(R) and HOMA(Rho) values used for Figures.

# units	HOMA(R)					HOMA(Rho)			
	CH ₂	O	S	NH	Se	CH ₂	O	S	NH
1	-0.7424	0.6468	0.7591	0.8715	0.7008	0.5344	0.8630	0.9397	0.9526
2	-0.6230	0.7119	0.7488	0.8251	0.7393	0.5738	0.8984	0.9239	0.9384
3	-0.5605	0.7503	0.7740	0.8307	0.7749	0.5942	0.9140	0.9277	0.9403
4	-0.5272	0.7715	0.7873	0.8340	0.7960	0.6051	0.9223	0.9299	0.9413
5	-0.5028	0.7843	0.7965	0.8357	0.8079	0.6130	0.9273	0.9317	0.9419
6	-0.4891	0.7929	0.8026	0.8364	0.8157	0.6177	0.9306	0.9329	0.9421
7	-0.4776	0.7990	0.8073	0.8373	0.8243	0.6215	0.9330	0.9339	0.9424
8	-0.4690	0.8035	0.8107	0.8380	0.8291	0.6244	0.9347	0.9346	0.9426
9	-0.4622	0.8070	0.8133	0.8385	0.8329	0.6266	0.9361	0.9351	0.9428
10	-0.4571	0.8097	0.8152	0.8389	0.8357	0.6298	0.9372	0.9355	0.9429

			
-4.5999	-0.5270	-4.6788	-0.7021
			
-2.6410	-0.5161	0.0539	0.5496
			
-0.1845	0.5429	-0.2736	0.4111
			
0.0295	0.5517	-2.7001	-0.5498

units	alkanes		allenes		cyclic-allenes		cyclic-polyenes		polyacetylenes		polyenes-all-cis		polyenes-all-trans		polyenes-cis-transoid		spiro cyclopropanes	
	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)	HOMA (R)	HOMA (Rho)
1	-3.6362	-0.1908							-8.3874	-1.0389	-0.1212	0.6873	-0.1212	0.6873	-0.1212	0.6873	-2.2372	-0.3371
2	-3.7547	-0.1356	-0.1212	0.6873					-4.8681	-0.2874	-0.0373	0.7192	0.1368	0.7576	0.1368	0.7576	-1.8856	-0.2424
3	-3.8026	-0.1364	-1.0776	0.6096	-0.9340	-0.396			-4.0587	-0.0816	-0.0164	0.7257	0.3062	0.8026	0.2920	0.7998	-1.7188	-0.2064
4	-3.8228	-0.1364	-1.4062	0.5791			-2.788	-0.3960	-3.6945	0.0171	0.3876	0.8263	0.4065	0.8299	0.3857	0.8261	-1.6530	-0.1948
5	-3.8318	-0.1362	-1.6422	0.5518	-1.8539	0.1458			-3.4823	0.0768	-0.0221	0.7298	0.4730	0.8484	0.4460	0.8431	-1.6148	-0.1878
6	-3.8382	-0.1361	-1.7711	0.5314			-2.620	0.1458	-3.3415	0.1177	0.2166	0.7851	0.5206	0.8616	0.4884	0.8549	-1.5888	-0.1830
7			-1.8655	0.5212	-2.0848	0.2753			-3.2417	0.1470	0.0295	0.7428	0.5565	0.8717	0.5190	0.8635	-1.5711	-0.1799
8			-1.9316	0.5101			-2.604	0.2753	-3.1713	0.1685	0.0120	0.7394	0.5809	0.8784	0.5432	0.8703	-1.5574	-0.1774
9			-1.9837	0.5043	-2.1757	0.3188			-3.1141	0.1860	-0.0031	0.7574	0.6071	0.8961	0.5604	0.8871	-1.5462	-0.1752
10	-3.8505	-0.1359	-2.0246	0.4971			-2.600	0.3188	-3.0687	0.2013	0.0112	0.7604	0.6253	0.8969	0.5751	0.8876	-1.5364	-0.1735
20			-2.0578	0.4933											0.6401	0.9039		

Polycyclopentadienes

1C				2C			
6	-1.183455000	-0.269759000	-0.000002000	6	3.016968000	-0.581291000	0.000064000
6	-0.724466000	0.998690000	-0.000024000	6	2.915950000	0.765568000	-0.000167000
6	0.745068000	0.983294000	0.000040000	6	1.508400000	1.148987000	-0.000124000
6	1.177669000	-0.294174000	-0.000040000	6	0.720095000	0.034551000	-0.000021000
6	-0.012711000	-1.216226000	0.000027000	6	-0.720101000	-0.034522000	0.000016000
1	-2.219052000	-0.587598000	-0.000002000	6	-1.508380000	-1.148975000	0.000068000
1	1.367269000	1.871640000	0.000069000	6	-2.915951000	-0.765586000	-0.000325000
1	-1.327901000	1.899759000	-0.000030000	6	-3.016968000	0.581265000	0.000092000
1	2.206387000	-0.633816000	-0.000072000	1	3.927965000	-1.167067000	0.000124000
1	-0.019670000	-1.880453000	-0.877089000	1	1.154068000	2.173923000	-0.000229000
1	-0.019661000	-1.880478000	0.877123000	1	3.740532000	1.470059000	-0.000295000
				1	-1.154031000	-2.173904000	0.000024000
				1	-3.740509000	-1.470101000	-0.000565000
				1	-3.928021000	1.167124000	0.000178000
				6	-1.633978000	1.176578000	0.000187000
				1	-1.462791000	1.814663000	-0.877981000
				1	-1.462837000	1.814215000	0.878695000
				6	1.633980000	-1.176582000	0.000144000
				1	1.462779000	-1.814553000	-0.878109000
				1	1.462750000	-1.814326000	0.878555000
3C				4C			
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6	0.000000000	4.495484000	1.322850000	6	3.398420000	5.598205000	0.000000000
6	0.000000000	3.038366000	1.327529000	6	2.952700000	4.211404000	0.000000000
6	0.000000000	2.565790000	0.044358000	6	1.585750000	4.158295000	0.000000000
6	0.000000000	1.197419000	-0.393982000	6	0.746847000	2.993157000	0.000000000
6	0.000000000	0.722228000	-1.677992000	6	-0.622452000	2.938421000	0.000000000
6	0.000000000	-0.722228000	-1.677992000	6	-1.070283000	1.568054000	0.000000000
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6	0.000000000	-2.565790000	0.044358000	6	-0.004922000	-0.715436000	0.000000000
6	0.000000000	-3.038366000	1.327529000	6	1.070283000	-1.568054000	0.000000000
6	0.000000000	-4.495484000	1.322850000	6	0.622452000	-2.938421000	0.000000000
6	0.000000000	-4.944054000	0.048150000	6	-0.746847000	-2.993157000	0.000000000
1	0.000000000	5.976196000	-0.279976000	6	-1.585750000	-4.158295000	0.000000000
1	0.000000000	2.429793000	2.225082000	6	-2.952700000	-4.211404000	0.000000000
1	0.000000000	5.108739000	2.217389000	6	-3.398420000	-5.598205000	0.000000000
1	0.000000000	1.331574000	-2.575180000	6	-2.324673000	-6.419018000	0.000000000
1	0.000000000	-1.331574000	-2.575180000	1	2.331834000	7.502021000	0.000000000
1	0.000000000	-5.108739000	2.217389000	1	3.618165000	3.355286000	0.000000000
1	0.000000000	-2.429793000	2.225082000	1	4.438688000	5.905015000	0.000000000
1	0.000000000	-5.976196000	-0.279976000	1	-1.286090000	3.796162000	0.000000000
6	0.000000000	-3.764114000	-0.887240000	1	-2.112176000	1.267240000	0.000000000
1	0.878256000	-3.765786000	-1.547771000	1	1.286090000	-3.796162000	0.000000000
1	-0.878256000	-3.765786000	-1.547771000	1	2.112176000	-1.267240000	0.000000000
6	0.000000000	0.000000000	0.537281000	1	-3.618165000	-3.355286000	0.000000000
1	-0.879208000	0.000000000	1.194342000	1	-4.438688000	-5.905015000	0.000000000
1	0.879208000	0.000000000	1.194342000	1	-2.331834000	-7.502021000	0.000000000
6	0.000000000	3.764114000	-0.887240000	6	1.070283000	5.586179000	0.000000000
1	-0.878256000	3.765786000	-1.547771000	1	0.442887000	5.792295000	0.878338000
1	0.878256000	3.765786000	-1.547771000	1	0.442887000	5.792295000	-0.878338000
				6	1.261873000	1.566168000	0.000000000
				1	1.886437000	1.363242000	-0.879364000
				1	1.886437000	1.363242000	0.879364000
				6	-1.261873000	-1.566168000	0.000000000
				1	-1.886437000	-1.363242000	-0.879364000
				1	-1.886437000	-1.363242000	0.879364000
				6	-1.070283000	-5.586179000	0.000000000
				1	-0.442887000	-5.792295000	0.878338000
				1	-0.442887000	-5.792295000	-0.878338000

5C				6C			
6	0.000000000	8.701878000	-0.117957000	6	-8.204315000	-0.022867000	-0.000207000
6	0.000000000	8.252931000	-1.392852000	6	-6.827072000	0.380700000	0.000064000
6	0.000000000	6.796571000	-1.397702000	6	-6.319776000	1.654644000	0.000457000
6	0.000000000	6.323367000	-0.113715000	6	-4.879807000	1.621656000	0.000586000
6	0.000000000	4.956125000	0.322936000	6	-4.432157000	0.323042000	0.000275000
6	0.000000000	4.479704000	1.608662000	6	-3.081021000	-0.141384000	0.000265000
6	0.000000000	3.039207000	1.610396000	6	-2.632900000	-1.440890000	0.000218000
6	0.000000000	2.560501000	0.323158000	6	-1.196046000	-1.475827000	0.000207000
6	0.000000000	1.198112000	-0.108903000	6	-0.685481000	-0.199053000	0.000235000
6	0.000000000	0.719067000	-1.396784000	6	0.685481000	0.199058000	0.000183000
6	0.000000000	-0.719067000	-1.396784000	6	1.196047000	1.475832000	-0.000001000
6	0.000000000	-1.198112000	-0.108903000	6	2.632901000	1.440893000	-0.000053000
6	0.000000000	-2.560501000	0.323158000	6	3.081021000	0.141388000	0.000128000
6	0.000000000	-3.039207000	1.610396000	6	4.432157000	-0.323039000	0.000161000
6	0.000000000	-4.479704000	1.608662000	6	4.879806000	-1.621653000	0.000510000
6	0.000000000	-4.956125000	0.322936000	6	6.319775000	-1.654643000	0.000453000
6	0.000000000	-6.323367000	-0.113715000	6	6.827072000	-0.380699000	0.000033000
6	0.000000000	-6.796571000	-1.397702000	6	8.204313000	0.022866000	-0.000180000
6	0.000000000	-8.252931000	-1.392852000	6	8.709035000	1.294783000	-0.000608000
6	0.000000000	-8.701878000	-0.117957000	6	10.164872000	1.253864000	-0.000678000
1	0.000000000	9.734068000	0.210035000	6	10.582122000	-0.031730000	-0.000351000
1	0.000000000	6.187670000	-2.294991000	1	-11.605983000	0.384818000	-0.000333000
1	0.000000000	8.866471000	-2.287189000	1	-8.122689000	-2.206956000	-0.001154000
1	0.000000000	5.090454000	2.504940000	1	-10.800179000	-2.132878000	-0.001328000
1	0.000000000	2.429935000	2.507511000	1	-6.908479000	2.565523000	0.000649000
1	0.000000000	-1.329220000	-2.293354000	1	-4.249566000	2.504162000	0.000881000
1	0.000000000	1.329220000	-2.293354000	1	-0.607940000	-2.386964000	0.000173000
1	0.000000000	-2.429935000	2.507511000	1	-3.264223000	-2.322686000	0.000191000
1	0.000000000	-5.090454000	2.504940000	1	0.607941000	2.386969000	-0.000113000
1	0.000000000	-8.866471000	-2.287189000	1	3.264225000	2.322689000	-0.000201000
1	0.000000000	-6.187670000	-2.294991000	1	6.908478000	-2.565523000	0.000699000
1	0.000000000	-9.734068000	0.210035000	1	4.249564000	-2.504159000	0.000811000
6	0.000000000	7.521882000	0.817697000	1	8.122703000	2.206962000	-0.000841000
1	0.878004000	7.524145000	1.478414000	1	10.800173000	2.132873000	-0.000973000
1	-0.878004000	7.524145000	1.478414000	1	11.605981000	-0.384834000	-0.000320000
6	0.000000000	3.758777000	-0.608607000	6	-9.379795000	0.937928000	0.000109000
1	-0.879085000	3.759631000	-1.265595000	1	-9.365355000	1.598673000	-0.877920000
1	0.879085000	3.759631000	-1.265595000	1	-9.365493000	1.597896000	0.878726000
6	0.000000000	0.000000000	0.823191000	6	-5.652658000	-0.579661000	-0.000067000
1	0.879211000	0.000000000	1.479856000	1	-5.669633000	-1.236399000	0.879171000
1	-0.879211000	0.000000000	1.479856000	1	-5.669434000	-1.235992000	-0.879611000
6	0.000000000	-3.758777000	-0.608607000	6	-1.860951000	0.761686000	0.000317000
1	0.879085000	-3.759631000	-1.265595000	1	-1.845254000	1.418124000	-0.879083000
1	-0.879085000	-3.759631000	-1.265595000	1	-1.845201000	1.417911000	0.879881000
6	0.000000000	-7.521882000	0.817697000	6	1.860951000	-0.761682000	0.000296000
1	-0.878004000	-7.524145000	1.478414000	1	1.845215000	-1.418155000	-0.879079000
1	0.878004000	-7.524145000	1.478414000	1	1.845239000	-1.417871000	0.879885000
				6	5.652658000	0.579663000	-0.000209000
				1	5.669591000	1.236520000	0.878939000
				1	5.669478000	1.235875000	-0.879843000
				6	9.379795000	-0.937932000	0.000010000
				1	9.365338000	-1.598542000	-0.878121000
				1	9.365484000	-1.598041000	0.878521000

7C							
6	0.000000000	12.457795000	0.147965000	1	0.000000000	2.429162000	2.324637000
6	0.000000000	12.009139000	1.422945000	1	0.000000000	5.085932000	2.323723000
6	0.000000000	10.552793000	1.428166000	1	0.000000000	1.328076000	-2.477261000
6	0.000000000	10.079311000	0.144241000	1	0.000000000	-1.328076000	-2.477261000
6	0.000000000	8.712363000	-0.292593000	1	0.000000000	-5.085932000	2.323723000
6	0.000000000	8.235965000	-1.578532000	1	0.000000000	-2.429162000	2.324637000
6	0.000000000	6.795812000	-1.580525000	1	0.000000000	-6.186951000	-2.477909000
6	0.000000000	6.316691000	-0.293005000	1	0.000000000	-8.846565000	-2.474900000
6	0.000000000	4.955003000	0.138622000	1	0.000000000	-12.622710000	2.317255000
6	0.000000000	4.475641000	1.427248000	1	0.000000000	-9.944356000	2.325758000
6	0.000000000	3.038910000	1.427829000	1	0.000000000	-13.489997000	-0.179978000
6	0.000000000	2.558666000	0.138818000	6	0.000000000	-11.277910000	-0.787457000
6	0.000000000	1.198235000	-0.291382000	1	0.878288000	-11.279804000	-1.447962000
6	0.000000000	0.717976000	-1.580677000	1	-0.878288000	-11.279804000	-1.447962000
6	0.000000000	-0.717976000	-1.580677000	6	0.000000000	-7.515025000	0.639009000
6	0.000000000	-1.198235000	-0.291382000	1	-0.879352000	-7.515919000	1.295788000
6	0.000000000	-2.558666000	0.138818000	1	0.879352000	-7.515919000	1.295788000
6	0.000000000	-3.038910000	1.427829000	6	0.000000000	-3.756938000	-0.793487000
6	0.000000000	-4.475641000	1.427248000	1	0.879453000	-3.757129000	-1.450024000
6	0.000000000	-4.955003000	0.138622000	1	-0.879453000	-3.757129000	-1.450024000
6	0.000000000	-6.316691000	-0.293005000	6	0.000000000	0.000000000	0.640867000
6	0.000000000	-6.795812000	-1.580525000	1	-0.879456000	0.000000000	1.297375000
6	0.000000000	-8.235965000	-1.578532000	1	0.879456000	0.000000000	1.297375000
6	0.000000000	-8.712363000	-0.292593000	6	0.000000000	3.756938000	-0.793487000
6	0.000000000	-10.079311000	0.144241000	1	-0.879453000	3.757129000	-1.450024000
6	0.000000000	-10.552793000	1.428166000	1	0.879453000	3.757129000	-1.450024000
6	0.000000000	-12.009139000	1.422945000	6	0.000000000	7.515025000	0.639009000
6	0.000000000	-12.457795000	0.147965000	1	0.879352000	7.515919000	1.295788000
1	0.000000000	13.489997000	-0.179978000	1	-0.879352000	7.515919000	1.295788000
1	0.000000000	9.944356000	2.325758000	6	0.000000000	11.277910000	-0.787457000
1	0.000000000	12.622710000	2.317255000	1	-0.878288000	11.279804000	-1.447962000
1	0.000000000	8.846565000	-2.474900000	1	0.878288000	11.279804000	-1.447962000
1	0.000000000	6.186951000	-2.477909000				

8C							
6	0.223776000	14.335674000	0.000000000	1	2.401093000	4.307416000	0.000000000
6	1.498803000	13.887115000	0.000000000	1	2.399996000	6.963972000	0.000000000
6	1.504154000	12.430787000	0.000000000	1	-2.400902000	3.206166000	0.000000000
6	0.220263000	11.957177000	0.000000000	1	-2.401051000	0.550408000	0.000000000
6	-0.216477000	10.590248000	0.000000000	1	2.400902000	-3.206166000	0.000000000
6	-1.502443000	10.113756000	0.000000000	1	2.401051000	-0.550408000	0.000000000
6	-1.504389000	8.673694000	0.000000000	1	-2.401093000	-4.307416000	0.000000000
6	-0.216771000	8.194581000	0.000000000	1	-2.399996000	-6.963972000	0.000000000
6	0.214821000	6.833016000	0.000000000	1	2.398831000	-10.724332000	0.000000000
6	1.503565000	6.353613000	0.000000000	1	2.401735000	-8.064784000	0.000000000
6	1.504247000	4.917113000	0.000000000	1	-2.401799000	-11.822419000	0.000000000
6	0.215096000	4.436639000	0.000000000	1	-2.393058000	-14.500763000	0.000000000
6	-0.214838000	3.076460000	0.000000000	1	0.104277000	-15.367839000	0.000000000
6	-1.504389000	2.595962000	0.000000000	6	0.711568000	-13.155678000	0.000000000
6	-1.504500000	1.160541000	0.000000000	1	1.372083000	-13.157535000	0.878288000
6	-0.214821000	0.679909000	0.000000000	1	1.372083000	-13.157535000	-0.878288000
6	0.214821000	-0.679909000	0.000000000	6	-0.715182000	-9.392959000	0.000000000
6	1.504500000	-1.160541000	0.000000000	1	-1.371939000	-9.393893000	-0.879351000
6	1.504389000	-2.595962000	0.000000000	1	-1.371939000	-9.393893000	0.879351000
6	0.214838000	-3.076460000	0.000000000	6	0.717282000	-5.634927000	0.000000000
6	-0.215096000	-4.436639000	0.000000000	1	1.373785000	-5.635131000	0.879455000
6	-1.504247000	-4.917113000	0.000000000	1	1.373785000	-5.635131000	-0.879455000
6	-1.503565000	-6.353613000	0.000000000	6	-0.717423000	-1.878228000	0.000000000
6	-0.214821000	-6.833016000	0.000000000	1	-1.373942000	-1.878309000	-0.879447000
6	0.216771000	-8.194581000	0.000000000	1	-1.373942000	-1.878309000	0.879447000
6	1.504389000	-8.673694000	0.000000000	6	0.717423000	1.878228000	0.000000000
6	1.502443000	-10.113756000	0.000000000	1	1.373942000	1.878309000	-0.879447000
6	0.216477000	-10.590248000	0.000000000	1	1.373942000	1.878309000	0.879447000
6	-0.220263000	-11.957177000	0.000000000	6	-0.717282000	5.634927000	0.000000000
6	-1.504154000	-12.430787000	0.000000000	1	-1.373785000	5.635131000	0.879455000
6	-1.498803000	-13.887115000	0.000000000	1	-1.373785000	5.635131000	-0.879455000
6	-0.223776000	-14.335674000	0.000000000	6	0.715182000	9.392959000	0.000000000
1	-0.104277000	15.367839000	0.000000000	1	1.371939000	9.393893000	-0.879351000
1	2.401799000	11.822419000	0.000000000	1	1.371939000	9.393893000	0.879351000
1	2.393058000	14.500763000	0.000000000	6	-0.711568000	13.155678000	0.000000000
1	-2.398831000	10.724332000	0.000000000	1	-1.372083000	13.157535000	0.878288000
1	-2.401735000	8.064784000	0.000000000	1	-1.372083000	13.157535000	-0.878288000

9-C							
6	0.000000000	16.213499000	-0.164754000	1	0.000000000	5.084224000	2.460396000
6	0.000000000	15.764876000	-1.439770000	1	0.000000000	2.428721000	2.460710000
6	0.000000000	14.308578000	-1.445039000	1	0.000000000	-1.327629000	-2.341466000
6	0.000000000	13.835053000	-0.161087000	1	0.000000000	1.327629000	-2.341466000
6	0.000000000	12.468146000	0.275651000	1	0.000000000	-2.428721000	2.460710000
6	0.000000000	11.991713000	1.561654000	1	0.000000000	-5.084224000	2.460396000
6	0.000000000	10.551691000	1.563652000	1	0.000000000	-8.841810000	-2.340656000
6	0.000000000	10.072531000	0.276010000	1	0.000000000	-6.185292000	-2.341624000
6	0.000000000	8.710978000	-0.155443000	1	0.000000000	-9.942793000	2.461004000
6	0.000000000	8.231471000	-1.444214000	1	0.000000000	-12.602347000	2.457997000
6	0.000000000	6.795065000	-1.444840000	1	0.000000000	-16.378487000	-2.334051000
6	0.000000000	6.314607000	-0.155589000	1	0.000000000	-13.700154000	-2.342645000
6	0.000000000	4.954546000	0.274252000	1	0.000000000	-17.245678000	0.163243000
6	0.000000000	4.473973000	1.563911000	6	0.000000000	15.033590000	0.770647000
6	0.000000000	3.038790000	1.564116000	1	0.878288000	15.035493000	1.431171000
6	0.000000000	2.557903000	0.274295000	1	-0.878288000	15.035493000	1.431171000
6	0.000000000	1.198333000	-0.155014000	6	0.000000000	11.270843000	-0.655936000
6	0.000000000	0.717434000	-1.444955000	1	-0.879333000	11.271775000	-1.312729000
6	0.000000000	-0.717434000	-1.444955000	1	0.879333000	11.271775000	-1.312729000
6	0.000000000	-1.198333000	-0.155014000	6	0.000000000	7.512938000	0.776708000
6	0.000000000	-2.557903000	0.274295000	1	0.879436000	7.513183000	1.433246000
6	0.000000000	-3.038790000	1.564116000	1	-0.879436000	7.513183000	1.433246000
6	0.000000000	-4.473973000	1.563911000	6	0.000000000	3.756273000	-0.658079000
6	0.000000000	-4.954546000	0.274252000	1	-0.879463000	3.756359000	-1.314577000
6	0.000000000	-6.314607000	-0.155589000	1	0.879463000	3.756359000	-1.314577000
6	0.000000000	-6.795065000	-1.444840000	6	0.000000000	0.000000000	0.777330000
6	0.000000000	-8.231471000	-1.444214000	1	0.879457000	0.000000000	1.433817000
6	0.000000000	-8.710978000	-0.155443000	1	-0.879457000	0.000000000	1.433817000
6	0.000000000	-10.072531000	0.276010000	6	0.000000000	-3.756273000	-0.658079000
6	0.000000000	-10.551691000	1.563652000	1	0.879463000	-3.756359000	-1.314577000
6	0.000000000	-11.991713000	1.561654000	1	-0.879463000	-3.756359000	-1.314577000
6	0.000000000	-12.468146000	0.275651000	6	0.000000000	-7.512938000	0.776708000
6	0.000000000	-13.835053000	-0.161087000	1	-0.879436000	-7.513183000	1.433246000
6	0.000000000	-14.308578000	-1.445039000	1	0.879436000	-7.513183000	1.433246000
6	0.000000000	-15.764876000	-1.439770000	6	0.000000000	-11.270843000	-0.655936000
6	0.000000000	-16.213499000	-0.164754000	1	0.879333000	-11.271775000	-1.312729000
1	0.000000000	17.245678000	0.163243000	1	-0.879333000	-11.271775000	-1.312729000
1	0.000000000	13.700154000	-2.342645000	6	0.000000000	-15.033590000	0.770647000
1	0.000000000	16.378487000	-2.334051000	1	-0.878288000	-15.035493000	1.431171000
1	0.000000000	12.602347000	2.457997000	1	0.878288000	-15.035493000	1.431171000
1	0.000000000	9.942793000	2.461004000				
1	0.000000000	6.185292000	-2.341624000				
1	0.000000000	8.841810000	-2.340656000				

10-C							
6	4.450113000	17.537046000	0.000000000	1	0.445718000	10.976233000	0.000000000
6	3.102500000	17.432705000	0.000000000	1	4.115025000	6.107469000	0.000000000
6	2.721563000	16.027089000	0.000000000	1	3.430514000	3.541819000	0.000000000
6	3.839813000	15.238245000	0.000000000	1	-2.177967000	1.151152000	0.000000000
6	3.909037000	13.804931000	0.000000000	1	-1.493212000	3.716350000	0.000000000
6	5.028587000	13.012843000	0.000000000	1	2.177967000	-1.151152000	0.000000000
6	4.658969000	11.621041000	0.000000000	1	1.493212000	-3.716350000	0.000000000
6	3.291302000	11.490312000	0.000000000	1	-4.115025000	-6.107469000	0.000000000
6	2.523260000	10.286108000	0.000000000	1	-3.430514000	-3.541819000	0.000000000
6	1.154402000	10.155330000	0.000000000	1	0.240533000	-8.409977000	0.000000000
6	0.783228000	8.767689000	0.000000000	1	-0.445718000	-10.976233000	0.000000000
6	1.904928000	7.970911000	0.000000000	1	-6.052156000	-13.371468000	0.000000000
6	1.969310000	6.546011000	0.000000000	1	-5.368897000	-10.801286000	0.000000000
6	3.091474000	5.749101000	0.000000000	1	-1.697334000	-15.670959000	0.000000000
6	2.721563000	4.362455000	0.000000000	1	-2.396907000	-18.256352000	0.000000000
6	1.351274000	4.230495000	0.000000000	6	-2.700025000	-12.888534000	0.000000000
6	0.586069000	3.027612000	0.000000000	1	-2.065757000	-13.058897000	0.879387000
6	-0.784375000	2.895608000	0.000000000	1	-2.065757000	-13.058897000	-0.879387000
6	-1.154401000	1.509451000	0.000000000	6	-3.114824000	-8.888164000	0.000000000
6	-0.031967000	0.712011000	0.000000000	1	-3.749164000	-8.719031000	-0.879487000
6	0.031967000	-0.712011000	0.000000000	1	-3.749164000	-8.719031000	0.879487000
6	1.154401000	-1.509451000	0.000000000	6	-0.759510000	-5.628759000	0.000000000
6	0.784375000	-2.895608000	0.000000000	1	-0.125280000	-5.798174000	0.879499000
6	-0.586069000	-3.027612000	0.000000000	1	-0.125280000	-5.798174000	-0.879499000
6	-1.351274000	-4.230495000	0.000000000	6	-1.177900000	-1.629397000	0.000000000
6	-2.721563000	-4.362455000	0.000000000	1	-1.812146000	-1.460128000	-0.879510000
6	-3.091474000	-5.749101000	0.000000000	1	-1.812146000	-1.460128000	0.879510000
6	-1.969310000	-6.546011000	0.000000000	6	1.177900000	1.629397000	0.000000000
6	-1.904928000	-7.970911000	0.000000000	1	1.812146000	1.460128000	-0.879510000
6	-0.783228000	-8.767689000	0.000000000	1	1.812146000	1.460128000	0.879510000
6	-1.154402000	-10.155330000	0.000000000	6	0.759510000	5.628759000	0.000000000
6	-2.523260000	-10.286108000	0.000000000	1	0.125280000	5.798174000	0.879499000
6	-3.291302000	-11.490312000	0.000000000	1	0.125280000	5.798174000	-0.879499000
6	-4.658969000	-11.621041000	0.000000000	6	3.114824000	8.888164000	0.000000000
6	-5.028587000	-13.012843000	0.000000000	1	3.749164000	8.719031000	-0.879487000
6	-3.909037000	-13.804931000	0.000000000	1	3.749164000	8.719031000	0.879487000
6	-3.839813000	-15.238245000	0.000000000	6	2.700025000	12.888534000	0.000000000
6	-2.721563000	-16.027089000	0.000000000	1	2.065757000	13.058897000	0.879387000
6	-3.102500000	-17.432705000	0.000000000	1	2.065757000	13.058897000	-0.879387000
6	-4.450113000	-17.537046000	0.000000000	6	5.049329000	16.155836000	0.000000000
1	5.033341000	18.449641000	0.000000000	1	5.687928000	15.987103000	-0.878313000
1	-5.033341000	-18.449641000	0.000000000	1	5.687928000	15.987103000	0.878313000
1	1.697334000	15.670959000	0.000000000	6	-5.049329000	-16.155836000	0.000000000
1	2.396907000	18.256352000	0.000000000	1	-5.687928000	-15.987103000	-0.878313000
1	6.052156000	13.371468000	0.000000000	1	-5.687928000	-15.987103000	0.878313000
1	5.368897000	10.801286000	0.000000000				
1	-0.240533000	8.409977000	0.000000000				

Polypyrroles

1-N				2-N			
6	0.000000000	1.125159000	0.331561000	6	-0.447376000	2.905248000	0.000000000
6	0.000000000	0.712562000	-0.983261000	6	0.928571000	2.837341000	0.000000000
6	0.000000000	-0.712562000	-0.983261000	6	1.286823000	1.461860000	0.000000000
6	0.000000000	-1.125159000	0.331561000	6	0.114926000	0.714953000	0.000000000
1	0.000000000	0.000000000	2.128959000	6	-0.114926000	-0.714953000	0.000000000
1	0.000000000	2.113635000	0.766092000	6	-1.286823000	-1.461860000	0.000000000
1	0.000000000	1.360611000	-1.848348000	6	-0.928571000	-2.837341000	0.000000000
1	0.000000000	-1.360611000	-1.848348000	6	0.447376000	-2.905248000	0.000000000
7	0.000000000	0.000000000	1.122278000	1	-1.902209000	1.361403000	0.000000000
1	0.000000000	-2.113635000	0.766092000	1	-1.117780000	3.751294000	0.000000000
				7	0.928571000	-1.617355000	0.000000000
				1	1.604335000	3.680599000	0.000000000
				1	2.293370000	1.065764000	0.000000000
				1	-2.293370000	-1.065764000	0.000000000
				1	1.902209000	-1.361403000	0.000000000
				1	-1.604335000	-3.680599000	0.000000000
				7	-0.928571000	1.617355000	0.000000000
				1	1.117780000	-3.751294000	0.000000000
3-N				4-N			
6	0.000000000	4.720331000	0.081991000	6	3.057865000	5.763196000	0.000000000
6	0.000000000	4.306540000	1.396448000	6	4.069698000	4.827496000	0.000000000
6	0.000000000	2.885994000	1.395050000	6	3.461656000	3.543850000	0.000000000
6	0.000000000	2.459572000	0.071784000	6	2.082925000	3.723597000	0.000000000
6	0.000000000	1.136214000	-0.509562000	6	0.992150000	2.775629000	0.000000000
6	0.000000000	0.708051000	-1.832168000	6	-0.387005000	2.953500000	0.000000000
6	0.000000000	-0.708051000	-1.832168000	6	-0.992150000	1.674094000	0.000000000
6	0.000000000	-1.136214000	-0.509562000	6	0.020986000	0.720940000	0.000000000
6	0.000000000	-2.459572000	0.071784000	6	-0.020986000	-0.720940000	0.000000000
6	0.000000000	-2.885994000	1.395050000	6	0.992150000	-1.674094000	0.000000000
6	0.000000000	-4.306540000	1.396448000	6	0.387005000	-2.953500000	0.000000000
6	0.000000000	-4.720331000	0.081991000	6	-0.992150000	-2.775629000	0.000000000
1	0.000000000	3.596655000	-1.716683000	6	-2.082925000	-3.723597000	0.000000000
1	0.000000000	5.708638000	-0.352056000	6	-3.461656000	-3.543850000	0.000000000
7	0.000000000	0.000000000	0.272515000	6	-4.069698000	-4.827496000	0.000000000
1	0.000000000	4.951266000	2.263680000	6	-3.057865000	-5.763196000	0.000000000
7	0.000000000	-3.596977000	-0.710048000	1	0.951494000	5.515723000	0.000000000
1	0.000000000	2.248077000	2.268419000	1	3.087704000	6.842181000	0.000000000
1	0.000000000	1.342875000	-2.707664000	7	1.214300000	1.414462000	0.000000000
1	0.000000000	0.000000000	1.279158000	1	5.129235000	5.039892000	0.000000000
1	0.000000000	-1.342875000	-2.707664000	7	-1.214300000	-1.414462000	0.000000000
1	0.000000000	-2.248077000	2.268419000	1	3.979014000	2.594112000	0.000000000
1	0.000000000	-3.596655000	-1.716683000	7	-1.861883000	-5.086059000	0.000000000
1	0.000000000	-4.951266000	2.263680000	1	-0.907410000	3.901413000	0.000000000
7	0.000000000	3.596977000	-0.710048000	1	2.125086000	0.985789000	0.000000000
1	0.000000000	-5.708638000	-0.352056000	1	-2.054897000	1.474444000	0.000000000
				1	2.054897000	-1.474444000	0.000000000
				1	-2.125086000	-0.985789000	0.000000000
				1	0.907410000	-3.901413000	0.000000000
				1	-3.979014000	-2.594112000	0.000000000
				7	1.861883000	5.086059000	0.000000000
				1	-0.951494000	-5.515723000	0.000000000
				1	-5.129235000	-5.039892000	0.000000000
				1	-3.087704000	-6.842181000	0.000000000

