

Supporting Information for “Optoelectronic Properties of Carbon Nanorings: Excitonic Effects from Time-Dependent Density Functional Theory”

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Table SI-1. $S_n \leftarrow S_0$ excitation energies and oscillator strengths up to S_4 for the cyclic paraphenylenes. All properties were computed from PBE0/6-31+G(d,p) TDDFT calculations at PBE0/6-31G(d,p)-optimized geometries.

Number of benzene rings	S_1 State		S_2 State		S_3 State		S_4 State	
	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength
5	2.08	0.0022	3.50	0.0168	3.53	0.0109	3.56	0.0004
6	2.29	0.0000	3.43	0.0056	3.57	0.0001	3.63	0.5459
7	2.50	0.0016	3.48	0.0002	3.53	0.0010	3.60	1.2204
8	2.96	0.0000	3.71	1.1785	3.71	1.1808	3.74	0.1596
9	3.00	0.0170	3.61	1.6001	3.66	1.4770	3.68	0.0133
10	2.98	0.0000	3.46	1.9694	3.58	0.0002	3.60	1.6925
11	3.16	0.0266	3.57	2.0466	3.61	1.9538	3.75	0.0042
12	3.24	0.0000	3.60	2.2387	3.60	2.2389	3.82	0.0044
13	3.20	0.0012	3.52	2.5531	3.53	2.4691	3.75	0.0018
14	3.30	0.0000	3.57	2.7355	3.57	2.7334	3.84	0.0023
15	3.29	0.0416	3.53	3.0027	3.56	2.9460	3.82	0.0017
16	3.30	0.0476	3.52	3.2317	3.53	3.2360	3.82	0.0010
17	3.30	0.0001	3.49	3.5386	3.51	3.5344	3.82	0.0015
18	3.35	0.0000	3.54	3.8007	3.54	3.8010	3.88	0.0010

Table SI-2. $S_n \leftarrow S_0$ excitation energies and oscillator strengths up to S_4 for the linear paraphenylenes. All properties were computed from PBE0/6-31+G(d,p) TDDFT calculations at PBE0/6-31G(d,p)-optimized geometries.

Number of benzene rings	S_1 State		S_2 State		S_3 State		S_4 State	
	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength	E_{opt} (eV)	Oscillator Strength
5	3.91	1.8285	4.59	0.0000	4.61	0.0000	4.62	0.0000
6	3.78	2.2541	4.37	0.0000	4.41	0.0000	4.57	0.0000
7	3.71	2.6725	4.20	0.0000	4.30	0.0000	4.64	0.4837
8	3.66	3.0789	4.08	0.0000	4.22	0.0000	4.48	0.5345
9	3.61	3.5264	3.97	0.0000	4.15	0.0000	4.32	0.5587
10	3.58	3.9501	3.89	0.0000	4.11	0.0000	4.21	0.5730
11	3.54	4.4077	3.82	0.0000	4.06	0.0000	4.11	0.5800
12	3.54	4.8329	3.78	0.0000	4.04	0.5959	4.05	0.0000
13	3.52	5.2740	3.74	0.0000	3.98	0.6066	4.03	0.0000
14	3.51	5.7074	3.70	0.0000	3.92	0.6424	4.01	0.0000
15	3.50	6.1498	3.67	0.0030	3.88	0.6591	4.00	0.0000
16	3.49	6.6009	3.65	0.0057	3.83	0.6811	3.98	0.0000
17	3.48	7.0545	3.62	0.0036	3.80	0.7112	3.97	0.0000
18	3.48	7.5154	3.61	0.0072	3.77	0.7229	3.94	0.0006

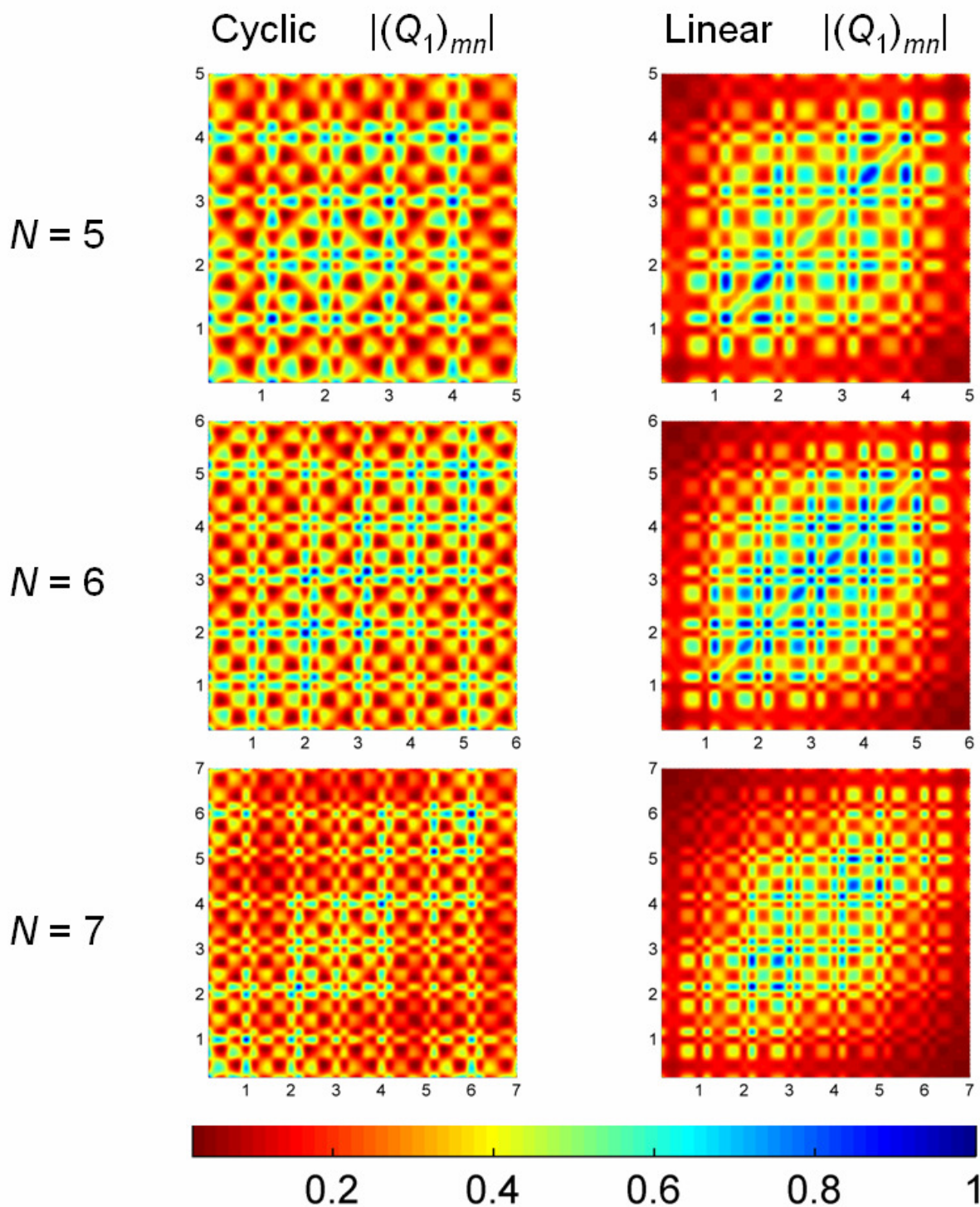


Figure SI-1. Contour plots of coordinate density matrices (\mathbf{Q}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the coordinate matrix, Q_{mn} , give a measure of exciton delocalization between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