5-N				6-N			
6	0.000000000	8.314281000	-0.169002000	6	0.087472000	10.116354000	0.000000000
6	0.000000000	7.900704000	-1.483651000	6	1.410602000	9.730859000	0.000000000
6	0.000000000	6.480380000	-1.482474000	6	1.439752000	8.310758000	0.000000000
6	0.000000000	6.053827000	-0.159122000	6	0.125849000	7.855997000	0.000000000
6	0.000000000	4.730576000	0.421671000	6	-0.426678000	6.520644000	0.000000000
6	0.000000000	4.302444000	1.744830000	6	-1.740514000	6.064585000	0.000000000
6	0.000000000	2.887330000	1.745591000	6	-1.711300000	4.649681000	0.000000000
6	0.000000000	2.458127000	0.422315000	6	-0.379276000	4.248473000	0.000000000
6	0.000000000	1.136389000	-0.154963000	6	0.225806000	2.939287000	0.000000000
6	0.000000000	0.707255000	-1.478553000	6	1.558318000	2.538316000	0.000000000
6	0.000000000	-0.707255000	-1.478553000	6	1.588489000	1.124134000	0.000000000
6	0.000000000	-1.136389000	-0.154963000	6	0.274232000	0.666796000	0.000000000
6	0.000000000	-2.458127000	0.422315000	6	-0.274232000	-0.666796000	0.000000000
6	0.000000000	-2.887330000	1.745591000	6	-1.588489000	-1.124134000	0.000000000
6	0.000000000	-4.302444000	1.744830000	6	-1.558318000	-2.538316000	0.000000000
6	0.000000000	-4.730576000	0.421671000	6	-0.225806000	-2.939287000	0.000000000
6	0.000000000	-6.053827000	-0.159122000	6	0.379276000	-4.248473000	0.000000000
6	0.000000000	-6.480380000	-1.482474000	6	1.711300000	-4.649681000	0.000000000
6	0.000000000	-7.900704000	-1.483651000	6	1.740514000	-6.064585000	0.000000000
6	0.000000000	-8.314281000	-0.169002000	6	0.426678000	-6.520644000	0.000000000
1	0.000000000	7.190968000	1.629722000	6	-0.125849000	-7.855997000	0.000000000
1	0.000000000	9.302518000	0.265120000	6	-1.439752000	-8.310758000	0.000000000
7	0.000000000	3.594847000	-0.360573000	6	-1.410602000	-9.730859000	0.000000000
1	0.000000000	8.545531000	-2.350767000	6	-0.087472000	-10.116354000	0.000000000
7	0.000000000	0.000000000	0.627992000	1	-1.686630000	8.954795000	0.000000000
1	0.000000000	5.842661000	-2.355992000	1	-0.367504000	11.095205000	0.000000000
7	0.000000000	-3.594847000	-0.360573000	7	0.379276000	5.401667000	0.000000000
1	0.000000000	4.937501000	2.620110000	1	2.263692000	10.394140000	0.000000000
7	0.000000000	-7.191148000	0.622954000	7	-0.532621000	1.786464000	0.000000000
1	0.000000000	3.595820000	-1.367286000	1	2.326525000	7.691571000	0.000000000
1	0.000000000	2.252902000	2.621269000	7	0.532621000	-1.786464000	0.000000000
1	0.000000000	1.341980000	-2.353977000	1	-2.628870000	6.681229000	0.000000000
1	0.000000000	0.000000000	1.634621000	7	-0.379276000	-5.401667000	0.000000000
1	0.000000000	-1.341980000	-2.353977000	1	1.385633000	5.423960000	0.000000000
1	0.000000000	-2.252902000	2.621269000	7	0.680199000	-8.976462000	0.000000000
7	0.000000000	7.191148000	0.622954000	1	-2.573380000	3.996914000	0.000000000
1	0.000000000	-3.595820000	-1.367286000	1	2.419974000	3.191578000	0.000000000
1	0.000000000	-4.937501000	2.620110000	1	-1.538935000	1.765193000	0.000000000
1	0.000000000	-5.842661000	-2.355992000	1	2.477081000	0.507932000	0.000000000
1	0.000000000	-7.190968000	1.629722000	1	-2.477081000	-0.507932000	0.000000000
1	0.000000000	-8.545531000	-2.350767000	7	-0.680199000	8.976462000	0.000000000
1	0.000000000	-9.302518000	0.265120000	1	1.538935000	-1.765193000	0.000000000
				1	-2.419974000	-3.191578000	0.000000000
				1	2.573380000	-3.996914000	0.000000000
				1	-1.385633000	-5.423960000	0.000000000
				1	2.628870000	-6.681229000	0.000000000
				1	-2.326525000	-7.691571000	0.000000000
				1	1.686630000	-8.954795000	0.000000000
				1	-2.263692000	-10.394140000	0.000000000
				1	0.367504000	-11.095205000	0.000000000

7-N				8-N			
6	0.000000000	11.909454000	0.206121000	6	-0.010921000	13.709942000	0.000000000
6	0.000000000	11.496047000	1.520818000	6	-1.334035000	13.324350000	0.000000000
6	0.000000000	10.075668000	1.519860000	6	-1.363070000	11.904263000	0.000000000
6	0.000000000	9.648786000	0.196651000	6	-0.049131000	11.449614000	0.000000000
6	0.000000000	8.325407000	-0.383951000	6	0.503458000	10.114290000	0.000000000
6	0.000000000	7.897115000	-1.707113000	6	1.817332000	9.658264000	0.000000000
6	0.000000000	6.481920000	-1.707767000	6	1.788146000	8.243387000	0.000000000
6	0.000000000	6.052784000	-0.384473000	6	0.456128000	7.842158000	0.000000000
6	0.000000000	4.731092000	0.192755000	6	-0.148914000	6.532977000	0.000000000
6	0.000000000	4.302101000	1.516551000	6	-1.481498000	6.132062000	0.000000000
6	0.000000000	2.887641000	1.516795000	6	-1.511734000	4.717953000	0.000000000
6	0.000000000	2.458136000	0.193175000	6	-0.197501000	4.260549000	0.000000000
6	0.000000000	1.136494000	-0.383352000	6	0.350753000	2.926939000	0.000000000
6	0.000000000	0.707185000	-1.707146000	6	1.665138000	2.469526000	0.000000000
6	0.000000000	-0.707185000	-1.707146000	6	1.634943000	1.055530000	0.000000000
6	0.000000000	-1.136494000	-0.383352000	6	0.302308000	0.654484000	0.000000000
6	0.000000000	-2.458136000	0.193175000	6	-0.302308000	-0.654484000	0.000000000
6	0.000000000	-2.887641000	1.516795000	6	-1.634943000	-1.055530000	0.000000000
6	0.000000000	-4.302101000	1.516551000	6	-1.665138000	-2.469526000	0.000000000
6	0.000000000	-4.731092000	0.192755000	6	-0.350753000	-2.926939000	0.000000000
6	0.000000000	-6.052784000	-0.384473000	6	0.197501000	-4.260549000	0.000000000
6	0.000000000	-6.481920000	-1.707767000	6	1.511734000	-4.717953000	0.000000000
6	0.000000000	-7.897115000	-1.707113000	6	1.481498000	-6.132062000	0.000000000
6	0.000000000	-8.325407000	-0.383951000	6	0.148914000	-6.532977000	0.000000000
6	0.000000000	-9.648786000	0.196651000	6	-0.456128000	-7.842158000	0.000000000
6	0.000000000	-10.075668000	1.519860000	6	-1.788146000	-8.243387000	0.000000000
6	0.000000000	-11.496047000	1.520818000	6	-1.817332000	-9.658264000	0.000000000
6	0.000000000	-11.909454000	0.206121000	6	-0.503458000	-10.114290000	0.000000000
1	0.000000000	10.785689000	-1.592171000	6	0.049131000	-11.449614000	0.000000000
1	0.000000000	12.897710000	-0.228053000	6	1.363070000	-11.904263000	0.000000000
7	0.000000000	7.189702000	0.398230000	6	1.334035000	-13.324350000	0.000000000
1	0.000000000	12.141094000	2.387774000	6	0.010921000	-13.709942000	0.000000000
7	0.000000000	3.594636000	-0.589872000	1	1.763281000	12.548582000	0.000000000
1	0.000000000	9.438025000	2.393441000	1	0.443978000	14.688829000	0.000000000
7	0.000000000	0.000000000	0.399473000	7	-0.302458000	8.995334000	0.000000000
1	0.000000000	8.532238000	-2.582336000	1	-2.187181000	13.987554000	0.000000000
7	0.000000000	-3.594636000	-0.589872000	7	0.609459000	5.380200000	0.000000000
1	0.000000000	7.190851000	1.404842000	1	-2.249820000	11.285041000	0.000000000
7	0.000000000	-7.189702000	0.398230000	7	-0.456128000	1.807459000	0.000000000
1	0.000000000	5.847289000	-2.583307000	1	2.705675000	10.274917000	0.000000000
7	0.000000000	-10.786074000	-0.585504000	7	0.456128000	-1.807459000	0.000000000
1	0.000000000	4.937170000	2.391715000	1	-1.308826000	9.017671000	0.000000000
1	0.000000000	3.594666000	-1.596410000	7	-0.609459000	-5.380200000	0.000000000
1	0.000000000	2.252965000	2.392273000	1	2.650247000	7.590646000	0.000000000
1	0.000000000	1.342082000	-2.582456000	7	0.302458000	-8.995334000	0.000000000
7	0.000000000	10.786074000	-0.585504000	1	-2.343114000	6.785359000	0.000000000
1	0.000000000	0.000000000	1.406027000	7	-0.756837000	-12.570137000	0.000000000
1	0.000000000	-1.342082000	-2.582456000	1	1.615784000	5.358979000	0.000000000
1	0.000000000	-2.252965000	2.392273000	1	-2.400397000	4.101849000	0.000000000
1	0.000000000	-3.594666000	-1.596410000	1	2.553724000	3.085712000	0.000000000
1	0.000000000	-4.937170000	2.391715000	7	0.756837000	12.570137000	0.000000000
1	0.000000000	-5.847289000	-2.583307000	1	-1.462453000	1.828969000	0.000000000
1	0.000000000	-7.190851000	1.404842000	1	2.496650000	0.402320000	0.000000000
1	0.000000000	-8.532238000	-2.582336000	1	-2.496650000	-0.402320000	0.000000000
1	0.000000000	-9.438025000	2.393441000	1	1.462453000	-1.828969000	0.000000000
1	0.000000000	-10.785689000	-1.592171000	1	-2.553724000	-3.085712000	0.000000000
1	0.000000000	-12.141094000	2.387774000	1	2.400397000	-4.101849000	0.000000000
1	0.000000000	-12.897710000	-0.228053000	1	-1.615784000	-5.358979000	0.000000000
				1	2.343114000	-6.785359000	0.000000000
				1	-2.650247000	-7.590646000	0.000000000
				1	1.308826000	-9.017671000	0.000000000
				1	-2.705675000	-10.274917000	0.000000000
				1	2.249820000	-11.285041000	0.000000000
				1	-1.763281000	-12.548582000	0.000000000
				1	2.187181000	-13.987554000	0.000000000
				1	-0.443978000	-14.688829000	0.000000000

9-N							
6	0.000000000	15.503871000	-0.226500000	1	0.000000000	16.492097000	0.207744000
6	0.000000000	15.090565000	-1.541237000	7	0.000000000	10.784194000	-0.419004000
6	0.000000000	13.670195000	-1.540381000	1	0.000000000	15.735671000	-2.408148000
6	0.000000000	13.243227000	-0.217201000	7	0.000000000	7.189083000	0.568801000
6	0.000000000	11.919801000	0.363280000	1	0.000000000	13.032624000	-2.414015000
6	0.000000000	11.491395000	1.686419000	7	0.000000000	3.594613000	-0.420929000
6	0.000000000	10.076217000	1.686941000	1	0.000000000	12.126431000	2.561701000
6	0.000000000	9.647209000	0.363613000	7	0.000000000	0.000000000	0.568190000
6	0.000000000	8.325568000	-0.213717000	1	0.000000000	10.785468000	-1.425620000
6	0.000000000	7.896704000	-1.537579000	7	0.000000000	-3.594613000	-0.420929000
6	0.000000000	6.482269000	-1.537946000	1	0.000000000	9.441526000	2.562439000
6	0.000000000	6.052653000	-0.214371000	7	0.000000000	-7.189083000	0.568801000
6	0.000000000	4.730958000	0.361995000	1	0.000000000	8.531846000	-2.412683000
6	0.000000000	4.301529000	1.685804000	7	0.000000000	-10.784194000	-0.419004000
6	0.000000000	2.887222000	1.685681000	1	0.000000000	7.189073000	1.575346000
6	0.000000000	2.458030000	0.361849000	7	0.000000000	-14.380451000	0.565045000
6	0.000000000	1.136458000	-0.214678000	1	0.000000000	5.847694000	-2.413502000
6	0.000000000	0.707140000	-1.538508000	1	0.000000000	4.936331000	2.561170000
6	0.000000000	-0.707140000	-1.538508000	7	0.000000000	14.380451000	0.565045000
6	0.000000000	-1.136458000	-0.214678000	1	0.000000000	3.594813000	-1.427487000
6	0.000000000	-2.458030000	0.361849000	1	0.000000000	2.252296000	2.560973000
6	0.000000000	-2.887222000	1.685681000	1	0.000000000	1.341976000	-2.413852000
6	0.000000000	-4.301529000	1.685804000	1	0.000000000	0.000000000	1.574740000
6	0.000000000	-4.730958000	0.361995000	1	0.000000000	-1.341976000	-2.413852000
6	0.000000000	-6.052653000	-0.214371000	1	0.000000000	-2.252296000	2.560973000
6	0.000000000	-6.482269000	-1.537946000	1	0.000000000	-3.594813000	-1.427487000
6	0.000000000	-7.896704000	-1.537579000	1	0.000000000	-4.936331000	2.561170000
6	0.000000000	-8.325568000	-0.213717000	1	0.000000000	-5.847694000	-2.413502000
6	0.000000000	-9.647209000	0.363613000	1	0.000000000	-7.189073000	1.575346000
6	0.000000000	-10.076217000	1.686941000	1	0.000000000	-8.531846000	-2.412683000
6	0.000000000	-11.491395000	1.686419000	1	0.000000000	-9.441526000	2.562439000
6	0.000000000	-11.919801000	0.363280000	1	0.000000000	-10.785468000	-1.425620000
6	0.000000000	-13.243227000	-0.217201000	1	0.000000000	-12.126431000	2.561701000
6	0.000000000	-13.670195000	-1.540381000	1	0.000000000	-13.032624000	-2.414015000
6	0.000000000	-15.090565000	-1.541237000	1	0.000000000	-14.380020000	1.571717000
6	0.000000000	-15.503871000	-0.226500000	1	0.000000000	-15.735671000	-2.408148000
1	0.000000000	14.380020000	1.571717000	1	0.000000000	-16.492097000	0.207744000

10-N							
6	0.301852000	-17.301004000	0.000000000	1	-0.132269000	-18.289284000	0.000000000
6	1.616536000	-16.887510000	0.000000000	7	0.493676000	-12.581316000	0.000000000
6	1.615471000	-15.467139000	0.000000000	1	2.483554000	-17.532473000	0.000000000
6	0.292231000	-15.040362000	0.000000000	7	-0.494580000	-8.986355000	0.000000000
6	-0.288458000	-13.717023000	0.000000000	1	2.489046000	-14.829477000	0.000000000
6	-1.611656000	-13.288792000	0.000000000	7	0.494741000	-5.391794000	0.000000000
6	-1.612370000	-11.873615000	0.000000000	1	-2.486885000	-13.923906000	0.000000000
6	-0.289096000	-11.444436000	0.000000000	7	-0.494592000	-1.797274000	0.000000000
6	0.288079000	-10.122735000	0.000000000	1	1.500295000	-12.582451000	0.000000000
6	1.611895000	-9.693711000	0.000000000	7	0.494592000	1.797274000	0.000000000
6	1.612081000	-8.279277000	0.000000000	1	-2.487973000	-11.239066000	0.000000000
6	0.288460000	-7.849824000	0.000000000	7	-0.494741000	5.391794000	0.000000000
6	-0.288079000	-6.528195000	0.000000000	1	2.487092000	-10.328728000	0.000000000
6	-1.611934000	-6.098885000	0.000000000	7	0.494580000	8.986355000	0.000000000
6	-1.611941000	-4.684583000	0.000000000	1	-1.501129000	-8.986491000	0.000000000
6	-0.288148000	-4.255280000	0.000000000	7	-0.493676000	12.581316000	0.000000000
6	0.288306000	-2.933686000	0.000000000	1	2.487598000	-7.644637000	0.000000000
6	1.612144000	-2.504334000	0.000000000	7	0.489852000	16.177700000	0.000000000
6	1.612094000	-1.090069000	0.000000000	1	-2.487283000	-6.733714000	0.000000000
6	0.288257000	-0.660788000	0.000000000	7	-0.489852000	-16.177700000	0.000000000
6	-0.288257000	0.660788000	0.000000000	1	1.501301000	-5.391916000	0.000000000
6	-1.612094000	1.090069000	0.000000000	1	-2.487314000	-4.049765000	0.000000000
6	-1.612144000	2.504334000	0.000000000	1	2.487513000	-3.139135000	0.000000000
6	-0.288306000	2.933686000	0.000000000	1	-1.501148000	-1.797342000	0.000000000
6	0.288148000	4.255280000	0.000000000	1	2.487465000	-0.455256000	0.000000000
6	1.611941000	4.684583000	0.000000000	1	-2.487465000	0.455256000	0.000000000
6	1.611934000	6.098885000	0.000000000	1	1.501148000	1.797342000	0.000000000
6	0.288079000	6.528195000	0.000000000	1	-2.487513000	3.139135000	0.000000000
6	-0.288460000	7.849824000	0.000000000	1	2.487314000	4.049765000	0.000000000
6	-1.612081000	8.279277000	0.000000000	1	-1.501301000	5.391916000	0.000000000
6	-1.611895000	9.693711000	0.000000000	1	2.487283000	6.733714000	0.000000000
6	-0.288079000	10.122735000	0.000000000	1	-2.487598000	7.644637000	0.000000000
6	0.289096000	11.444436000	0.000000000	1	1.501129000	8.986491000	0.000000000
6	1.612370000	11.873615000	0.000000000	1	-2.487092000	10.328728000	0.000000000
6	1.611656000	13.288792000	0.000000000	1	2.487973000	11.239066000	0.000000000
6	0.288458000	13.717023000	0.000000000	1	-1.500295000	12.582451000	0.000000000
6	-0.292231000	15.040362000	0.000000000	1	2.486885000	13.923906000	0.000000000
6	-1.615471000	15.467139000	0.000000000	1	-2.489046000	14.829477000	0.000000000
6	-1.616536000	16.887510000	0.000000000	1	1.496528000	16.177444000	0.000000000
6	-0.301852000	17.301004000	0.000000000	1	-2.483554000	17.532473000	0.000000000
1	-1.496528000	-16.177444000	0.000000000	1	0.132269000	18.289284000	0.000000000

Polyfurans

1-O				2-O			
6	0.000000000	1.095028000	0.347528000	6	-0.678988000	2.775237000	0.000000000
6	0.000000000	0.717894000	-0.959701000	6	0.678988000	2.874255000	0.000000000
6	0.000000000	-0.717894000	-0.959701000	6	1.180421000	1.534757000	0.000000000
6	0.000000000	-1.095028000	0.347528000	6	0.082306000	0.714571000	0.000000000
1	0.000000000	2.050791000	0.847588000	6	-0.082306000	-0.714571000	0.000000000
1	0.000000000	-1.373737000	-1.818523000	6	-1.180421000	-1.534757000	0.000000000
1	0.000000000	1.373737000	-1.818523000	6	-0.678988000	-2.874255000	0.000000000
1	0.000000000	-2.050791000	0.847588000	6	0.678988000	-2.775237000	0.000000000
8	0.000000000	0.000000000	1.160994000	1	-1.480197000	3.497105000	0.000000000
				1	2.210856000	1.213300000	0.000000000
				1	1.255216000	3.788074000	0.000000000
				1	-2.210856000	-1.213300000	0.000000000
				1	-1.255216000	-3.788074000	0.000000000
				1	1.480197000	-3.497105000	0.000000000
				8	-1.062498000	1.464873000	0.000000000
				8	1.062498000	-1.464873000	0.000000000
3-O				4-O			
6	0.000000000	4.580481000	0.089687000	6	3.144597000	5.493207000	0.000000000
6	0.000000000	4.204193000	1.398396000	6	4.141776000	4.565712000	0.000000000
6	0.000000000	2.774678000	1.406871000	6	3.503071000	3.287021000	0.000000000
6	0.000000000	2.383256000	0.092235000	6	2.153310000	3.532344000	0.000000000
6	0.000000000	1.102306000	-0.554983000	6	0.997186000	2.682785000	0.000000000
6	0.000000000	0.711494000	-1.870894000	6	-0.353889000	2.928951000	0.000000000
6	0.000000000	-0.711494000	-1.870894000	6	-0.997186000	1.660802000	0.000000000
6	0.000000000	-1.102306000	-0.554983000	6	0.000431000	0.715756000	0.000000000
6	0.000000000	-2.383256000	0.092235000	6	-0.000431000	-0.715756000	0.000000000
6	0.000000000	-2.774678000	1.406871000	6	0.997186000	-1.660802000	0.000000000
6	0.000000000	-4.204193000	1.398396000	6	0.353889000	-2.928951000	0.000000000
6	0.000000000	-4.580481000	0.089687000	6	-0.997186000	-2.682785000	0.000000000
1	0.000000000	5.534761000	-0.412615000	6	-2.153310000	-3.532344000	0.000000000
1	0.000000000	2.118122000	2.263608000	6	-3.503071000	-3.287021000	0.000000000
1	0.000000000	4.862547000	2.254930000	6	-4.141776000	-4.565712000	0.000000000
1	0.000000000	1.371317000	-2.725257000	6	-3.144597000	-5.493207000	0.000000000
1	0.000000000	-1.371317000	-2.725257000	1	3.128151000	6.571489000	0.000000000
1	0.000000000	-4.862547000	2.254930000	1	3.970551000	2.314126000	0.000000000
1	0.000000000	-2.118122000	2.263608000	1	5.203431000	4.765569000	0.000000000
1	0.000000000	-5.534761000	-0.412615000	1	-0.817623000	3.903763000	0.000000000
8	0.000000000	3.483579000	-0.723285000	1	-2.057692000	1.459374000	0.000000000
8	0.000000000	0.000000000	0.259436000	1	0.817623000	-3.903763000	0.000000000
8	0.000000000	-3.483579000	-0.723285000	1	2.057692000	-1.459374000	0.000000000
				1	-3.970551000	-2.314126000	0.000000000
				1	-5.203431000	-4.765569000	0.000000000
				1	-3.128151000	-6.571489000	0.000000000
				8	1.923529000	4.882588000	0.000000000
				8	1.225487000	1.331589000	0.000000000
				8	-1.225487000	-1.331589000	0.000000000
				8	-1.923529000	-4.882588000	0.000000000

5-O				6-O			
6	0.000000000	8.063096000	-0.178966000	6	0.142714000	9.808287000	0.000000000
6	0.000000000	7.688089000	-1.488193000	6	1.458400000	9.456569000	0.000000000
6	0.000000000	6.258830000	-1.498106000	6	1.493677000	8.027737000	0.000000000
6	0.000000000	5.866079000	-0.183612000	6	0.186319000	7.611753000	0.000000000
6	0.000000000	4.585014000	0.462131000	6	-0.436618000	6.319469000	0.000000000
6	0.000000000	4.193810000	1.778719000	6	-1.746149000	5.904997000	0.000000000
6	0.000000000	2.772135000	1.779292000	6	-1.721507000	4.483607000	0.000000000
6	0.000000000	2.380042000	0.461998000	6	-0.397448000	4.114879000	0.000000000
6	0.000000000	1.102779000	-0.183256000	6	0.270383000	2.849422000	0.000000000
6	0.000000000	0.710432000	-1.500891000	6	1.595094000	2.481075000	0.000000000
6	0.000000000	-0.710432000	-1.500891000	6	1.621071000	1.060744000	0.000000000
6	0.000000000	-1.102779000	-0.183256000	6	0.310578000	0.644248000	0.000000000
6	0.000000000	-2.380042000	0.461998000	6	-0.310578000	-0.644248000	0.000000000
6	0.000000000	-2.772135000	1.779292000	6	-1.621071000	-1.060744000	0.000000000
6	0.000000000	-4.193810000	1.778719000	6	-1.595094000	-2.481075000	0.000000000
6	0.000000000	-4.585014000	0.462131000	6	-0.270383000	-2.849422000	0.000000000
6	0.000000000	-5.866079000	-0.183612000	6	0.397448000	-4.114879000	0.000000000
6	0.000000000	-6.258830000	-1.498106000	6	1.721507000	-4.483607000	0.000000000
6	0.000000000	-7.688089000	-1.488193000	6	1.746149000	-5.904997000	0.000000000
6	0.000000000	-8.063096000	-0.178966000	6	0.436618000	-6.319469000	0.000000000
1	0.000000000	9.016940000	0.324172000	6	-0.186319000	-7.611753000	0.000000000
1	0.000000000	5.603166000	-2.355530000	6	-1.493677000	-8.027737000	0.000000000
1	0.000000000	8.347319000	-2.344032000	6	-1.458400000	-9.456569000	0.000000000
1	0.000000000	4.853947000	2.632830000	6	-0.142714000	-9.808287000	0.000000000
1	0.000000000	2.112862000	2.634040000	1	-0.377209000	10.753087000	0.000000000
1	0.000000000	-1.369988000	-2.355422000	1	2.362592000	7.387371000	0.000000000
1	0.000000000	1.369988000	-2.355422000	1	2.302389000	10.130898000	0.000000000
1	0.000000000	-2.112862000	2.634040000	1	-2.611814000	6.549908000	0.000000000
1	0.000000000	-4.853947000	2.632830000	1	-2.564449000	3.809305000	0.000000000
1	0.000000000	-8.347319000	-2.344032000	1	2.487556000	0.416965000	0.000000000
1	0.000000000	-5.603166000	-2.355530000	1	2.437461000	3.156082000	0.000000000
1	0.000000000	-9.016940000	0.324172000	1	-2.487556000	-0.416965000	0.000000000
8	0.000000000	-6.965673000	0.633017000	1	-2.437461000	-3.156082000	0.000000000
8	0.000000000	-3.483225000	-0.352573000	1	2.611814000	-6.549908000	0.000000000
8	0.000000000	0.000000000	0.631424000	1	2.564449000	-3.809305000	0.000000000
8	0.000000000	3.483225000	-0.352573000	1	-2.362592000	-7.387371000	0.000000000
8	0.000000000	6.965673000	0.633017000	1	-2.302389000	-10.130898000	0.000000000
				1	0.377209000	-10.753087000	0.000000000
				8	0.649674000	-8.696696000	0.000000000
				8	-0.397448000	-5.232334000	0.000000000
				8	0.524156000	-1.732159000	0.000000000
				8	-0.524156000	1.732159000	0.000000000
				8	0.397448000	5.232334000	0.000000000
				8	-0.649674000	8.696696000	0.000000000

7-0				8-0			
6	0.000000000	11.545620000	0.213938000	6	0.031413000	13.290306000	0.000000000
6	0.000000000	11.171783000	1.523531000	6	-1.287319000	12.950133000	0.000000000
6	0.000000000	9.742575000	1.534691000	6	-1.335099000	11.521676000	0.000000000
6	0.000000000	9.348697000	0.220519000	6	-0.031413000	11.094295000	0.000000000
6	0.000000000	8.067128000	-0.424151000	6	0.580275000	9.796656000	0.000000000
6	0.000000000	7.674998000	-1.740556000	6	1.886219000	9.370889000	0.000000000
6	0.000000000	6.253432000	-1.740114000	6	1.849276000	7.949819000	0.000000000
6	0.000000000	5.862246000	-0.422482000	6	0.522082000	7.592551000	0.000000000
6	0.000000000	4.585584000	0.223618000	6	-0.156540000	6.332893000	0.000000000
6	0.000000000	4.194484000	1.541883000	6	-1.484404000	5.975779000	0.000000000
6	0.000000000	2.773971000	1.543393000	6	-1.522432000	4.555813000	0.000000000
6	0.000000000	2.380057000	0.225896000	6	-0.215463000	4.128164000	0.000000000
6	0.000000000	1.102738000	-0.417658000	6	0.395077000	2.834765000	0.000000000
6	0.000000000	0.710124000	-1.735685000	6	1.702640000	2.408295000	0.000000000
6	0.000000000	-0.710124000	-1.735685000	6	1.666015000	0.988563000	0.000000000
6	0.000000000	-1.102738000	-0.417658000	6	0.338303000	0.629997000	0.000000000
6	0.000000000	-2.380057000	0.225896000	6	-0.338303000	-0.629997000	0.000000000
6	0.000000000	-2.773971000	1.543393000	6	-1.666015000	-0.988563000	0.000000000
6	0.000000000	-4.194484000	1.541883000	6	-1.702640000	-2.408295000	0.000000000
6	0.000000000	-4.585584000	0.223618000	6	-0.395077000	-2.834765000	0.000000000
6	0.000000000	-5.862246000	-0.422482000	6	0.215463000	-4.128164000	0.000000000
6	0.000000000	-6.253432000	-1.740114000	6	1.522432000	-4.555813000	0.000000000
6	0.000000000	-7.674998000	-1.740556000	6	1.484404000	-5.975779000	0.000000000
6	0.000000000	-8.067128000	-0.424151000	6	0.156540000	-6.332893000	0.000000000
6	0.000000000	-9.348697000	0.220519000	6	-0.522082000	-7.592551000	0.000000000
6	0.000000000	-9.742575000	1.534691000	6	-1.849276000	-7.949819000	0.000000000
6	0.000000000	-11.171783000	1.523531000	6	-1.886219000	-9.370889000	0.000000000
6	0.000000000	-11.545620000	0.213938000	6	-0.580275000	-9.796656000	0.000000000
1	0.000000000	12.499025000	-0.290033000	6	0.031413000	-11.094295000	0.000000000
1	0.000000000	9.087674000	2.392702000	6	1.335099000	-11.521676000	0.000000000
1	0.000000000	11.831774000	2.378776000	6	1.287319000	-12.950133000	0.000000000
1	0.000000000	8.334552000	-2.595110000	6	-0.031413000	-13.290306000	0.000000000
1	0.000000000	5.593583000	-2.594423000	1	0.559587000	14.230521000	0.000000000
1	0.000000000	2.115372000	2.398671000	1	-2.209581000	10.888931000	0.000000000
1	0.000000000	4.854942000	2.395704000	1	-2.125353000	13.631842000	0.000000000
1	0.000000000	1.369694000	-2.590200000	1	2.757450000	10.008254000	0.000000000
1	0.000000000	-1.369694000	-2.590200000	1	2.686405000	7.268310000	0.000000000
1	0.000000000	-4.854942000	2.395704000	1	-2.394415000	3.919486000	0.000000000
1	0.000000000	-2.115372000	2.398671000	1	-2.321010000	6.657905000	0.000000000
1	0.000000000	-5.593583000	-2.594423000	1	2.573828000	3.045674000	0.000000000
1	0.000000000	-8.334552000	-2.595110000	1	2.503246000	0.307183000	0.000000000
1	0.000000000	-11.831774000	2.378776000	1	-2.573828000	-3.045674000	0.000000000
1	0.000000000	-9.087674000	2.392702000	1	-2.503246000	-0.307183000	0.000000000
1	0.000000000	-12.499025000	-0.290033000	1	2.394415000	-3.919486000	0.000000000
8	0.000000000	-10.447551000	-0.597084000	1	2.321010000	-6.657905000	0.000000000
8	0.000000000	-6.966025000	0.391329000	1	-2.757450000	-10.008254000	0.000000000
8	0.000000000	-3.482189000	-0.589981000	1	-2.686405000	-7.268310000	0.000000000
8	0.000000000	0.000000000	0.397217000	1	2.209581000	-10.888931000	0.000000000
8	0.000000000	3.482189000	-0.589981000	1	2.125353000	-13.631842000	0.000000000
8	0.000000000	6.966025000	0.391329000	1	-0.559587000	-14.230521000	0.000000000
8	0.000000000	10.447551000	-0.597084000	8	-0.814048000	-12.171868000	0.000000000
				8	0.263179000	-8.716812000	0.000000000
				8	-0.628479000	-5.209011000	0.000000000
				8	0.447855000	-1.753405000	0.000000000
				8	-0.447855000	1.753405000	0.000000000
				8	0.628479000	5.209011000	0.000000000
				8	-0.263179000	8.716812000	0.000000000
				8	0.814048000	12.171868000	0.000000000

9-0							
6	0.000000000	15.028186000	-0.228068000	6	0.000000000	-13.226560000	-1.550741000
6	0.000000000	14.655749000	-1.538072000	6	0.000000000	-14.655749000	-1.538072000
6	0.000000000	13.226560000	-1.550741000	6	0.000000000	-15.028186000	-0.228068000
6	0.000000000	12.831307000	-0.236982000	1	0.000000000	15.981064000	0.276902000
6	0.000000000	11.549079000	0.406381000	1	0.000000000	12.572569000	-2.409447000
6	0.000000000	11.155659000	1.722423000	1	0.000000000	15.316651000	-2.392610000
6	0.000000000	9.734115000	1.720562000	1	0.000000000	11.814363000	2.577629000
6	0.000000000	9.344245000	0.402542000	1	0.000000000	9.073434000	2.574231000
6	0.000000000	8.068233000	-0.244824000	1	0.000000000	5.600293000	-2.422431000
6	0.000000000	7.678472000	-1.563524000	1	0.000000000	8.339783000	-2.416680000
6	0.000000000	6.257998000	-1.566459000	1	0.000000000	4.850241000	2.565822000
6	0.000000000	5.862759000	-0.249350000	1	0.000000000	2.110973000	2.563832000
6	0.000000000	4.584879000	0.393009000	1	0.000000000	-1.369594000	-2.425702000
6	0.000000000	4.191287000	1.710840000	1	0.000000000	1.369594000	-2.425702000
6	0.000000000	2.771148000	1.709776000	1	0.000000000	-2.110973000	2.563832000
6	0.000000000	2.379464000	0.391410000	1	0.000000000	-4.850241000	2.565822000
6	0.000000000	1.102759000	-0.253009000	1	0.000000000	-8.339783000	-2.416680000
6	0.000000000	0.710082000	-1.571137000	1	0.000000000	-5.600293000	-2.422431000
6	0.000000000	-0.710082000	-1.571137000	1	0.000000000	-9.073434000	2.574231000
6	0.000000000	-1.102759000	-0.253009000	1	0.000000000	-11.814363000	2.577629000
6	0.000000000	-2.379464000	0.391410000	1	0.000000000	-15.316651000	-2.392610000
6	0.000000000	-2.771148000	1.709776000	1	0.000000000	-12.572569000	-2.409447000
6	0.000000000	-4.191287000	1.710840000	1	0.000000000	-15.981064000	0.276902000
6	0.000000000	-4.584879000	0.393009000	8	0.000000000	-13.929289000	0.581787000
6	0.000000000	-5.862759000	-0.249350000	8	0.000000000	-10.448819000	-0.410188000
6	0.000000000	-6.257998000	-1.566459000	8	0.000000000	-6.964072000	0.567656000
6	0.000000000	-7.678472000	-1.563524000	8	0.000000000	-3.482855000	-0.422675000
6	0.000000000	-8.068233000	-0.244824000	8	0.000000000	0.000000000	0.561785000
6	0.000000000	-9.344245000	0.402542000	8	0.000000000	3.482855000	-0.422675000
6	0.000000000	-9.734115000	1.720562000	8	0.000000000	6.964072000	0.567656000
6	0.000000000	-11.155659000	1.722423000	8	0.000000000	10.448819000	-0.410188000
6	0.000000000	-11.549079000	0.406381000	8	0.000000000	13.929289000	0.581787000
6	0.000000000	-12.831307000	-0.236982000				

10-O							
6	4.176406000	16.243198000	0.000000000	6	-2.424426000	-14.855398000	0.000000000
6	2.814530000	16.230366000	0.000000000	6	-2.814530000	-16.230366000	0.000000000
6	2.424426000	14.855398000	0.000000000	6	-4.176406000	-16.243198000	0.000000000
6	3.586918000	14.126840000	0.000000000	1	4.915384000	17.028624000	0.000000000
6	3.867884000	12.720034000	0.000000000	1	-4.915384000	-17.028624000	0.000000000
6	5.032440000	11.991662000	0.000000000	1	1.423356000	14.451756000	0.000000000
6	4.653708000	10.621484000	0.000000000	1	2.165185000	17.093718000	0.000000000
6	3.279502000	10.595019000	0.000000000	1	6.031781000	12.399814000	0.000000000
6	2.316363000	9.536861000	0.000000000	1	5.301778000	9.758198000	0.000000000
6	0.941472000	9.511961000	0.000000000	1	-0.439319000	7.737235000	0.000000000
6	0.560790000	8.143480000	0.000000000	1	0.294959000	10.376377000	0.000000000
6	1.725306000	7.412084000	0.000000000	1	4.168833000	5.684779000	0.000000000
6	2.003988000	6.009240000	0.000000000	1	3.435786000	3.045648000	0.000000000
6	3.168918000	5.278108000	0.000000000	1	-2.304125000	1.026363000	0.000000000
6	2.788818000	3.909754000	0.000000000	1	-1.570683000	3.665120000	0.000000000
6	1.413745000	3.884166000	0.000000000	1	2.304125000	-1.026363000	0.000000000
6	0.451365000	2.826287000	0.000000000	1	1.570683000	-3.665120000	0.000000000
6	-0.923797000	2.800969000	0.000000000	1	-4.168833000	-5.684779000	0.000000000
6	-1.304078000	1.432734000	0.000000000	1	-3.435786000	-3.045648000	0.000000000
6	-0.139290000	0.701338000	0.000000000	1	0.439319000	-7.737235000	0.000000000
6	0.139290000	-0.701338000	0.000000000	1	-0.294959000	-10.376377000	0.000000000
6	1.304078000	-1.432734000	0.000000000	1	-6.031781000	-12.399814000	0.000000000
6	0.923797000	-2.800969000	0.000000000	1	-5.301778000	-9.758198000	0.000000000
6	-0.451365000	-2.826287000	0.000000000	1	-1.423356000	-14.451756000	0.000000000
6	-1.413745000	-3.884166000	0.000000000	1	-2.165185000	-17.093718000	0.000000000
6	-2.788818000	-3.909754000	0.000000000	8	-0.941139000	-1.545650000	0.000000000
6	-3.168918000	-5.278108000	0.000000000	8	0.941139000	1.545650000	0.000000000
6	-2.003988000	-6.009240000	0.000000000	8	0.923797000	5.164857000	0.000000000
6	-1.725306000	-7.412084000	0.000000000	8	2.805839000	8.256353000	0.000000000
6	-0.560790000	-8.143480000	0.000000000	8	-0.923797000	-5.164857000	0.000000000
6	-0.941472000	-9.511961000	0.000000000	8	2.788819000	11.875620000	0.000000000
6	-2.316363000	-9.536861000	0.000000000	8	4.666857000	14.969255000	0.000000000
6	-3.279502000	-10.595019000	0.000000000	8	-2.805839000	-8.256353000	0.000000000
6	-4.653708000	-10.621484000	0.000000000	8	-2.788819000	-11.875620000	0.000000000
6	-5.032440000	-11.991662000	0.000000000	8	-4.666857000	-14.969255000	0.000000000
6	-3.867884000	-12.720034000	0.000000000				
6	-3.586918000	-14.126840000	0.000000000				

Polythiophenes

1-S				2-S			
6	1.243160000	-0.011415000	0.000000000	6	-0.122876000	3.211432000	0.000000000
6	0.714874000	-1.272534000	0.000000000	6	1.182900000	2.807060000	0.000000000
6	-0.714824000	-1.272493000	0.000000000	6	1.323964000	1.390412000	0.000000000
6	-1.243257000	-0.011656000	0.000000000	6	0.122876000	0.714773000	0.000000000
16	0.000000000	1.199280000	0.000000000	6	-0.122876000	-0.714773000	0.000000000
1	1.320307000	-2.171656000	0.000000000	6	-1.323964000	-1.390412000	0.000000000
1	-1.320311000	-2.171653000	0.000000000	6	-1.182900000	-2.807060000	0.000000000
1	2.283671000	0.281156000	0.000000000	6	0.122876000	-3.211432000	0.000000000
1	-2.283389000	0.282263000	0.000000000	16	-1.210435000	1.859139000	0.000000000
				1	2.020358000	3.495031000	0.000000000
				16	1.210435000	-1.859139000	0.000000000
				1	2.282824000	0.884269000	0.000000000
				1	-2.282824000	-0.884269000	0.000000000
				1	-2.020358000	-3.495031000	0.000000000
				1	-0.517439000	4.217673000	0.000000000
				1	0.517439000	-4.217673000	0.000000000
3-S				4-S			
6	0.000000000	5.169480000	0.125956000	6	0.042515000	7.133570000	0.000000000
6	0.000000000	4.641646000	1.387453000	6	-1.235309000	6.646318000	0.000000000
6	0.000000000	3.218793000	1.392653000	6	-1.286007000	5.224546000	0.000000000
6	0.000000000	2.661230000	0.130887000	6	-0.042515000	4.626790000	0.000000000
6	0.000000000	1.265915000	-0.250656000	6	0.293701000	3.220258000	0.000000000
6	0.000000000	0.707832000	-1.512064000	6	1.536929000	2.621388000	0.000000000
6	0.000000000	-0.707832000	-1.512064000	6	1.492163000	1.207637000	0.000000000
6	0.000000000	-1.265915000	-0.250656000	6	0.212311000	0.689253000	0.000000000
6	0.000000000	-2.661230000	0.130887000	6	-0.212311000	-0.689253000	0.000000000
6	0.000000000	-3.218793000	1.392653000	6	-1.492163000	-1.207637000	0.000000000
6	0.000000000	-4.641646000	1.387453000	6	-1.536929000	-2.621388000	0.000000000
6	0.000000000	-5.169480000	0.125956000	6	-0.293701000	-3.220258000	0.000000000
16	0.000000000	3.929240000	-1.086863000	6	0.042515000	-4.626790000	0.000000000
1	0.000000000	5.246714000	2.286629000	6	1.286007000	-5.224546000	0.000000000
16	0.000000000	0.000000000	0.968201000	6	1.235309000	-6.646318000	0.000000000
1	0.000000000	2.623309000	2.298696000	6	-0.042515000	-7.133570000	0.000000000
16	0.000000000	-3.929240000	-1.086863000	16	1.215167000	5.855412000	0.000000000
1	0.000000000	1.302869000	-2.418420000	1	-2.114605000	7.279895000	0.000000000
1	0.000000000	-1.302869000	-2.418420000	16	-0.965914000	1.994753000	0.000000000
1	0.000000000	-2.623309000	2.298696000	1	-2.210496000	4.658186000	0.000000000
1	0.000000000	-5.246714000	2.286629000	16	0.965914000	-1.994753000	0.000000000
1	0.000000000	6.209078000	-0.168082000	1	2.461661000	3.187321000	0.000000000
1	0.000000000	-6.209078000	-0.168082000	16	-1.215167000	-5.855412000	0.000000000
				1	2.379252000	0.584276000	0.000000000
				1	-2.379252000	-0.584276000	0.000000000
				1	-2.461661000	-3.187321000	0.000000000
				1	2.210496000	-4.658186000	0.000000000
				1	2.114605000	-7.279895000	0.000000000
				1	0.369614000	8.163308000	0.000000000
				1	-0.369614000	-8.163308000	0.000000000

5-S				6-S			
6	0.000000000	9.093007000	-0.147149000	6	2.737874000	10.710975000	0.000000000
6	0.000000000	8.566086000	-1.409051000	6	1.381929000	10.533037000	0.000000000
6	0.000000000	7.143539000	-1.415180000	6	1.003458000	9.161877000	0.000000000
6	0.000000000	6.584851000	-0.153552000	6	2.074707000	8.292238000	0.000000000
6	0.000000000	5.189696000	0.226114000	6	2.074707000	6.846302000	0.000000000
6	0.000000000	4.630260000	1.487740000	6	3.144512000	5.974309000	0.000000000
6	0.000000000	3.215997000	1.487597000	6	2.771781000	4.610055000	0.000000000
6	0.000000000	2.657264000	0.224522000	6	1.406016000	4.403865000	0.000000000
6	0.000000000	1.266510000	-0.155327000	6	0.672343000	3.162996000	0.000000000
6	0.000000000	0.706736000	-1.418409000	6	-0.694137000	2.957654000	0.000000000
6	0.000000000	-0.706736000	-1.418409000	6	-1.068457000	1.595083000	0.000000000
6	0.000000000	-1.266510000	-0.155327000	6	0.001444000	0.720496000	0.000000000
6	0.000000000	-2.657264000	0.224522000	6	-0.001444000	-0.720496000	0.000000000
6	0.000000000	-3.215997000	1.487597000	6	1.068457000	-1.595083000	0.000000000
6	0.000000000	-4.630260000	1.487740000	6	0.694137000	-2.957654000	0.000000000
6	0.000000000	-5.189696000	0.226114000	6	-0.672343000	-3.162996000	0.000000000
6	0.000000000	-6.584851000	-0.153552000	6	-1.406016000	-4.403865000	0.000000000
6	0.000000000	-7.143539000	-1.415180000	6	-2.771781000	-4.610055000	0.000000000
6	0.000000000	-8.566086000	-1.409051000	6	-3.144512000	-5.974309000	0.000000000
6	0.000000000	-9.093007000	-0.147149000	6	-2.074707000	-6.846302000	0.000000000
16	0.000000000	7.851928000	1.065249000	6	-2.074707000	-8.292238000	0.000000000
1	0.000000000	9.171552000	-2.307928000	6	-1.003458000	-9.161877000	0.000000000
16	0.000000000	3.925149000	-0.994322000	6	-1.381929000	-10.533037000	0.000000000
1	0.000000000	6.549008000	-2.321883000	6	-2.737874000	-10.710975000	0.000000000
16	0.000000000	0.000000000	1.064791000	16	3.582837000	9.195649000	0.000000000
1	0.000000000	5.224898000	2.394300000	1	0.673061000	11.352820000	0.000000000
16	0.000000000	-3.925149000	-0.994322000	16	0.564351000	5.948110000	0.000000000
1	0.000000000	2.621012000	2.393910000	1	-0.027228000	8.825357000	0.000000000
16	0.000000000	-7.851928000	1.065249000	16	1.513651000	1.618672000	0.000000000
1	0.000000000	1.301665000	-2.324748000	1	4.175606000	6.309398000	0.000000000
1	0.000000000	-1.301665000	-2.324748000	16	-1.513651000	-1.618672000	0.000000000
1	0.000000000	-2.621012000	2.393910000	1	3.489151000	3.797180000	0.000000000
1	0.000000000	-5.224898000	2.394300000	16	-0.564351000	-5.948110000	0.000000000
1	0.000000000	-6.549008000	-2.321883000	1	-1.410360000	3.771506000	0.000000000
1	0.000000000	-9.171552000	-2.307928000	16	-3.582837000	-9.195649000	0.000000000
1	0.000000000	10.132349000	0.149350000	1	-2.099936000	1.261266000	0.000000000
1	0.000000000	-10.132349000	0.149350000	1	2.099936000	-1.261266000	0.000000000
				1	1.410360000	-3.771506000	0.000000000
				1	-3.489151000	-3.797180000	0.000000000
				1	-4.175606000	-6.309398000	0.000000000
				1	0.027228000	-8.825357000	0.000000000
				1	-0.673061000	-11.352820000	0.000000000
				1	3.296294000	11.636352000	0.000000000
				1	-3.296294000	-11.636352000	0.000000000

7-S				8-S			
6	0.000000000	13.015607000	0.151575000	6	0.019569000	14.978216000	0.000000000
6	0.000000000	12.489832000	1.413991000	6	-1.249068000	14.467791000	0.000000000
6	0.000000000	11.067347000	1.421350000	6	-1.273815000	13.045448000	0.000000000
6	0.000000000	10.507627000	0.160153000	6	-0.019569000	12.470373000	0.000000000
6	0.000000000	9.112186000	-0.218251000	6	0.341486000	11.070280000	0.000000000
6	0.000000000	8.551721000	-1.479541000	6	1.595737000	10.494170000	0.000000000
6	0.000000000	7.137602000	-1.478230000	6	1.576884000	9.080182000	0.000000000
6	0.000000000	6.579940000	-0.214575000	6	0.306364000	8.538273000	0.000000000
6	0.000000000	5.189731000	0.166313000	6	-0.091996000	7.153004000	0.000000000
6	0.000000000	4.631136000	1.430253000	6	-1.363061000	6.610650000	0.000000000
6	0.000000000	3.218140000	1.431764000	6	-1.382710000	5.197891000	0.000000000
6	0.000000000	2.656834000	0.168883000	6	-0.127109000	4.620408000	0.000000000
6	0.000000000	1.266507000	-0.208871000	6	0.232326000	3.225315000	0.000000000
6	0.000000000	0.706337000	-1.472419000	6	1.488340000	2.648235000	0.000000000
6	0.000000000	-0.706337000	-1.472419000	6	1.469224000	1.235835000	0.000000000
6	0.000000000	-1.266507000	-0.208871000	6	0.198058000	0.692414000	0.000000000
6	0.000000000	-2.656834000	0.168883000	6	-0.198058000	-0.692414000	0.000000000
6	0.000000000	-3.218140000	1.431764000	6	-1.469224000	-1.235835000	0.000000000
6	0.000000000	-4.631136000	1.430253000	6	-1.488340000	-2.648235000	0.000000000
6	0.000000000	-5.189731000	0.166313000	6	-0.232326000	-3.225315000	0.000000000
6	0.000000000	-6.579940000	-0.214575000	6	0.127109000	-4.620408000	0.000000000
6	0.000000000	-7.137602000	-1.478230000	6	1.382710000	-5.197891000	0.000000000
6	0.000000000	-8.551721000	-1.479541000	6	1.363061000	-6.610650000	0.000000000
6	0.000000000	-9.112186000	-0.218251000	6	0.091996000	-7.153004000	0.000000000
6	0.000000000	-10.507627000	0.160153000	6	-0.306364000	-8.538273000	0.000000000
6	0.000000000	-11.067347000	1.421350000	6	-1.576884000	-9.080182000	0.000000000
6	0.000000000	-12.489832000	1.413991000	6	-1.595737000	-10.494170000	0.000000000
6	0.000000000	-13.015607000	0.151575000	6	-0.341486000	-11.070280000	0.000000000
16	0.000000000	11.773590000	-1.059770000	6	0.019569000	-12.470373000	0.000000000
1	0.000000000	13.096094000	2.312320000	6	1.273815000	-13.045448000	0.000000000
16	0.000000000	7.848813000	1.003268000	6	1.249068000	-14.467791000	0.000000000
1	0.000000000	10.473611000	2.328578000	6	-0.019569000	-14.978216000	0.000000000
16	0.000000000	3.922271000	-1.052707000	1	0.329655000	16.013609000	0.000000000
1	0.000000000	9.145639000	-2.386558000	16	1.215696000	13.721291000	0.000000000
16	0.000000000	0.000000000	1.011567000	1	-2.139998000	15.084879000	0.000000000
1	0.000000000	6.541888000	-2.384072000	16	-0.895574000	9.822173000	0.000000000
16	0.000000000	-3.922271000	-1.052707000	1	-2.188210000	12.462840000	0.000000000
1	0.000000000	5.227032000	2.335947000	16	1.110666000	5.870062000	0.000000000
16	0.000000000	-7.848813000	1.003268000	1	2.509952000	11.076923000	0.000000000
1	0.000000000	2.624213000	2.338771000	16	-1.005075000	1.975433000	0.000000000
16	0.000000000	-11.773590000	-1.059770000	1	2.475256000	8.473248000	0.000000000
1	0.000000000	1.301246000	-2.378761000	16	1.005075000	-1.975433000	0.000000000
1	0.000000000	-1.301246000	-2.378761000	1	-2.261022000	7.218141000	0.000000000
1	0.000000000	-2.624213000	2.338771000	16	-1.110666000	-5.870062000	0.000000000
1	0.000000000	-5.227032000	2.335947000	1	-2.297195000	4.615555000	0.000000000
1	0.000000000	-6.541888000	-2.384072000	16	0.895574000	-9.822173000	0.000000000
1	0.000000000	-9.145639000	-2.386558000	1	2.402485000	3.231067000	0.000000000
1	0.000000000	-10.473611000	2.328578000	16	-1.215696000	-13.721291000	0.000000000
1	0.000000000	-13.096094000	2.312320000	1	2.367503000	0.628804000	0.000000000
1	0.000000000	-14.054704000	-0.145796000	1	-2.367503000	-0.628804000	0.000000000
1	0.000000000	14.054704000	-0.145796000	1	-2.402485000	-3.231067000	0.000000000
				1	2.297195000	-4.615555000	0.000000000
				1	2.261022000	-7.218141000	0.000000000
				1	-2.475256000	-8.473248000	0.000000000
				1	-2.509952000	-11.076923000	0.000000000
				1	2.188210000	-12.462840000	0.000000000
				1	2.139998000	-15.084879000	0.000000000
				1	-0.329655000	-16.013609000	0.000000000

9-S							
6	0.000000000	16.938789000	-0.150263000	6	0.000000000	-14.991224000	-1.421252000
6	0.000000000	16.413758000	-1.412929000	6	0.000000000	-16.413758000	-1.412929000
6	0.000000000	14.991224000	-1.421252000	6	0.000000000	-16.938789000	-0.150263000
6	0.000000000	14.430674000	-0.160435000	1	0.000000000	17.977693000	0.147849000
6	0.000000000	13.034889000	0.216832000	16	0.000000000	15.695759000	1.060290000
6	0.000000000	12.473483000	1.477747000	1	0.000000000	17.020520000	-2.310922000
6	0.000000000	11.059392000	1.475422000	16	0.000000000	11.772418000	-1.005562000
6	0.000000000	10.502666000	0.211346000	1	0.000000000	14.398165000	-2.328915000
6	0.000000000	9.112747000	-0.170531000	16	0.000000000	7.844454000	1.047526000
6	0.000000000	8.555092000	-1.434966000	1	0.000000000	13.066811000	2.385145000
6	0.000000000	7.142179000	-1.437525000	16	0.000000000	3.923915000	-1.019722000
6	0.000000000	6.579947000	-0.175003000	1	0.000000000	10.462962000	2.380794000
6	0.000000000	5.189425000	0.201670000	16	0.000000000	0.000000000	1.041436000
6	0.000000000	4.628350000	1.464954000	1	0.000000000	9.151735000	-2.340158000
6	0.000000000	3.215856000	1.463957000	16	0.000000000	-3.923915000	-1.019722000
6	0.000000000	2.656518000	0.199897000	1	0.000000000	6.548889000	-2.344954000
6	0.000000000	1.266758000	-0.178729000	16	0.000000000	-7.844454000	1.047526000
6	0.000000000	0.706189000	-1.442468000	1	0.000000000	5.222692000	2.371659000
6	0.000000000	-0.706189000	-1.442468000	16	0.000000000	-11.772418000	-1.005562000
6	0.000000000	-1.266758000	-0.178729000	1	0.000000000	2.620294000	2.369882000
6	0.000000000	-2.656518000	0.199897000	16	0.000000000	-15.695759000	1.060290000
6	0.000000000	-3.215856000	1.463957000	1	0.000000000	1.301294000	-2.348718000
6	0.000000000	-4.628350000	1.464954000	1	0.000000000	-1.301294000	-2.348718000
6	0.000000000	-5.189425000	0.201670000	1	0.000000000	-2.620294000	2.369882000
6	0.000000000	-6.579947000	-0.175003000	1	0.000000000	-5.222692000	2.371659000
6	0.000000000	-7.142179000	-1.437525000	1	0.000000000	-6.548889000	-2.344954000
6	0.000000000	-8.555092000	-1.434966000	1	0.000000000	-9.151735000	-2.340158000
6	0.000000000	-9.112747000	-0.170531000	1	0.000000000	-10.462962000	2.380794000
6	0.000000000	-10.502666000	0.211346000	1	0.000000000	-13.066811000	2.385145000
6	0.000000000	-11.059392000	1.475422000	1	0.000000000	-14.398165000	-2.328915000
6	0.000000000	-12.473483000	1.477747000	1	0.000000000	-17.020520000	-2.310922000
6	0.000000000	-13.034889000	0.216832000	1	0.000000000	-17.977693000	0.147849000
6	0.000000000	-14.430674000	-0.160435000				

10-S							
6	0.180547000	-18.899329000	0.000000000	6	-0.187343000	16.391295000	0.000000000
6	1.442536000	-18.372654000	0.000000000	6	-1.448941000	16.950117000	0.000000000
6	1.448941000	-16.950117000	0.000000000	6	-1.442536000	18.372654000	0.000000000
6	0.187343000	-16.391295000	0.000000000	6	-0.180547000	18.899329000	0.000000000
6	-0.191810000	-14.996021000	0.000000000	1	-0.116397000	-19.938549000	0.000000000
6	-1.453493000	-14.436306000	0.000000000	16	-1.031688000	-17.657882000	0.000000000
6	-1.453054000	-13.022221000	0.000000000	1	2.341284000	-18.978278000	0.000000000
6	-0.189688000	-12.463847000	0.000000000	16	1.028921000	-13.731948000	0.000000000
6	0.190451000	-11.073446000	0.000000000	1	2.355745000	-16.355779000	0.000000000
6	1.454228000	-10.514247000	0.000000000	16	-1.029171000	-9.806671000	0.000000000
6	1.455046000	-9.101369000	0.000000000	1	-2.360025000	-15.030935000	0.000000000
6	0.191810000	-8.540686000	0.000000000	16	1.033725000	-5.883966000	0.000000000
6	-0.186454000	-7.150596000	0.000000000	1	-2.359134000	-12.426895000	0.000000000
6	-1.450316000	-6.590718000	0.000000000	16	-1.030423000	-1.961857000	0.000000000
6	-1.450640000	-5.178221000	0.000000000	1	2.360068000	-11.109875000	0.000000000
6	-0.187070000	-4.617746000	0.000000000	16	1.030423000	1.961857000	0.000000000
6	0.190643000	-3.227684000	0.000000000	1	2.361671000	-8.506873000	0.000000000
6	1.454170000	-2.666895000	0.000000000	16	-1.033725000	5.883966000	0.000000000
6	1.453493000	-1.254452000	0.000000000	1	-2.356382000	-7.186010000	0.000000000
6	0.189443000	-0.694841000	0.000000000	16	1.029171000	9.806671000	0.000000000
6	-0.189443000	0.694841000	0.000000000	1	-2.357037000	-4.583407000	0.000000000
6	-1.453493000	1.254452000	0.000000000	16	-1.028921000	13.731948000	0.000000000
6	-1.454170000	2.666895000	0.000000000	1	2.360659000	-3.261546000	0.000000000
6	-0.190643000	3.227684000	0.000000000	16	1.031688000	17.657882000	0.000000000
6	0.187070000	4.617746000	0.000000000	1	2.359446000	-0.658963000	0.000000000
6	1.450640000	5.178221000	0.000000000	1	-2.359446000	0.658963000	0.000000000
6	1.450316000	6.590718000	0.000000000	1	-2.360659000	3.261546000	0.000000000
6	0.186454000	7.150596000	0.000000000	1	2.357037000	4.583407000	0.000000000
6	-0.191810000	8.540686000	0.000000000	1	2.356382000	7.186010000	0.000000000
6	-1.455046000	9.101369000	0.000000000	1	-2.361671000	8.506873000	0.000000000
6	-1.454228000	10.514247000	0.000000000	1	-2.360068000	11.109875000	0.000000000
6	-0.190451000	11.073446000	0.000000000	1	2.359134000	12.426895000	0.000000000
6	0.189688000	12.463847000	0.000000000	1	2.360025000	15.030935000	0.000000000
6	1.453054000	13.022221000	0.000000000	1	-2.355745000	16.355779000	0.000000000
6	1.453493000	14.436306000	0.000000000	1	-2.341284000	18.978278000	0.000000000
6	0.191810000	14.996021000	0.000000000	1	0.116397000	19.938549000	0.000000000

Polyselenophenes

1-Se				2-Se			
6	0.000000000	1.290044000	-0.439289000	6	0.670186000	3.245919000	0.000000000
6	0.000000000	0.716439000	-1.676273000	6	-0.670186000	2.994218000	0.000000000
6	0.000000000	-0.716439000	-1.676273000	6	-1.023249000	1.612796000	0.000000000
6	0.000000000	-1.290044000	-0.439289000	6	0.023457000	0.721682000	0.000000000
1	0.000000000	2.344540000	-0.203326000	6	-0.023457000	-0.721682000	0.000000000
1	0.000000000	-1.301913000	-2.589913000	6	1.023249000	-1.612796000	0.000000000
1	0.000000000	1.301913000	-2.589913000	6	0.670186000	-2.994218000	0.000000000
1	0.000000000	-2.344540000	-0.203326000	6	-0.670186000	-3.245919000	0.000000000
34	0.000000000	0.000000000	0.910977000	1	1.161318000	4.208397000	0.000000000
				1	-2.056408000	1.278558000	0.000000000
				1	-1.414205000	3.783856000	0.000000000
				1	2.056408000	-1.278558000	0.000000000
				1	1.414205000	-3.783856000	0.000000000
				1	-1.161318000	-4.208397000	0.000000000
				34	1.663530000	1.663642000	0.000000000
				34	-1.663530000	-1.663642000	0.000000000
3-Se				4-Se			
6	0.000000000	5.328019000	0.249160000	6	-0.162748000	7.344921000	0.000000000
6	0.000000000	4.753707000	1.486649000	6	-1.399482000	6.768621000	0.000000000
6	0.000000000	3.328765000	1.488864000	6	-1.399482000	5.343956000	0.000000000
6	0.000000000	2.723032000	0.253338000	6	-0.162672000	4.740097000	0.000000000
6	0.000000000	1.316319000	-0.056026000	6	0.148482000	3.334479000	0.000000000
6	0.000000000	0.708413000	-1.290928000	6	1.385005000	2.727948000	0.000000000
6	0.000000000	-0.708413000	-1.290928000	6	1.387929000	1.312468000	0.000000000
6	0.000000000	-1.316319000	-0.056026000	6	0.152453000	0.701537000	0.000000000
6	0.000000000	-2.723032000	0.253338000	6	-0.152453000	-0.701537000	0.000000000
6	0.000000000	-3.328765000	1.488864000	6	-1.387929000	-1.312468000	0.000000000
6	0.000000000	-4.753707000	1.486649000	6	-1.385005000	-2.727948000	0.000000000
6	0.000000000	-5.328019000	0.249160000	6	-0.148482000	-3.334479000	0.000000000
1	0.000000000	6.382047000	0.011261000	6	0.162672000	-4.740097000	0.000000000
1	0.000000000	2.750667000	2.408033000	6	1.399482000	-5.343956000	0.000000000
1	0.000000000	5.336007000	2.402056000	6	1.399482000	-6.768621000	0.000000000
1	0.000000000	1.284720000	-2.211093000	6	0.162748000	-7.344921000	0.000000000
1	0.000000000	-1.284720000	-2.211093000	1	0.073516000	8.399311000	0.000000000
1	0.000000000	-5.336007000	2.402056000	1	-2.317766000	4.764452000	0.000000000
1	0.000000000	-2.750667000	2.408033000	1	-2.315771000	7.349509000	0.000000000
1	0.000000000	-6.382047000	0.011261000	1	2.303958000	3.306166000	0.000000000
34	0.000000000	4.041469000	-1.104233000	1	2.309203000	0.737907000	0.000000000
34	0.000000000	0.000000000	1.302784000	1	-2.303958000	-3.306166000	0.000000000
34	0.000000000	-4.041469000	-1.104233000	1	-2.309203000	-0.737907000	0.000000000
				1	2.317766000	-4.764452000	0.000000000
				1	2.315771000	-7.349509000	0.000000000
				1	-0.073516000	-8.399311000	0.000000000
				34	1.192891000	6.060840000	0.000000000
				34	-1.209080000	2.016798000	0.000000000
				34	1.209080000	-2.016798000	0.000000000
				34	-1.192891000	-6.060840000	0.000000000

5-Se				6-Se			
6	0.000000000	9.363224000	-0.207844000	6	2.297679000	11.146725000	0.000000000
6	0.000000000	8.789451000	-1.445758000	6	0.965584000	10.851696000	0.000000000
6	0.000000000	7.364705000	-1.449204000	6	0.656918000	9.460599000	0.000000000
6	0.000000000	6.757711000	-0.213895000	6	1.733567000	8.603121000	0.000000000
6	0.000000000	5.351549000	0.094464000	6	1.733567000	7.163509000	0.000000000
6	0.000000000	4.742297000	1.329885000	6	2.809762000	6.303535000	0.000000000
6	0.000000000	3.327075000	1.329970000	6	2.506281000	4.921134000	0.000000000
6	0.000000000	2.718446000	0.092989000	6	1.167526000	4.592080000	0.000000000
6	0.000000000	1.316682000	-0.214218000	6	0.567047000	3.288956000	0.000000000
6	0.000000000	0.707087000	-1.451312000	6	-0.772351000	2.959567000	0.000000000
6	0.000000000	-0.707087000	-1.451312000	6	-1.076407000	1.578732000	0.000000000
6	0.000000000	-1.316682000	-0.214218000	6	0.001035000	0.717098000	0.000000000
6	0.000000000	-2.718446000	0.092989000	6	-0.001035000	-0.717098000	0.000000000
6	0.000000000	-3.327075000	1.329970000	6	1.076407000	-1.578732000	0.000000000
6	0.000000000	-4.742297000	1.329885000	6	0.772351000	-2.959567000	0.000000000
6	0.000000000	-5.351549000	0.094464000	6	-0.567047000	-3.288956000	0.000000000
6	0.000000000	-6.757711000	-0.213895000	6	-1.167526000	-4.592080000	0.000000000
6	0.000000000	-7.364705000	-1.449204000	6	-2.506281000	-4.921134000	0.000000000
6	0.000000000	-8.789451000	-1.445758000	6	-2.809762000	-6.303535000	0.000000000
6	0.000000000	-9.363224000	-0.207844000	6	-1.733567000	-7.163509000	0.000000000
1	0.000000000	10.416957000	0.031278000	6	-1.733567000	-8.603121000	0.000000000
1	0.000000000	6.787672000	-2.369026000	6	-0.656918000	-9.460599000	0.000000000
1	0.000000000	9.372227000	-2.360866000	6	-0.965584000	-10.851696000	0.000000000
1	0.000000000	5.318380000	2.250158000	6	-2.297679000	-11.146725000	0.000000000
1	0.000000000	2.750910000	2.250256000	1	2.756646000	12.124956000	0.000000000
1	0.000000000	-1.283338000	-2.371535000	1	-0.365225000	9.094106000	0.000000000
1	0.000000000	1.283338000	-2.371535000	1	0.196510000	11.616898000	0.000000000
1	0.000000000	-2.750910000	2.250256000	1	3.832227000	6.668800000	0.000000000
1	0.000000000	-5.318380000	2.250158000	1	3.281580000	4.160992000	0.000000000
1	0.000000000	-9.372227000	-2.360866000	1	-2.099025000	1.213809000	0.000000000
1	0.000000000	-6.787672000	-2.369026000	1	-1.547100000	3.720242000	0.000000000
1	0.000000000	-10.416957000	0.031278000	1	2.099025000	-1.213809000	0.000000000
34	0.000000000	-8.075174000	1.145362000	1	1.547100000	-3.720242000	0.000000000
34	0.000000000	-4.036718000	-1.266237000	1	-3.832227000	-6.668800000	0.000000000
34	0.000000000	0.000000000	1.146413000	1	-3.281580000	-4.160992000	0.000000000
34	0.000000000	4.036718000	-1.266237000	1	0.365225000	-9.094106000	0.000000000
34	0.000000000	8.075174000	1.145362000	1	-0.196510000	-11.616898000	0.000000000
				1	-2.756646000	-12.124956000	0.000000000
				34	-3.343333000	-9.598703000	0.000000000
				34	-0.122732000	-6.171156000	0.000000000
				34	-1.612866000	-1.710728000	0.000000000
				34	1.612866000	1.710728000	0.000000000
				34	0.122732000	6.171156000	0.000000000
				34	3.343333000	9.598703000	0.000000000