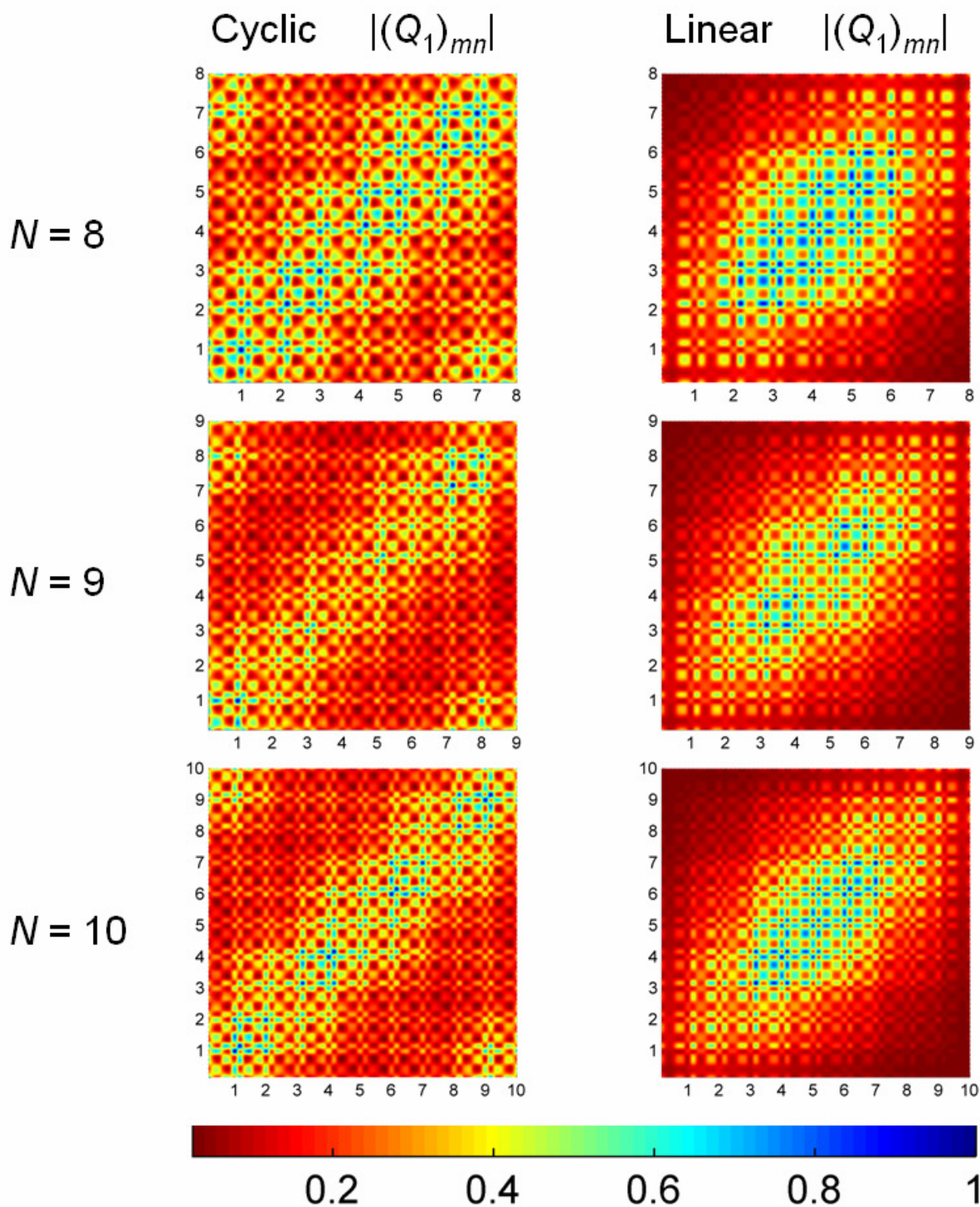


Figure SI-1 (continued). Contour plots of coordinate density matrices (\mathbf{Q}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the coordinate matrix, Q_{mn} , give a measure of exciton delocalization between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

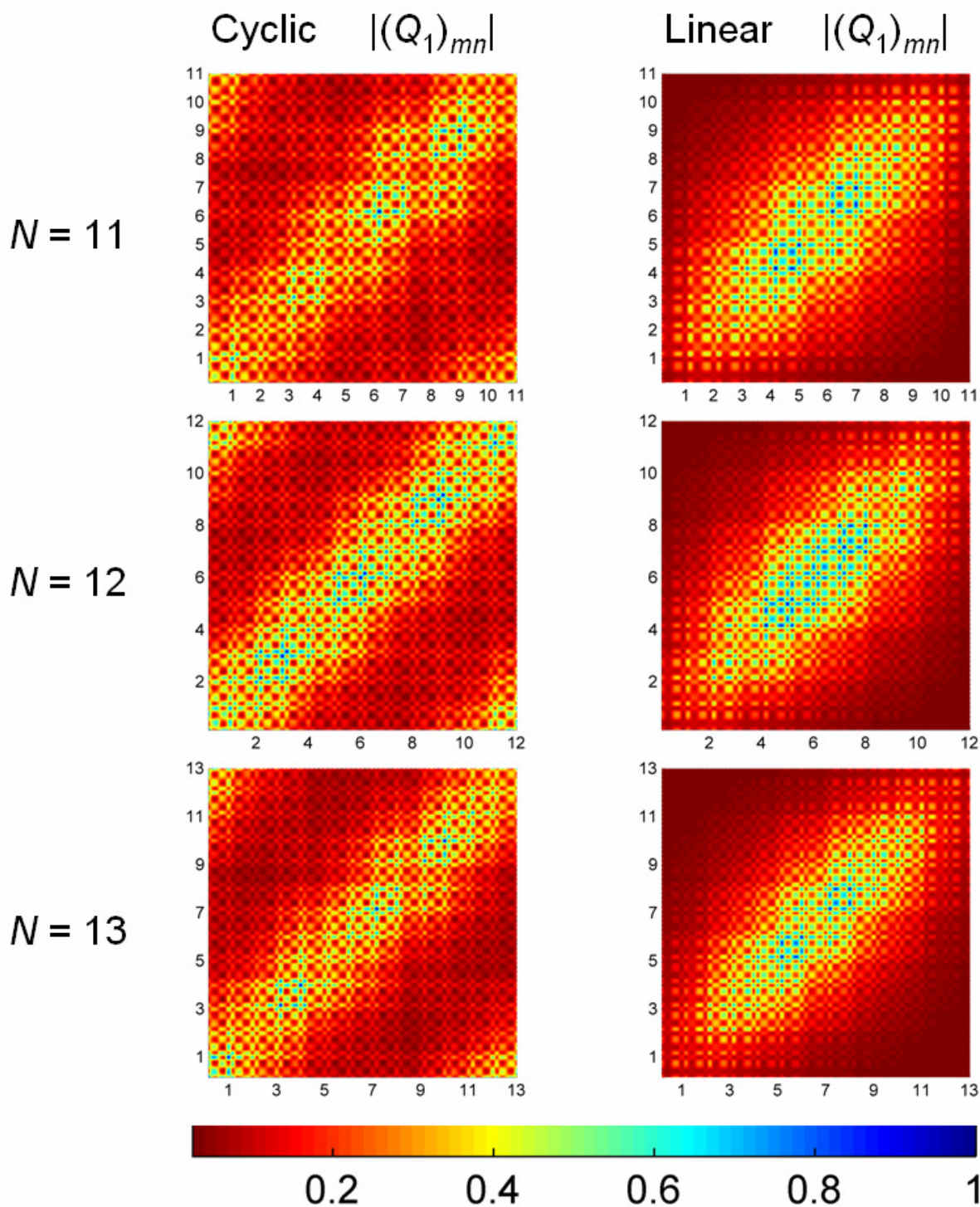


Figure SI-1 (continued). Contour plots of coordinate density matrices (\mathbf{Q}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the coordinate matrix, Q_{mn} , give a measure of exciton delocalization between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

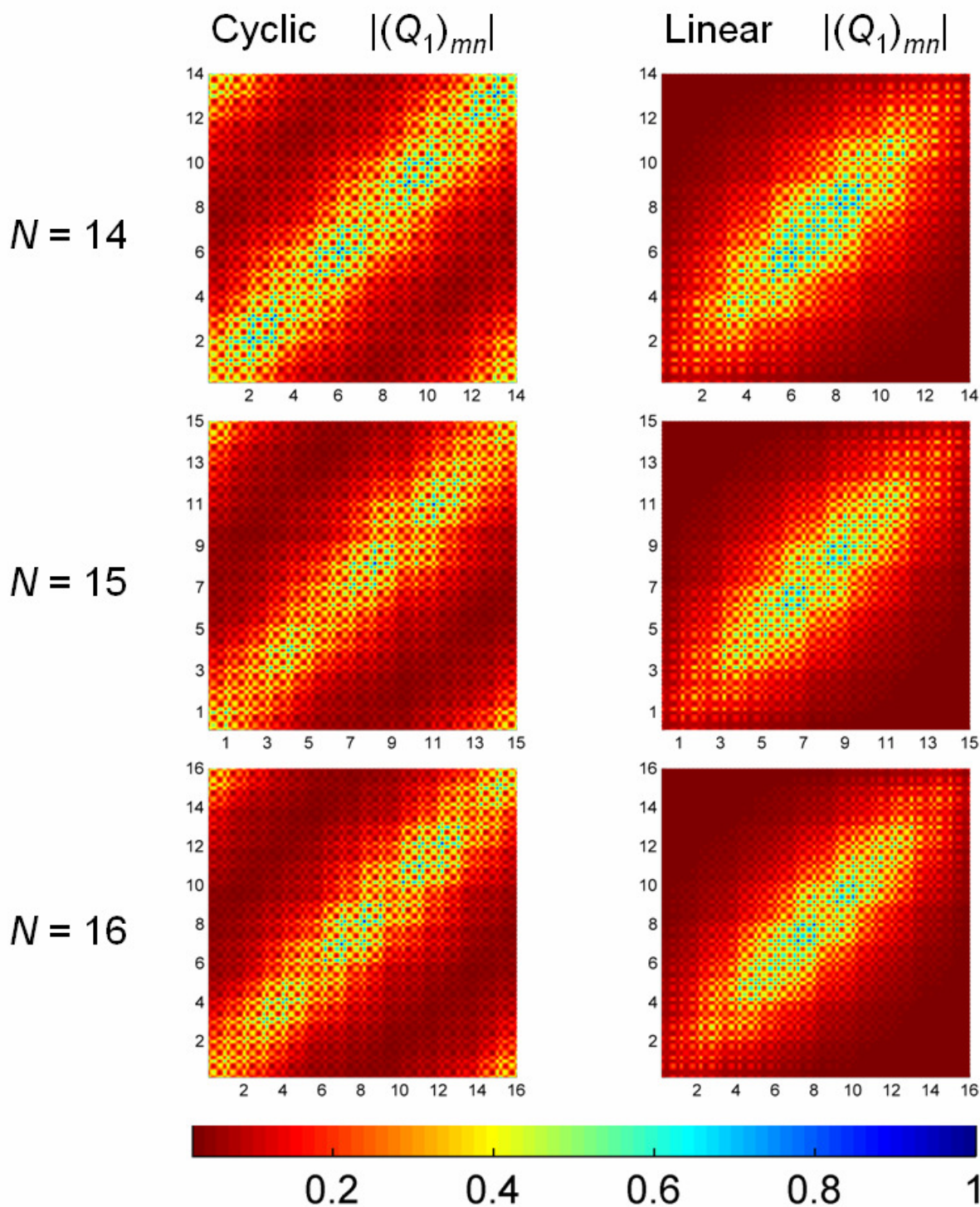


Figure SI-1 (continued). Contour plots of coordinate density matrices (\mathbf{Q}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the coordinate matrix, Q_{mn} , give a measure of exciton delocalization between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

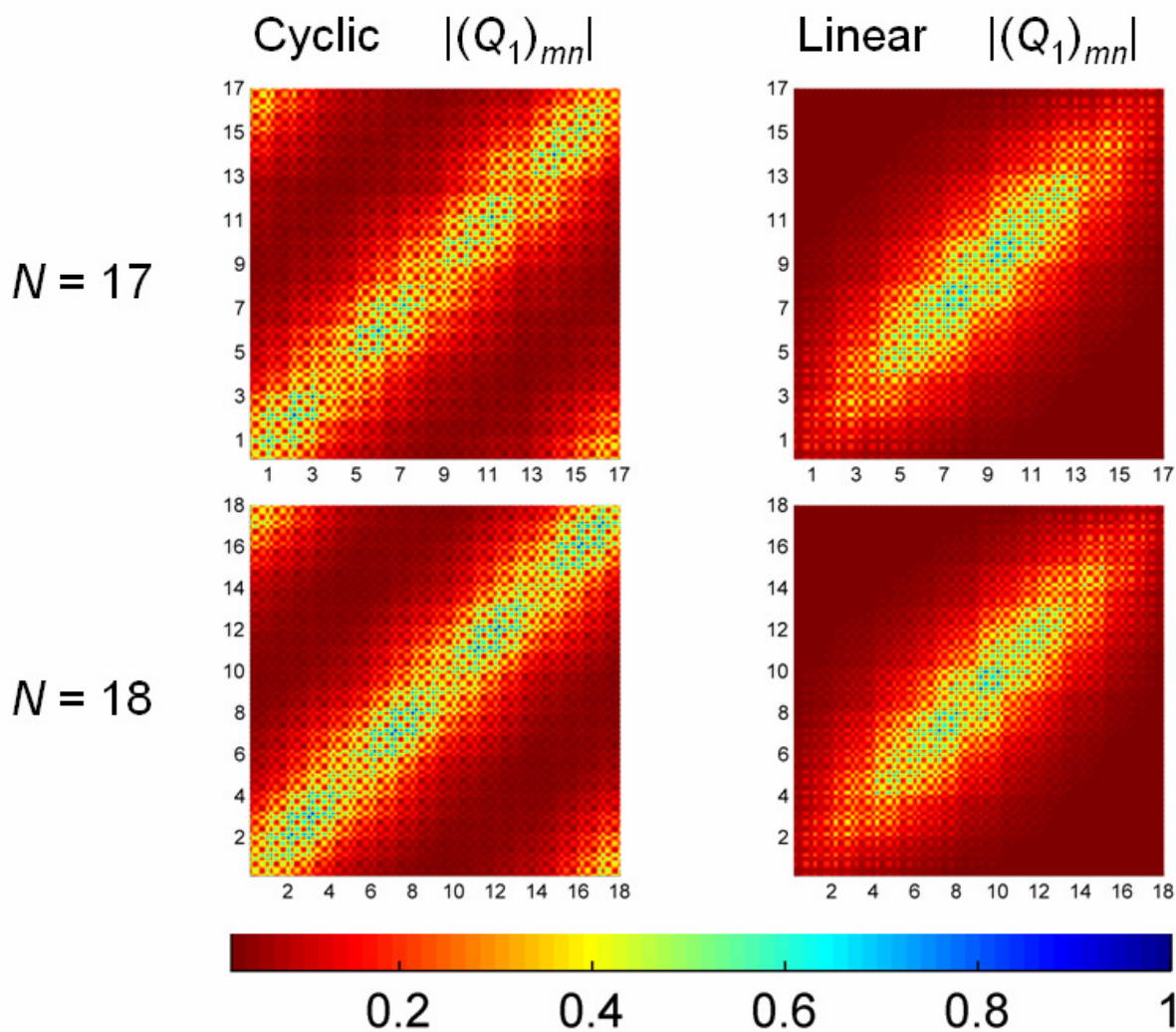


Figure SI-1 (continued). Contour plots of coordinate density matrices (\mathbf{Q}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the coordinate matrix, Q_{mn} , give a measure of exciton delocalization between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

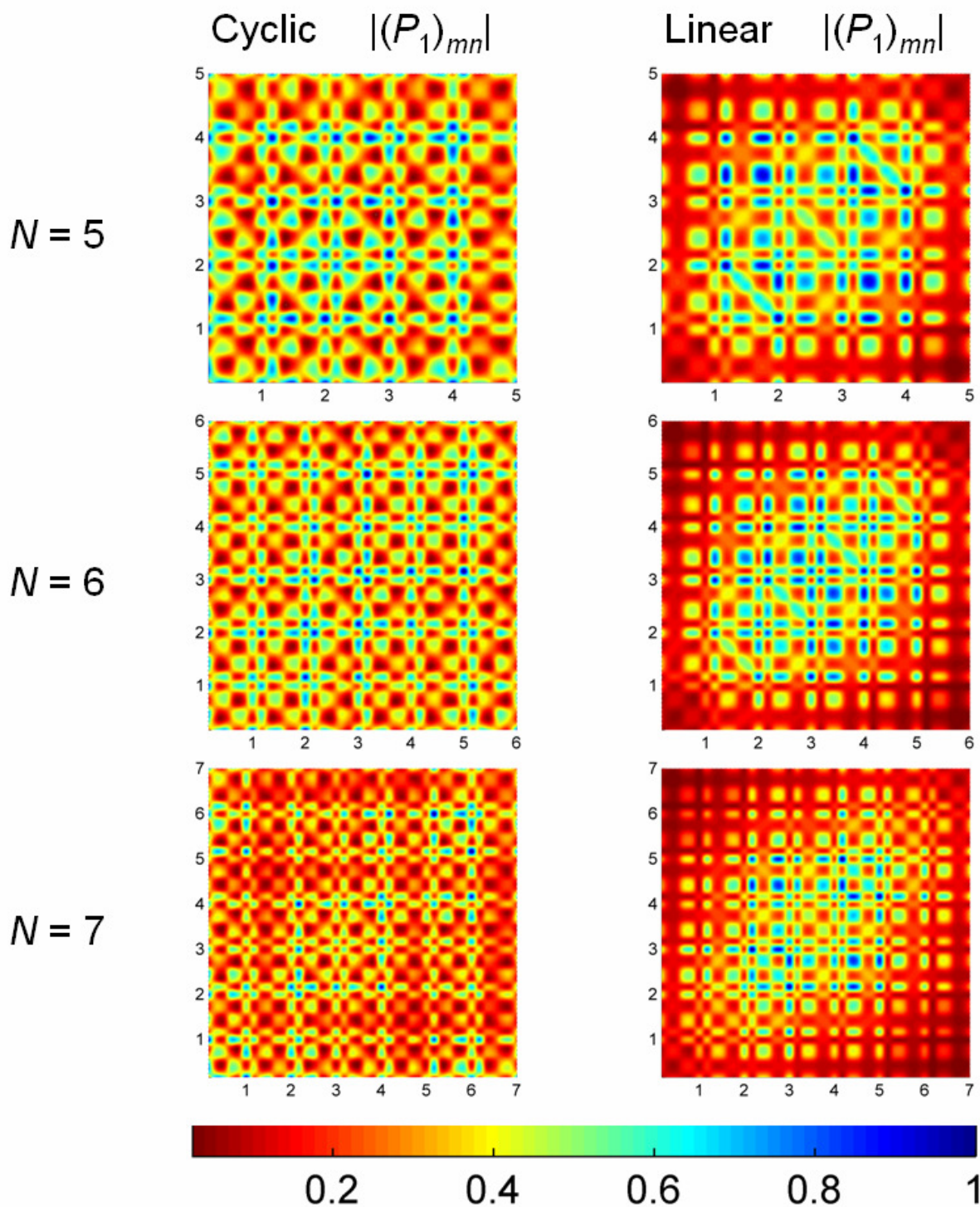


Figure SI-2. Contour plots of momentum density matrices (\mathbf{P}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the momentum matrix, P_{mn} , represent the probability amplitude of an electron-hole pair oscillation between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