7-Se				8-Se			
6	0.000000000	13.396222000	0.185806000	6	-0.150830000	15.412958000	0.000000000
6	0.000000000	12.823860000	1.424463000	6	-1.388854000	14.839214000	0.000000000
6	0.000000000	11.399348000	1.428917000	6	-1.391708000	13.414725000	0.000000000
6	0.000000000	10.791725000	0.193831000	6	-0.155941000	12.808465000	0.000000000
6	0.000000000	9.385404000	-0.112953000	6	0.152339000	11.402501000	0.000000000
6	0.000000000	8.775432000	-1.348192000	6	1.388213000	10.793762000	0.000000000
6	0.000000000	7.360536000	-1.347409000	6	1.388852000	9.378892000	0.000000000
6	0.000000000	6.752576000	-0.109842000	6	0.151889000	8.769695000	0.000000000
6	0.000000000	5.351224000	0.197544000	6	-0.154257000	7.368111000	0.000000000
6	0.000000000	4.742325000	1.435483000	6	-1.391760000	6.758245000	0.000000000
6	0.000000000	3.328809000	1.436676000	6	-1.391856000	5.344813000	0.000000000
6	0.000000000	2.717817000	0.199573000	6	-0.154257000	4.734727000	0.000000000
6	0.000000000	1.316776000	-0.105281000	6	0.151347000	3.333944000	0.000000000
6	0.000000000	0.706573000	-1.342969000	6	1.389361000	2.724157000	0.000000000
6	0.000000000	-0.706573000	-1.342969000	6	1.389897000	1.311121000	0.000000000
6	0.000000000	-1.316776000	-0.105281000	6	0.152332000	0.700407000	0.000000000
6	0.000000000	-2.717817000	0.199573000	6	-0.152332000	-0.700407000	0.000000000
6	0.000000000	-3.328809000	1.436676000	6	-1.389897000	-1.311121000	0.000000000
6	0.000000000	-4.742325000	1.435483000	6	-1.389361000	-2.724157000	0.000000000
6	0.000000000	-5.351224000	0.197544000	6	-0.151347000	-3.333944000	0.000000000
6	0.000000000	-6.752576000	-0.109842000	6	0.154257000	-4.734727000	0.000000000
6	0.000000000	-7.360536000	-1.347409000	6	1.391856000	-5.344813000	0.000000000
6	0.000000000	-8.775432000	-1.348192000	6	1.391760000	-6.758245000	0.000000000
6	0.000000000	-9.385404000	-0.112953000	6	0.154257000	-7.368111000	0.000000000
6	0.000000000	-10.791725000	0.193831000	6	-0.151889000	-8.769695000	0.000000000
6	0.000000000	-11.399348000	1.428917000	6	-1.388852000	-9.378892000	0.000000000
6	0.000000000	-12.823860000	1.424463000	6	-1.388213000	-10.793762000	0.000000000
6	0.000000000	-13.396222000	0.185806000	6	-0.152339000	-11.402501000	0.000000000
1	0.000000000	14.449914000	-0.053569000	6	0.155941000	-12.808465000	0.000000000
1	0.000000000	10.822664000	2.348974000	6	1.391708000	-13.414725000	0.000000000
1	0.000000000	13.407704000	2.338848000	6	1.388854000	-14.839214000	0.000000000
1	0.000000000	9.351324000	-2.268572000	6	0.150830000	-15.412958000	0.000000000
1	0.000000000	6.783606000	-2.267209000	1	0.087448000	16.466897000	0.000000000
1	0.000000000	2.753068000	2.357211000	1	-2.311148000	12.837049000	0.000000000
1	0.000000000	5.319629000	2.355014000	1	-2.303886000	15.422043000	0.000000000
1	0.000000000	1.283080000	-2.263004000	1	2.308026000	11.370560000	0.000000000
1	0.000000000	-1.283080000	-2.263004000	1	2.309209000	8.802848000	0.000000000
1	0.000000000	-5.319629000	2.355014000	1	-2.311980000	4.768408000	0.000000000
1	0.000000000	-2.753068000	2.357211000	1	-2.311705000	7.334880000	0.000000000
1	0.000000000	-6.783606000	-2.267209000	1	2.309169000	3.301023000	0.000000000
1	0.000000000	-9.351324000	-2.268572000	1	2.310127000	0.734915000	0.000000000
1	0.000000000	-13.407704000	2.338848000	1	-2.309169000	-3.301023000	0.000000000
1	0.000000000	-10.822664000	2.348974000	1	-2.310127000	-0.734915000	0.000000000
1	0.000000000	-14.449914000	-0.053569000	1	2.311980000	-4.768408000	0.000000000
34	0.000000000	-12.108266000	-1.165892000	1	2.311705000	-7.334880000	0.000000000
34	0.000000000	-8.071691000	1.248335000	1	-2.308026000	-11.370560000	0.000000000
34	0.000000000	-4.033740000	-1.161897000	1	-2.309209000	-8.802848000	0.000000000
34	0.000000000	0.000000000	1.255285000	1	2.311148000	-12.837049000	0.000000000
34	0.000000000	4.033740000	-1.161897000	1	2.303886000	-15.422043000	0.000000000
34	0.000000000	8.071691000	1.248335000	1	-0.087448000	-16.466897000	0.000000000
34	0.000000000	12.108266000	-1.165892000	34	-1.202319000	-14.126530000	0.000000000
				34	1.207638000	-10.087445000	0.000000000
				34	-1.206233000	-6.051697000	0.000000000
				34	1.208761000	-2.016750000	0.000000000
				34	-1.208761000	2.016750000	0.000000000
				34	1.206233000	6.051697000	0.000000000
				34	-1.207638000	10.087445000	0.000000000
				34	1.202319000	14.126530000	0.000000000

9-Se							
6	0.000000000	17.430108000	-0.170468000	6	0.000000000	-14.825626000	-0.180011000
6	0.000000000	16.858459000	-1.409483000	6	0.000000000	-15.434015000	-1.414761000
6	0.000000000	15.434015000	-1.414761000	6	0.000000000	-16.858459000	-1.409483000
6	0.000000000	14.825626000	-0.180011000	6	0.000000000	-17.430108000	-0.170468000
6	0.000000000	13.419148000	0.125871000	1	0.000000000	18.483645000	0.069586000
6	0.000000000	12.808438000	1.360799000	1	0.000000000	14.857824000	-2.335130000
6	0.000000000	11.393614000	1.359183000	1	0.000000000	17.442903000	-2.323484000
6	0.000000000	10.786367000	0.121242000	1	0.000000000	13.383836000	2.281483000
6	0.000000000	9.385234000	-0.186837000	1	0.000000000	10.816123000	2.278639000
6	0.000000000	8.777073000	-1.425216000	1	0.000000000	6.788459000	-2.348123000
6	0.000000000	7.363670000	-1.427250000	1	0.000000000	9.354971000	-2.344368000
6	0.000000000	6.751915000	-0.190465000	1	0.000000000	5.315820000	2.271149000
6	0.000000000	5.350777000	0.113359000	1	0.000000000	2.749785000	2.269678000
6	0.000000000	4.739785000	1.350827000	1	0.000000000	-1.283055000	-2.351510000
6	0.000000000	3.326856000	1.349985000	1	0.000000000	1.283055000	-2.351510000
6	0.000000000	2.717300000	0.111792000	1	0.000000000	-2.749785000	2.269678000
6	0.000000000	1.316738000	-0.193617000	1	0.000000000	-5.315820000	2.271149000
6	0.000000000	0.706464000	-1.431523000	1	0.000000000	-9.354971000	-2.344368000
6	0.000000000	-0.706464000	-1.431523000	1	0.000000000	-6.788459000	-2.348123000
6	0.000000000	-1.316738000	-0.193617000	1	0.000000000	-10.816123000	2.278639000
6	0.000000000	-2.717300000	0.111792000	1	0.000000000	-13.383836000	2.281483000
6	0.000000000	-3.326856000	1.349985000	1	0.000000000	-17.442903000	-2.323484000
6	0.000000000	-4.739785000	1.350827000	1	0.000000000	-14.857824000	-2.335130000
6	0.000000000	-5.350777000	0.113359000	1	0.000000000	-18.483645000	0.069586000
6	0.000000000	-6.751915000	-0.190465000	34	0.000000000	-16.141454000	1.180415000
6	0.000000000	-7.363670000	-1.427250000	34	0.000000000	-12.106262000	-1.236198000
6	0.000000000	-8.777073000	-1.425216000	34	0.000000000	-8.067006000	1.171855000
6	0.000000000	-9.385234000	-0.186837000	34	0.000000000	-4.034941000	-1.248067000
6	0.000000000	-10.786367000	0.121242000	34	0.000000000	0.000000000	1.167019000
6	0.000000000	-11.393614000	1.359183000	34	0.000000000	4.034941000	-1.248067000
6	0.000000000	-12.808438000	1.360799000	34	0.000000000	8.067006000	1.171855000
6	0.000000000	-13.419148000	0.125871000	34	0.000000000	12.106262000	-1.236198000
				34	0.000000000	16.141454000	1.180415000

10- ^{Se}							
6	-0.146208000	19.447125000	0.000000000	6	-0.154820000	-15.436370000	0.000000000
6	-1.384535000	18.873955000	0.000000000	6	0.152629000	-16.842540000	0.000000000
6	-1.388108000	17.449482000	0.000000000	6	1.388108000	-17.449482000	0.000000000
6	-0.152629000	16.842540000	0.000000000	6	1.384535000	-18.873955000	0.000000000
6	0.154820000	15.436370000	0.000000000	6	0.146208000	-19.447125000	0.000000000
6	1.390462000	14.827056000	0.000000000	1	0.092417000	20.500991000	0.000000000
6	1.390462000	13.412214000	0.000000000	1	-0.092417000	-20.500991000	0.000000000
6	0.153204000	12.803580000	0.000000000	1	-2.307793000	16.872214000	0.000000000
6	-0.153263000	11.402083000	0.000000000	1	-2.299227000	19.457312000	0.000000000
6	-1.391049000	10.792696000	0.000000000	1	2.310498000	15.403469000	0.000000000
6	-1.391649000	9.379305000	0.000000000	1	2.310572000	12.835764000	0.000000000
6	-0.154236000	8.768792000	0.000000000	1	-2.311956000	8.803196000	0.000000000
6	0.150720000	7.367883000	0.000000000	1	-2.310779000	11.369670000	0.000000000
6	1.388685000	6.757824000	0.000000000	1	2.308576000	7.334531000	0.000000000
6	1.388889000	5.344885000	0.000000000	1	2.309008000	4.768490000	0.000000000
6	0.151119000	4.734451000	0.000000000	1	-2.310589000	0.733383000	0.000000000
6	-0.153423000	3.333711000	0.000000000	1	-2.311345000	3.299382000	0.000000000
6	-1.391192000	2.723066000	0.000000000	1	2.310589000	-0.733383000	0.000000000
6	-1.390757000	1.310213000	0.000000000	1	2.311345000	-3.299382000	0.000000000
6	-0.152630000	0.700273000	0.000000000	1	-2.308576000	-7.334531000	0.000000000
6	0.152630000	-0.700273000	0.000000000	1	-2.309008000	-4.768490000	0.000000000
6	1.390757000	-1.310213000	0.000000000	1	2.311956000	-8.803196000	0.000000000
6	1.391192000	-2.723066000	0.000000000	1	2.310779000	-11.369670000	0.000000000
6	0.153423000	-3.333711000	0.000000000	1	-2.310498000	-15.403469000	0.000000000
6	-0.151119000	-4.734451000	0.000000000	1	-2.310572000	-12.835764000	0.000000000
6	-1.388889000	-5.344885000	0.000000000	1	2.307793000	-16.872214000	0.000000000
6	-1.388685000	-6.757824000	0.000000000	1	2.299227000	-19.457312000	0.000000000
6	-0.150720000	-7.367883000	0.000000000	34	-1.207700000	-2.017410000	0.000000000
6	0.154236000	-8.768792000	0.000000000	34	1.207700000	2.017410000	0.000000000
6	1.391649000	-9.379305000	0.000000000	34	-1.209791000	6.051082000	0.000000000
6	1.391049000	-10.792696000	0.000000000	34	1.206832000	10.085235000	0.000000000
6	0.153263000	-11.402083000	0.000000000	34	1.209791000	-6.051082000	0.000000000
6	-0.153204000	-12.803580000	0.000000000	34	-1.205800000	14.121933000	0.000000000
6	-1.390462000	-13.412214000	0.000000000	34	1.206239000	18.160038000	0.000000000
6	-1.390462000	-14.827056000	0.000000000	34	-1.206832000	-10.085235000	0.000000000
				34	1.205800000	-14.121933000	0.000000000
				34	-1.206239000	-18.160038000	0.000000000

Polyenes-all-cis *cisoid*; n=number of C=C bonds

n=1				n=2			
6	0.000000000	0.000000000	0.665124000	6	0.249353000	1.523443000	-0.493851000
1	0.000000000	0.923317000	1.238130000	1	0.655029000	2.527355000	-0.419856000
6	0.000000000	0.000000000	-0.665124000	6	0.249353000	0.691389000	0.554737000
1	0.000000000	-0.923317000	-1.238130000	1	0.629156000	1.056293000	1.508973000
1	0.000000000	0.923317000	-1.238130000	6	-0.249353000	-0.691389000	0.554737000
1	0.000000000	-0.923317000	1.238130000	1	-0.629156000	-1.056293000	1.508973000
				6	-0.249353000	-1.523443000	-0.493851000
				1	0.166138000	-1.231772000	-1.454432000
				1	-0.655029000	-2.527355000	-0.419856000
				1	-0.166138000	1.231772000	-1.454432000
n=3				n=4			
6	-0.333601000	1.671796000	-1.096897000	6	0.759654000	-1.329795000	-1.352892000
1	-0.149808000	2.469063000	-1.810405000	1	1.034985000	-1.697046000	-2.336731000
6	0.333601000	1.618913000	0.062474000	6	-0.269190000	-1.880199000	-0.681341000
1	1.041093000	2.420201000	0.279720000	1	-0.809666000	-2.691809000	-1.167636000
6	0.159721000	0.655941000	1.159893000	6	-0.759654000	-1.556614000	0.646204000
1	0.307184000	1.098564000	2.145505000	1	-1.489419000	-2.274714000	1.018256000
6	-0.159721000	-0.655941000	1.159893000	6	-0.444912000	-0.574613000	1.537598000
1	-0.307184000	-1.098564000	2.145505000	1	-0.898154000	-0.721371000	2.519744000
6	-0.333601000	-1.618913000	0.062474000	6	0.444912000	0.574613000	1.537598000
1	-1.041093000	-2.420201000	0.279720000	1	0.898154000	0.721371000	2.519744000
6	0.333601000	-1.671796000	-1.096897000	6	0.759654000	1.556614000	0.646204000
1	1.076716000	-0.929267000	-1.367639000	1	1.489419000	2.274714000	1.018256000
1	0.149808000	-2.469063000	-1.810405000	6	0.269190000	1.880199000	-0.681341000
1	-1.076716000	0.929267000	-1.367639000	1	0.809666000	2.691809000	-1.167636000
				6	-0.759654000	1.329795000	-1.352892000
				1	-1.375133000	0.547145000	-0.931045000
				1	-1.034985000	1.697046000	-2.336731000
				1	1.375133000	-0.547145000	-0.931045000
n=5				n=6			
6	0.049499000	2.994112000	-0.094634000	6	-0.523944000	1.869651000	1.814990000
1	-0.567719000	3.825120000	-0.421962000	1	-1.183482000	1.729055000	2.665689000
6	0.664198000	2.201910000	-0.982111000	6	-0.720112000	2.880098000	0.955608000
1	0.550425000	2.438217000	-2.040675000	1	-1.550756000	3.557769000	1.153213000
6	1.557388000	1.069742000	-0.707353000	6	0.096321000	3.261100000	-0.199872000
1	2.321802000	0.913793000	-1.468599000	1	-0.033712000	4.303818000	-0.488920000
6	1.573096000	0.208829000	0.328628000	6	1.013392000	2.580604000	-0.928804000
1	2.391935000	-0.512933000	0.344992000	1	1.567364000	3.189908000	-1.645745000
6	0.664198000	0.105041000	1.481436000	6	1.451868000	1.184221000	-0.929087000
1	1.157259000	0.131046000	2.455166000	1	2.528850000	1.065718000	-1.054061000
6	-0.664198000	-0.105041000	1.481436000	6	0.720112000	0.041789000	-0.936428000
1	-1.157259000	-0.131046000	2.455166000	1	1.260778000	-0.897967000	-0.994975000
6	-1.573096000	-0.208829000	0.328628000	6	-0.720112000	-0.041789000	-0.936428000
1	-2.391935000	0.512933000	0.344992000	1	-1.260778000	0.897967000	-0.994975000
6	-1.557388000	-1.069742000	-0.707353000	6	-1.451868000	-1.184221000	-0.929087000
1	-2.321802000	-0.913793000	-1.468599000	1	-2.528850000	-1.065718000	-1.054061000
6	-0.664198000	-2.201910000	-0.982111000	6	-1.013392000	-2.580604000	-0.928804000
1	-0.550425000	-2.438217000	-2.040675000	1	-1.567364000	-3.189908000	-1.645745000
6	-0.049499000	-2.994112000	-0.094634000	6	-0.096321000	-3.261100000	-0.199872000
1	-0.145242000	-2.842954000	0.975282000	1	0.033712000	-4.303818000	-0.488920000
1	0.567719000	-3.825120000	-0.421962000	6	0.720112000	-2.880098000	0.955608000
1	0.145242000	2.842954000	0.975282000	1	1.550756000	-3.557769000	1.153213000
				6	0.523944000	-1.869651000	1.814990000
				1	-0.297769000	-1.170936000	1.706353000
				1	1.183482000	-1.729055000	2.665689000
				1	0.297769000	1.170936000	1.706353000

n=7				n=8			
6	-3.088641000	-2.014017000	-1.409566000	6	2.938869000	3.479862000	-0.575226000
1	-3.501671000	-2.242087000	-2.387341000	1	2.896404000	4.416257000	-1.122956000
6	-3.531088000	-0.958203000	-0.711379000	6	3.400127000	2.365887000	-1.161519000
1	-4.321805000	-0.357220000	-1.160969000	1	3.739018000	2.446813000	-2.194605000
6	-3.144294000	-0.514777000	0.630898000	6	3.581871000	1.031444000	-0.582558000
1	-3.870624000	0.156562000	1.088189000	1	4.281708000	0.410514000	-1.141216000
6	-2.072916000	-0.808195000	1.399380000	6	3.056867000	0.455361000	0.520113000
1	-2.096765000	-0.399693000	2.411499000	1	3.449131000	-0.533408000	0.765545000
6	-0.891772000	-1.643602000	1.142177000	6	2.079629000	0.951023000	1.499436000
1	-0.679267000	-2.366147000	1.932593000	1	2.392711000	0.835638000	2.538993000
6	-0.001824000	-1.580367000	0.134381000	6	0.838870000	1.430917000	1.295867000
1	0.800933000	-2.319423000	0.139037000	1	0.285407000	1.755937000	2.178602000
6	0.001824000	-0.671726000	-1.019590000	6	0.145081000	1.633676000	0.016293000
1	0.044829000	-1.166428000	-1.991602000	1	-0.193147000	2.655952000	-0.163733000
6	-0.001824000	0.671726000	-1.019590000	6	-0.145081000	0.720195000	-0.926002000
1	-0.044829000	1.166428000	-1.991602000	1	-0.622846000	1.086286000	-1.835880000
6	0.001824000	1.580367000	0.134381000	6	0.145081000	-0.720195000	-0.926002000
1	-0.800933000	2.319423000	0.139037000	1	0.622846000	-1.086286000	-1.835880000
6	0.891772000	1.643602000	1.142177000	6	-0.145081000	-1.633676000	0.016293000
1	0.679267000	2.366147000	1.932593000	1	0.193147000	-2.655952000	-0.163733000
6	2.072916000	0.808195000	1.399380000	6	-0.838870000	-1.430917000	1.295867000
1	2.096765000	0.399693000	2.411499000	1	-0.285407000	-1.755937000	2.178602000
6	3.144294000	0.514777000	0.630898000	6	-2.079629000	-0.951023000	1.499436000
1	3.870624000	-0.156562000	1.088189000	1	-2.392711000	-0.835638000	2.538993000
6	3.531088000	0.958203000	-0.711379000	6	-3.056867000	-0.455361000	0.520113000
1	4.321805000	0.357220000	-1.160969000	1	-3.449131000	0.533408000	0.765545000
6	3.088641000	2.014017000	-1.409566000	6	-3.581871000	-1.031444000	-0.582558000
1	2.324851000	2.682468000	-1.029202000	1	-4.281708000	-0.410514000	-1.141216000
1	3.501671000	2.242087000	-2.387341000	6	-3.400127000	-2.365887000	-1.161519000
1	-2.324851000	-2.682468000	-1.029202000	1	-3.739018000	-2.446813000	-2.194605000
				6	-2.938869000	-3.479862000	-0.575226000
				1	-2.607538000	-3.496802000	0.456826000
				1	-2.896404000	-4.416257000	-1.122956000
				1	2.607538000	3.496802000	0.456826000
n=9							
6	-3.815000000	3.536518000	-0.736286000	6	2.130765000	-0.539946000	-1.315027000
1	-3.831118000	4.554035000	-1.114535000	1	2.099513000	-0.037973000	-2.283550000
6	-3.659086000	3.297320000	0.573556000	6	3.159879000	-0.232847000	-0.504267000
1	-3.565869000	4.160457000	1.233106000	1	3.824842000	0.565029000	-0.840888000
6	-3.659086000	2.011763000	1.278650000	6	3.472352000	-0.750182000	0.835838000
1	-3.863539000	2.104036000	2.345004000	1	3.619121000	0.036376000	1.578531000
6	-3.472352000	0.750182000	0.835838000	6	3.659086000	-2.011763000	1.278650000
1	-3.619121000	-0.036376000	1.578531000	1	3.863539000	-2.104036000	2.345004000
6	-3.159879000	0.232847000	-0.504267000	6	3.659086000	-3.297320000	0.573556000
1	-3.824842000	-0.565029000	-0.840888000	1	3.565869000	-4.160457000	1.233106000
6	-2.130765000	0.539946000	-1.315027000	6	3.815000000	-3.536518000	-0.736286000
1	-2.099513000	0.037973000	-2.283550000	1	3.942125000	-2.739365000	-1.459859000
6	-1.060500000	1.520745000	-1.087347000	1	3.831118000	-4.554035000	-1.114535000
1	-0.955543000	2.274837000	-1.869639000	1	-3.942125000	2.739365000	-1.459859000
6	-0.189700000	1.574932000	-0.064935000				
1	0.502911000	2.417988000	-0.050929000				
6	-0.079729000	0.667532000	1.087104000				
1	-0.095634000	1.163239000	2.059054000				
6	0.079729000	-0.667532000	1.087104000				
1	0.095634000	-1.163239000	2.059054000				
6	0.189700000	-1.574932000	-0.064935000				
1	-0.502911000	-2.417988000	-0.050929000				
6	1.060500000	-1.520745000	-1.087347000				
1	0.955543000	-2.274837000	-1.869639000				

n=10						
6	-0.665455000	4.863936000	-0.835385000	6	-0.536548000	-2.213510000
1	-1.484051000	5.174032000	-1.484221000	1	-0.793267000	-2.449515000
6	0.216533000	4.008880000	-1.396841000	6	-1.558710000	-2.586154000
1	0.046156000	3.786365000	-2.452016000	1	-2.562535000	-2.216134000
6	1.420657000	3.361709000	-0.858170000	6	-1.420657000	-3.361709000
1	2.304487000	3.472494000	-1.489570000	1	-2.304487000	-3.472494000
6	1.558710000	2.586154000	0.233385000	6	-0.216533000	-4.008880000
1	2.562535000	2.216134000	0.448988000	1	-0.046156000	-3.786365000
6	0.536548000	2.213510000	1.219885000	6	0.665455000	-4.863936000
1	0.793267000	2.449515000	2.254372000	1	1.484051000	-5.174032000
6	-0.638201000	1.593942000	1.010965000	6	0.712777000	-5.484483000
1	-1.280189000	1.454191000	1.882105000	1	1.668853000	-5.955606000
6	-1.214242000	1.120839000	-0.255321000	6	-0.259869000	-5.590663000
1	-2.240288000	1.446340000	-0.433928000	1	-1.249144000	-5.175077000
6	-0.665455000	0.312670000	-1.179754000	1	-0.084486000	-6.119214000
1	-1.258215000	0.118254000	-2.075347000	6	-0.712777000	5.484483000
6	0.665455000	-0.312670000	-1.179754000	1	-1.668853000	5.955606000
1	1.258215000	-0.118254000	-2.075347000	6	0.259869000	5.590663000
6	1.214242000	-1.120839000	-0.255321000	1	0.084486000	6.119214000
1	2.240288000	-1.446340000	-0.433928000	1	1.249144000	5.175077000
6	0.638201000	-1.593942000	1.010965000			
1	1.280189000	-1.454191000	1.882105000			
n=20						
6	0.086543000	3.521901000	-1.420715000	1	-1.654754000	-6.597783000
1	-0.040656000	3.549806000	-2.504262000	6	-1.143077000	-6.760053000
6	1.269548000	3.013441000	-0.997868000	1	-2.154959000	-6.597572000
1	1.983214000	2.812955000	-1.798403000	6	-0.290818000	-7.406689000
6	1.823461000	2.720686000	0.313386000	1	-0.648584000	-7.644002000
1	2.908390000	2.840631000	0.327591000	6	-0.054667000	5.450229000
6	1.308775000	2.297148000	1.499033000	1	-0.073601000	5.240833000
1	2.046358000	2.256582000	2.302439000	6	0.911640000	6.274234000
6	-0.011372000	1.927704000	1.971772000	1	1.654754000	6.597783000
1	-0.119248000	2.109729000	3.042576000	6	1.143077000	6.760053000
6	-1.116635000	1.382130000	1.398886000	1	2.154959000	6.597572000
1	-1.977929000	1.322623000	2.066555000	6	0.290818000	7.406689000
6	-1.425368000	0.880094000	0.072186000	1	0.648584000	7.644002000
1	-2.475779000	1.016766000	-0.189920000	6	1.099569000	-7.802486000
6	-0.689616000	0.233624000	-0.863786000	1	1.819807000	-7.468824000
1	-1.204542000	0.039565000	-1.805852000	6	1.577120000	-8.560378000
6	0.689616000	-0.233624000	-0.863786000	1	2.659292000	-8.699636000
1	1.204542000	-0.039565000	-1.805852000	6	0.847009000	-9.170785000
6	1.425368000	-0.880094000	0.072186000	1	1.246860000	-8.909232000
1	2.475779000	-1.016766000	-0.189920000	6	-0.198453000	-10.020866000
6	1.116635000	-1.382130000	1.398886000	1	-0.596583000	-10.301145000
1	1.977929000	-1.322623000	2.066555000	6	-1.099569000	7.802486000
6	0.011372000	-1.927704000	1.971772000	1	-1.819807000	7.468824000
1	0.119248000	-2.109729000	3.042576000	6	-1.577120000	8.560378000
6	-1.308775000	-2.297148000	1.499033000	1	-2.659292000	8.699636000
1	-2.046358000	-2.256582000	2.302439000	6	-0.847009000	9.170785000
6	-1.823461000	-2.720686000	0.313386000	1	-1.246860000	8.909232000
1	-2.908390000	-2.840631000	0.327591000	6	0.198453000	10.020866000
6	-1.269548000	-3.013441000	-0.997868000	1	0.596583000	10.301145000
1	-1.983214000	-2.812955000	-1.798403000	6	-0.900197000	-10.636875000
6	-0.086543000	-3.521901000	-1.420715000	1	-1.965151000	-10.809253000
1	0.040656000	-3.549806000	-2.504262000	6	-0.360463000	-11.064858000
6	1.072778000	-4.027803000	-0.699921000	1	0.698787000	-10.958414000
1	2.024288000	-3.754070000	-1.156667000	6	-0.969742000	-11.536669000
6	1.143077000	-4.828085000	0.381958000	1	0.900197000	10.636875000
1	2.143210000	-5.039324000	0.763724000	6	1.965151000	10.809253000
6	-1.072778000	4.027803000	-0.699921000	1	0.360463000	11.064858000
1	-2.024288000	3.754070000	-1.156667000	6	0.969742000	11.536669000
6	-1.143077000	4.828085000	0.381958000	1	-0.698787000	10.958414000
1	-2.143210000	5.039324000	0.763724000			
6	0.054667000	-5.450229000	1.146704000			
1	0.073601000	-5.240833000	2.217596000			
6	-0.911640000	-6.274234000	0.704869000			

Polyenes-all-*cis transoid*; n=number of C=C bonds

n=3				n=4			
6	-2.369870000	1.689735000	0.000000000	6	0.148642000	-4.034412000	0.000000000
1	-3.427046000	1.446288000	0.000000000	1	-0.624136000	-4.795731000	0.000000000
6	-1.424864000	0.736160000	0.000000000	6	-0.148639000	-2.724475000	0.000000000
1	-1.737433000	-0.305941000	0.000000000	1	-1.195615000	-2.429253000	0.000000000
6	0.000000000	1.016486000	0.000000000	6	0.853213000	-1.675658000	0.000000000
1	0.267251000	2.072334000	0.000000000	1	1.886236000	-2.020536000	0.000000000
6	1.010194000	0.113519000	0.000000000	6	0.640869000	-0.333646000	0.000000000
1	2.029649000	0.496713000	0.000000000	1	1.524549000	0.299354000	0.000000000
6	0.890740000	-1.333660000	0.000000000	6	-0.640877000	0.333646000	0.000000000
1	-0.109931000	-1.760508000	0.000000000	1	-1.524566000	-0.299340000	0.000000000
6	1.944257000	-2.165792000	0.000000000	6	-0.853211000	1.675659000	0.000000000
1	1.820998000	-3.243599000	0.000000000	1	-1.886231000	2.020548000	0.000000000
1	-2.110431000	2.745435000	0.000000000	6	0.148642000	2.724476000	0.000000000
1	2.964202000	-1.789414000	0.000000000	1	1.195619000	2.429254000	0.000000000
				6	-0.148639000	4.034407000	0.000000000
				1	0.624140000	4.795725000	0.000000000
				1	-1.178739000	4.381900000	0.000000000
				1	1.178742000	-4.381904000	0.000000000
n=5				n=6			
6	-2.563392000	-4.447773000	0.000000000	6	0.507101000	-6.232384000	0.000000000
1	-2.185445000	-5.464591000	0.000000000	1	1.393468000	-6.857777000	0.000000000
6	-1.739405000	-3.386598000	0.000000000	6	0.587793000	-4.891150000	0.000000000
1	-0.665933000	-3.562499000	0.000000000	1	1.573495000	-4.430924000	0.000000000
6	-2.202606000	-2.012798000	0.000000000	6	-0.569588000	-4.018583000	0.000000000
1	-3.284418000	-1.887410000	0.000000000	1	-1.533597000	-4.525276000	0.000000000
6	-1.441359000	-0.885914000	0.000000000	6	-0.577336000	-2.658209000	0.000000000
1	-1.975126000	0.060923000	0.000000000	1	-1.552426000	-2.178055000	0.000000000
6	0.000000000	-0.824984000	0.000000000	6	0.577362000	-1.794872000	0.000000000
1	0.530561000	-1.773657000	0.000000000	1	1.550684000	-2.278640000	0.000000000
6	0.768336000	0.300780000	0.000000000	6	0.577043000	-0.430490000	0.000000000
1	1.845141000	0.152837000	0.000000000	1	1.550822000	0.052349000	0.000000000
6	0.299587000	1.665205000	0.000000000	6	-0.577062000	0.430493000	0.000000000
1	-0.776666000	1.816836000	0.000000000	1	-1.550862000	-0.052304000	0.000000000
6	1.071637000	2.784709000	0.000000000	6	-0.577336000	1.794874000	0.000000000
1	0.560472000	3.746366000	0.000000000	1	-1.550641000	2.278681000	0.000000000
6	2.519738000	2.853879000	0.000000000	6	0.577361000	2.658215000	0.000000000
1	3.074814000	1.918308000	0.000000000	1	1.552467000	2.178090000	0.000000000
6	3.208279000	4.007550000	0.000000000	6	0.569596000	4.018582000	0.000000000
1	4.292928000	4.025301000	0.000000000	1	1.533601000	4.525289000	0.000000000
1	2.702536000	4.969844000	0.000000000	6	-0.587791000	4.891147000	0.000000000
1	-3.643741000	-4.326587000	0.000000000	1	-1.573484000	4.430892000	0.000000000
				6	-0.507137000	6.232368000	0.000000000
				1	-1.393525000	6.857728000	0.000000000
				1	0.452610000	6.742873000	0.000000000
				1	-0.452662000	-6.742855000	0.000000000
n=7							
6	-4.786289000	5.588927000	0.000000000	1	3.410251000	-1.428731000	0.000000000
1	-4.581298000	6.654182000	0.000000000	6	2.137582000	-3.175695000	0.000000000
6	-3.797834000	4.678612000	0.000000000	1	1.101592000	-3.504574000	0.000000000
1	-2.768503000	5.030482000	0.000000000	6	3.084980000	-4.152257000	0.000000000
6	-4.026651000	3.247476000	0.000000000	1	2.740187000	-5.185267000	0.000000000
1	-5.072546000	2.943924000	0.000000000	6	4.524209000	-3.981036000	0.000000000
6	-3.088623000	2.261893000	0.000000000	1	4.917120000	-2.966727000	0.000000000
1	-3.458042000	1.239713000	0.000000000	6	5.393305000	-5.005922000	0.000000000
6	-1.658428000	2.440845000	0.000000000	1	6.466127000	-4.845183000	0.000000000
1	-1.292748000	3.464381000	0.000000000	1	-5.831754000	5.291067000	0.000000000
6	-0.712055000	1.457239000	0.000000000	1	5.052452000	-6.038214000	0.000000000
1	0.324297000	1.784883000	0.000000000				

6	-0.946492000	0.037573000	0.000000000
1	-1.982923000	-0.289735000	0.000000000
6	0.000000000	-0.947210000	0.000000000
1	-0.367733000	-1.969952000	0.000000000
6	1.427846000	-0.769011000	0.000000000
1	1.795990000	0.253602000	0.000000000
6	2.373039000	-1.753745000	0.000000000

n=8				n=9			
6	-7.076214000	-4.666789000	0.000000000	6	6.092783000	7.399216000	0.000000000
1	-8.108455000	-4.333638000	0.000000000	1	7.177164000	7.369314000	0.000000000
6	-6.052212000	-3.796601000	0.000000000	6	5.354257000	6.276552000	0.000000000
1	-6.275655000	-2.731955000	0.000000000	1	5.868124000	5.317746000	0.000000000
6	-4.660045000	-4.198976000	0.000000000	6	3.905024000	6.271146000	0.000000000
1	-4.487541000	-5.274278000	0.000000000	1	3.436639000	7.254317000	0.000000000
6	-3.566447000	-3.389254000	0.000000000	6	3.083520000	5.186347000	0.000000000
1	-2.597839000	-3.882492000	0.000000000	1	2.015177000	5.386354000	0.000000000
6	-3.566996000	-1.948204000	0.000000000	6	3.490528000	3.803958000	0.000000000
1	-4.537353000	-1.458440000	0.000000000	1	4.559622000	3.607965000	0.000000000
6	-2.473992000	-1.130091000	0.000000000	6	2.672409000	2.710858000	0.000000000
1	-2.671449000	-0.061274000	0.000000000	1	3.163509000	1.741188000	0.000000000
6	-1.094401000	-1.537184000	0.000000000	6	1.234277000	2.712582000	0.000000000
1	-0.897120000	-2.605996000	0.000000000	1	0.743500000	3.682360000	0.000000000
6	0.000000000	-0.718796000	0.000000000	6	0.414567000	1.618870000	0.000000000
1	0.969186000	-1.210825000	0.000000000	1	-0.654002000	1.817608000	0.000000000
6	-0.000019000	0.718892000	0.000000000	6	0.819884000	0.239956000	0.000000000
1	-0.969171000	1.210985000	0.000000000	1	1.888436000	0.041178000	0.000000000
6	1.094434000	1.537213000	0.000000000	6	0.000000000	-0.854090000	0.000000000
1	0.897231000	2.606042000	0.000000000	1	0.491193000	-1.823684000	0.000000000
6	2.474016000	1.130096000	0.000000000	1	-1.437207000	-0.852647000	0.000000000
1	2.671513000	0.061287000	0.000000000	6	-1.928521000	0.116900000	0.000000000
6	3.567001000	1.948236000	0.000000000	6	-2.256603000	-1.946605000	0.000000000
1	4.537378000	1.458512000	0.000000000	1	-3.325263000	-1.748523000	0.000000000
6	3.566452000	3.389289000	0.000000000	6	-1.850567000	-3.326292000	0.000000000
1	2.597856000	3.882550000	0.000000000	1	-0.781942000	-3.524740000	0.000000000
6	4.660052000	4.199020000	0.000000000	6	-2.669751000	-4.418588000	0.000000000
1	4.487604000	5.274331000	0.000000000	1	-2.180850000	-5.389377000	0.000000000
6	6.052175000	3.796552000	0.000000000	6	-4.110733000	-4.416813000	0.000000000
1	6.275559000	2.731895000	0.000000000	1	-4.603359000	-3.447906000	0.000000000
6	7.076157000	4.666608000	0.000000000	6	-4.920973000	-5.510092000	0.000000000
1	8.108368000	4.333374000	0.000000000	1	-5.996150000	-5.337023000	0.000000000
1	-6.907533000	-5.740750000	0.000000000	6	-4.519149000	-6.902520000	0.000000000
1	6.907644000	5.740603000	0.000000000	1	-3.454704000	-7.126542000	0.000000000
				6	-5.390030000	-7.925954000	0.000000000
				1	-5.057935000	-8.958663000	0.000000000
				1	-6.463821000	-7.756507000	0.000000000
				1	5.629778000	8.382731000	0.000000000
n=10							
6	7.136170000	-6.066922000	0.000000000	1	-4.537240000	1.458213000	0.000000000
1	6.178026000	-6.581992000	0.000000000	6	-3.567747000	3.388106000	0.000000000
6	8.259790000	-6.803930000	0.000000000	1	-2.598570000	3.880146000	0.000000000
1	8.231444000	-7.888352000	0.000000000	6	-4.661633000	4.205224000	0.000000000
1	9.242699000	-6.339584000	0.000000000	1	-4.466376000	5.274443000	0.000000000
6	7.129196000	-4.617568000	0.000000000	6	-6.043690000	3.797073000	0.000000000
1	8.112039000	-4.148426000	0.000000000	1	-6.242894000	2.728604000	0.000000000
6	6.043734000	-3.796989000	0.000000000	6	-7.129202000	4.617678000	0.000000000
1	6.242926000	-2.728515000	0.000000000	1	-8.111954000	4.148324000	0.000000000
6	4.661653000	-4.205142000	0.000000000	6	-7.136281000	6.066557000	0.000000000
1	4.466417000	-5.274365000	0.000000000	1	-6.178198000	6.581764000	0.000000000
6	3.567778000	-3.388027000	0.000000000	6	-8.259890000	6.803653000	0.000000000
1	2.598598000	-3.880064000	0.000000000	1	-8.231485000	7.888069000	0.000000000
6	3.568021000	-1.949930000	0.000000000	1	-9.242821000	6.339352000	0.000000000
1	4.537271000	-1.458131000	0.000000000				
6	2.473444000	-1.131166000	0.000000000				
1	2.671530000	-0.062477000	0.000000000				
6	1.095027000	-1.537381000	0.000000000				
1	0.896857000	-2.606035000	0.000000000				
6	0.000000000	-0.718329000	0.000000000				
1	-0.969042000	-1.210606000	0.000000000				
6	0.000025000	0.718398000	0.000000000				