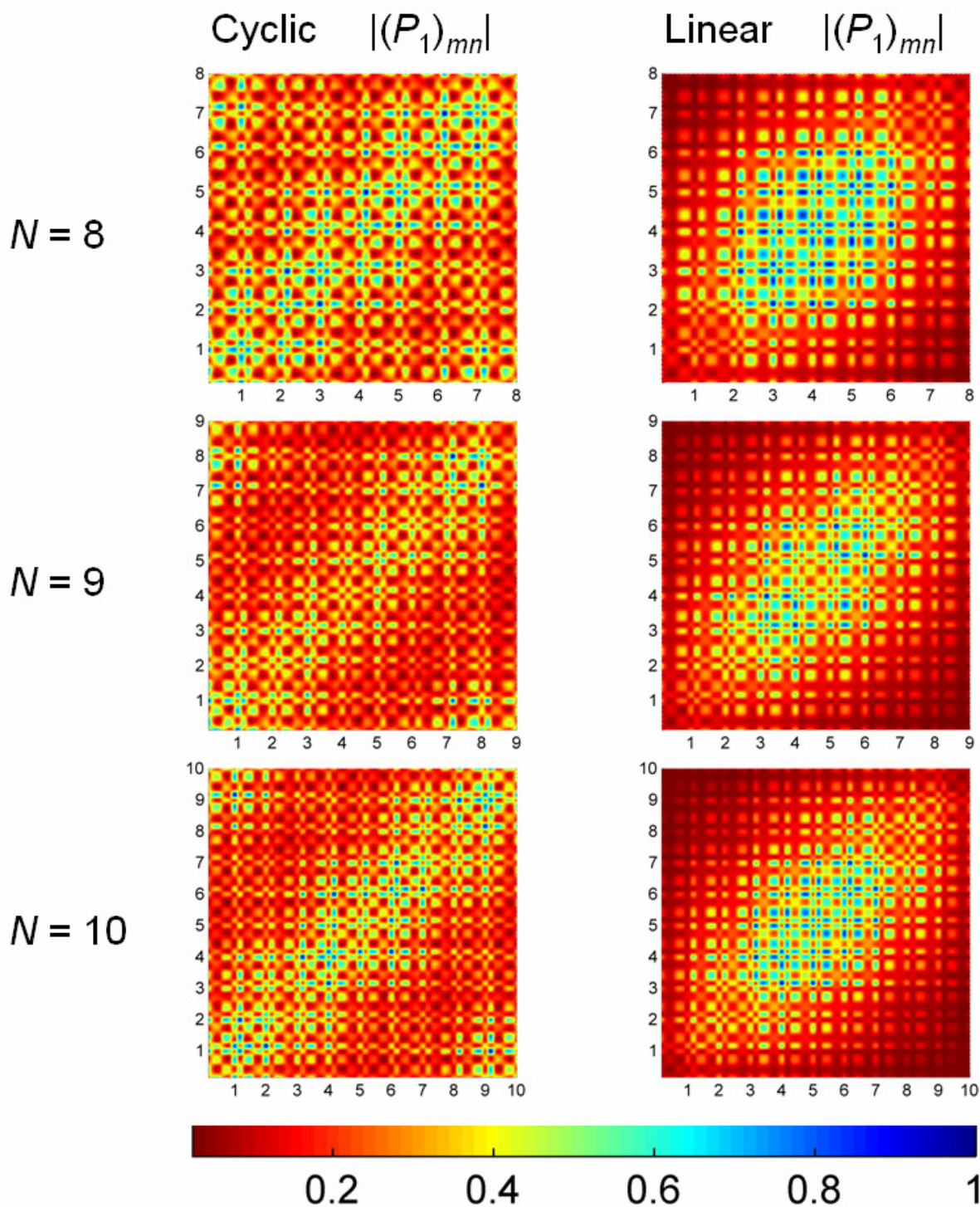


Figure SI-2 (continued). Contour plots of momentum density matrices (\mathbf{P}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the momentum matrix, P_{mn} , represent the probability amplitude of an electron-hole pair oscillation between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

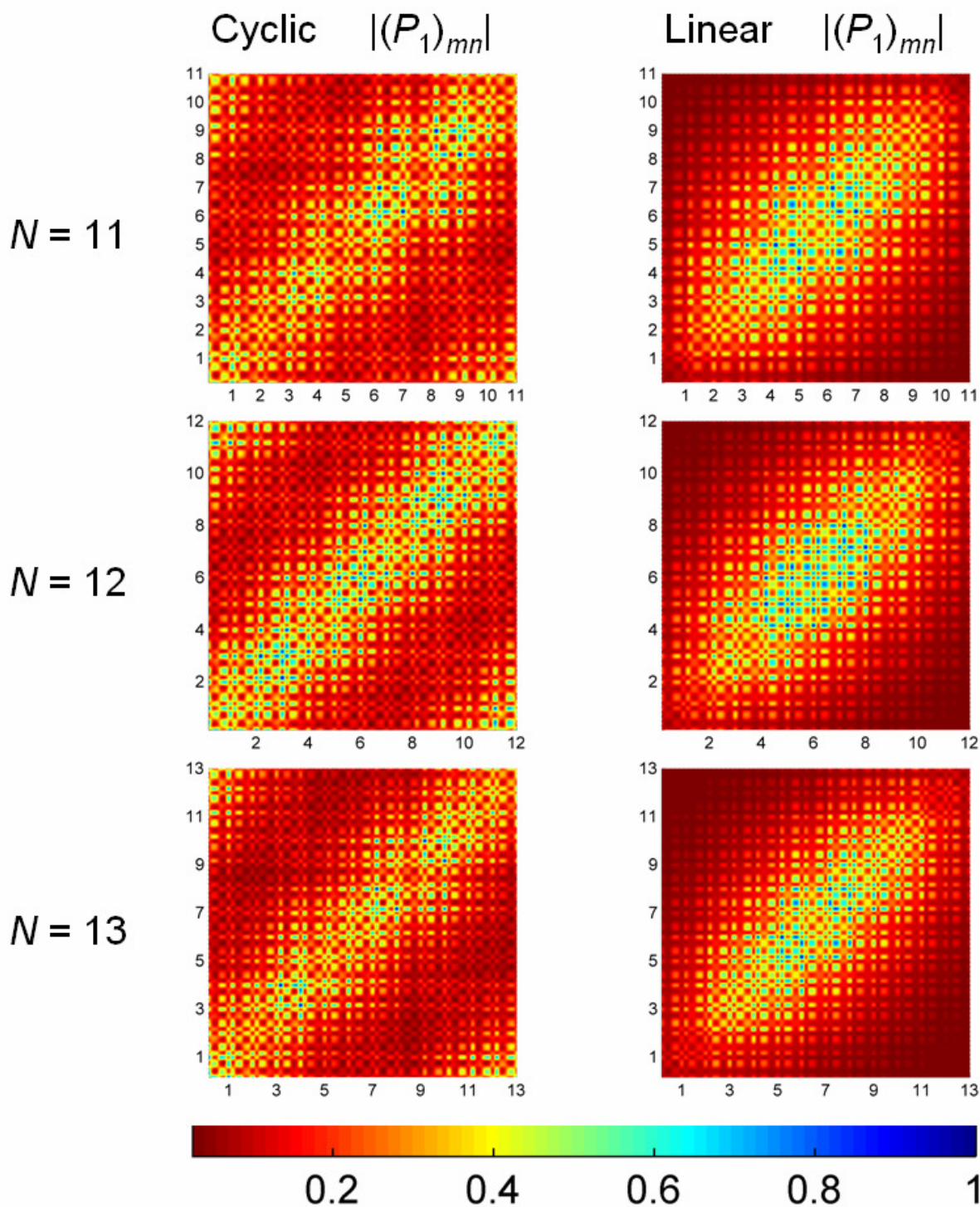


Figure SI-2 (continued). Contour plots of momentum density matrices (\mathbf{P}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x- and y-axis labels represent the number of benzene repeat units in the molecule. The elements of the momentum matrix, P_{mn} , represent the probability amplitude of an electron-hole pair oscillation between sites m (x-axis) and n (y-axis). The color scale is given at the bottom.

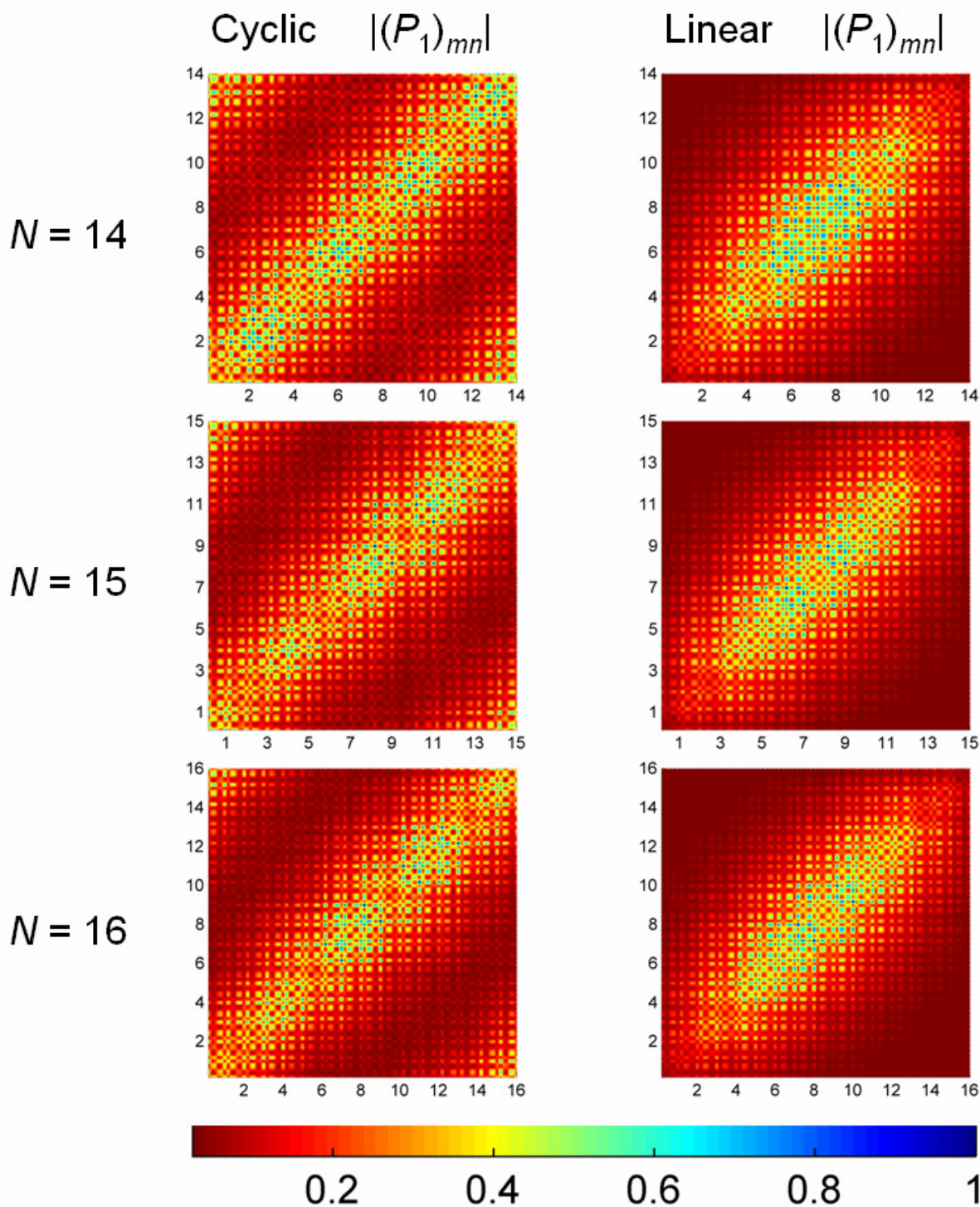


Figure SI-2 (continued). Contour plots of momentum density matrices (\mathbf{P}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x- and y-axis labels represent the number of benzene repeat units in the molecule. The elements of the momentum matrix, P_{mn} , represent the probability amplitude of an electron-hole pair oscillation between sites m (x-axis) and n (y-axis). The color scale is given at the bottom.

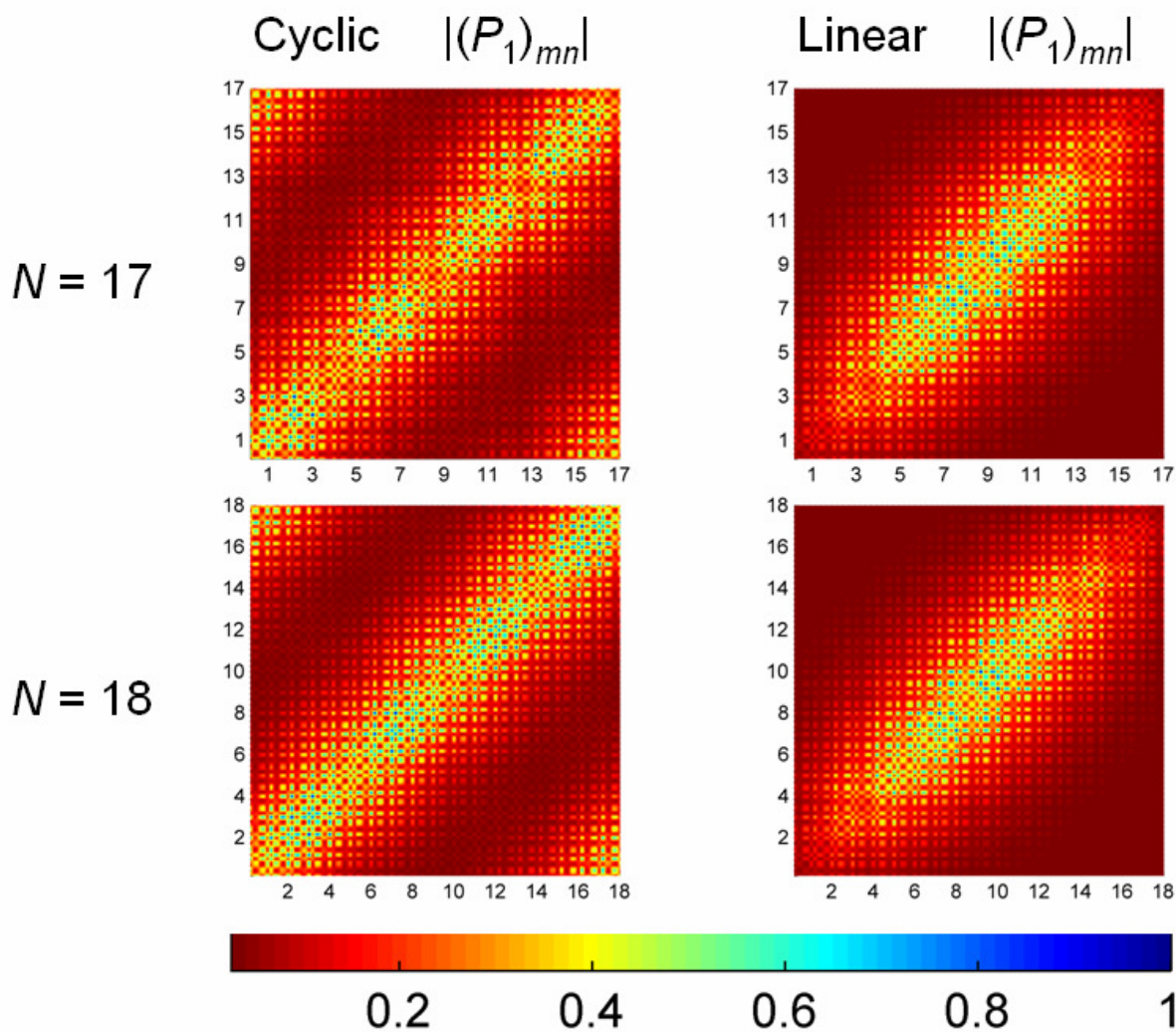


Figure SI-2 (continued). Contour plots of momentum density matrices (\mathbf{P}_1) for the lowest excitation energy ($S_1 \leftarrow S_0$) in the cyclic and linear paraphenylenes. The x - and y -axis labels represent the number of benzene repeat units in the molecule. The elements of the momentum matrix, P_{mn} , represent the probability amplitude of an electron-hole pair oscillation between sites m (x -axis) and n (y -axis). The color scale is given at the bottom.

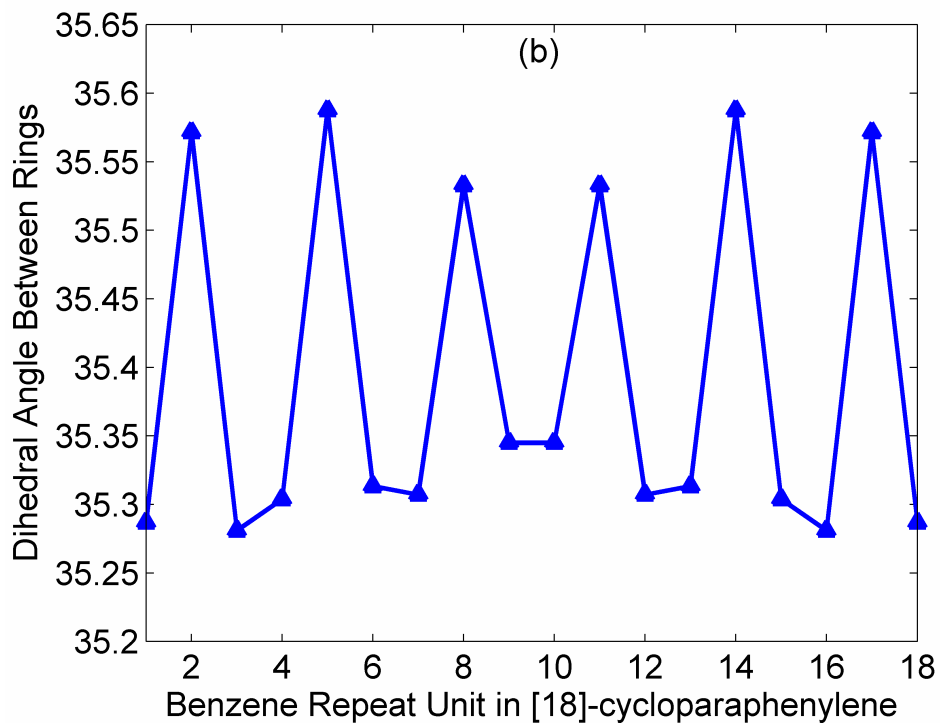
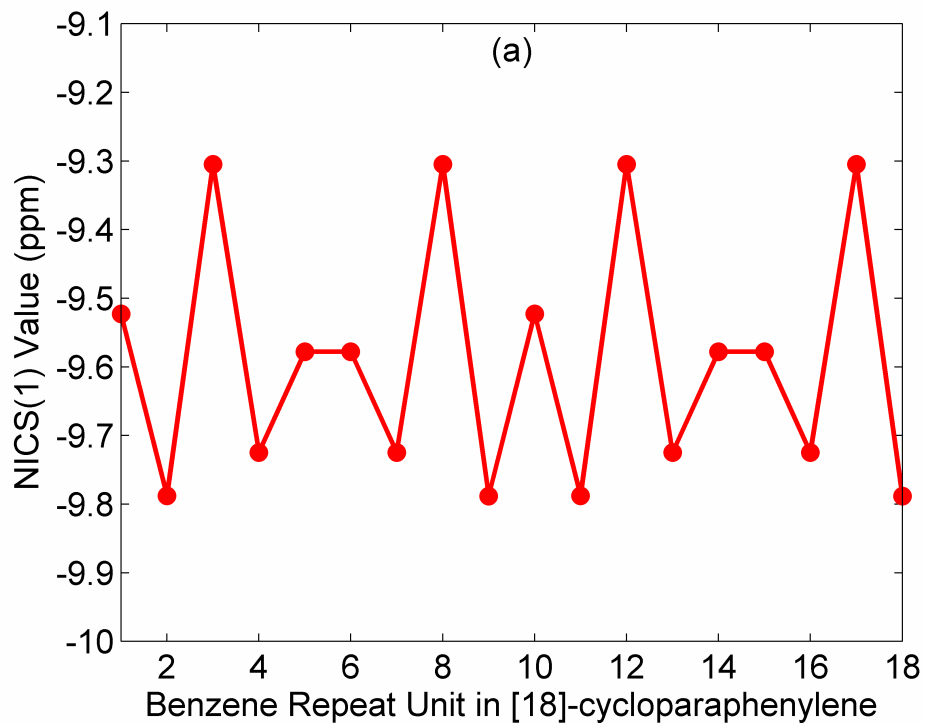