1	0.969074000	1.210663000	0.000000000
6	-1.094994000	1.537464000	0.000000000
1	-0.896804000	2.606115000	0.000000000
6	-2.473408000	1.131257000	0.000000000
1	-2.671490000	0.062567000	0.000000000
6	-3.567994000	1.950021000	0.000000000

n=20							
6	0.583621000	-20.486567000	0.000000000	6	-0.574721000	4.026293000	0.000000000
1	1.569685000	-20.027149000	0.000000000	1	-1.549290000	4.507627000	0.000000000
6	0.501190000	-21.827836000	0.000000000	6	0.575118000	4.885792000	0.000000000
1	1.386817000	-22.454307000	0.000000000	1	1.549706000	4.404495000	0.000000000
1	-0.459197000	-22.337134000	0.000000000	6	0.575083000	6.254232000	0.000000000
6	-0.572982000	-19.613328000	0.000000000	1	1.549660000	6.735543000	0.000000000
1	-1.537325000	-20.119302000	0.000000000	6	-0.574772000	7.113846000	0.000000000
6	-0.579786000	-18.252544000	0.000000000	1	-1.549382000	6.632599000	0.000000000
1	-1.554647000	-17.771787000	0.000000000	6	-0.574599000	8.482192000	0.000000000
6	0.574924000	-17.390686000	0.000000000	1	-1.549106000	8.963637000	0.000000000
1	1.547956000	-17.875090000	0.000000000	6	0.575472000	9.341778000	0.000000000
6	0.575838000	-16.025169000	0.000000000	1	1.550013000	8.860388000	0.000000000
1	1.550130000	-15.543281000	0.000000000	6	0.575385000	10.709952000	0.000000000
6	-0.576144000	-15.164626000	0.000000000	1	1.549869000	11.191430000	0.000000000
1	-1.550253000	-15.646771000	0.000000000	6	-0.574894000	11.569757000	0.000000000
6	-0.576286000	-13.797492000	0.000000000	1	-1.549421000	11.088339000	0.000000000
1	-1.550643000	-13.315729000	0.000000000	6	-0.574647000	12.937587000	0.000000000
6	0.574647000	-12.937587000	0.000000000	1	-1.548974000	13.419349000	0.000000000
1	1.548974000	-13.419349000	0.000000000	6	0.576286000	13.797492000	0.000000000
6	0.574894000	-11.569757000	0.000000000	1	1.550643000	13.315729000	0.000000000
1	1.549421000	-11.088339000	0.000000000	6	0.576144000	15.164626000	0.000000000
6	-0.575385000	-10.709952000	0.000000000	1	1.550253000	15.646771000	0.000000000
1	-1.549869000	-11.191430000	0.000000000	6	-0.575838000	16.025169000	0.000000000
6	-0.575472000	-9.341778000	0.000000000	1	-1.550130000	15.543281000	0.000000000
1	-1.550013000	-8.860388000	0.000000000	6	-0.574924000	17.390686000	0.000000000
6	0.574599000	-8.482192000	0.000000000	1	-1.547956000	17.875090000	0.000000000
1	1.549106000	-8.963637000	0.000000000	6	0.579786000	18.252544000	0.000000000
6	0.574772000	-7.113846000	0.000000000	1	1.554647000	17.771787000	0.000000000
1	1.549382000	-6.632599000	0.000000000	6	0.572982000	19.613328000	0.000000000
6	-0.575083000	-6.254232000	0.000000000	1	1.537325000	20.119302000	0.000000000
1	-1.549660000	-6.735543000	0.000000000	6	-0.583621000	20.486567000	0.000000000
6	-0.575118000	-4.885792000	0.000000000	1	-1.569685000	20.027149000	0.000000000
1	-1.549706000	-4.404495000	0.000000000	6	-0.501190000	21.827836000	0.000000000
6	0.574721000	-4.026293000	0.000000000	1	0.459197000	22.337134000	0.000000000
1	1.549290000	-4.507627000	0.000000000	1	-1.386817000	22.454307000	0.000000000
6	0.574819000	-2.657807000	0.000000000				
1	1.549444000	-2.176586000	0.000000000				
6	-0.574924000	-1.798247000	0.000000000				
1	-1.549537000	-2.279492000	0.000000000				
6	-0.574895000	-0.429740000	0.000000000				
1	-1.549485000	0.051552000	0.000000000				
6	0.574924000	1.798247000	0.000000000				
1	1.549537000	2.279492000	0.000000000				
6	0.574895000	0.429740000	0.000000000				
1	1.549485000	-0.051552000	0.000000000				
6	-0.574819000	2.657807000	0.000000000				
1	-1.549444000	2.176586000	0.000000000				

Polyenes-all-*trans*; n=number of C=C bonds

n=2				n=3		
6	-0.000006000	-0.728635000	0.000000000	6	-0.326736000	1.885777000
1	-0.977448000	-1.210965000	0.000000000	1	-1.416690000	1.877190000
6	1.106751000	-1.484060000	0.000000000	6	0.318571000	3.063028000
1	1.058970000	-2.567926000	0.000000000	1	-0.216221000	4.006761000
1	2.098219000	-1.038198000	0.000000000	1	1.404290000	3.115003000
6	0.000000000	0.728627000	0.000000000	6	0.326736000	0.591698000
1	0.977446000	1.210953000	0.000000000	1	1.417206000	0.592726000
6	-1.106747000	1.484066000	0.000000000	6	-0.326736000	-0.591698000
1	-2.098222000	1.038216000	0.000000000	1	-1.417206000	-0.592726000
1	-1.058954000	2.567931000	0.000000000	6	0.326736000	-1.885777000
				1	1.416690000	-1.877190000
				6	-0.318571000	-3.063028000
				1	-1.404290000	-3.115003000
				1	0.216221000	-4.006761000
n=4				n=5		
6	2.229899000	3.692005000	0.000000000	6	-0.341052000	4.355489000
1	2.176523000	4.775365000	0.000000000	1	-1.430954000	4.337738000
1	3.222883000	3.250031000	0.000000000	6	0.293019000	5.540476000
6	1.123156000	1.482897000	0.000000000	1	-0.251599000	6.478508000
1	2.096195000	0.990928000	0.000000000	1	1.378068000	5.603552000
6	0.002858000	0.720241000	0.000000000	6	0.321909000	3.069915000
1	-0.968141000	1.216624000	0.000000000	1	1.412134000	3.077697000
6	-0.002858000	-0.720241000	0.000000000	6	-0.325862000	1.877763000
1	0.968141000	-1.216624000	0.000000000	1	-1.416405000	1.875989000
6	-1.123156000	-1.482897000	0.000000000	6	0.325862000	0.596411000
1	-2.096195000	-0.990928000	0.000000000	1	1.416211000	0.596495000
6	-1.123156000	-2.930343000	0.000000000	6	-0.325862000	-0.596411000
1	-0.146433000	-3.414360000	0.000000000	1	-1.416211000	-0.596495000
6	-2.229899000	-3.692005000	0.000000000	6	0.325862000	-1.877763000
1	-3.222883000	-3.250031000	0.000000000	1	1.416405000	-1.875989000
1	-2.176523000	-4.775365000	0.000000000	6	-0.321909000	-3.069915000
				1	-1.412134000	-3.077697000
				6	0.341052000	-4.355489000
				1	1.430954000	-4.337738000
				6	-0.293019000	-5.540476000
				1	-1.378068000	-5.603552000
				1	0.251599000	-6.478508000
n=6				n=7		
6	2.233721000	5.137744000	0.000000000	6	-0.354512000	6.826862000
1	1.254270000	5.616225000	0.000000000	1	-1.444359000	6.804833000
6	3.336110000	5.906939000	0.000000000	6	0.274651000	8.014897000
1	3.275586000	6.989909000	0.000000000	1	-0.274035000	8.950533000
1	4.331939000	5.471508000	0.000000000	1	1.359411000	8.082540000
6	2.242073000	3.691825000	0.000000000	6	0.313161000	5.544631000
1	3.217398000	3.204638000	0.000000000	1	1.403334000	5.556260000
6	1.123994000	2.921956000	0.000000000	6	-0.330603000	4.349025000
1	0.151267000	3.415058000	0.000000000	1	-1.421183000	4.344122000
6	1.123994000	1.485769000	0.000000000	6	0.324176000	3.071638000
1	2.095522000	0.990874000	0.000000000	1	1.414475000	3.073946000
6	0.000861000	0.717075000	0.000000000	6	-0.325529000	1.874690000
1	-0.970292000	1.212941000	0.000000000	1	-1.415981000	1.873954000
6	-0.000861000	-0.717075000	0.000000000	6	0.325529000	0.598690000
1	0.970292000	-1.212941000	0.000000000	1	1.415917000	0.598809000
6	-1.123994000	-1.485769000	0.000000000	6	-0.325529000	-0.598690000
1	-2.095522000	-0.990874000	0.000000000	1	-1.415917000	-0.598809000
6	-1.123994000	-2.921956000	0.000000000	6	0.325529000	-1.874690000
1	-0.151267000	-3.415058000	0.000000000	1	1.415981000	-1.873954000
6	-2.242073000	-3.691825000	0.000000000	6	-0.324176000	-3.071638000
1	-3.217398000	-3.204638000	0.000000000	1	-1.414475000	-3.073946000
6	-2.233721000	-5.137744000	0.000000000	6	0.330603000	-4.349025000
1	-1.254270000	-5.616225000	0.000000000	1	1.421183000	-4.344122000
6	-3.336110000	-5.906939000	0.000000000	6	-0.313161000	-5.544631000
1	-4.331939000	-5.471508000	0.000000000	1	-1.403334000	-5.556260000
1	-3.275586000	-6.989909000	0.000000000	6	0.354512000	-6.826862000

				1	1.444359000	-6.804833000	0.000000000
				6	-0.274651000	-8.014897000	0.000000000
				1	-1.359411000	-8.082540000	0.000000000
				1	0.274035000	-8.950533000	0.000000000
n=8				n=9			
6	3.350376000	7.343920000	0.000000000	6	-0.366900000	9.298565000	0.000000000
1	2.369657000	7.820177000	0.000000000	1	-1.456701000	9.273907000	0.000000000
6	4.450976000	8.116011000	0.000000000	6	0.259299000	10.488317000	0.000000000
1	4.387755000	9.198823000	0.000000000	1	-0.291794000	11.422533000	0.000000000
1	5.447965000	7.682984000	0.000000000	1	1.343881000	10.558705000	0.000000000
6	3.362009000	5.898114000	0.000000000	6	0.303736000	8.018204000	0.000000000
1	4.338458000	5.412706000	0.000000000	1	1.393876000	8.032311000	0.000000000
6	2.245210000	5.125353000	0.000000000	6	-0.337384000	6.820742000	0.000000000
1	1.271441000	5.616912000	0.000000000	1	-1.427967000	6.813587000	0.000000000
6	2.248031000	3.690088000	0.000000000	6	0.319822000	5.545385000	0.000000000
1	3.220394000	3.196401000	0.000000000	1	1.410107000	5.549678000	0.000000000
6	1.125193000	2.918601000	0.000000000	6	-0.327832000	4.346389000	0.000000000
1	0.153462000	3.413905000	0.000000000	1	-1.418309000	4.344084000	0.000000000
6	1.125193000	1.486742000	0.000000000	6	0.324695000	3.072740000	0.000000000
1	2.096474000	0.990746000	0.000000000	1	1.415064000	3.073948000	0.000000000
6	0.000370000	0.715482000	0.000000000	6	-0.325383000	1.872996000	0.000000000
1	-0.970735000	1.211915000	0.000000000	1	-1.415820000	1.872565000	0.000000000
6	-0.000370000	-0.715482000	0.000000000	6	0.325383000	0.599974000	0.000000000
1	0.970735000	-1.211915000	0.000000000	1	1.415791000	0.600097000	0.000000000
6	-1.125193000	-1.486742000	0.000000000	6	-0.325383000	-0.599974000	0.000000000
1	-2.096474000	-0.990746000	0.000000000	1	-1.415791000	-0.600097000	0.000000000
6	-1.125193000	-2.918601000	0.000000000	6	0.325383000	-1.872996000	0.000000000
1	-0.153462000	-3.413905000	0.000000000	1	1.415820000	-1.872565000	0.000000000
6	-2.248031000	-3.690088000	0.000000000	6	-0.324695000	-3.072740000	0.000000000
1	-3.220394000	-3.196401000	0.000000000	1	-1.415064000	-3.073948000	0.000000000
6	-2.245210000	-5.125353000	0.000000000	6	0.327832000	-4.346389000	0.000000000
1	-1.271441000	-5.616912000	0.000000000	1	1.418309000	-4.344084000	0.000000000
6	-3.362009000	-5.898114000	0.000000000	6	-0.319822000	-5.545385000	0.000000000
1	-4.338458000	-5.412706000	0.000000000	1	-1.410107000	-5.549678000	0.000000000
6	-3.350376000	-7.343920000	0.000000000	6	0.337384000	-6.820742000	0.000000000
1	-2.369657000	-7.820177000	0.000000000	1	1.427967000	-6.813587000	0.000000000
6	-4.450976000	-8.116011000	0.000000000	6	-0.303736000	-8.018204000	0.000000000
1	-5.447965000	-7.682984000	0.000000000	1	-1.393876000	-8.032311000	0.000000000
1	-4.387755000	-9.198823000	0.000000000	6	0.366900000	-9.298565000	0.000000000
				1	1.456701000	-9.273907000	0.000000000
				6	-0.259299000	-10.488317000	0.000000000
				1	-1.343881000	-10.558705000	0.000000000
				1	0.291794000	-11.422533000	0.000000000

n=10							
6	4.469982000	9.547162000	0.000000000	6	-1.126233000	-1.487061000	0.000000000
1	3.488747000	10.022028000	0.000000000	1	-2.097069000	-0.990607000	0.000000000
6	5.569564000	10.320887000	0.000000000	6	-1.126233000	-2.916203000	0.000000000
1	5.504720000	11.403596000	0.000000000	1	-0.155162000	-3.412294000	0.000000000
1	6.567088000	9.889357000	0.000000000	6	-2.251234000	-3.689045000	0.000000000
6	4.483707000	8.101934000	0.000000000	1	-3.222630000	-3.193766000	0.000000000
1	5.460688000	7.618087000	0.000000000	6	-2.249873000	-5.119813000	0.000000000
6	3.367710000	7.327517000	0.000000000	1	-1.277880000	-5.614179000	0.000000000
1	2.393494000	7.817757000	0.000000000	6	-3.372283000	-5.892941000	0.000000000
6	3.372283000	5.892941000	0.000000000	1	-4.345003000	-5.400435000	0.000000000
1	4.345003000	5.400435000	0.000000000	6	-3.367710000	-7.327517000	0.000000000
6	2.249873000	5.119813000	0.000000000	1	-2.393494000	-7.817757000	0.000000000
1	1.277880000	5.614179000	0.000000000	6	-4.483707000	-8.101934000	0.000000000
6	2.251234000	3.689045000	0.000000000	1	-5.460688000	-7.618087000	0.000000000
1	3.222630000	3.193766000	0.000000000	6	-4.469982000	-9.547162000	0.000000000
6	1.126233000	2.916203000	0.000000000	1	-3.488747000	-10.022028000	0.000000000
1	0.155162000	3.412294000	0.000000000	6	-5.569564000	-10.320887000	0.000000000
6	1.126233000	1.487061000	0.000000000	1	-6.567088000	-9.889357000	0.000000000
1	2.097069000	0.990607000	0.000000000	1	-5.504720000	-11.403596000	0.000000000
6	0.000196000	0.714337000	0.000000000				
1	-0.970546000	1.211024000	0.000000000				
6	-0.000196000	-0.714337000	0.000000000				
1	0.970546000	-1.211024000	0.000000000				

n=20							
C	10.07048700	20.56512000	0.00000000	H	-7.72971900	-11.99926600	0.00000000
H	9.08673300	21.03468000	0.00000000	C	-6.75351800	-13.92139100	0.00000000
C	11.16595400	21.34482300	0.00000000	H	-5.78106300	-14.41473200	0.00000000
H	11.09524400	22.42716900	0.00000000	C	-7.87663500	-14.69833000	0.00000000
H	12.16578600	20.91869500	0.00000000	H	-8.84959900	-14.20623900	0.00000000
C	10.09157100	19.12007200	0.00000000	C	-7.87000900	-16.12841200	0.00000000
H	11.07079700	18.64086600	0.00000000	H	-6.89621900	-16.61918700	0.00000000
C	8.97894100	18.34038800	0.00000000	C	-8.98975300	-16.90619100	0.00000000
H	8.00256000	18.82625800	0.00000000	H	-9.96441700	-16.41763400	0.00000000
C	8.98975300	16.90619100	0.00000000	C	-8.97894100	-18.34038800	0.00000000
H	9.96441700	16.41763400	0.00000000	H	-8.00256000	-18.82625800	0.00000000
C	7.87000900	16.12841200	0.00000000	C	-10.09157100	-19.12007200	0.00000000
H	6.89621900	16.61918700	0.00000000	H	-11.07079700	-18.64086600	0.00000000
C	7.87663500	14.69833000	0.00000000	C	-10.07048700	-20.56512000	0.00000000
H	8.84959900	14.20623900	0.00000000	H	-9.08673300	-21.03468000	0.00000000
C	6.75351800	13.92139100	0.00000000	C	-11.16595400	-21.34482300	0.00000000
H	5.78106300	14.41473200	0.00000000	H	-12.16578600	-20.91869500	0.00000000
C	6.75776300	12.49341200	0.00000000	H	-11.09524400	-22.42716900	0.00000000
H	7.72971900	11.99926600	0.00000000				
C	5.63264900	11.71711900	0.00000000				
H	4.66101800	12.21204700	0.00000000				
C	5.63533100	10.29035000	0.00000000				
H	6.60663300	9.79488500	0.00000000				
C	4.50893200	9.51457400	0.00000000				
H	3.53785000	10.01056200	0.00000000				
C	4.51052700	8.08854400	0.00000000				
H	5.48138400	7.59218600	0.00000000				
C	3.38327100	7.31317700	0.00000000				
H	2.41256600	7.80989000	0.00000000				
C	3.38410300	5.88760700	0.00000000				
H	4.35465500	5.39063900	0.00000000				
C	2.25627700	5.11254800	0.00000000				
H	1.28582800	5.60975100	0.00000000				
C	2.25659300	3.68725900	0.00000000				
H	3.22694500	3.18989300	0.00000000				
C	1.12841000	2.91241400	0.00000000				
H	0.15812100	3.40992400	0.00000000				
C	1.12841000	1.48727800	0.00000000				
H	2.09864900	0.98968400	0.00000000				
C	0.00005600	0.71254600	0.00000000				
H	-0.97017000	1.21017800	0.00000000				
C	-1.12841000	-1.48727800	0.00000000				
H	-2.09864900	-0.98968400	0.00000000				
C	-0.00005600	-0.71254600	0.00000000				
H	0.97017000	-1.21017800	0.00000000				
C	-1.12841000	-2.91241400	0.00000000				
H	-0.15812100	-3.40992400	0.00000000				
C	-2.25659300	-3.68725900	0.00000000				
H	-3.22694500	-3.18989300	0.00000000				
C	-2.25627700	-5.11254800	0.00000000				
H	-1.28582800	-5.60975100	0.00000000				
C	-3.38410300	-5.88760700	0.00000000				
H	-4.35465500	-5.39063900	0.00000000				
C	-3.38327100	-7.31317700	0.00000000				
H	-2.41256600	-7.80989000	0.00000000				
C	-4.51052700	-8.08854400	0.00000000				
H	-5.48138400	-7.59218600	0.00000000				
C	-4.50893200	-9.51457400	0.00000000				
H	-3.53785000	-10.01056200	0.00000000				
C	-5.63533100	-10.29035000	0.00000000				
H	-6.60663300	-9.79488500	0.00000000				
C	-5.63264900	-11.71711900	0.00000000				
H	-4.66101800	-12.21204700	0.00000000				
C	-6.75776300	-12.49341200	0.00000000				

Alkanes; n=number of C-atoms

n=2				n=4			
6	0.765170000	-0.000002000	0.000008000	6	-1.961892000	0.120817000	0.000001000
1	1.164086000	0.421921000	-0.928412000	1	-2.109694000	0.752082000	-0.883665000
1	1.164268000	-1.014944000	0.098862000	1	-2.109652000	0.752193000	0.883593000
6	-0.765170000	-0.000007000	-0.000001000	6	-0.568457000	-0.514414000	0.000007000
1	-1.164242000	1.014974000	-0.098574000	1	-0.463541000	-1.167634000	-0.877154000
1	-1.164113000	-0.422188000	0.928289000	1	-0.463534000	-1.167594000	0.877173000
1	-1.164064000	-0.592904000	-0.829730000	6	0.568457000	0.514418000	-0.000007000
1	1.164066000	0.593193000	0.829524000	1	0.463551000	1.167595000	-0.877176000
				1	0.463557000	1.167636000	0.877156000
				6	1.961887000	-0.120820000	-0.000001000
				1	2.109647000	-0.752197000	-0.883594000
				1	2.109689000	-0.752086000	0.883666000
				1	2.749690000	0.639597000	-0.000054000
				1	-2.749690000	-0.639604000	0.000054000
n=6				n=8			
6	-3.223296000	0.208380000	0.000003000	6	4.497668000	0.256146000	-0.000015000
1	-3.313715000	0.850337000	-0.883645000	1	4.568432000	0.900610000	0.883591000
1	-3.313658000	0.850471000	0.883554000	1	4.568416000	0.900649000	-0.883602000
6	-1.892204000	-0.549243000	0.000022000	6	3.190019000	-0.541276000	-0.000021000
1	-1.846866000	-1.208946000	-0.877118000	1	3.164363000	-1.201989000	0.877129000
1	-1.846860000	-1.208917000	0.877187000	1	3.164346000	-1.201953000	-0.877205000
6	-0.668627000	0.375171000	-0.000014000	6	1.939304000	0.346241000	0.000016000
1	-0.714596000	1.035871000	-0.877686000	1	1.965471000	1.007957000	0.877673000
1	-0.714573000	1.035881000	0.877645000	1	1.965452000	1.007985000	-0.877610000
6	0.668624000	-0.375153000	-0.000026000	6	0.625114000	-0.444070000	0.000011000
1	0.714584000	-1.035858000	-0.877710000	1	0.600009000	-1.105678000	0.877642000
1	0.714579000	-1.035878000	0.877618000	1	0.600006000	-1.105689000	-0.877615000
6	1.892210000	0.549243000	0.000006000	6	-0.625112000	0.444068000	0.000027000
1	1.846888000	1.208936000	-0.877132000	1	-0.599996000	1.105685000	0.877653000
1	1.846874000	1.208928000	0.877177000	1	-0.600004000	1.105669000	-0.877604000
6	3.223294000	-0.208395000	0.000008000	6	-1.939304000	-0.346237000	0.000036000
1	3.313649000	-0.850459000	-0.883563000	1	-1.965471000	-1.007951000	0.877706000
1	3.313698000	-0.850372000	0.883640000	1	-1.965449000	-1.007991000	-0.877577000
1	4.075962000	0.478520000	-0.000037000	6	-3.190020000	0.541275000	-0.000019000
1	-4.075972000	-0.478528000	0.000071000	1	-3.164375000	1.201985000	0.877125000
				1	-3.164344000	1.201960000	-0.877210000
				6	-4.497670000	-0.256145000	-0.000026000
				1	-4.568406000	-0.900671000	0.883542000
				1	-4.568448000	-0.900594000	-0.883648000
				1	-5.370788000	0.404580000	0.000010000
				1	5.370786000	-0.404580000	-0.000052000

n=10				n=12			
6	-5.777280000	0.286328000	-0.000001000	6	-7.058110000	0.307472000	-0.000016000
1	-5.839466000	0.931812000	-0.883577000	1	-7.115397000	0.953419000	-0.883585000
1	-5.839468000	0.931810000	0.883575000	1	-7.115408000	0.953413000	0.883556000
6	-4.480558000	-0.528750000	0.000002000	6	-5.767564000	-0.517347000	-0.000012000
1	-4.463678000	-1.190041000	-0.877055000	1	-5.755613000	-1.178745000	-0.877068000
1	-4.463677000	-1.190043000	0.877058000	1	-5.755623000	-1.178750000	0.877041000
6	-3.217635000	0.341339000	-0.000006000	6	-4.498156000	0.343272000	0.000002000
1	-3.234755000	1.003648000	-0.877541000	1	-4.510349000	1.005695000	-0.877528000
1	-3.234756000	1.003650000	0.877528000	1	-4.510360000	1.005692000	0.877534000
6	-1.914232000	-0.466526000	-0.000001000	6	-3.200788000	-0.474247000	0.000010000
1	-1.898161000	-1.128700000	-0.877523000	1	-3.189598000	-1.136516000	-0.877515000
1	-1.898165000	-1.128695000	0.877525000	1	-3.189602000	-1.136515000	0.877536000
6	-0.651706000	0.404077000	0.000003000	6	-1.931856000	0.387014000	0.000003000
1	-0.667761000	1.066234000	-0.877494000	1	-1.943045000	1.049271000	-0.877492000
1	-0.667763000	1.066238000	0.877496000	1	-1.943050000	1.049275000	0.877494000
6	0.651709000	-0.404085000	0.000002000	6	-0.634417000	-0.430706000	0.000011000
1	0.667763000	-1.066242000	-0.877494000	1	-0.623184000	-1.092968000	-0.877487000
1	0.667760000	-1.066243000	0.877496000	1	-0.623189000	-1.092958000	0.877517000
6	1.914230000	0.466523000	0.000009000	6	0.634416000	0.430695000	0.000013000
1	1.898157000	1.128696000	-0.877513000	1	0.623182000	1.092948000	-0.877492000
1	1.898159000	1.128690000	0.877536000	1	0.623181000	1.092955000	0.877512000
6	3.217637000	-0.341332000	0.000004000	6	1.931859000	-0.387015000	0.000011000
1	3.234758000	-1.003638000	-0.877535000	1	1.943052000	-1.049277000	-0.877481000
1	3.234764000	-1.003653000	0.877531000	1	1.943054000	-1.049273000	0.877504000
6	4.480558000	0.528755000	-0.000004000	6	3.200786000	0.474253000	0.000013000
1	4.463679000	1.190053000	-0.877055000	1	3.189593000	1.136523000	-0.877510000
1	4.463683000	1.190043000	0.877056000	1	3.189602000	1.136518000	0.877541000
6	5.777276000	-0.286327000	-0.000006000	6	4.498155000	-0.343263000	0.000003000
1	5.839454000	-0.931826000	-0.883571000	1	4.510350000	-1.005681000	-0.877533000
1	5.839480000	-0.931795000	0.883581000	1	4.510363000	-1.005694000	0.877528000
1	6.659350000	0.362338000	-0.000026000	6	5.767566000	0.517350000	-0.000012000
1	-6.659349000	-0.362341000	-0.000006000	1	5.755615000	1.178756000	-0.877062000
				1	5.755628000	1.178748000	0.877045000
				6	7.058108000	-0.307476000	-0.000020000
				1	7.115381000	-0.953435000	-0.883580000
				1	7.115416000	-0.953403000	0.883562000
				1	7.945076000	0.334483000	-0.000046000
				1	-7.945076000	-0.334488000	-0.000026000
n=14							
6	-8.339906000	0.323183000	-0.000071000	1	0.655247000	-1.074000000	0.877551000
1	-8.394188000	0.969386000	-0.883641000	6	1.919552000	0.444086000	0.000042000
1	-8.394226000	0.969392000	0.883491000	1	1.911237000	1.106388000	-0.877459000
6	-7.053155000	-0.507569000	-0.000043000	1	1.911250000	1.106392000	0.877542000
1	-7.044195000	-1.169026000	-0.877091000	6	3.213338000	-0.379391000	0.000028000
1	-7.044234000	-1.169023000	0.877008000	1	3.221568000	-1.041703000	-0.877459000
6	-5.779803000	0.347223000	-0.000013000	1	3.221587000	-1.041700000	0.877516000
1	-5.788988000	1.009701000	-0.877539000	6	4.486139000	0.476156000	0.000019000
1	-5.789023000	1.009700000	0.877513000	1	4.477912000	1.138475000	-0.877500000
6	-4.486139000	-0.476152000	0.000010000	1	4.477944000	1.138466000	0.877545000
1	-4.477914000	-1.138468000	-0.877511000	6	5.779802000	-0.347220000	-0.000011000
1	-4.477945000	-1.138466000	0.877534000	1	5.788984000	-1.009690000	-0.877543000
6	-3.213338000	0.379393000	0.000034000	1	5.789023000	-1.009706000	0.877508000
1	-3.221565000	1.041703000	-0.877454000	6	7.053156000	0.507567000	-0.000044000
1	-3.221589000	1.041702000	0.877523000	1	7.044197000	1.169030000	-0.877088000
6	-1.919552000	-0.444087000	0.000051000	1	7.044237000	1.169018000	0.877011000
1	-1.911239000	-1.106393000	-0.877447000	6	8.339906000	-0.323186000	-0.000073000
1	-1.911250000	-1.106386000	0.877555000	1	8.394177000	-0.969405000	-0.883631000
6	-0.646919000	0.411697000	0.000043000	1	8.394238000	-0.969379000	0.883501000
1	-0.655243000	1.074001000	-0.877457000	1	9.229839000	0.314655000	-0.000110000
1	-0.655246000	1.074005000	0.877539000	1	-9.229839000	-0.314659000	-0.000091000
6	0.646920000	-0.411699000	0.000048000				
1	0.655244000	-1.074012000	-0.877444000				

n=16							
6	-9.621921000	-0.335562000	-0.000176000	6	1.929223000	0.400917000	0.000058000
1	-9.674032000	-0.981947000	0.883355000	1	1.935672000	1.063276000	0.877436000
1	-9.673954000	-0.981917000	-0.883743000	1	1.935636000	1.063249000	-0.877349000
6	-8.338087000	0.499245000	-0.000107000	6	3.204423000	-0.451158000	0.000054000
1	-8.331491000	1.160655000	0.876910000	1	3.198045000	-1.113489000	0.877468000
1	-8.331404000	1.160674000	-0.877119000	1	3.198011000	-1.113506000	-0.877332000
6	-7.062181000	-0.351634000	-0.000048000	6	4.495848000	0.376076000	0.000018000
1	-7.069378000	-1.014127000	0.877418000	1	4.502196000	1.038406000	0.877420000
1	-7.069301000	-1.014110000	-0.877514000	1	4.502157000	1.038417000	-0.877382000
6	-5.771109000	0.475772000	0.000013000	6	5.771096000	-0.475765000	0.000011000
1	-5.764906000	1.138088000	0.877474000	1	5.764854000	-1.138090000	0.877474000
1	-5.764836000	1.138109000	-0.877445000	1	5.764815000	-1.138079000	-0.877450000
6	-4.495839000	-0.376065000	0.000058000	6	7.062183000	0.351622000	-0.000023000
1	-4.502207000	-1.038414000	0.877457000	1	7.069393000	1.014109000	0.877463000
1	-4.502150000	-1.038405000	-0.877336000	1	7.069329000	1.014126000	-0.877462000
6	-3.204412000	0.451165000	0.000100000	6	8.338090000	-0.499251000	-0.000101000
1	-3.198048000	1.113482000	0.877506000	1	8.331517000	-1.160664000	0.876904000
1	-3.198008000	1.113504000	-0.877302000	1	8.331439000	-1.160670000	-0.877135000
6	-1.929234000	-0.400917000	0.000128000	6	9.621908000	0.335564000	-0.000155000
1	-1.935687000	-1.063250000	0.877531000	1	9.673982000	0.981997000	0.883351000
1	-1.935675000	-1.063265000	-0.877254000	1	9.673981000	0.981894000	-0.883741000
6	-0.637590000	0.426059000	0.000121000	1	10.513956000	-0.299384000	-0.000140000
1	-0.631114000	1.088423000	0.877509000	1	-10.513957000	0.299399000	-0.000229000
1	-0.631121000	1.088385000	-0.877273000				
6	0.637600000	-0.426076000	0.000099000				
1	0.631169000	-1.088383000	0.877507000				
1	0.631140000	-1.088443000	-0.877284000				
n=18							
6	-10.904985000	0.345199000	-0.000187000	1	1.916554000	1.097243000	0.877604000
1	-10.955899000	0.991677000	-0.883753000	6	3.211533000	-0.394756000	0.000096000
1	-10.955974000	0.991699000	0.883356000	1	3.216616000	-1.057117000	-0.877384000
6	-9.622518000	-0.492187000	-0.000120000	1	3.216651000	-1.057111000	0.877580000
1	-9.616930000	-1.153703000	-0.877147000	6	4.488401000	0.454728000	0.000069000
1	-9.617002000	-1.153681000	0.876924000	1	4.483337000	1.117079000	-0.877417000
6	-8.344736000	0.356010000	-0.000090000	1	4.483386000	1.117070000	0.877562000
1	-8.350524000	1.018527000	-0.877609000	6	5.778096000	-0.375164000	0.000023000
1	-8.350593000	1.018546000	0.877415000	1	5.782996000	-1.037519000	-0.877454000
6	-7.055244000	-0.473920000	-0.000027000	1	5.783052000	-1.037529000	0.877491000
1	-7.050337000	-1.136288000	-0.877530000	6	7.055243000	0.473922000	-0.000007000
1	-7.050408000	-1.136270000	0.877490000	1	7.050340000	1.136292000	-0.877507000
6	-5.778095000	0.375162000	0.000019000	1	7.050412000	1.136266000	0.877514000
1	-5.782997000	1.037518000	-0.877457000	6	8.344736000	-0.356005000	-0.000075000
1	-5.783060000	1.037526000	0.877488000	1	8.350524000	-1.018521000	-0.877599000
6	-4.488400000	-0.454736000	0.000065000	1	8.350605000	-1.018550000	0.877423000
1	-4.483335000	-1.117088000	-0.877419000	6	9.622520000	0.492185000	-0.000132000
1	-4.483389000	-1.117076000	0.877560000	1	9.616923000	1.153707000	-0.877155000
6	-3.211535000	0.394750000	0.000099000	1	9.617005000	1.153681000	0.876914000
1	-3.216620000	1.057109000	-0.877383000	6	10.904986000	-0.345206000	-0.000201000
1	-3.216660000	1.057108000	0.877581000	1	10.955883000	-0.991699000	-0.883754000
6	-1.921685000	-0.434888000	0.000124000	1	10.955988000	-0.991689000	0.883356000
1	-1.916528000	-1.097242000	-0.877360000	1	11.798241000	0.287976000	-0.000253000
1	-1.916554000	-1.097234000	0.877615000	1	-11.798239000	-0.287985000	-0.000220000
6	-0.644951000	0.414784000	0.000140000				
1	-0.650113000	1.077140000	-0.877344000				
1	-0.650121000	1.077137000	0.877626000				
6	0.644948000	-0.414773000	0.000142000				
1	0.650115000	-1.077131000	-0.877339000				
1	0.650126000	-1.077122000	0.877632000				
6	1.921687000	0.434895000	0.000115000				
1	1.916528000	1.097245000	-0.877372000				

n=20							
6	-12.187669000	-0.353206000	-0.000622000	1	0.634727000	-1.086297000	0.877920000
1	-12.237699000	-0.999776000	0.882922000	1	0.634703000	-1.086317000	-0.877062000
1	-12.237475000	-0.999717000	-0.884223000	6	1.927726000	0.407398000	0.000388000
1	-13.081846000	0.278668000	-0.000714000	1	1.931987000	1.069758000	0.877877000
6	-10.906524000	0.486125000	-0.000432000	1	1.931930000	1.069759000	-0.877101000
1	-10.902107000	1.147595000	0.876644000	6	3.205713000	-0.440412000	0.000338000
1	-10.901883000	1.147649000	-0.877466000	1	3.201577000	-1.102746000	0.877846000
6	-9.627501000	-0.360182000	-0.000295000	1	3.201479000	-1.102781000	-0.877142000
1	-9.632424000	-1.022736000	0.877212000	6	4.494357000	0.391111000	0.000243000
1	-9.632209000	-1.022692000	-0.877836000	1	4.498548000	1.053480000	0.877724000
6	-8.339329000	0.471744000	-0.000117000	1	4.498419000	1.053465000	-0.877251000
1	-8.335574000	1.134077000	0.877427000	6	5.772495000	-0.456461000	0.000151000
1	-8.335367000	1.134124000	-0.877625000	1	5.768535000	-1.118786000	0.877667000
6	-7.060913000	-0.375394000	0.000007000	1	5.768373000	-1.118829000	-0.877332000
1	-7.064940000	-1.037767000	0.877481000	6	7.060913000	0.375396000	0.000006000
1	-7.064756000	-1.037740000	-0.877488000	1	7.064939000	1.037769000	0.877479000
6	-5.772494000	0.456461000	0.000151000	1	7.064754000	1.037742000	-0.877489000
1	-5.768534000	1.118786000	0.877667000	6	8.339330000	-0.471740000	-0.000118000
1	-5.768372000	1.118828000	-0.877332000	1	8.335574000	-1.134074000	0.877426000
6	-4.494358000	-0.391113000	0.000244000	1	8.335368000	-1.134121000	-0.877625000
1	-4.498550000	-1.053482000	0.877726000	6	9.627500000	0.360187000	-0.000294000
1	-4.498421000	-1.053467000	-0.877249000	1	9.632422000	1.022741000	0.877213000
6	-3.205712000	0.440407000	0.000340000	1	9.632208000	1.022698000	-0.877834000
1	-3.201575000	1.102741000	0.877848000	6	10.906524000	-0.486119000	-0.000431000
1	-3.201476000	1.102776000	-0.877141000	1	10.902107000	-1.147588000	0.876646000
6	-1.927726000	-0.407405000	0.000388000	1	10.901882000	-1.147644000	-0.877464000
1	-1.931988000	-1.069765000	0.877877000	6	12.187669000	0.353212000	-0.000622000
1	-1.931931000	-1.069766000	-0.877100000	1	12.237693000	0.999790000	0.882918000
6	-0.638967000	0.423942000	0.000423000	1	12.237477000	0.999715000	-0.884229000
1	-0.634725000	1.086287000	0.877922000	1	13.081845000	-0.278662000	-0.000705000
1	-0.634703000	1.086309000	-0.877060000				
6	0.638967000	-0.423950000	0.000422000				