Figure SI-3. (a) NICS(1) values of individual benzene rings for the $N = 18$ cycloparaphenylene and (b) dihedral angle between adjacent benzene rings for the same $N = 18$ cycloparaphenylene. The NICS(1) values were obtained by computing the absolute magnetic shielding at 1 Å outside each of the benzene rings (i.e., oriented outside the nanoring). The 4 maxima in Figure SI-3(a) are located at the same positions corresponding to maxima in the $N = 18$ coordinate transition matrix (cf. Figure SI-1).

Cartesian coordinates (in Å) of [5]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-2.3252756395	-2.6110264855	-0.1574978962
C	-1.5684445871	-2.8241165455	-1.3219029524
C	-1.8279391499	-3.2324140852	1.0041766003
C	-0.2519194994	-3.2516129261	-1.2505278401
C	-0.5112700429	-3.6698896635	1.0750241248
C	0.3641117361	-3.4968212405	-0.0130734630
C	1.7650542363	-3.0275729786	0.1573569431
C	2.6221858670	-2.7836906170	-0.9324253204
C	2.0594969347	-2.3220714612	1.3343995267
C	3.4363205994	-1.6567815219	-0.9582731692
C	2.8716318724	-1.1982974549	1.3092847521
C	3.4246115314	-0.7360841736	0.1052336853
C	3.4246104722	0.7360847193	-0.1052344405
C	2.8716290352	1.1982985692	-1.3092842622
C	3.4363213725	1.6567823800	0.9582723129
C	2.0595023672	2.3220786822	-1.3344014924
C	2.6221883531	2.7836927998	0.9324257882
C	1.7650578778	3.0275767186	-0.1573571492
C	0.3641135092	3.4968188214	0.0130739510
C	-0.5112690508	3.6698903078	-1.0750223776
C	-0.2519174543	3.2516079239	1.2505278246
C	-1.8279386262	3.2324155954	-1.0041754807
C	-1.5684428200	2.8241129135	1.3219037569
C	-2.3252739757	2.6110257482	0.1574981650
C	-3.2088952054	1.4153892532	0.0903830273
C	-3.4133015137	0.7663264447	-1.1402161224
C	-3.4309527508	0.6181085434	1.2277537327
C	-3.4309510064	-0.6181093836	-1.2277550481
C	-3.4133015922	-0.7663271384	1.1402153922
C	-3.2088985590	-1.4153909364	-0.0903839831
H	-1.9229145308	-2.4580914305	-2.2794826576
H	0.3530151037	-3.1823726587	-2.1493415773
H	-0.1280731748	-4.0043052759	2.0355647129
H	-2.4187624963	-3.2396325940	1.9157813608
H	2.5488040049	-3.3908986685	-1.8309710549
H	3.9683900691	-1.4187313486	-1.8759299156
H	2.8802077016	-0.5589481649	2.1864210822
H	1.4773686977	-2.5053167216	2.2318960724
H	2.8802083463	0.5589516781	-2.1864221798
H	1.4773677981	2.5053185219	-2.2318952754
H	2.5488046414	3.3908984563	1.8309729244
H	3.9683913131	1.4187319135	1.8759287209
H	-0.1280729316	4.0043102794	-2.0355617819
H	-2.4187608633	3.2396329126	-1.9157809130
H	-1.9229105624	2.4580828536	2.2794822772
H	0.3530169390	3.1823707512	2.1493418645
H	-3.3787768131	1.3303714188	-2.0671985475
H	-3.4389830688	-1.0631729505	-2.2180134812
H	-3.3787825911	-1.3303732271	2.0671972541
H	-3.4389826481	1.0631714462	2.2180125290

Cartesian coordinates (in Å) of [6]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-2.7107954474	3.1896279164	-0.0174436438
C	-3.4442286181	2.6715502356	-1.0984711314
C	-3.0019848797	2.6364498166	1.2387990999
C	-4.1355799236	1.4738159388	-0.9836721919
C	-3.7109440695	1.4509541000	1.3550115456
C	-4.1399492597	0.7435941396	0.2190983963
C	-4.1399476869	-0.7435930756	0.2190983848
C	-4.1355787418	-1.4738150590	-0.9836719719
C	-3.7109423456	-1.4509539444	1.3550109775
C	-3.4442293296	-2.6715504495	-1.0984713330
C	-3.0019850891	-2.6364508853	1.2387990695
C	-2.7107951885	-3.1896274654	-0.0174441964
C	-1.4197171332	-3.8947895196	-0.2032129360
C	-0.6926137677	-3.6254720286	-1.3723909311
C	-0.6946559482	-4.4597637119	0.8611190840
C	0.6926050958	-3.6255083352	-1.3724218937
C	0.6946859977	-4.4597963233	0.8610920185
C	1.4197265833	-3.8948094092	-0.2032453769
C	2.7106934939	-3.1894684057	-0.0174899735
C	3.4443212692	-2.6715990395	-1.0984821362
C	3.0021598768	-2.6365473484	1.2387947427
C	4.1354815292	-1.4737493166	-0.9837319687
C	3.7108808240	-1.4509043762	1.3549671269
C	4.1400784882	-0.7436055016	0.2190876424
C	4.1400774071	0.7436047265	0.2190876080
C	4.1354800663	1.4737483747	-0.9837319767
C	3.7108797612	1.4509046851	1.3549665129
C	3.4443222406	2.6715994851	-1.0984826602
C	3.0021607658	2.6365488849	1.2387948129
C	2.7106942937	3.1894685629	-0.0174904614
C	1.4197274150	3.8948097011	-0.2032453021
C	0.6926052147	3.6255074809	-1.3724211338
C	0.6946859634	4.4597956850	0.8610922136
C	-0.6926136254	3.6254714512	-1.3723908127
C	-0.6946560129	4.4597637483	0.8611193527
C	-1.4197166182	3.8947887686	-0.2032124489
H	-3.3688740523	3.1357380225	-2.0780367883
H	-4.5586205085	1.0433975564	-1.8860680027
H	-3.7744398040	0.9997777695	2.3392545246
H	-2.5215879021	3.0333956100	2.1278936909
H	-4.5586202798	-1.0433974849	-1.8860677843
H	-3.3688735496	-3.1357374482	-2.0780371145
H	-2.5215866814	-3.0333954291	2.1278934680
H	-3.7744391446	-0.9997780348	2.3392539989
H	-1.2017666325	-3.2237800222	-2.2423525342
H	1.2017341802	-3.2237284227	-2.2423585993
H	1.2154556876	-4.8020030063	1.7515966933
H	-1.2154141631	-4.8020371663	1.7516048817
H	3.3687582484	-3.1356396411	-2.0781014735
H	4.5585230740	-1.0433334577	-1.8861275559
H	3.7746182100	-0.9998445550	2.3392461098
H	2.5217004413	-3.0334458881	2.1278777269
H	4.5585231619	1.0433333858	-1.8861273134
H	3.3687579627	3.1356390709	-2.0781022906
H	2.5217002899	3.0334463410	2.1278778165
H	3.7746181759	0.9998451720	2.3392455127
H	1.2017338685	3.2237274915	-2.2423581391
H	-1.2017669480	3.2237799711	-2.2423522927
H	-1.2154142778	4.8020369142	1.7516052761
H	1.2154557480	4.8020037452	1.7515962068

Cartesian coordinates (in Å) of [7]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	3.9922847356	-2.7178098336	0.3197766572
C	3.1880259395	-2.9224778730	1.4509293423
C	3.8019735101	-3.6170644578	-0.7442092070
C	2.1025822183	-3.7797810664	1.4220400654
C	2.7113932248	-4.4786632417	-0.7738179899
C	1.7591649162	-4.4855190144	0.2594156318
C	0.3375767564	-4.8493966265	0.0595249780
C	-0.5620085307	-4.9220590779	1.1353389548
C	-0.2364199288	-4.7561540592	-1.2180178431
C	-1.8999086585	-4.5964847023	0.9715806317
C	-1.5830690981	-4.4676388860	-1.3841649300
C	-2.4141752933	-4.2175898430	-0.2796179072
C	-3.5547063121	-3.2719891717	-0.3642597759
C	-4.3481521982	-2.9452392356	0.7501428550
C	-3.6397373740	-2.3994895889	-1.4602765778
C	-4.9504179188	-1.6990649005	0.8656888684
C	-4.2488058543	-1.1596659566	-1.3508996546
C	-4.7998684666	-0.7274953260	-0.1365509144
C	-4.7998638495	0.7274940664	0.1365509734
C	-4.2488204491	1.1596721798	1.3509055835
C	-4.9504320907	1.6990683334	-0.8656815841
C	-3.6397292267	2.3994856945	1.4602741637
C	-4.3481418363	2.9452322660	-0.7501497126
C	-3.5547090825	3.2719895754	0.3642600786
C	-2.4141696341	4.2175779731	0.2796152523
C	-1.5830789048	4.4676656401	1.3841651765
C	-1.8999190300	4.5965149805	-0.9715764243
C	-0.2364178255	4.7561261614	1.2180173896
C	-0.5620062677	4.9220322841	-1.1353445240
C	0.3375746131	4.8494105097	-0.0595247881
C	1.7591467735	4.4854746623	-0.2593974312
C	2.7114186780	4.4787046139	0.7737947045
C	2.1026475869	3.7798835033	-1.4220856957
C	3.8019377732	3.6170269881	0.7442330899
C	3.1879368500	2.9223827398	-1.4508781861
C	3.9923242823	2.7178352483	-0.3197949621
C	4.6748087911	1.4101560096	-0.1719584315
C	4.8232760580	0.8318228837	1.0988661532
C	4.8454751766	0.5447056516	-1.2653886088
C	4.8454884928	-0.5447069188	1.2653886922
C	4.8232992986	-0.8318243599	-1.0988667173
C	4.6747898214	-1.4101471127	0.1719572164
H	3.3009227704	-2.2809377319	2.3179587515
H	1.4214918713	-3.7639065036	2.2660991194
H	2.5541724284	-5.0886489766	-1.6593811269
H	4.4597650513	-3.5852556543	-1.6084171906
H	-0.1948095413	-5.1133894958	2.1394458426
H	-2.5145815986	-4.5070637752	1.8616691435
H	-1.9512886316	-4.3077615263	-2.3927803024
H	0.3999883680	-4.7620745431	-2.0978484560
H	-4.4157177395	-3.6312086470	1.5894281729
H	-5.4631208340	-1.4444935310	1.7897268954
H	-4.1375807846	-0.4532313946	-2.1679774433
H	-3.0829861073	-2.6093572599	-2.3669374675
H	-4.1375765439	0.4532325428	2.1679770809
H	-3.0829853591	2.6093595446	2.3669377231
H	-4.4157187972	3.6312085830	-1.5894281279
H	-5.4631177439	1.4444917411	-1.7897279209
H	-1.9512888251	4.3077610855	2.3927798193
H	0.3999878388	4.7620838767	2.0978490461
H	-0.1948095266	5.1133903989	-2.1394463351
H	-2.5145791675	4.5070553344	-1.8616708054
H	2.5541699238	5.0886488606	1.6593816766
H	4.4597666680	3.5852609232	1.6084141714
H	3.3009395678	2.2809544787	-2.3179727719
H	1.4214803925	3.7638848530	-2.2660847534
H	4.7776101702	1.4557719982	1.9863352759
H	4.8647270724	-0.9415969533	2.2759658701
H	4.7776074233	-1.4557741570	-1.9863343150

H 4.8647253187 0.9415952166 -2.2759661651

Cartesian coordinates (in Å) of [8]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	2.7825082730	4.7885678316	-0.0562048106
C	3.6248881179	4.6066362510	1.0524034279
C	3.1229649741	4.1032531481	-1.2307739980
C	4.6070896747	3.6248711765	1.0522565181
C	4.1036824179	3.1231113411	-1.2309386155
C	4.7888234368	2.7824384738	-0.0563411554
C	5.3539281341	1.4183200379	0.0560908480
C	5.1107518266	0.6932591475	1.2308168143
C	5.8213210229	0.6943650184	-1.0525593236
C	5.1107502928	-0.6932591856	1.2308161167
C	5.8213206074	-0.6943659807	-1.0525587359
C	5.3539261234	-1.4183192582	0.0560906423
C	4.7888225211	-2.7824373577	-0.0563413733
C	4.6070884764	-3.6248687530	1.0522561695
C	4.1036791779	-3.1231086800	-1.2309369061
C	3.6248902085	-4.6066370775	1.0524034426
C	3.1229672528	-4.1032560004	-1.2307756034
C	2.7825089867	-4.7885688040	-0.0562047743
C	1.4183003915	-5.3534699237	0.0563482163
C	0.6932188248	-5.1103385219	1.2310739423
C	0.6943623936	-5.8209757664	-1.0522643056
C	-0.6933084908	-5.1103409403	1.2310447053
C	-0.6943625082	-5.8210333716	-1.0522827214
C	-1.4183623993	-5.3536147654	0.0563261663
C	-2.7825979775	-4.7887691707	-0.0562218117
C	-3.6249299142	-4.6067717992	1.0524143244
C	-3.1232428638	-4.1036564625	-1.2308554919
C	-4.6069612615	-3.6248428237	1.0523348757
C	-4.1037346072	-3.1232864295	-1.2309355175
C	-4.7888448458	-2.7825344557	-0.0563372290
C	-5.3537855696	-1.4183391874	0.0561044201
C	-5.1106414680	-0.6932606507	1.2308311142
C	-5.8210965273	-0.6943624891	-1.0525673590
C	-5.1106397313	0.6932606739	1.2308304054
C	-5.8210960585	0.6943634030	-1.0525668428
C	-5.3537837776	1.4183385202	0.0561042659
C	-4.7888441059	2.7825335630	-0.0563374358
C	-4.6069599317	3.6248404051	1.0523347695
C	-4.1037311443	3.1232836876	-1.2309337531
C	-3.6249322702	4.6067730661	1.0524144351
C	-3.1232458022	4.1036601278	-1.2308573804
C	-2.7825989033	4.7887699680	-0.0562216728
C	-1.4183628318	5.3536157728	0.0563260441
C	-0.6933085591	5.1103441547	1.2310458408
C	-0.6943616787	5.8210346489	-1.0522830396
C	0.6932187567	5.1103348306	1.2310723856
C	0.6943632460	5.8209740779	-1.0522642337
C	1.4183001745	5.3534687380	0.0563480339
H	3.4567834353	5.1865015864	1.9561648978
H	5.1869226585	3.4566751760	1.9560224185
H	4.2227936528	2.5062343419	-2.1165684333
H	2.5062415565	4.2226008767	-2.1164696335
H	4.7592441671	1.2136912814	2.1165391472
H	4.7592444454	-1.2136901483	2.1165394129
H	6.1127240590	-1.2233969088	-1.9561420525
H	6.1127246408	1.2233971094	-1.9561422185
H	5.1869223455	-3.4566753875	1.9560216456
H	3.4567834533	-5.1865019430	1.9561651073
H	2.5062402466	-4.2226015301	-2.1164694980
H	4.2227928821	-2.5062355602	-2.1165685374
H	1.2136017284	-4.7586673432	2.1167684301
H	-1.2137416647	-4.7587992630	2.1167566272
H	-1.2233589035	-6.1126165018	-1.9558253064
H	1.2234180751	-6.1124633717	-1.9558042970
H	-3.4567672690	-5.1865483585	1.9562217106
H	-5.1867592829	-3.4566031145	1.9561139357
H	-4.2229961347	-2.5065964258	-2.1166724955
H	-2.5065579003	-4.2230093159	-2.1165817962
H	-4.7591698668	-1.2136729232	2.1165819587

H	-4.7591700967	1.2136718675	2.1165822515
H	-6.1125068482	1.2233842704	-1.9561520036
H	-6.1125074361	-1.2233844301	-1.9561521242
H	-5.1867590352	3.4566031818	1.9561132860
H	-3.4567670719	5.1865484549	1.9562224346
H	-2.5065567626	4.2230101353	-2.1165817635
H	-4.2229953935	2.5065976157	-2.1166725659
H	-1.2137426432	4.7587982299	2.1167560065
H	1.2136006361	4.7586680284	2.1167687209
H	1.2234178850	6.1124629599	-1.9558040663
H	-1.2233591276	6.1126172013	-1.9558254820