Allenenes, n=number of C=C bonds

n=1				n=2			
6	0.000000000	0.665036000	0.000000000	6	0.000000000	0.000000000	1.306424000
1	0.923445000	1.237979000	0.000000000	6	0.000000000	0.000000000	0.000000000
1	-0.923403000	1.238027000	0.000000000	1	0.000000000	0.927678000	1.873541000
6	0.000000000	-0.665036000	0.000000000	1	0.000000000	-0.927678000	1.873541000
1	-0.923445000	-1.237979000	0.000000000	6	0.000000000	0.000000000	-1.306424000
1	0.923403000	-1.238027000	0.000000000	1	-0.927678000	0.000000000	-1.873541000
				1	0.927678000	0.000000000	-1.873541000
n=3				n=4			
6	0.000000000	0.000000000	-1.953082000	6	0.000000000	0.000000000	-2.592835000
6	0.000000000	0.000000000	-0.635588000	6	0.000000000	0.000000000	-1.279267000
6	0.000000000	0.000000000	0.635537000	6	0.000000000	0.000000000	0.000022000
6	0.000000000	0.000000000	1.953194000	6	0.000000000	0.000000000	1.279298000
1	0.000000000	0.927042000	-2.521668000	6	0.000000000	0.000000000	2.592807000
1	0.000000000	-0.927042000	-2.521668000	1	0.000000000	0.927632000	-3.160623000
1	0.000000000	-0.927307000	2.521487000	1	0.000000000	-0.927632000	-3.160623000
1	0.000000000	0.927307000	2.521487000	1	-0.927655000	0.000000000	3.160549000
				1	0.927655000	0.000000000	3.160549000
n=5				n=6			
C	0.00002900	3.23627500	0.00000000	6	-3.236284000	-0.000149000	0.000083000
C	0.00000800	1.91822900	0.00000000	6	-1.918234000	0.000069000	0.000008000
C	0.00000000	0.64528300	0.00000000	6	-0.645297000	0.000177000	-0.000060000
C	0.00003400	-0.64529100	0.00000000	6	0.645273000	0.000126000	-0.000150000
C	-0.00010500	-1.91822700	0.00000000	6	1.918215000	0.000082000	-0.000060000
C	0.00000400	-3.23627300	0.00000000	6	3.236285000	-0.000148000	0.000033000
H	-0.92724900	3.80496900	0.00000000	1	-3.805057000	0.927074000	0.000160000
H	0.92732600	3.80494000	0.00000000	1	-3.804764000	-0.927551000	-0.000004000
H	0.92734100	-3.80486900	0.00000000	1	3.804895000	-0.927478000	0.000438000
H	-0.92723800	-3.80502400	0.00000000	1	3.805180000	0.927011000	0.000275000
n=7				n=8			
C	-4.51897400	0.00027200	-0.00010900	6	5.159313000	-0.000068000	0.000112000
C	-3.20051900	-0.00000600	-0.00002900	6	3.842076000	-0.000030000	-0.000004000
C	-1.92668800	-0.00018800	0.00004100	6	2.566021000	0.000006000	-0.000078000
C	-0.63769100	-0.00023800	0.00010500	6	1.280612000	0.000041000	-0.000109000
C	0.63769100	-0.00019700	0.00015200	6	-0.000001000	0.000074000	-0.000058000
H	-5.08753200	-0.92714000	-0.00015000	1	5.726929000	-0.004257000	0.927989000
H	-5.08714800	0.92791900	-0.00015100	1	5.727092000	0.004091000	-0.927664000
C	1.92668700	-0.00015300	0.00010900	6	-1.280605000	0.000107000	-0.000029000
C	3.20052300	0.00001600	-0.00001400	6	-2.566017000	0.000018000	0.000001000
C	4.51896600	0.00024700	-0.00015300	6	-3.842078000	0.000102000	0.000029000
H	5.08752700	-0.92716300	-0.00015800	6	-5.159323000	-0.000141000	0.000057000
H	5.08718800	0.92786800	-0.00015700	1	-5.727167000	0.927598000	0.004248000
				1	-5.726836000	-0.928081000	-0.004101000
n=9				n=10			
6	5.801271000	-0.000127000	-0.000090000	6	6.441677000	0.000226000	0.000253000
6	4.482614000	-0.000135000	-0.000056000	6	5.123890000	0.000089000	0.000051000
6	3.208443000	-0.000073000	-0.000017000	6	3.848250000	-0.000022000	-0.000092000
6	1.919836000	0.000094000	0.000035000	6	2.561925000	-0.000103000	-0.000160000
6	0.643393000	0.000201000	0.000091000	6	1.282390000	-0.000168000	-0.000193000
1	6.369367000	-0.927824000	-0.000119000	1	7.009439000	-0.355304000	-0.856737000
1	6.369360000	0.927575000	-0.000107000	1	7.009107000	0.355895000	0.857406000
6	-0.643391000	0.000189000	0.000148000	6	-0.000003000	-0.000211000	-0.000171000
6	-1.919836000	0.000190000	0.000129000	6	-1.282396000	-0.000222000	-0.000071000
6	-3.208441000	0.000100000	0.000053000	6	-2.561922000	-0.000099000	-0.000025000
6	-4.482617000	0.000017000	-0.000043000	6	-3.848247000	0.000025000	0.000020000
6	-5.801272000	-0.000279000	-0.000147000	6	-5.123888000	0.000049000	0.000105000
1	-6.369160000	-0.928103000	-0.000184000	6	-6.441679000	0.000233000	0.000124000
1	-6.369569000	0.927294000	-0.000198000	1	-7.009372000	-0.856765000	0.355741000
				1	-7.009148000	0.857397000	-0.355452000

Polyynes, n=number of triple bonds

n=1				n=2			
6	0.000000000	0.000000000	0.602676000	6	0.000000000	0.000000000	1.896785000
1	0.000000000	0.000000000	1.668402000	1	0.000000000	0.000000000	2.962279000
6	0.000000000	0.000000000	-0.602676000	6	0.000000000	0.000000000	0.684362000
1	0.000000000	0.000000000	-1.668402000	6	0.000000000	0.000000000	-0.684362000
				6	0.000000000	0.000000000	-1.896785000
				1	0.000000000	0.000000000	-2.962279000
n=3				n=4			
6	0.000000000	0.000000000	3.186671000	6	0.000000000	0.000000000	4.474162000
1	0.000000000	0.000000000	4.252039000	1	0.000000000	0.000000000	5.539726000
6	0.000000000	0.000000000	1.971669000	6	0.000000000	0.000000000	3.258249000
6	0.000000000	0.000000000	0.611725000	6	0.000000000	0.000000000	1.901337000
6	0.000000000	0.000000000	-0.611725000	6	0.000000000	0.000000000	0.674103000
6	0.000000000	0.000000000	-1.971669000	6	0.000000000	0.000000000	-0.674103000
6	0.000000000	0.000000000	-3.186671000	6	0.000000000	0.000000000	-1.901337000
1	0.000000000	0.000000000	-4.252039000	6	0.000000000	0.000000000	-3.258249000
				6	0.000000000	0.000000000	-4.474162000
				1	0.000000000	0.000000000	-5.539726000
n=5				n=6			
6	0.000000000	0.000000000	3.188951000	6	0.000000000	0.000000000	1.903473000
6	0.000000000	0.000000000	1.960193000	6	0.000000000	0.000000000	0.669865000
6	0.000000000	0.000000000	0.615821000	6	0.000000000	0.000000000	-0.669865000
6	0.000000000	0.000000000	-0.615821000	6	0.000000000	0.000000000	-1.903473000
6	0.000000000	0.000000000	-1.960193000	6	0.000000000	0.000000000	-3.245864000
6	0.000000000	0.000000000	-3.188951000	6	0.000000000	0.000000000	-4.475439000
6	0.000000000	0.000000000	-4.544562000	6	0.000000000	0.000000000	-5.830536000
6	0.000000000	0.000000000	-5.760901000	6	0.000000000	0.000000000	-7.047109000
1	0.000000000	0.000000000	-6.826525000	1	0.000000000	0.000000000	-8.112784000
6	0.000000000	0.000000000	4.544562000	6	0.000000000	0.000000000	3.245864000
6	0.000000000	0.000000000	5.760901000	6	0.000000000	0.000000000	4.475439000
1	0.000000000	0.000000000	6.826525000	6	0.000000000	0.000000000	5.830536000
				6	0.000000000	0.000000000	7.047109000
				1	0.000000000	0.000000000	8.112784000
n=7				n=8			
6	0.000000000	0.000000000	0.617879000	6	0.000000000	0.000000000	0.667867000
6	0.000000000	0.000000000	-0.617879000	6	0.000000000	0.000000000	1.904496000
6	0.000000000	0.000000000	-1.955468000	6	0.000000000	0.000000000	3.241356000
6	0.000000000	0.000000000	-3.190079000	6	0.000000000	0.000000000	4.476328000
6	0.000000000	0.000000000	-4.531478000	6	0.000000000	0.000000000	5.817448000
6	0.000000000	0.000000000	-5.761479000	6	0.000000000	0.000000000	7.047589000
6	0.000000000	0.000000000	-7.116314000	6	0.000000000	0.000000000	8.401943000
6	0.000000000	0.000000000	-8.333011000	6	0.000000000	0.000000000	9.618666000
1	0.000000000	0.000000000	-9.398719000	1	0.000000000	0.000000000	10.684384000
6	0.000000000	0.000000000	1.955468000	6	0.000000000	0.000000000	-0.667867000
6	0.000000000	0.000000000	3.190079000	6	0.000000000	0.000000000	-1.904496000
6	0.000000000	0.000000000	4.531478000	6	0.000000000	0.000000000	-3.241356000
6	0.000000000	0.000000000	5.761479000	6	0.000000000	0.000000000	-4.476328000
6	0.000000000	0.000000000	7.116314000	6	0.000000000	0.000000000	-5.817448000
6	0.000000000	0.000000000	8.333011000	6	0.000000000	0.000000000	-7.047589000
1	0.000000000	0.000000000	9.398719000	6	0.000000000	0.000000000	-8.401943000
				6	0.000000000	0.000000000	-9.618666000
				1	0.000000000	0.000000000	-10.684384000

Cyclic allenes; n=number of C=C bonds

n=6				n=10			
C	-0.65478800	1.13412800	0.00000000	6	0.645373000	1.986639000	0.000000000
C	-1.30957800	0.00000000	0.00000000	6	1.689975000	1.227692000	0.000000000
C	-0.65478900	-1.13412700	0.00000000	6	2.088838000	0.000119000	0.000000000
C	0.65478800	1.13412800	0.00000000	6	1.689835000	-1.227884000	0.000000000
C	0.65478900	-1.13412700	0.00000000	6	-0.645373000	1.986639000	0.000000000
C	1.30957800	0.00000000	0.00000000	6	0.645600000	-1.986566000	0.000000000
				6	-2.088838000	0.000119000	0.000000000
				6	-1.689975000	1.227692000	0.000000000
				6	-1.689835000	-1.227884000	0.000000000
				6	-0.645600000	-1.986566000	0.000000000
n=14				n=18			
C	-0.64336600	2.81881700	0.00000000	C	0.00000700	3.73474700	0.00000000
C	-1.80270800	2.26050800	0.00000000	C	1.24814600	3.42835500	0.00000000
C	-2.60497200	1.25450000	0.00000000	C	2.40147200	2.86119300	0.00000000
C	-2.89130600	-0.00001000	0.00000000	C	3.16073500	1.82422100	0.00000000
C	0.64336600	2.81881700	0.00000000	C	-1.24821300	3.42857600	0.00000000
C	-2.60498100	-1.25448200	0.00000000	C	3.67984000	0.64849400	0.00000000
C	0.64338600	-2.81881300	0.00000000	C	2.34617600	-2.79543200	0.00000000
C	1.80269200	-2.26052000	0.00000000	C	1.27773000	-3.50971200	0.00000000
C	-0.64338600	-2.81881300	0.00000000	C	3.23603500	-1.86806100	0.00000000
C	-1.80269200	-2.26052000	0.00000000	C	3.59489100	-0.63393900	0.00000000
C	1.80270800	2.26050800	0.00000000	C	-2.40157900	2.86154200	0.00000000
C	2.60497200	1.25450000	0.00000000	C	-3.16117200	1.82480200	0.00000000
C	2.89130600	-0.00001000	0.00000000	C	-3.68002400	0.64894100	0.00000000
C	2.60498100	-1.25448200	0.00000000	C	-3.59464000	-0.63345900	0.00000000
				C	-3.23587200	-1.86759200	0.00000000
				C	0.00000000	-3.64836500	0.00000000
				C	-2.34584000	-2.79479200	0.00000000
				C	-1.27769300	-3.50951900	0.00000000

Cyclic polyynes, n=number of triple bonds

n=4				n=6			
C	0.61330600	1.61840300	0.00000000	C	0.61491500	2.44100400	0.00000000
C	1.61840300	0.61330600	0.00000000	C	1.80651400	1.75303400	0.00000000
C	1.61840300	-0.61330600	0.00000000	C	2.42142900	0.68797000	0.00000000
C	0.61330600	-1.61840300	0.00000000	C	2.42142900	-0.68797000	0.00000000
C	-0.61330600	1.61840300	0.00000000	C	-0.61491500	2.44100400	0.00000000
C	-0.61330600	-1.61840300	0.00000000	C	1.80651400	-1.75303400	0.00000000
C	-1.61840300	-0.61330600	0.00000000	C	-1.80651400	-1.75303400	0.00000000
C	-1.61840300	0.61330600	0.00000000	C	-2.42142900	-0.68797000	0.00000000
n=8				n=10			
C	2.34738000	2.34738000	0.00000000	6	0.618130000	4.082955000	0.000000000
C	1.21233500	3.09163500	0.00000000	6	1.899823000	3.666507000	0.000000000
C	-0.00000800	3.31947700	0.00000000	6	2.899978000	2.939852000	0.000000000
C	-1.32890500	3.04337100	0.00000000	6	3.692108000	1.849579000	0.000000000
C	3.04337100	1.32890500	0.00000000	6	-0.618130000	4.082955000	0.000000000
C	-2.34738000	2.34738000	0.00000000	6	4.074133000	0.673826000	0.000000000
C	-3.04337100	-1.32890500	0.00000000	6	2.899978000	-2.939852000	0.000000000
C	-2.34738000	-2.34738000	0.00000000	6	1.899823000	-3.666507000	0.000000000
C	-3.31947700	-0.00000800	0.00000000	6	3.692108000	-1.849579000	0.000000000
C	-3.09163500	1.21233500	0.00000000	6	4.074133000	-0.673826000	0.000000000
C	3.31947700	0.00000800	0.00000000	6	-1.899823000	3.666507000	0.000000000
C	3.09163500	-1.21233500	0.00000000	6	-2.899978000	2.939852000	0.000000000
C	2.34738000	-2.34738000	0.00000000	6	-3.692108000	1.849579000	0.000000000
C	1.32890500	-3.04337100	0.00000000	6	-4.074133000	0.673826000	0.000000000
C	0.00000800	-3.31947700	0.00000000	6	-4.074133000	-0.673826000	0.000000000
C	-1.21233500	-3.09163500	0.00000000	6	0.618130000	-4.082955000	0.000000000
				6	-1.899823000	-3.666507000	0.000000000
				6	-0.618130000	-4.082955000	0.000000000
				6	-3.692108000	-1.849579000	0.000000000
				6	-2.899978000	-2.939852000	0.000000000

n=9				n=10			
6	0.000000000	0.000000000	1.953439000	6	0.000000000	0.000000000	3.238918000
6	0.000000000	0.000000000	3.190655000	6	0.000000000	0.000000000	4.476479000
6	0.000000000	0.000000000	4.526909000	6	0.000000000	0.000000000	5.812364000
6	0.000000000	0.000000000	5.762176000	6	0.000000000	0.000000000	7.047808000
6	0.000000000	0.000000000	7.103012000	6	0.000000000	0.000000000	8.388469000
6	0.000000000	0.000000000	8.333275000	6	0.000000000	0.000000000	9.618806000
6	0.000000000	0.000000000	9.687525000	6	0.000000000	0.000000000	10.972979000
6	0.000000000	0.000000000	10.904280000	6	0.000000000	0.000000000	12.189752000
1	0.000000000	0.000000000	11.970018000	1	0.000000000	0.000000000	13.255508000
6	0.000000000	0.000000000	0.618878000	6	0.000000000	0.000000000	1.905042000
6	0.000000000	0.000000000	-0.618878000	6	0.000000000	0.000000000	0.666656000
6	0.000000000	0.000000000	-1.953439000	6	0.000000000	0.000000000	-0.666656000
6	0.000000000	0.000000000	-3.190655000	6	0.000000000	0.000000000	-1.905042000
6	0.000000000	0.000000000	-4.526909000	6	0.000000000	0.000000000	-3.238918000
6	0.000000000	0.000000000	-5.762176000	6	0.000000000	0.000000000	-4.476479000
6	0.000000000	0.000000000	-7.103012000	6	0.000000000	0.000000000	-5.812364000
6	0.000000000	0.000000000	-8.333275000	6	0.000000000	0.000000000	-7.047808000
6	0.000000000	0.000000000	-9.687525000	6	0.000000000	0.000000000	-8.388469000
6	0.000000000	0.000000000	-10.904280000	6	0.000000000	0.000000000	-9.618806000
1	0.000000000	0.000000000	-11.970018000	6	0.000000000	0.000000000	-10.972979000
				6	0.000000000	0.000000000	-12.189752000
				1	0.000000000	0.000000000	-13.255508000
n=20							
6	0.000000000	0.000000000	16.092790000				
6	0.000000000	0.000000000	17.330779000				
6	0.000000000	0.000000000	18.666129000				
6	0.000000000	0.000000000	19.901761000				
6	0.000000000	0.000000000	21.242087000				
6	0.000000000	0.000000000	22.472480000				
6	0.000000000	0.000000000	23.826496000				
6	0.000000000	0.000000000	25.043263000				
1	0.000000000	0.000000000	26.109079000				
6	0.000000000	0.000000000	14.759831000				
6	0.000000000	0.000000000	13.520616000				
6	0.000000000	0.000000000	12.188934000				
6	0.000000000	0.000000000	10.949043000				
6	0.000000000	0.000000000	9.618092000				
6	0.000000000	0.000000000	8.377798000				
6	0.000000000	0.000000000	7.047316000				
6	0.000000000	0.000000000	5.806731000				
6	0.000000000	0.000000000	4.476657000				
6	0.000000000	0.000000000	3.235767000				
6	0.000000000	0.000000000	1.905989000				
6	0.000000000	0.000000000	0.664828000				
6	0.000000000	0.000000000	-9.618092000				
6	0.000000000	0.000000000	-8.377798000				
6	0.000000000	0.000000000	-7.047316000				
6	0.000000000	0.000000000	-5.806731000				
6	0.000000000	0.000000000	-4.476657000				
6	0.000000000	0.000000000	-3.235767000				
6	0.000000000	0.000000000	-1.905989000				
6	0.000000000	0.000000000	-0.664828000				
6	0.000000000	0.000000000	-10.949043000				
6	0.000000000	0.000000000	-12.188934000				
6	0.000000000	0.000000000	-13.520616000				
6	0.000000000	0.000000000	-14.759831000				
6	0.000000000	0.000000000	-16.092790000				
6	0.000000000	0.000000000	-17.330779000				
6	0.000000000	0.000000000	-18.666129000				
6	0.000000000	0.000000000	-19.901761000				
6	0.000000000	0.000000000	-21.242087000				
6	0.000000000	0.000000000	-22.472480000				
6	0.000000000	0.000000000	-23.826496000				
6	0.000000000	0.000000000	-25.043263000				

Spiro polycyclopropanes, n=number of cyclopropane units

n=1				n=2		
6	0.000000000	0.000000000	0.870895000	6	1.272355000	0.548630000
6	0.000000000	0.754064000	-0.435462000	6	-0.000006000	-0.000128000
6	0.000000000	-0.754064000	-0.435462000	6	1.272570000	-0.548562000
1	0.910532000	0.000000000	1.462358000	1	1.576596000	-0.274166000
1	-0.910532000	0.000000000	1.462358000	1	1.576549000	-1.547387000
1	0.910435000	1.266592000	-0.731137000	6	-1.272428000	0.533287000
1	-0.910435000	1.266592000	-0.731137000	1	-1.576157000	1.540449000
1	0.910435000	-1.266592000	-0.731137000	1	-1.576537000	0.230208000
1	-0.910435000	-1.266592000	-0.731137000	6	-1.272494000	-0.533277000
				1	-1.576520000	-1.540325000
				1	-1.576391000	-0.230258000
				1	1.576333000	0.274206000
				1	1.576145000	1.547567000
						-0.230041000
n=3				n=4		
6	-1.840030000	-0.443435000	-0.764595000	6	-2.571684000	0.158395000
6	-0.732230000	0.185242000	-0.000013000	6	-2.052491000	1.242915000
6	-1.840012000	-0.443441000	0.764591000	1	-1.579222000	2.115444000
1	-1.650953000	-1.386510000	1.272060000	1	-2.631645000	1.453622000
1	-2.554630000	0.200516000	1.271305000	6	-1.364026000	-0.070250000
6	0.732228000	0.185229000	-0.000002000	6	-0.000001000	-0.578312000
6	0.000012000	1.498209000	0.000021000	6	-0.858549000	-1.132097000
1	0.000015000	2.087235000	0.915677000	1	-0.622605000	-0.847814000
1	0.000021000	2.087236000	-0.915634000	1	-1.248003000	-2.142977000
6	1.840009000	-0.443464000	0.764590000	6	1.364027000	-0.070250000
1	1.650969000	-1.386534000	1.272065000	6	0.858555000	-1.132106000
1	2.554585000	0.200523000	1.271326000	1	1.248006000	-2.142986000
6	1.840028000	-0.443429000	-0.764596000	1	0.622622000	-0.847833000
1	2.554620000	0.200546000	-1.271325000	6	2.571685000	0.158403000
1	1.650973000	-1.386489000	-1.272085000	1	2.442855000	0.311800000
1	-2.554625000	0.200538000	-1.271320000	1	3.494302000	-0.348908000
1	-1.651002000	-1.386521000	-1.272043000	6	2.052484000	1.242918000
				1	2.631630000	1.453643000
				1	1.579203000	2.115435000
				1	-3.494305000	-0.348917000
				1	-2.442836000	0.311797000
						1.734755000
n=5				n=6		
6	3.319359000	0.195329000	0.259640000	6	3.965725000	-0.206709000
6	1.968170000	-0.159572000	-0.246252000	6	2.639352000	-0.117827000
6	2.669740000	-1.139860000	0.623564000	6	3.452329000	1.121998000
1	2.320288000	-1.270961000	1.644516000	1	3.926809000	1.512696000
1	3.075585000	-2.040621000	0.169668000	1	3.145103000	1.883267000
6	1.258494000	-0.170166000	-1.570659000	6	1.262049000	-0.548288000
1	0.843192000	-1.112100000	-1.924601000	6	1.895639000	-0.859200000
1	1.626663000	0.485943000	-2.357682000	1	1.557727000	-0.301154000
6	0.644815000	0.461130000	-0.348807000	1	2.178835000	-1.890242000
6	-0.644813000	0.461056000	0.348924000	6	0.509534000	-1.304107000
6	-0.000004000	1.774956000	0.000189000	1	-0.004383000	-2.219878000
1	-0.438459000	2.364821000	-0.803349000	1	0.915502000	-1.311562000
1	0.438438000	2.364694000	0.803827000	6	-0.000003000	-0.000001000
6	-1.968169000	-0.159624000	0.246219000	6	-1.262052000	0.548292000
6	-1.258507000	-0.170505000	1.570631000	6	-0.509534000	1.304110000
1	-1.626682000	0.485427000	2.357799000	1	-0.915492000	1.311590000
1	-0.843206000	-1.112518000	1.924363000	1	0.004396000	2.219865000
6	-3.319351000	0.195385000	-0.259613000	6	-2.639352000	0.117827000
1	-3.399959000	0.949621000	-1.038714000	6	-1.895638000	0.859196000
1	-4.155416000	0.178506000	0.435232000	1	-2.178833000	1.890234000
6	-2.669729000	-1.139731000	-0.623810000	1	-1.557718000	0.301136000
1	-3.075585000	-2.040580000	-0.170099000	6	-3.965724000	0.206708000
1	-2.320275000	-1.270621000	-1.644786000	1	-3.998429000	0.326448000
1	4.155413000	0.178599000	-0.435224000	1	-4.780036000	0.695553000
1	3.399982000	0.949405000	1.038893000	6	-3.452330000	-1.121998000
				1	-3.926808000	-1.512694000
						1.042347000

	1	-3.145108000	-1.883270000	-0.567024000
	1	4.780028000	-0.695552000	0.119609000
	1	3.998439000	-0.326443000	-1.489915000

n=7				n=8			
6	-4.597467000	-0.341889000	-0.484440000	6	-5.272727000	-0.037541000	-0.455628000
6	-4.040802000	-1.000465000	0.778015000	6	-3.956992000	-0.141854000	0.226545000
1	-3.640453000	-2.007186000	0.689138000	6	-4.615001000	-1.397561000	-0.220472000
1	-4.548785000	-0.801665000	1.718527000	1	-4.207123000	-1.918420000	-1.083002000
6	-3.315338000	0.113348000	0.112475000	1	-5.055222000	-2.049418000	0.530087000
6	-1.954049000	0.420969000	-0.334557000	6	-3.325757000	0.386253000	1.483791000
6	-2.693905000	1.421367000	0.513500000	1	-2.939323000	-0.330559000	2.206126000
1	-3.055371000	2.331186000	0.037117000	1	-3.733136000	1.295526000	1.922732000
1	-2.380487000	1.546615000	1.548394000	6	-2.636358000	0.488591000	0.149041000
6	-0.628121000	-0.203812000	-0.377889000	6	-1.309514000	0.226024000	-0.417103000
6	-1.181535000	0.433038000	-1.624951000	6	-1.960585000	1.561858000	-0.659356000
1	-0.746840000	1.374291000	-1.956513000	1	-2.346971000	1.774283000	-1.655026000
1	-1.517978000	-0.217800000	-2.430591000	1	-1.563071000	2.428930000	-0.134972000
6	0.000001000	-1.518563000	-0.000027000	6	-0.000001000	-0.285089000	0.000032000
1	0.473719000	-2.106603000	-0.784090000	6	-0.639103000	-0.836470000	-1.246192000
1	-0.473735000	-2.106592000	0.784034000	1	-0.218617000	-0.549866000	-2.208469000
6	0.628123000	-0.203828000	0.377865000	1	-1.045136000	-1.845871000	-1.211732000
6	1.954051000	0.420962000	0.334559000	6	0.639101000	-0.836369000	1.246293000
6	1.181529000	0.432993000	1.624949000	1	1.045126000	-1.845776000	1.211912000
1	1.517964000	-0.217853000	2.430585000	1	0.218642000	-0.549678000	2.208554000
1	0.746822000	1.374241000	1.956508000	6	1.309517000	0.226050000	0.417102000
6	3.315345000	0.113354000	-0.112467000	6	2.636358000	0.488577000	-0.149071000
6	2.693908000	1.421386000	-0.513462000	6	1.960590000	1.561901000	0.659251000
1	3.055366000	2.331198000	-0.037064000	1	2.346985000	1.774400000	1.654901000
1	2.380497000	1.546635000	-1.548358000	1	1.563074000	2.428939000	0.134812000
6	4.597466000	-0.341897000	0.484448000	6	3.956993000	-0.141872000	-0.226547000
1	4.565622000	-0.911482000	1.410166000	6	3.325729000	0.386140000	-1.483826000
1	5.473745000	0.293131000	0.379628000	1	3.733101000	1.295377000	-1.922846000
6	4.040803000	-1.000453000	-0.778022000	1	2.939281000	-0.330743000	-2.206082000
1	4.548792000	-0.801676000	-1.718534000	6	5.272730000	-0.037498000	0.455601000
1	3.640429000	-2.007164000	-0.689127000	1	5.300707000	0.343739000	1.473571000
1	-5.473753000	0.293130000	-0.379627000	1	6.148214000	0.210872000	-0.139356000
1	-4.565604000	-0.911467000	-1.410163000	6	4.615017000	-1.397543000	0.220539000
				1	5.055238000	-2.049419000	-0.530004000
				1	4.207170000	-1.918374000	1.083100000
				1	-6.148206000	0.210854000	0.139325000
				1	-5.300707000	0.343631000	-1.473621000
n=9							
1	5.725615000	-1.118703000	-1.757589000	6	-1.371006000	1.471390000	0.498975000
6	5.309498000	-1.095260000	-0.753410000	1	-1.797962000	2.228491000	-0.156310000
6	5.950028000	-0.146868000	0.260255000	1	-0.983253000	1.854525000	1.441228000
6	4.605212000	0.134694000	-0.305163000	6	-1.981803000	0.095650000	0.488845000
1	4.955048000	-2.057394000	-0.392549000	6	-3.276450000	-0.519029000	0.178662000
6	3.276450000	0.519030000	0.178649000	6	-2.613467000	-0.832759000	1.491800000
6	3.903493000	1.298251000	-0.946888000	1	-3.037418000	-0.400993000	2.397166000
1	3.498906000	1.166784000	-1.948846000	1	-2.175605000	-1.820391000	1.625031000
1	4.269446000	2.301480000	-0.734848000	6	-4.605210000	-0.134703000	-0.305166000
6	2.613467000	0.832764000	1.491790000	6	-3.903488000	-1.298267000	-0.946869000
1	2.175613000	1.820399000	1.625037000	1	-4.269441000	-2.301492000	-0.734808000
1	3.037430000	0.401001000	2.397153000	1	-3.498895000	-1.166827000	-1.948828000
6	1.981803000	-0.095642000	0.488846000	6	-5.950033000	0.146860000	0.260247000
6	0.669406000	-0.299120000	-0.132642000	1	-6.019107000	0.479672000	1.293115000
6	1.371002000	-1.471381000	0.498948000	1	-6.790658000	-0.457003000	-0.072607000
1	1.797974000	-2.228467000	-0.156343000	6	-5.309496000	1.095241000	-0.753428000
1	0.983239000	-1.854540000	1.441188000	1	-5.725615000	1.118667000	-1.757608000
6	-0.669405000	0.299135000	-0.132625000	1	-4.955053000	2.057386000	-0.392587000
6	-0.000004000	0.000021000	-1.447055000	1	6.790664000	0.456990000	-0.072585000
1	-0.374850000	-0.835813000	-2.035085000	1	6.019107000	-0.479664000	1.293130000
1	0.374831000	0.835866000	-2.035076000				

n=10						
1	0.778682000	4.999039000	2.202263000	1	0.056061000	-1.568399000
6	0.000000000	4.617599000	1.543852000	6	-0.277129000	-2.626022000
6	-0.184956000	5.274728000	0.205125000	6	-0.418101000	-3.940601000
6	0.418101000	3.940601000	0.265635000	6	-1.644493000	-3.247095000
1	-0.881808000	4.239503000	2.058051000	1	-2.106308000	-3.637853000
6	0.277129000	2.626022000	-0.368535000	1	-2.345450000	-2.824332000
6	1.644493000	3.247095000	-0.260773000	6	0.184956000	-5.274728000
1	2.345450000	2.824332000	0.456693000	6	0.000000000	-4.617599000
1	2.106308000	3.637853000	-1.166262000	1	-0.778682000	-4.999039000
6	-0.562459000	1.990743000	-1.444236000	1	0.881808000	-4.239503000
1	-0.056061000	1.568399000	-2.310321000	6	-1.276045000	5.967484000
1	-1.538006000	2.424449000	-1.656699000	1	-1.573405000	5.582065000
6	-0.353778000	1.328239000	-0.108974000	1	-2.085682000	6.414275000
6	0.000000000	0.000000000	0.402169000	6	0.112525000	6.595347000
6	-1.214220000	0.698060000	0.952971000	1	0.736026000	6.626024000
1	-1.161048000	1.102453000	1.962185000	1	0.222334000	7.457878000
1	-2.195403000	0.324402000	0.665774000	6	-0.112525000	-6.595347000
6	0.353778000	-1.328239000	-0.108974000	1	-0.736026000	-6.626024000
6	1.214220000	-0.698060000	0.952971000	1	-0.222334000	-7.457878000
1	1.161048000	-1.102453000	1.962185000	6	1.276045000	-5.967484000
1	2.195403000	-0.324402000	0.665774000	1	2.085682000	-6.414275000
6	0.562459000	-1.990743000	-1.444236000	1	1.573405000	-5.582065000
1	1.538006000	-2.424449000	-1.656699000			

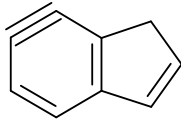
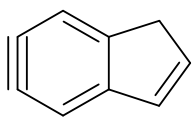
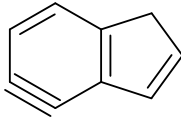
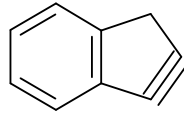
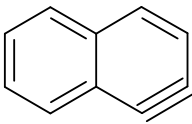
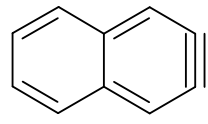
Cyclic and bicyclic hydrocarbons, n=number of C-atoms in the cycle, m=number of double bonds

n=3, m=1				n1=4, n2=3, m=0 bicyclo[2.1.0]pentane			
6	0.000002000	-0.501287000	0.647466000	6	0.245628000	0.995713000	0.782930000
6	0.000002000	0.861572000	0.000000000	6	0.245628000	-0.537992000	0.765945000
6	0.000002000	-0.501287000	-0.647466000	6	-0.943069000	-1.050112000	0.000000000
1	-0.000026000	-1.041608000	1.581070000	6	0.245628000	-0.537992000	-0.765945000
1	0.912693000	1.464610000	0.000000000	6	0.245628000	0.995713000	-0.782930000
1	-0.912674000	1.464617000	0.000000000	1	-0.608681000	1.469640000	-1.280531000
1	-0.000026000	-1.041608000	-1.581070000	1	1.165172000	1.421343000	-1.193157000
				1	0.799815000	-1.175126000	1.448269000
				1	0.799815000	-1.175126000	-1.448269000
				1	1.165172000	1.421343000	1.193157000
				1	-0.608681000	1.469640000	1.280531000
				1	-1.880950000	-0.494246000	0.000000000
				1	-1.068327000	-2.129450000	0.000000000
n1=4, n2=3, m=1 bicyclo[2.1.0]pent-1(5)ene				n1=4, n2=3, m=1 bicyclo[2.1.0]pent-1(4)ene			
6	-0.887083000	0.775593000	0.327990000	6	-0.252182000	-1.029979000	0.773756000
6	0.508280000	0.779141000	-0.357490000	6	-0.252182000	0.514300000	0.677941000
6	1.467838000	-0.222889000	0.268189000	6	0.765164000	1.389404000	0.000000000
6	0.421126000	-0.714374000	-0.353978000	6	-0.252182000	0.514300000	-0.677941000
6	-1.049935000	-0.780710000	-0.052736000	6	-0.252182000	-1.029979000	-0.773756000
1	-1.382507000	-1.493144000	0.710401000	1	0.656998000	-1.427047000	-1.236737000
1	-1.678049000	-0.878601000	-0.942376000	1	-1.121914000	-1.450794000	-1.283425000
1	0.747294000	1.402265000	-1.215842000	1	-1.121914000	-1.450794000	1.283425000
1	-1.646193000	1.429018000	-0.114154000	1	0.656998000	-1.427047000	1.236737000
1	-0.869952000	0.921514000	1.415068000	1	1.834990000	1.152095000	0.000000000
1	2.068047000	-0.401625000	1.155056000	1	0.556230000	2.455314000	0.000000000
n1=4, n2=3, m=1 bicyclo[2.1.0]pent-2-ene				n1=4, n2=3, m=2 bicyclo[2.1.0]pent-1(5),3-diene			
6	0.267703000	1.057977000	0.672054000	6	-1.179414000	0.392167000	0.000000000
6	0.267703000	-0.460796000	0.760945000	6	0.000000000	1.041658000	0.000000000
6	-0.925452000	-1.015181000	0.000000000	6	1.330180000	0.511500000	0.000000000
6	0.267703000	-0.460796000	-0.760945000	6	0.836178000	-0.711925000	0.000000000
6	0.267703000	1.057977000	-0.672054000	6	-0.696613000	-0.998800000	0.000000000
1	0.126933000	1.828177000	-1.424269000	1	-0.937335000	-1.601345000	0.883637000
1	0.884745000	-1.082275000	1.400163000	1	-0.937335000	-1.601345000	-0.883637000
1	0.884745000	-1.082275000	-1.400163000	1	-2.171460000	0.822054000	0.000000000
1	0.126933000	1.828177000	1.424269000	1	2.304144000	0.973036000	0.000000000
1	-1.865015000	-0.466847000	0.000000000				
1	-1.030507000	-2.100041000	0.000000000				
n=1,m=4 cyclopenta-1,2,3,4-tetraene				n1=4, n2=3, m=2 bicyclo[2.1.0]pent-1(4),2-diene			
6	0.838353000	0.793199000	-0.026646000	6	0.000000000	0.668055000	-1.233034000
6	-0.625921000	0.895737000	-0.020991000	6	0.000000000	0.663808000	0.339668000
6	-1.248663000	-0.354044000	-0.163908000	6	0.000000000	0.000000000	1.679284000
6	-0.137740000	-1.088041000	0.229860000	6	0.000000000	-0.663808000	0.339668000
6	1.147915000	-0.540909000	-0.081141000	6	0.000000000	-0.668055000	-1.233034000
1	2.096323000	-1.052016000	-0.137368000	1	0.000000000	-1.460867000	-1.972852000
1	-1.143170000	1.753114000	0.406103000	1	0.000000000	1.460867000	-1.972852000
1	1.503114000	1.630999000	0.151756000	1	-0.910557000	0.000000000	2.295196000
1	-2.299939000	-0.567751000	-0.043536000	1	0.910557000	0.000000000	2.295196000
cyclopentadiene							
6	-0.000002000	-1.008691000	0.725383000				
6	-0.000002000	0.307237000	1.048550000				
6	0.000005000	1.354389000	0.000000000				
6	-0.000002000	0.307237000	-1.048550000				
6	-0.000002000	-1.008691000	-0.725383000				
1	-0.000006000	-1.828656000	-1.434998000				
1	-0.000006000	-1.828656000	1.434998000				
1	0.898847000	1.974198000	0.000000000				
1	-0.898826000	1.974235000	0.000000000				

n1=5, n2=3, m=0 bicyclo[3.1.0]hexane				n1=5, n2=3, m=1 bicyclo[3.1.0]hex-1(6)-ene			
6	0.287962000	0.634854000	1.229692000	6	-0.405255000	1.319388000	0.016436000
6	0.287962000	-0.814891000	0.757900000	6	0.906503000	0.647632000	-0.446354000
6	-0.922834000	-1.307313000	0.000000000	6	1.616500000	-0.318720000	0.468421000
6	0.287962000	-0.814891000	-0.757900000	6	0.641022000	-0.815883000	-0.244875000
6	0.287962000	0.634854000	-1.229692000	6	-0.788439000	-1.201296000	-0.249424000
6	-0.176333000	1.452085000	0.000000000	6	-1.378427000	0.134679000	0.352884000
1	0.871262000	-1.541062000	1.317355000	1	1.385594000	1.031383000	-1.347937000
1	1.310311000	0.917377000	1.511319000	1	-0.802884000	1.930666000	-0.801638000
1	-0.347934000	0.807522000	2.105990000	1	-0.292360000	1.981568000	0.882529000
1	-1.267627000	1.542917000	0.000000000	1	-1.451188000	0.006356000	1.436960000
1	0.220705000	2.471547000	0.000000000	1	-2.388883000	0.319489000	-0.023895000
1	1.310311000	0.917377000	-1.511319000	1	-1.158632000	-1.369940000	-1.266299000
1	-0.347934000	0.807522000	-2.105990000	1	-1.040081000	-2.073304000	0.361372000
1	0.871262000	-1.541062000	-1.317355000	1	2.197010000	-0.421014000	1.376369000
1	-1.832734000	-0.712194000	0.000000000				
1	-1.103699000	-2.378136000	0.000000000				
n1=5, n2=3, m=1 bicyclo[3.1.0]hex-1(5)-ene				n1=5, n2=3, m=1 bicyclo[3.1.0]hex-1-ene			
6	-0.095020000	-0.645889000	1.238500000	6	-0.577644000	1.245639000	0.007615000
6	-0.095020000	0.745099000	0.658686000	6	0.627506000	0.746016000	-0.280162000
6	0.786767000	1.776547000	0.000000000	6	1.816401000	0.075121000	0.266333000
6	-0.095020000	0.745099000	-0.658686000	6	0.649822000	-0.728679000	-0.367870000
6	-0.095020000	-0.645889000	-1.238500000	6	-0.690298000	-1.131640000	0.268579000
6	-0.560717000	-1.481455000	0.000000000	6	-1.600989000	0.103891000	-0.056968000
1	-0.728303000	-0.788354000	2.120114000	1	-0.807000000	2.236394000	0.390393000
1	0.930080000	-0.907652000	1.539454000	1	-2.412785000	0.242588000	0.666902000
1	-0.179011000	-2.507137000	0.000000000	1	-2.073373000	0.005105000	-1.045865000
1	-1.654547000	-1.542042000	0.000000000	1	-1.080954000	-2.076938000	-0.123048000
1	-0.728303000	-0.788354000	-2.120114000	1	-0.597437000	-1.238940000	1.356879000
1	0.930080000	-0.907652000	-1.539454000	1	0.915686000	-1.192199000	-1.318597000
1	1.878642000	1.658489000	0.000000000	1	1.958872000	0.121729000	1.345165000
1	0.475534000	2.821624000	0.000000000	1	2.748203000	0.040171000	-0.296994000
n1=5, n2=3, m=1 bicyclo[3.1.0]hex-2-ene				n1=5, n2=3, m=2 bicyclo[3.1.0]hexa-1(6),4-diene			
6	-0.652545000	1.210295000	-0.054124000	6	0.531358000	1.259726000	0.000757000
6	0.714533000	0.748634000	-0.440459000	6	-0.720077000	0.785745000	0.000463000
6	1.460561000	-0.023491000	0.633254000	6	-1.897432000	-0.041036000	-0.000462000
6	0.645633000	-0.773187000	-0.388589000	6	-0.749775000	-0.682029000	-0.000457000
6	-0.793963000	-1.156001000	-0.034526000	6	0.645359000	-1.210524000	0.000748000
6	-1.468652000	0.181263000	0.205076000	6	1.540382000	0.096475000	-0.001058000
1	1.283312000	1.282519000	-1.196661000	1	0.841318000	2.298305000	0.001060000
1	-0.917406000	2.259184000	0.038246000	1	2.201419000	0.109772000	-0.879720000
1	-2.489335000	0.266025000	0.565113000	1	2.205442000	0.109609000	0.874552000
1	-1.276694000	-1.702759000	-0.856889000	1	0.815572000	-1.842274000	0.878955000
1	-0.848446000	-1.811848000	0.845120000	1	0.817426000	-1.846978000	-0.873653000
1	-1.179617000	-1.374744000	-1.117251000	1	-2.980073000	-0.078576000	-0.001147000
1	1.094179000	0.048125000	1.654124000				
1	2.541367000	-0.091577000	0.544409000				
n1=5, n2=3, m=2 bicyclo[3.1.0]hexa-1(6),3-diene				n1=5, n2=3, m=2 bicyclo[3.1.0]hexa-1(6),2-diene			
6	0.498777000	1.240990000	-0.108645000	6	-0.593928000	1.199664000	0.142858000
6	-0.824379000	0.721904000	0.408580000	6	0.765215000	0.711140000	-0.407941000
6	-1.599457000	-0.278488000	-0.421088000	6	1.668349000	-0.217135000	0.361785000
6	-0.610766000	-0.768117000	0.278546000	6	0.646431000	-0.783942000	-0.230655000
6	0.822581000	-1.152604000	0.136234000	6	-0.748572000	-1.195256000	-0.127529000
6	1.384744000	0.237417000	-0.227250000	6	-1.451257000	-0.068909000	0.123099000
1	-1.259393000	1.189979000	1.292970000	1	1.080377000	1.126676000	-1.366403000
1	0.738093000	2.287382000	-0.273817000	1	-1.015553000	2.002033000	-0.472021000
1	2.426042000	0.349248000	-0.514048000	1	-0.555141000	1.584206000	1.175064000
1	1.299170000	-1.529032000	1.051731000	1	-2.490332000	-0.073688000	0.441507000
1	0.977246000	-1.900456000	-0.648931000	1	-1.128174000	-2.209428000	-0.109916000
1	-2.210155000	-0.403727000	-1.306168000	1	2.391398000	-0.303172000	1.162066000
n=1, m=4 cyclohexa-1,2,3,4-tetraene							
6	-0.664937000	1.169193000	0.000112000				
6	0.666238000	0.799848000	0.000020000				
6	1.753689000	-0.000178000	-0.000227000				
6	0.666287000	-0.799682000	0.000110000				
6	-0.665105000	-1.169125000	0.000075000				

6	-1.458090000	-0.000063000	-0.000205000			
1	-1.041210000	2.184750000	0.000276000			
1	-2.547119000	-0.000057000	-0.000128000			
1	-1.040866000	-2.184824000	0.000197000			
1	2.840697000	0.000183000	0.000346000			
n1=5, n2=3, m=2 bicyclo[3.1.0]hexa-1(5),2-diene				n1=5, n2=3, m=2 bicyclo[3.1.0]hexa-1,4-diene		
6	-0.715581000	1.191355000	0.008176000	6	0.000000000	1.202072000 -0.643147000
6	0.620890000	0.686963000	-0.317344000	6	0.000000000	0.720784000 0.606809000
6	1.842084000	0.014848000	0.249110000	6	0.000000000	0.000000000 1.904921000
6	0.629765000	-0.643660000	-0.369076000	6	0.000000000	-0.720784000 0.606809000
6	-0.731879000	-1.170762000	0.018070000	6	0.000000000	-1.202072000 -0.643147000
6	-1.533642000	0.117030000	0.131930000	6	0.000000000	0.000000000 -1.589266000
1	-1.011997000	2.231644000	0.085589000	1	0.000000000	2.232839000 -0.983257000
1	-2.612611000	0.146970000	0.258516000	1	-0.876398000	0.000000000 -2.256702000
1	-1.170337000	-1.905903000	-0.668738000	1	0.876398000	0.000000000 -2.256702000
1	-0.656256000	-1.674091000	0.992158000	1	0.000000000	-2.232839000 -0.983257000
1	2.013521000	0.001480000	1.333019000	1	-0.908570000	0.000000000 2.511025000
1	2.767867000	0.025257000	-0.325745000	1	0.908570000	0.000000000 2.511025000

Cyclic hydrocarbynes, n=number of C-atoms in the cycle, m=number of double bonds

							
1	-1.560341000	2.136651000	0.000000000	1	0.778230000	-2.693465000	0.000000000
6	-1.337559000	1.072630000	0.000000000	6	0.905361000	-1.616069000	0.000000000
6	-0.759621000	-1.555725000	0.000000000	6	1.267937000	1.309038000	0.000000000
6	0.000000000	0.639872000	0.000000000	6	-0.180143000	-0.711476000	0.000000000
6	-2.411898000	0.152235000	0.000000000	6	2.097630000	-0.908818000	0.000000000
6	-1.946483000	-1.151790000	0.000000000	6	2.255798000	0.331644000	0.000000000
6	0.354966000	-0.744876000	0.000000000	6	0.000000000	0.705340000	0.000000000
1	-3.446712000	0.475457000	0.000000000	1	1.413129000	2.384683000	0.000000000
6	1.256631000	1.400055000	0.000000000	6	-1.622431000	-0.979732000	0.000000000
1	1.311344000	2.483125000	0.000000000	1	-2.051395000	-1.975787000	0.000000000
6	2.308940000	0.558206000	0.000000000	6	-2.309607000	0.178321000	0.000000000
1	3.353413000	0.846570000	0.000000000	1	-3.388878000	0.280329000	0.000000000
6	1.852783000	-0.883164000	0.000000000	6	-1.367276000	1.358563000	0.000000000
1	2.217873000	-1.433232000	0.878385000	1	-1.517346000	2.001690000	0.878413000
1	2.217873000	-1.433232000	-0.878385000	1	-1.517346000	2.001690000	-0.878413000
							
6	0.745583000	-1.595109000	0.000000000	1	-0.284797000	-2.710606000	0.000000000
6	1.332543000	1.035454000	0.000000000	6	0.172556000	-1.726745000	0.000000000
6	-0.367335000	-0.768737000	0.000000000	6	1.377911000	0.846642000	0.000000000
6	1.930685000	-1.190985000	0.000000000	6	-0.606397000	-0.577907000	0.000000000
6	2.406370000	0.109331000	0.000000000	6	1.567178000	-1.581654000	0.000000000
6	0.000000000	0.612885000	0.000000000	6	2.161847000	-0.319617000	0.000000000
1	3.442602000	0.427344000	0.000000000	6	0.000000000	0.721970000	0.000000000
1	1.564219000	2.098027000	0.000000000	1	2.194067000	-2.468504000	0.000000000
6	-1.822933000	-0.881393000	0.000000000	1	3.244490000	-0.236100000	0.000000000
1	-2.364999000	-1.819295000	0.000000000	1	1.851621000	1.825406000	0.000000000
6	-2.359209000	0.355388000	0.000000000	6	-2.042063000	-0.294524000	0.000000000
1	-3.417273000	0.589579000	0.000000000	6	-2.329847000	0.904524000	0.000000000
6	-1.282447000	1.416521000	0.000000000	6	-1.113308000	1.807240000	0.000000000
1	-1.362043000	2.072113000	0.878573000	1	-1.066320000	2.455112000	0.882039000
1	-1.362043000	2.072113000	-0.878573000	1	-1.066320000	2.455112000	-0.882039000
							
1	-3.418525000	0.732751000	0.000000000	1	0.000000000	1.246218000	3.253069000
6	-2.417247000	0.312605000	0.000000000	6	0.000000000	0.708033000	2.309861000
1	-1.463186000	2.228421000	0.000000000	1	0.000000000	2.488804000	1.121789000
6	-1.322103000	1.150997000	0.000000000	6	0.000000000	1.402047000	1.122393000
6	-0.990143000	-1.649518000	0.000000000	6	0.000000000	-1.402047000	1.122393000
6	0.000000000	0.632897000	0.000000000	6	0.000000000	0.724106000	-0.128616000
6	-2.251813000	-1.090930000	0.000000000	6	0.000000000	-0.708033000	2.309861000
6	0.149832000	-0.816867000	0.000000000	6	0.000000000	-0.724106000	-0.128616000
6	1.145250000	1.496702000	0.000000000	6	0.000000000	1.467238000	-1.364408000
1	-3.127398000	-1.733299000	0.000000000	1	0.000000000	-1.246218000	3.253069000
1	-0.855232000	-2.726105000	0.000000000	1	0.000000000	-2.552498000	-1.365502000
6	2.454994000	1.030788000	0.000000000	1	0.000000000	-2.488804000	1.121789000

1	0.969024000	2.569910000	0.000000000	6	0.000000000	0.629992000	-2.440789000
1	3.312878000	1.693400000	0.000000000	1	0.000000000	2.552498000	-1.365502000
6	2.478633000	-0.372254000	0.000000000	6	0.000000000	-0.629992000	-2.440789000
6	1.516337000	-1.155266000	0.000000000	6	0.000000000	-1.467238000	-1.364408000

cyclopropane				cyclopropene			
6	0.000000000	0.870813000	0.000000000	6	0.000000000	0.000000000	0.861658000
6	0.754146000	-0.435407000	0.000000000	1	-0.912584000	0.000000000	1.464717000
6	-0.754146000	-0.435407000	0.000000000	1	0.912584000	0.000000000	1.464717000
1	0.000000000	1.462325000	0.910550000	6	0.000000000	0.647478000	-0.501241000
1	0.000000000	1.462325000	-0.910550000	1	0.000000000	1.580635000	-1.042246000
1	1.266411000	-0.731163000	0.910550000	6	0.000000000	-0.647478000	-0.501241000
1	1.266411000	-0.731163000	-0.910550000	1	0.000000000	-1.580635000	-1.042246000
1	-1.266411000	-0.731163000	-0.910550000				
1	-1.266411000	-0.731163000	0.910550000				
cyclopent-1-en-3-yne				cyclopent-1-yne			
1	1.816286000	0.232183000	0.881412000	6	0.000000000	0.000000000	1.124059000
6	1.175702000	0.115393000	0.000000000	6	0.000000000	1.284450000	0.185422000
6	0.469869000	-1.251506000	0.000000000	6	0.000000000	0.599342000	-1.156643000
6	-0.734321000	-0.968128000	0.000000000	6	0.000000000	-0.599342000	-1.156643000
6	-1.171106000	0.418478000	0.000000000	6	0.000000000	-1.284450000	0.185422000
6	0.000000000	1.108783000	0.000000000	1	-0.869067000	0.000000000	1.774821000
1	1.816286000	0.232183000	-0.881412000	1	0.874587000	1.904042000	0.340162000
1	-2.180387000	0.806450000	0.000000000	1	-0.874587000	1.904042000	0.340162000
1	0.106957000	2.191058000	0.000000000	1	0.874587000	-1.904042000	0.340162000
				1	-0.874587000	-1.904042000	0.340162000
				1	0.869067000	0.000000000	1.774821000
3-methylene cyclopropene				cyclopropyne			
6	0.000000000	0.630267000	-1.171656000	6	0.000000000	0.000000000	0.781271000
6	0.000000000	-0.630267000	-1.171656000	1	-0.911885000	0.000000000	1.389843000
6	0.000000000	0.000000000	0.179356000	1	0.911885000	0.000000000	1.389843000
6	0.000000000	0.000000000	1.486326000	6	0.000000000	0.621829000	-0.622276000
1	0.000000000	-0.937616000	2.032889000	6	0.000000000	-0.621829000	-0.622276000
1	0.000000000	0.937616000	2.032889000				
cycloheptyne				cyclohexyne			
6	-0.083806000	1.778589000	-0.541359000	6	0.234090000	0.563781000	-1.301649000
6	0.000000000	0.607448000	-1.430049000	6	-0.234090000	-0.563781000	-1.301649000
6	0.000000000	-0.607448000	-1.430049000	6	-0.555956000	-1.494748000	-0.198244000
6	-0.710014000	1.189945000	0.755593000	6	-0.555956000	-0.537869000	1.054566000
6	0.083806000	-1.778589000	-0.541359000	6	0.555956000	0.537869000	1.054566000
6	0.000000000	0.000000000	1.481814000	6	0.555956000	1.494748000	-0.198244000
6	0.710014000	-1.189945000	0.755593000	1	-1.522687000	-2.002503000	-0.285746000
1	0.912247000	2.203242000	-0.360100000	1	-1.533192000	-0.042003000	1.098013000
1	-0.912247000	-2.203242000	-0.360100000	1	-0.465317000	-1.144660000	1.964283000
1	-1.723080000	0.876267000	0.482439000	1	0.465317000	1.144660000	1.964283000
1	-0.763278000	-0.419200000	2.150114000	1	1.533192000	0.042003000	1.098013000
1	-0.709908000	2.593751000	-0.922614000	1	-0.209033000	2.275393000	-0.104589000
1	-0.825691000	1.990006000	1.499606000	1	1.522687000	2.002503000	-0.285746000
1	0.709908000	-2.593751000	-0.922614000	1	0.209033000	-2.275393000	-0.104589000
1	0.763278000	0.419200000	2.150114000				
1	0.825691000	-1.990006000	1.499606000				
1	1.723080000	-0.876267000	0.482439000				
cyclohex-1-en-3-yne				cyclohex-1-en-4-yne			
6	0.566461000	-1.273455000	0.128192000	6	-0.610076000	-1.259023000	0.000210000
6	-0.658510000	-1.297046000	0.078597000	6	-0.669032000	1.105453000	-0.000207000
6	1.506651000	-0.174915000	-0.183140000	6	0.669413000	1.105282000	0.000030000
1	2.436923000	-0.155614000	0.392057000	6	0.609531000	-1.258801000	-0.000129000
1	1.781563000	-0.201938000	-1.246173000	1	-1.192894000	2.060333000	0.000372000
6	-1.543411000	-0.156708000	-0.048375000	1	1.193574000	2.059997000	0.000426000
1	-2.618249000	-0.212692000	-0.183309000	6	-1.577322000	-0.144267000	-0.000012000
6	-0.856625000	1.010624000	-0.072736000	1	-2.237455000	-0.135717000	-0.877793000
1	-1.394979000	1.946936000	-0.208442000	1	-2.237635000	-0.135429000	0.877635000
6	0.643869000	1.112590000	0.161819000	6	1.577372000	-0.144751000	-0.000016000
1	0.788066000	1.320516000	1.233041000	1	2.237637000	-0.136191000	-0.877695000
1	1.056074000	1.976250000	-0.373323000	1	2.237466000	-0.136358000	0.877793000
cyclohexa-1,3-dien-5-yne				cyclobutyne			
1	0.000000000	2.546212000	-0.134029000	6	0.000000000	0.624099000	0.968947000
6	0.000000000	1.461690000	-0.133615000	6	0.000000000	0.749274000	-0.639337000
6	0.000000000	-1.461690000	-0.133615000	6	0.000000000	-0.749274000	-0.639337000

6	0.000000000	0.625447000	-1.237197000	6	0.000000000	-0.624099000	0.968947000
6	0.000000000	0.703431000	1.058046000	1	0.903712000	1.248007000	-0.988830000
6	0.000000000	-0.703431000	1.058046000	1	-0.903712000	1.248007000	-0.988830000
6	0.000000000	-0.625447000	-1.237197000	1	0.903712000	-1.248007000	-0.988830000
1	0.000000000	1.227837000	2.010625000	1	-0.903712000	-1.248007000	-0.988830000
1	0.000000000	-1.227837000	2.010625000				
1	0.000000000	-2.546212000	-0.134029000				

R and Rho values

etane	1.5303	0.2430	cyc=cyclic polyynes		
			cyc-2	1.4131	0.3150
butane	1.5314	0.2441	cyc-2	1.4758	0.2325
butane	1.5333	0.2455	cyc-2	1.4131	0.3150
butane	1.5314	0.2441	cyc-2	1.4758	0.2325
hexane	1.5316	0.2440	cyc-4	1.2266	0.4092
hexane	1.5335	0.2450	cyc-4	1.4214	0.2705
hexane	1.5334	0.2448	cyc-4	1.2266	0.4092
hexane	1.5335	0.2450	cyc-4	1.4214	0.2705
hexane	1.5316	0.2440	cyc-4	1.2266	0.4092
			cyc-4	1.4214	0.2705
heptane	1.5316	0.2440	cyc-4	1.2266	0.4092
heptane	1.5336	0.2450	cyc-4	1.4214	0.2705
heptane	1.5335	0.2447			
heptane	1.5336	0.2446	cyc-6	1.2298	0.3939
heptane	1.5335	0.2447	cyc-6	1.3759	0.3006
heptane	1.5336	0.2450	cyc-6	1.2298	0.3939
heptane	1.5316	0.2440	cyc-6	1.3759	0.3006
			cyc-6	1.2298	0.3939
decane	1.5316	0.2440	cyc-6	1.3759	0.3006
decane	1.5336	0.2450	cyc-6	1.2298	0.3939
decane	1.5335	0.2447	cyc-6	1.3759	0.3006
decane	1.5336	0.2446	cyc-6	1.2298	0.3939
decane	1.5336	0.2446	cyc-6	1.3759	0.3006
decane	1.5336	0.2446	cyc-6	1.2298	0.3939
decane	1.5335	0.2447	cyc-6	1.3759	0.3006
decane	1.5336	0.2450			
decane	1.5316	0.2440	cyc-8	1.2336	0.3881
			cyc-8	1.3573	0.3131
dodecane	1.5316	0.2440	cyc-8	1.2336	0.3881
dodecane	1.5336	0.2450	cyc-8	1.3573	0.3131
dodecane	1.5335	0.2447	cyc-8	1.2336	0.3881
dodecane	1.5336	0.2446	cyc-8	1.3573	0.3131
dodecane	1.5336	0.2446	cyc-8	1.2336	0.3881
dodecane	1.5336	0.2446	cyc-8	1.3573	0.3131
dodecane	1.5336	0.2446	cyc-8	1.2336	0.3881
dodecane	1.5336	0.2446	cyc-8	1.3573	0.3131
dodecane	1.5335	0.2447	cyc-8	1.2336	0.3881
dodecane	1.5336	0.2450	cyc-8	1.3573	0.3131
dodecane	1.5316	0.2440	cyc-8	1.2336	0.3881
			cyc-8	1.3573	0.3131
icosane	1.5316	0.2440	cyc-8	1.2336	0.3881
icosane	1.5337	0.2450	cyc-8	1.3573	0.3131
icosane	1.5335	0.2447			
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196

icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5336	0.2446	cyc-10	1.3477	0.3196
icosane	1.5336	0.2446	cyc-10	1.2363	0.3855
icosane	1.5335	0.2447	cyc-10	1.3477	0.3196
icosane	1.5337	0.2450	cyc-10	1.2363	0.3855
icosane	1.5316	0.2440	cyc-10	1.3477	0.3196
			cyc-10	1.2363	0.3855
eten	1.3301	0.3475	cyc-10	1.3477	0.3196
			cyc-10	1.2363	0.3855
allene	1.3064	0.3515	cyc-10	1.3477	0.3196
allene	1.3064	0.3515	cyc-al=cyclic allenes		
			cyc-al-3	1.3096	0.3424
allen-3	1.3175	0.3663	cyc-al-3	1.3096	0.3424
allen-3	1.2711	0.3445	cyc-al-3	1.3096	0.3424
allen-3	1.3177	0.3444	cyc-al-3	1.3096	0.3424
			cyc-al-3	1.3096	0.3424
allen-4	1.3136	0.3610	cyc-al-3	1.3096	0.3424
allen-4	1.2793	0.3464			
allen-4	1.2793	0.3610	cyc-al-5	1.2910	0.3512
allen-4	1.3135	0.3464	cyc-al-5	1.2910	0.3512
			cyc-al-5	1.2910	0.3512
allen-5	1.3181	0.3650	cyc-al-5	1.2910	0.3512
allen-5	1.2730	0.3440	cyc-al-5	1.2910	0.3512
allen-5	1.2906	0.3533	cyc-al-5	1.2910	0.3512
allen-5	1.2729	0.3650	cyc-al-5	1.2910	0.3512
allen-5	1.3181	0.3440	cyc-al-5	1.2910	0.3512
			cyc-al-5	1.2910	0.3512
allen-6	1.3162	0.3450	cyc-al-5	1.2910	0.3512
allen-6	1.2769	0.3576			
allen-6	1.2835	0.3627	cyc-al-7	1.2868	0.3540
allen-6	1.2835	0.3576	cyc-al-7	1.2868	0.3540
allen-6	1.2769	0.3627	cyc-al-7	1.2868	0.3540
allen-6	1.3162	0.3450	cyc-al-7	1.2868	0.3540
			cyc-al-7	1.2868	0.3540
allen-7	1.3185	0.3544	cyc-al-7	1.2868	0.3540
allen-7	1.2738	0.3646	cyc-al-7	1.2868	0.3540
allen-7	1.2890	0.3438	cyc-al-7	1.2868	0.3540
allen-7	1.2754	0.3625	cyc-al-7	1.2868	0.3540
allen-7	1.2890	0.3544	cyc-al-7	1.2868	0.3540
allen-7	1.2738	0.3646	cyc-al-7	1.2868	0.3540
allen-7	1.3184	0.3438	cyc-al-7	1.2868	0.3540
			cyc-al-7	1.2868	0.3540
allen-8	1.3173	0.3566	cyc-al-7	1.2868	0.3540
allen-8	1.2761	0.3634			
allen-8	1.2854	0.3444	cyc-al-9	1.2852	0.3563
allen-8	1.2806	0.3594	cyc-al-9	1.2852	0.3563

allen-8	1.2806	0.3594	cyc-al-9	1.2852	0.3563
allen-8	1.2854	0.3566	cyc-al-9	1.2852	0.3563
allen-8	1.2761	0.3634	cyc-al-9	1.2852	0.3563
allen-8	1.3172	0.3444	cyc-al-9	1.2852	0.3563
			cyc-al-9	1.2852	0.3563
allen-9	1.3187	0.3547	cyc-al-9	1.2852	0.3563
allen-9	1.2742	0.3645	cyc-al-9	1.2852	0.3563
allen-9	1.2886	0.3438	cyc-al-9	1.2852	0.3563
allen-9	1.2765	0.3620	cyc-al-9	1.2852	0.3563
allen-9	1.2868	0.3558	cyc-al-9	1.2852	0.3563
allen-9	1.2764	0.3620	cyc-al-9	1.2852	0.3563
allen-9	1.2886	0.3547	cyc-al-9	1.2852	0.3563
allen-9	1.2742	0.3645	cyc-al-9	1.2852	0.3563
allen-9	1.3187	0.3438	cyc-al-9	1.2852	0.3563
			cyc-al-9	1.2852	0.3563
allen-10	1.3178	0.3602	cyc-al-9	1.2852	0.3563
allen-10	1.2756	0.3637			
allen-10	1.2863	0.3442	benzene	1.3962	0.3120
allen-10	1.2795	0.3561			
allen-10	1.2824	0.3584	cyclopent-1-en-3-yne	1.3594	0.244874
allen-10	1.2824	0.3584	cyclopent-1-en-3-yne	1.4538	0.216887
allen-10	1.2795	0.3602	cyclopent-1-en-3-yne	1.2371	0.428769
allen-10	1.2863	0.3561	cyclopent-1-en-3-yne	1.5384	0.259498
allen-10	1.2756	0.3637	cyclopent-1-en-3-yne	1.5392	0.331508
allen-10	1.3178	0.3442			
			benzyn	1.4069	0.305463
acetylene	1.2054	0.4023	benzyn	1.4125	0.299199
ply=polyyne			benzyn	1.3846	0.297218
ply-2	1.2124	0.3999	benzyn	1.2509	0.412002
ply-2	1.3687	0.3119	benzyn	1.3846	0.297218
ply-2	1.2124	0.3999	benzyn	1.4125	0.299199
ply-3	1.2150	0.3989	cyclohex-1-en-4-yne	1.3385	0.342296
ply-3	1.3599	0.3161	cyclohex-1-en-4-yne	1.5449	0.236389
ply-3	1.2235	0.3926	cyclohex-1-en-4-yne	1.4759	0.252727
ply-3	1.3599	0.3161	cyclohex-1-en-4-yne	1.2196	0.427353
ply-3	1.2150	0.3989	cyclohex-1-en-4-yne	1.4759	0.252727
			cyclohex-1-en-4-yne	1.5449	0.236389
ply-4	1.2159	0.3986			
ply-4	1.3569	0.3176	cyclohex-1-en-3-yne	1.3546	0.218905
ply-4	1.2272	0.3906	cyclohex-1-en-3-yne	1.4490	0.250896
ply-4	1.3482	0.3220	cyclohex-1-en-3-yne	1.2262	0.424958
ply-4	1.2272	0.3906	cyclohex-1-en-3-yne	1.4791	0.264165
ply-4	1.3569	0.3176	cyclohex-1-en-3-yne	1.5878	0.33232
ply-4	1.2159	0.3986	cyclohex-1-en-3-yne	1.5221	0.249172
ply-5	1.2163	0.3984	naphthyn-1A	1.4345	0.278741
ply-5	1.3556	0.3183	naphthyn-1A	1.3902	0.29135
ply-5	1.2288	0.3899	naphthyn-1A	1.4032	0.311699
ply-5	1.3444	0.3240	naphthyn-1A	1.2406	0.287512
ply-5	1.2316	0.3881	naphthyn-1A	1.4078	0.418324
ply-5	1.3444	0.3240	naphthyn-1A	1.4575	0.285616

ply-5	1.2288	0.3899			
ply-5	1.3556	0.3183	naphthyn-1B	1.4575	0.2787
ply-5	1.2163	0.3984	naphthyn-1B	1.4117	0.2992
			naphthyn-1B	1.3798	0.3215
ply-6	1.2166	0.3983	naphthyn-1B	1.4133	0.3025
ply-6	1.3551	0.3186	naphthyn-1B	1.3792	0.3210
ply-6	1.2296	0.3894	naphthyn-1B	1.4200	0.3048
ply-6	1.3424	0.3251			
ply-6	1.2336	0.3871	naphthyn-2A	1.4482	0.285357
ply-6	1.3397	0.3266	naphthyn-2A	1.4420	0.284357
ply-6	1.2336	0.3871	naphthyn-2A	1.3637	0.309154
ply-6	1.3424	0.3251	naphthyn-2A	1.2600	0.40536
ply-6	1.2296	0.3894	naphthyn-2A	1.3637	0.309154
ply-6	1.3551	0.3186	naphthyn-2A	1.4420	0.284357
ply-6	1.2166	0.3983			
			naphthyn-2B	1.4482	0.2854
ply-7	1.2167	0.3983	naphthyn-2B	1.4229	0.2975
ply-7	1.3548	0.3188	naphthyn-2B	1.3754	0.3232
ply-7	1.2300	0.3892	naphthyn-2B	1.4161	0.3010
ply-7	1.3414	0.3257	naphthyn-2B	1.3754	0.3232
ply-7	1.2346	0.3865	naphthyn-2B	1.4229	0.2975
ply-7	1.3376	0.3277			
ply-7	1.2358	0.3859	indyn-1A	1.4295	0.294737
ply-7	1.3376	0.3277	indyn-1A	1.3783	0.298384
ply-7	1.2346	0.3865	indyn-1A	1.2537	0.409029
ply-7	1.3414	0.3257	indyn-1A	1.3846	0.297139
ply-7	1.2300	0.3892	indyn-1A	1.4147	0.296743
ply-7	1.3548	0.3188	indyn-1A	1.4058	0.305125
ply-7	1.2167	0.3983			
			indyn-1B	1.4295	0.294737
ply-8	1.2167	0.3983	indyn-1B	1.4687	0.257936
ply-8	1.3544	0.3191	indyn-1B	1.3476	0.254008
ply-8	1.2301	0.3891	indyn-1B	1.5118	0.339699
ply-8	1.3411	0.3259	indyn-1B	1.5042	0.272923
ply-8	1.2350	0.3863			
ply-8	1.3369	0.3281	indyn-2A	1.4282	0.29812
ply-8	1.2366	0.3854	indyn-2A	1.4043	0.298799
ply-8	1.3357	0.3287	indyn-2A	1.3897	0.296277
ply-8	1.2366	0.3854	indyn-2A	1.2505	0.411265
ply-8	1.3369	0.3281	indyn-2A	1.3863	0.294308
ply-8	1.2350	0.3863	indyn-2A	1.4130	0.303206
ply-8	1.3411	0.3259			
ply-8	1.2301	0.3891	indyn-2B	1.4282	0.29812
ply-8	1.3544	0.3191	indyn-2B	1.5153	0.27456
ply-8	1.2167	0.3983	indyn-2B	1.5103	0.340369
			indyn-2B	1.3466	0.2549
ply-9	1.2168	0.3983	indyn-2B	1.4670	0.25235
ply-9	1.3543	0.3191			
ply-9	1.2303	0.3890	indyn-3A	1.4296	0.294847
ply-9	1.3408	0.3261	indyn-3A	1.3979	0.308792
ply-9	1.2353	0.3861	indyn-3A	1.4180	0.294713
ply-9	1.3363	0.3285	indyn-3A	1.3846	0.297205

ply-9	1.2372	0.3851	indyn-3A	1.2521	0.410153
ply-9	1.3346	0.3294	indyn-3A	1.3862	0.294602
ply-9	1.2378	0.3848			
ply-9	1.3346	0.3294	indyn-3B	1.4296	0.2948
ply-9	1.2372	0.3851	indyn-3B	1.5134	0.2525
ply-9	1.3363	0.3285	indyn-3B	1.5118	0.2544
ply-9	1.2353	0.3861	indyn-3B	1.3480	0.3395
ply-9	1.3408	0.3261	indyn-3B	1.4600	0.2785
ply-9	1.2303	0.3890			
ply-9	1.3543	0.3191	indyn-4A	1.4344	0.2956
ply-9	1.2168	0.3983	indyn-4A	1.3880	0.3198
			indyn-4A	1.4022	0.3053
ply-10	1.2168	0.3983	indyn-4A	1.3951	0.3121
ply-10	1.3542	0.3192	indyn-4A	1.4053	0.3076
ply-10	1.2303	0.3890	indyn-4A	1.3835	0.3167
ply-10	1.3407	0.3261			
ply-10	1.2354	0.3861	indyn-4B	1.4344	0.2956
ply-10	1.3359	0.3287	indyn-4B	1.4634	0.2365
ply-10	1.2376	0.3849	indyn-4B	1.2331	0.2300
ply-10	1.3339	0.3298	indyn-4B	1.5149	0.4340
ply-10	1.2384	0.3844	indyn-4B	1.5548	0.2533
ply-10	1.3333	0.3301			
ply-10	1.2384	0.3844	naphthalene-A	1.3763	0.3231
ply-10	1.3339	0.3298	naphthalene-A	1.4169	0.3004
ply-10	1.2376	0.3849	naphthalene-A	1.3763	0.3231
ply-10	1.3359	0.3287	naphthalene-A	1.4213	0.2991
ply-10	1.2354	0.3861	naphthalene-A	1.4337	0.2937
ply-10	1.3407	0.3261	naphthalene-A	1.4213	0.2991
ply-10	1.2303	0.3890			
ply-10	1.3542	0.3192	naphthalene-B	1.4212	0.2991
ply-10	1.2168	0.3983	naphthalene-B	1.3762	0.3232
sp=all-cis-polyene			naphthalene-B	1.4169	0.3004
sp-2	1.3386	0.3426	naphthalene-B	1.3762	0.3232
sp-2	1.4700	0.2734	naphthalene-B	1.4212	0.2991
sp-2	1.3386	0.3426	naphthalene-B	1.4337	0.2937
sp-3	1.3387	0.3422	1,2-dihydronaphthalene-A	1.3946	0.3126
sp-3	1.4703	0.2722	1,2-dihydronaphthalene-A	1.3948	0.3125
sp-3	1.3502	0.3339	1,2-dihydronaphthalene-A	1.3981	0.3105
sp-3	1.4703	0.2722	1,2-dihydronaphthalene-A	1.3939	0.3133
sp-3	1.3387	0.3422	1,2-dihydronaphthalene-A	1.4135	0.3040
			1,2-dihydronaphthalene-A	1.4015	0.3094
sp-4	1.3463	0.3387			
sp-4	1.4518	0.2810	1,2-dihydronaphthalene-B	1.5155	0.2530
sp-4	1.3631	0.3262	1,2-dihydronaphthalene-B	1.5367	0.2431
sp-4	1.4535	0.2787	1,2-dihydronaphthalene-B	1.5097	0.2549
sp-4	1.3631	0.3262	1,2-dihydronaphthalene-B	1.3419	0.3426
sp-4	1.4518	0.2810	1,2-dihydronaphthalene-B	1.4677	0.2749
sp-4	1.3463	0.3387	1,2-dihydronaphthalene-B	1.4135	0.3040

sp-5	1.3391	0.3422	1,4-dihydronaphthalene-A	1.3916	0.3141
sp-5	1.4680	0.2736	1,4-dihydronaphthalene-A	1.3968	0.3115
sp-5	1.3471	0.3357	1,4-dihydronaphthalene-A	1.3916	0.3141
sp-5	1.4717	0.2717	1,4-dihydronaphthalene-A	1.4022	0.3092
sp-5	1.3449	0.3360	1,4-dihydronaphthalene-A	1.4030	0.3083
sp-5	1.4717	0.2717	1,4-dihydronaphthalene-A	1.4022	0.3092
sp-5	1.3471	0.3357			
sp-5	1.4680	0.2736	1,4-dihydronaphthalene-B	1.5173	0.2517
sp-5	1.3391	0.3422	1,4-dihydronaphthalene-B	1.5023	0.2580
			1,4-dihydronaphthalene-B	1.3330	0.3466
sp-6	1.3409	0.3413	1,4-dihydronaphthalene-B	1.5023	0.2580
sp-6	1.4652	0.2744	1,4-dihydronaphthalene-B	1.5173	0.2517
sp-6	1.3548	0.3312	1,4-dihydronaphthalene-B	1.4030	0.3083
sp-6	1.4636	0.2748			
sp-6	1.3567	0.3315	tetrahydronaphthalene-A	1.5087	0.2549
sp-6	1.4427	0.2869	tetrahydronaphthalene-A	1.3419	0.3423
sp-6	1.3567	0.3315	tetrahydronaphthalene-A	1.4646	0.2749
sp-6	1.4636	0.2748	tetrahydronaphthalene-A	1.3446	0.3403
sp-6	1.3548	0.3312	tetrahydronaphthalene-A	1.5173	0.2541
sp-6	1.4652	0.2744	tetrahydronaphthalene-A	1.5458	0.2399
sp-6	1.3409	0.3413			
			tetrahydronaphthalene-B	1.5052	0.2578
sp-7	1.3409	0.3413	tetrahydronaphthalene-B	1.5162	0.2505
sp-7	1.4656	0.2743	tetrahydronaphthalene-B	1.3372	0.3441
sp-7	1.3507	0.3336	tetrahydronaphthalene-B	1.5104	0.2543
sp-7	1.4694	0.2725	tetrahydronaphthalene-B	1.5483	0.2380
sp-7	1.3460	0.3359	tetrahydronaphthalene-B	1.5173	0.2541
sp-7	1.4688	0.2735			
sp-7	1.3435	0.3375	tetrahydronaphthalene-A-2	1.5095	0.2549
sp-7	1.4688	0.2735	tetrahydronaphthalene-A-2	1.3431	0.3417
sp-7	1.3460	0.3359	tetrahydronaphthalene-A-2	1.4637	0.2756
sp-7	1.4694	0.2725	tetrahydronaphthalene-A-2	1.3461	0.3397
sp-7	1.3507	0.3336	tetrahydronaphthalene-A-2	1.5231	0.2512
sp-7	1.4656	0.2743	tetrahydronaphthalene-A-2	1.5466	0.2389
sp-7	1.3409	0.3413			
			tetrahydronaphthalene-B-2	1.5033	0.2586
sp-8	1.3407	0.3414	tetrahydronaphthalene-B-2	1.5414	0.2400
sp-8	1.4659	0.2742	tetrahydronaphthalene-B-2	1.5079	0.2556
sp-8	1.3503	0.3339	tetrahydronaphthalene-B-2	1.3363	0.3446
sp-8	1.4696	0.2724	tetrahydronaphthalene-B-2	1.5107	0.2549
sp-8	1.3458	0.3359	tetrahydronaphthalene-B-2	1.5231	0.2512
sp-8	1.4696	0.2731			
sp-8	1.3441	0.3371	hexahydronaphthalene-A	1.5073	0.2557
sp-8	1.4693	0.2731	hexahydronaphthalene-A	1.3419	0.3425
sp-8	1.3441	0.3371	hexahydronaphthalene-A	1.4629	0.2759
sp-8	1.4696	0.2731	hexahydronaphthalene-A	1.3471	0.3392

sp-8	1.3458	0.3359	hexahydronaphthalene-A	1.5248	0.2501
sp-8	1.4696	0.2724	hexahydronaphthalene-A	1.5454	0.2403
sp-8	1.3503	0.3339			
sp-8	1.4659	0.2742	hexahydronaphthalene-B	1.5102	0.2552
sp-8	1.3407	0.3414	hexahydronaphthalene-B	1.5378	0.2426
			hexahydronaphthalene-B	1.5335	0.2454
sp-9	1.3406	0.3415	hexahydronaphthalene-B	1.5328	0.2454
sp-9	1.4662	0.2741	hexahydronaphthalene-B	1.5452	0.2401
sp-9	1.3500	0.3341	hexahydronaphthalene-B	1.5248	0.2501
sp-9	1.4701	0.2722			
sp-9	1.3456	0.3361	hexahydronaphthalene-A-2	1.3340	0.3460
sp-9	1.4695	0.2732	hexahydronaphthalene-A-2	1.5041	0.2572
sp-9	1.3441	0.3372	hexahydronaphthalene-A-2	1.5048	0.2564
sp-9	1.4706	0.2725	hexahydronaphthalene-A-2	1.3375	0.3435
sp-9	1.3446	0.3368	hexahydronaphthalene-A-2	1.5176	0.2535
sp-9	1.4706	0.2725	hexahydronaphthalene-A-2	1.5064	0.2573
sp-9	1.3441	0.3372			
sp-9	1.4695	0.2732	hexahydronaphthalene-B-2	1.5104	0.2556
sp-9	1.3456	0.3361	hexahydronaphthalene-B-2	1.5422	0.2402
sp-9	1.4701	0.2722	hexahydronaphthalene-B-2	1.5357	0.2444
sp-9	1.3500	0.3341	hexahydronaphthalene-B-2	1.5349	0.2445
sp-9	1.4662	0.2741	hexahydronaphthalene-B-2	1.5528	0.2357
sp-9	1.3406	0.3415	hexahydronaphthalene-B-2	1.5176	0.2535
sp-10	1.3410	0.3413	hexahydronaphthalene-A-3	1.3437	0.3413
sp-10	1.4656	0.2743	hexahydronaphthalene-A-3	1.4666	0.2744
sp-10	1.3507	0.3337	hexahydronaphthalene-A-3	1.3437	0.3413
sp-10	1.4693	0.2725	hexahydronaphthalene-A-3	1.5127	0.2546
sp-10	1.3461	0.3358	hexahydronaphthalene-A-3	1.5440	0.2432
sp-10	1.4686	0.2735	hexahydronaphthalene-A-3	1.5127	0.2546
sp-10	1.3445	0.3370			
sp-10	1.4694	0.2730	hexahydronaphthalene-B-3	1.5370	0.2441
sp-10	1.3450	0.3366	hexahydronaphthalene-B-3	1.5365	0.2438
sp-10	1.4705	0.2724	hexahydronaphthalene-B-3	1.5376	0.2435
sp-10	1.3450	0.3366	hexahydronaphthalene-B-3	1.5365	0.2438
sp-10	1.4694	0.2730	hexahydronaphthalene-B-3	1.5370	0.2441
sp-10	1.3445	0.3370	hexahydronaphthalene-B-3	1.5440	0.2432
sp-10	1.4686	0.2735			
sp-10	1.3461	0.3358	hexahydronaphthalene-A-4	1.3415	0.3425
sp-10	1.4693	0.2725	hexahydronaphthalene-A-4	1.5093	0.2550
sp-10	1.3507	0.3337	hexahydronaphthalene-A-4	1.5363	0.2436
sp-10	1.4656	0.2743	hexahydronaphthalene-A-4	1.5168	0.2524
sp-10	1.3410	0.3413	hexahydronaphthalene-A-4	1.3507	0.3369
ctc=cis-transoid polyene			hexahydronaphthalene-A-4	1.4719	0.2724
ctc-2	1.3400	0.3428			
ctc-2	1.4573	0.2802	hexahydronaphthalene-B-4	1.5099	0.2550

ctc-2	1.3400	0.3428	hexahydronaphthalene-B-4	1.5349	0.2443
			hexahydronaphthalene-B-4	1.5327	0.2456
ctc-3	1.3425	0.3412	hexahydronaphthalene-B-4	1.5336	0.2449
ctc-3	1.4522	0.2819	hexahydronaphthalene-B-4	1.5152	0.2525
ctc-3	1.3549	0.3341	hexahydronaphthalene-B-4	1.3507	0.3369
ctc-3	1.4522	0.2819	HHN=hexahydronaphthalene		
ctc-3	1.3425	0.3412	letter identifies the ring		
			number identifies structure		
ctc-4	1.3432	0.3408	HHN-34-A	1.3360	0.3448
ctc-4	1.4504	0.2828	HHN-34-A	1.5077	0.2557
ctc-4	1.3587	0.3317	HHN-34-A	1.5416	0.2400
ctc-4	1.4450	0.2848	HHN-34-A	1.5085	0.2564
ctc-4	1.3587	0.3317	HHN-34-A	1.5213	0.2517
ctc-4	1.4504	0.2828	HHN-34-A	1.5144	0.2531
ctc-4	1.3432	0.3408			
			HHN-34-B	1.3390	0.3426
ctc-5	1.3435	0.3406	HHN-34-B	1.5081	0.2551
ctc-5	1.4498	0.2832	HHN-34-B	1.5358	0.2440
ctc-5	1.3599	0.3310	HHN-34-B	1.5323	0.2456
ctc-5	1.4427	0.2861	HHN-34-B	1.5426	0.2410
ctc-5	1.3630	0.3290	HHN-34-B	1.5213	0.2517
ctc-5	1.4427	0.2861			
ctc-5	1.3599	0.3310	HHN-35-A	1.3370	0.3442
ctc-5	1.4498	0.2832	HHN-35-A	1.5109	0.2541
ctc-5	1.3435	0.3406	HHN-35-A	1.5401	0.2418
			HHN-35-A	1.5368	0.2441
ctc-6	1.3437	0.3405	HHN-35-A	1.5397	0.2445
ctc-6	1.4495	0.2833	HHN-35-A	1.5101	0.2556
ctc-6	1.3604	0.3307			
ctc-6	1.4418	0.2866	HHN-35-B	1.5101	0.2556
ctc-6	1.3644	0.3282	HHN-35-B	1.3370	0.3442
ctc-6	1.4399	0.2876	HHN-35-B	1.5109	0.2541
ctc-6	1.3644	0.3282	HHN-35-B	1.5401	0.2418
ctc-6	1.4418	0.2866	HHN-35-B	1.5368	0.2441
ctc-6	1.3604	0.3307	HHN-35-B	1.5397	0.2445
ctc-6	1.4495	0.2833			
ctc-6	1.3437	0.3405	HHN-36-A	1.3365	0.3444
			HHN-36-A	1.5091	0.2550
ctc-7	1.3438	0.3405	HHN-36-A	1.5369	0.2432
ctc-7	1.4493	0.2834	HHN-36-A	1.5336	0.2461
ctc-7	1.3606	0.3306	HHN-36-A	1.5410	0.2444
ctc-7	1.4414	0.2868	HHN-36-A	1.5103	0.2555
ctc-7	1.3650	0.3278			
ctc-7	1.4389	0.2881	HHN-36-B	1.5355	0.2450
ctc-7	1.3659	0.3273	HHN-36-B	1.5095	0.2546
ctc-7	1.4389	0.2881	HHN-36-B	1.3369	0.3443
ctc-7	1.3650	0.3278	HHN-36-B	1.5087	0.2550
ctc-7	1.4414	0.2868	HHN-36-B	1.5409	0.2419
ctc-7	1.3606	0.3306	HHN-36-B	1.5410	0.2444
ctc-7	1.4493	0.2834			
ctc-7	1.3438	0.3405	HHN-37-A	1.3362	0.3446

			HHN-37-A	1.5107	0.2541
ctc-8	1.3438	0.3405	HHN-37-A	1.5410	0.2413
ctc-8	1.4492	0.2835	HHN-37-A	1.5325	0.2466
ctc-8	1.3607	0.3305	HHN-37-A	1.5418	0.2434
ctc-8	1.4411	0.2869	HHN-37-A	1.5136	0.2535
ctc-8	1.3653	0.3276			
ctc-8	1.4384	0.2883	HHN-37-B	1.5325	0.2466
ctc-8	1.3666	0.3269	HHN-37-B	1.5410	0.2413
ctc-8	1.4377	0.2887	HHN-37-B	1.5107	0.2541
ctc-8	1.3666	0.3269	HHN-37-B	1.3362	0.3446
ctc-8	1.4384	0.2883	HHN-37-B	1.5136	0.2535
ctc-8	1.3653	0.3276	HHN-37-B	1.5418	0.2434
ctc-8	1.4411	0.2869			
ctc-8	1.3607	0.3305	HHN-38-A	1.3438	0.3411
ctc-8	1.4492	0.2835	HHN-38-A	1.5070	0.2559
ctc-8	1.3438	0.3405	HHN-38-A	1.5359	0.2436
			HHN-38-A	1.5390	0.2432
ctc-9	1.3438	0.3404	HHN-38-A	1.5238	0.2505
ctc-9	1.4493	0.2835	HHN-38-A	1.4631	0.2770
ctc-9	1.3608	0.3305			
ctc-9	1.4410	0.2869	HHN-38-B	1.5351	0.2454
ctc-9	1.3654	0.3276	HHN-38-B	1.5333	0.2450
ctc-9	1.4382	0.2885	HHN-38-B	1.5367	0.2435
ctc-9	1.3668	0.3267	HHN-38-B	1.5051	0.2565
ctc-9	1.4372	0.2889	HHN-38-B	1.3469	0.3389
ctc-9	1.3672	0.3265	HHN-38-B	1.5238	0.2505
ctc-9	1.4372	0.2889			
ctc-9	1.3668	0.3267	cyclopropyn	1.5351	0.2291
ctc-9	1.4382	0.2885	cyclopropyn	1.2437	0.4275
ctc-9	1.3654	0.3276	cyclopropyn	1.5351	0.2291
ctc-9	1.4410	0.2869			
ctc-9	1.3608	0.3305	cyclopropen	1.5089	0.2330
ctc-9	1.4493	0.2835	cyclopropen	1.2950	0.3527
ctc-9	1.3438	0.3404	cyclopropen	1.5089	0.2330
ctc-10	1.3438	0.3404	cyclobuten	1.6132	0.1751
ctc-10	1.4489	0.2836	cyclobuten	1.2482	0.4380
ctc-10	1.3608	0.3305	cyclobuten	1.6132	0.1751
ctc-10	1.4411	0.2869	cyclobuten	1.4986	0.2653
ctc-10	1.3654	0.3276			
ctc-10	1.4381	0.2885	cyclobut-1-en-3-yne	1.4908	0.2432
ctc-10	1.3669	0.3267	cyclobut-1-en-3-yne	1.2605	0.4178
ctc-10	1.4370	0.2890	cyclobut-1-en-3-yne	1.4908	0.2432
ctc-10	1.3675	0.3264	cyclobut-1-en-3-yne	1.3070	0.3517
ctc-10	1.4367	0.2892			
ctc-10	1.3675	0.3264	cpent-1-en-3-yne	1.5909	0.2311
ctc-10	1.4370	0.2890	cpent-1-en-3-yne	1.5068	0.2384
ctc-10	1.3669	0.3267	cpent-1-en-3-yne	1.1987	0.4666
ctc-10	1.4381	0.2885	cpent-1-en-3-yne	1.5068	0.2384
ctc-10	1.3654	0.3276	cpent-1-en-3-yne	1.5909	0.2311
ctc-10	1.4411	0.2869			
ctc-10	1.3608	0.3305	cyclohexyne	1.5764	0.2245

ctc-10	1.4489	0.2836	cyclohexyne	1.4791	0.2511
ctc-10	1.3438	0.3404	cyclohexyne	1.2209	0.4253
			cyclohexyne	1.4791	0.2511
ctc-20	1.3438	0.3404	cyclohexyne	1.5764	0.2245
ctc-20	1.4492	0.2835	cyclohexyne	1.5471	0.2394
ctc-20	1.3608	0.3305			
ctc-20	1.4409	0.2870	cyclohexan	1.5368	0.2439
ctc-20	1.3655	0.3275			
ctc-20	1.4379	0.2886	cyclohexadiene	1.5394	0.2422
ctc-20	1.3671	0.3266	cyclohexadiene	1.3430	0.3418
ctc-20	1.4367	0.2892	cyclohexadiene	1.4671	0.2742
ctc-20	1.3678	0.3261	cyclohexadiene	1.3430	0.3418
ctc-20	1.4361	0.2895	cyclohexadiene	1.5117	0.2541
ctc-20	1.3682	0.3259	cyclohexadiene	1.5117	0.2541
ctc-20	1.4358	0.2897			
ctc-20	1.3684	0.3258	cyclopentadiene	1.5056	0.2568
ctc-20	1.4357	0.2898	cyclopentadiene	1.3490	0.3384
ctc-20	1.3684	0.3258	cyclopentadiene	1.4695	0.2728
ctc-20	1.4356	0.2898	cyclopentadiene	1.3490	0.3384
ctc-20	1.3685	0.3258	cyclopentadiene	1.5056	0.2568
ctc-20	1.4355	0.2898			
ctc-20	1.3685	0.3258	cyclopentene	1.5122	0.2535
ctc-20	1.4355	0.2898	cyclopentene	1.3350	0.3470
tp=all-trans polyene			cyclopentene	1.5122	0.2535
tp-2	1.3400	0.3428	cyclopentene	1.5526	0.2366
tp-2	1.4573	0.2802	cyclopentene	1.5525	0.2366
tp-2	1.3400	0.3428			
			cyclopentane	1.5424	0.2412
tp-3	1.3425	0.3411	cyclopentane	1.5366	0.2439
tp-3	1.4497	0.2835	cyclopentane	1.5401	0.2423
tp-3	1.3518	0.3370	cyclopentane	1.5549	0.2356
tp-3	1.4497	0.2835	cyclopentane	1.5574	0.2344
tp-3	1.3425	0.3411			
			cyclopropane	1.5083	0.2389
tp-4	1.3435	0.3405	cyclopropane	1.5083	0.2389
tp-4	1.4475	0.2846	cyclopropane	1.5083	0.2389
tp-4	1.3553	0.3349	c3=spirocyclopropane		
tp-4	1.4405	0.2878	c3-2	1.4847	0.2486
tp-4	1.3553	0.3349	c3-2	1.5301	0.2291
tp-4	1.4475	0.2846	c3-2	1.4847	0.2486
tp-4	1.3435	0.3405	c3-2	1.4847	0.2486
			c3-2	1.5301	0.2291
tp-5	1.3440	0.3402	c3-2	1.4847	0.2486
tp-5	1.4465	0.2851			
tp-5	1.3568	0.3340	c3-3	1.4856	0.2479
tp-5	1.4376	0.2893	c3-3	1.5292	0.2297
tp-5	1.3593	0.3325	c3-3	1.4856	0.2479
tp-5	1.4376	0.2893	c3-3	1.5034	0.2399
tp-5	1.3568	0.3340	c3-3	1.4645	0.2566
tp-5	1.4465	0.2851	c3-3	1.5034	0.2399
tp-5	1.3440	0.3402	c3-3	1.4856	0.2479
			c3-3	1.5292	0.2297

tp-6	1.3442	0.3401	c3-3	1.4856	0.2479
tp-6	1.4459	0.2854			
tp-6	1.3575	0.3336	c3-4	1.4856	0.2479
tp-6	1.4362	0.2900	c3-4	1.5288	0.2299
tp-6	1.3610	0.3315	c3-4	1.4868	0.2472
tp-6	1.4342	0.2911	c3-4	1.5032	0.2401
tp-6	1.3610	0.3315	c3-4	1.4653	0.2560
tp-6	1.4362	0.2900	c3-4	1.5047	0.2391
tp-6	1.3575	0.3336	c3-4	1.5047	0.2391
tp-6	1.4459	0.2854	c3-4	1.4653	0.2560
tp-6	1.3442	0.3401	c3-4	1.5032	0.2401
			c3-4	1.4868	0.2472
tp-7	1.3444	0.3400	c3-4	1.5288	0.2299
tp-7	1.4457	0.2855	c3-4	1.4856	0.2479
tp-7	1.3579	0.3333			
tp-7	1.4354	0.2904	c3-5	1.4865	0.2473
tp-7	1.3619	0.3309	c3-5	1.5288	0.2299
tp-7	1.4325	0.2919	c3-5	1.4858	0.2477
tp-7	1.3629	0.3303	c3-5	1.5026	0.2405
tp-7	1.4325	0.2919	c3-5	1.4653	0.2559
tp-7	1.3619	0.3309	c3-5	1.5060	0.2383
tp-7	1.4354	0.2904	c3-5	1.5046	0.2393
tp-7	1.3579	0.3333	c3-5	1.4663	0.2552
tp-7	1.4457	0.2855	c3-5	1.5046	0.2393
tp-7	1.3444	0.3400	c3-5	1.5060	0.2383
			c3-5	1.4653	0.2559
tp-8	1.3444	0.3400	c3-5	1.5026	0.2405
tp-8	1.4459	0.2854	c3-5	1.4858	0.2477
tp-8	1.3581	0.3332	c3-5	1.5288	0.2299
tp-8	1.4353	0.2905	c3-5	1.4865	0.2473
tp-8	1.3623	0.3307			
tp-8	1.4319	0.2922	c3-6	1.4866	0.2478
tp-8	1.3638	0.3298	c3-6	1.5288	0.2299
tp-8	1.4310	0.2927	c3-6	1.4857	0.2473
tp-8	1.3638	0.3298	c3-6	1.5027	0.2404
tp-8	1.4319	0.2922	c3-6	1.4654	0.2558
tp-8	1.3623	0.3307	c3-6	1.5057	0.2385
tp-8	1.4353	0.2905	c3-6	1.5041	0.2396
tp-8	1.3581	0.3332	c3-6	1.4662	0.2552
tp-8	1.4459	0.2854	c3-6	1.5059	0.2386
tp-8	1.3444	0.3400	c3-6	1.5059	0.2386
			c3-6	1.4662	0.2552
tp-9	1.3445	0.3399	c3-6	1.5041	0.2396
tp-9	1.4454	0.2857	c3-6	1.5057	0.2385
tp-9	1.3583	0.3331	c3-6	1.4654	0.2558
tp-9	1.4347	0.2908	c3-6	1.5027	0.2404
tp-9	1.3627	0.3305	c3-6	1.4857	0.2473
tp-9	1.4311	0.2927	c3-6	1.5288	0.2299
tp-9	1.3646	0.3294	c3-6	1.4866	0.2478
tp-9	1.4297	0.2934			
tp-9	1.3651	0.3291	c3-7	1.4866	0.2473
tp-9	1.4297	0.2934	c3-7	1.5289	0.2299

tp-9	1.3646	0.3294	c3-7	1.4857	0.2478
tp-9	1.4311	0.2927	c3-7	1.5026	0.2404
tp-9	1.3627	0.3305	c3-7	1.4655	0.2558
tp-9	1.4347	0.2908	c3-7	1.5058	0.2384
tp-9	1.3583	0.3331	c3-7	1.5040	0.2396
tp-9	1.4454	0.2857	c3-7	1.4664	0.2551
tp-9	1.3445	0.3399	c3-7	1.5057	0.2387
			c3-7	1.5053	0.2388
tp-10	1.3445	0.3399	c3-7	1.4661	0.2552
tp-10	1.4453	0.2857	c3-7	1.5053	0.2388
tp-10	1.3584	0.3331	c3-7	1.5057	0.2387
tp-10	1.4346	0.2908	c3-7	1.4664	0.2551
tp-10	1.3629	0.3303	c3-7	1.5040	0.2396
tp-10	1.4308	0.2928	c3-7	1.5058	0.2384
tp-10	1.3649	0.3292	c3-7	1.4655	0.2558
tp-10	1.4291	0.2937	c3-7	1.5026	0.2404
tp-10	1.3657	0.3287	c3-7	1.4857	0.2478
tp-10	1.4287	0.2939	c3-7	1.5289	0.2299
tp-10	1.3657	0.3287	c3-7	1.4866	0.2473
tp-10	1.4291	0.2937			
tp-10	1.3649	0.3292	c3-8	1.4865	0.2478
tp-10	1.4308	0.2928	c3-8	1.5289	0.2298
tp-10	1.3629	0.3303	c3-8	1.4857	0.2473
tp-10	1.4346	0.2908	c3-8	1.5027	0.2404
tp-10	1.3584	0.3331	c3-8	1.4655	0.2558
tp-10	1.4453	0.2857	c3-8	1.5058	0.2384
tp-10	1.3445	0.3399	c3-8	1.5040	0.2396
			c3-8	1.4663	0.2551
			c3-8	1.5057	0.2387
			c3-8	1.5052	0.2389
			c3-8	1.4663	0.2551
			c3-8	1.5052	0.2389
			c3-9	1.4865	0.2477
			c3-9	1.5288	0.2299
			c3-9	1.4858	0.2473
			c3-9	1.5027	0.2404
			c3-9	1.4654	0.2558
			c3-9	1.5057	0.2385
			c3-9	1.5041	0.2396
			c3-9	1.4663	0.2551
			c3-9	1.5056	0.2387
			c3-9	1.5053	0.2389
			c3-9	1.4663	0.2551
			c3-9	1.5051	0.2390
			c3-9	1.5051	0.2390
			c3-9	1.4664	0.2549
			c3-10	1.4865	0.2478
			c3-10	1.5288	0.2299
			c3-10	1.4857	0.2473
			c3-10	1.5027	0.2404

			c3-10	1.4653	0.2558
			c3-10	1.5057	0.2385
			c3-10	1.5040	0.2396
			c3-10	1.4663	0.2551
			c3-10	1.5057	0.2386
			c3-10	1.5052	0.2389
			c3-10	1.4662	0.2551
			c3-10	1.5051	0.2389
			c3-10	1.5051	0.2390
			c3-10	1.4665	0.2549
			c3-10	1.5050	0.2390