Cartesian coordinates (in Å) of [9]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	2.7971078063	5.5083594885	0.2331475514
C	3.1451589013	4.7316989455	1.3480950539
C	3.6978634443	5.5043128071	-0.8445215621
C	4.2210793176	3.8603574525	1.3130487378
C	4.7680673008	4.6189825316	-0.8875160165
C	4.9970086424	3.7101700211	0.1561799889
C	5.7540085880	2.4492763744	-0.0055610005
C	6.3443687454	1.7820678739	1.0786286155
C	5.6161908506	1.7322822320	-1.2011289228
C	6.5883656924	0.4164772535	1.0303992696
C	5.8540221798	0.3659275803	-1.2467747786
C	6.2450191684	-0.3404540525	-0.1008771698
C	5.9761711463	-1.7940413144	-0.0294609724
C	5.4135982532	-2.3110050677	1.1458072227
C	5.9727095893	-2.6275733933	-1.1587114833
C	4.7113429256	-3.5060180009	1.1416697522
C	5.2690016104	-3.8249085164	-1.1628962921
C	4.5387158478	-4.2410953651	-0.0390078683
C	3.4032128435	-5.1856654608	-0.1247852373
C	2.9057557550	-5.8742610309	0.9926774064
C	2.6035185133	-5.1761821219	-1.2759427129
C	1.5999278972	-6.3455087833	1.0216690261
C	1.3003706616	-5.6491147404	-1.2480233151
C	0.7365824253	-6.1516663525	-0.0675835406
C	-0.7367291327	-6.1518381729	0.0676182441
C	-1.3005116072	-5.6491137358	1.2480070308
C	-1.6000832994	-6.3454643620	-1.0216506144
C	-2.6036312869	-5.1761002511	1.2759348960
C	-2.9058575083	-5.8741097313	-0.9927330338
C	-3.4033818362	-5.1856932921	0.1248144024
C	-4.5387965276	-4.2410116110	0.0389743524
C	-5.2690641477	-3.8247869971	1.1628667428
C	-4.7114265276	-3.5058888029	-1.1416634648
C	-5.9727405117	-2.6274254743	1.1587396616
C	-5.4135778409	-2.3108208423	-1.1458128507
C	-5.9761685391	-1.7939150832	0.0294663982
C	-6.2451184492	-0.3403490756	0.1008913835
C	-5.8540196936	0.3660659961	1.2467332634
C	-6.5884437277	0.4166477414	-1.0303410404
C	-5.6159502182	1.7323732611	1.2010875810
C	-6.3443148193	1.7822110799	-1.0786805032
C	-5.7539775943	2.4493828715	0.0055610717
C	-4.9970944247	3.7103496294	-0.1562397471
C	-4.7679994802	4.6191179232	0.8874619657
C	-4.2209713701	3.8604238045	-1.3129953350
C	-3.6977271327	5.5043725033	0.8445720554
C	-3.1449781971	4.7316679078	-1.3480744696
C	-2.7969519400	5.5082684057	-0.2330882270
C	-1.4172503648	6.0354692576	-0.1250052108
C	-0.7943660511	6.1445200067	1.1277357292
C	-0.5866188483	6.1638005994	-1.2487084522
C	0.5867485945	6.1636743870	1.2487547539
C	0.7945013864	6.1445834749	-1.1277697327
C	1.4172876284	6.0352345730	0.1249894483
H	2.4886250007	4.6986709227	2.2110006841
H	4.3708476437	3.1789581202	2.1451356501
H	5.3978684891	4.5911245662	-1.7729335804
H	3.5229363685	6.1550417502	-1.6966124332
H	6.5477839402	2.3270525716	1.9967329799
H	6.9842533380	-0.0820089409	1.9112245942
H	5.5870090767	-0.1808566597	-2.1462292475
H	5.1717340535	2.2181948046	-2.0649877267
H	5.3977440613	-1.7002669031	2.0434039901
H	4.1673990372	-3.7952780106	2.0358345326
H	5.2325628876	-4.4141759069	-2.0753752681
H	6.4724847451	-2.3041883026	-2.0680327289
H	3.5275664279	-5.9817988315	1.8775695152
H	1.2243457860	-6.8115678309	1.9288615796
H	0.6665890992	-5.4886772407	-2.1151882667

H	2.9517440322	-4.6583416000	-2.1646926516
H	-0.6667314459	-5.4886347978	2.1151775240
H	-2.9518494024	-4.6582455678	2.1646727997
H	-3.5277045022	-5.9817295537	-1.8775792044
H	-1.2244951510	-6.8115439567	-1.9288481513
H	-5.2326747549	-4.4140725606	2.0753493145
H	-6.4725636221	-2.3040646605	2.0680247226
H	-5.3978036210	-1.7001161039	-2.0434159862
H	-4.1674899478	-3.7951660286	-2.0358427643
H	-5.5870470918	-0.1807099644	2.1462301650
H	-5.1717414448	2.2183563117	2.0650036112
H	-6.5477554010	2.3271911139	-1.9967552706
H	-6.9842448729	-0.0818493806	-1.9112262984
H	-5.3977571369	4.5912189978	1.7729305286
H	-3.5228221366	6.1551258332	1.6966228098
H	-2.4885322987	4.6987710408	-2.2110254336
H	-4.3707929284	3.1790854851	-2.1451462580
H	-1.3910439078	6.0991215467	2.0336621088
H	1.0204807645	6.1820882166	2.2440865026
H	1.3911840385	6.0990608065	-2.0336564059
H	-1.0203272521	6.1820130687	-2.2440795031

Cartesian coordinates (in Å) of [10]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-6.8663661513	-0.7405391632	-0.2628380098
C	-6.4686333175	-1.4658437088	-1.3968665480
C	-7.0124021784	-1.4802917539	0.9226685514
C	-6.0416062690	-2.7812548940	-1.3053996788
C	-6.5933873912	-2.7997986025	1.0148281617
C	-6.0004724182	-3.4516051702	-0.0758792843
C	-5.1218466055	-4.6297952820	0.0816251139
C	-4.8141751966	-5.4967809949	-0.9784611532
C	-4.3532821853	-4.7478514469	1.2478438117
C	-3.6873404239	-6.3074307808	-0.9387428768
C	-3.2308117046	-5.5599092887	1.2891237871
C	-2.8216999753	-6.2899620759	0.1651411905
C	-1.4194054633	-6.7548566625	0.0939260361
C	-0.6951542027	-6.5490848482	-1.0877869224
C	-0.6957440766	-7.1418428437	1.2320597570
C	0.6920045446	-6.5492805122	-1.0877392837
C	0.6922977278	-7.1421016698	1.2320597763
C	1.4161083637	-6.7550667242	0.0940576144
C	2.8187486620	-6.2913071855	0.1651709795
C	3.6843934643	-6.3093256825	-0.9386863569
C	3.2282814436	-5.5615605020	1.2891956882
C	4.8114677355	-5.4989987441	-0.9785225318
C	4.3509697815	-4.7498231277	1.2477824340
C	5.1196816257	-4.6322613844	0.0816088479
C	5.9989868027	-3.4545658437	-0.0759034355
C	6.0402904605	-2.7841538319	-1.3053835552
C	6.5920497392	-2.8029590969	1.0148521400
C	6.4680156680	-1.4689663046	-1.3968651280
C	7.0116988161	-1.4836524229	0.9226715277
C	6.8657647050	-0.7437821277	-0.2627693447
C	6.8665743059	0.7405777548	-0.2629020416
C	6.4686561388	1.4658215993	-1.3969097927
C	7.0126664693	1.4803467101	0.9225881036
C	6.0414408601	2.7811590911	-1.3053968047
C	6.5933926855	2.7997747677	1.0147852132
C	6.0002652438	3.4514805377	-0.0758626413
C	5.1217870823	4.6297693502	0.0816340172
C	4.8142596188	5.4968527327	-0.9784233442
C	4.3533218169	4.7479595647	1.2478883622
C	3.6873067262	6.3073413080	-0.9387996680
C	3.2307294482	5.5598495691	1.2890674613
C	2.8217150956	6.2900317535	0.1651157528
C	1.4193932878	6.7548467214	0.0939155889
C	0.6951491195	6.5491450250	-1.0877979878
C	0.6957560361	7.1419424263	1.2320409046
C	-0.6919990023	6.5493404538	-1.0877506988
C	-0.6923097810	7.1422012035	1.2320408717
C	-1.4160962761	6.7550525721	0.0940482758
C	-2.8187644142	6.2913767722	0.1651457613
C	-3.6843599583	6.3092373117	-0.9387425915
C	-3.2282006234	5.5615025485	1.2891398700
C	-4.8115505068	5.4990690532	-0.9784858336
C	-4.3510087691	4.7499300398	1.2478262017
C	-5.1196236634	4.6322369350	0.0816179014
C	-5.9987743435	3.4544378435	-0.0758860697
C	-6.0401253145	2.7840574964	-1.3053811507
C	-6.5920584630	2.8029362205	1.0148079467
C	-6.4680354884	1.4689428880	-1.3969081721
C	-7.0119625188	1.4837071880	0.9225909480
C	-6.8659790591	0.7438213855	-0.2628347722
H	-6.3844364397	-0.9768187586	-2.3607922420
H	-5.6159823692	-3.2523237387	-2.1864680275
H	-6.6664321152	-3.3078627028	1.9725628347
H	-7.3870953960	-1.0032142712	1.8222102671
H	-5.4339435649	-5.4955877229	-1.8710684709
H	-3.4444805095	-6.9227226963	-1.8010637707
H	-2.5871869225	-5.5207771041	2.1628630653
H	-4.5567335792	-4.0940401847	2.0903783924
H	-1.2203483816	-6.2479948306	-1.9894269507

H	1.2173649710	-6.2485958229	-1.9894534783
H	1.2244675772	-7.3893047390	2.1468349293
H	-1.2280144966	-7.3887251243	2.1468574364
H	3.4411326994	-6.9243250035	-1.8010926333
H	5.4313274921	-5.4981914729	-1.8710681664
H	4.5548344649	-4.0962359556	2.0903830411
H	2.5845595280	-5.5219105359	2.1628503922
H	5.6144112845	-3.2549806497	-2.1864549694
H	6.3838740672	-0.9798660021	-2.3607577276
H	7.3865646157	-1.0067295960	1.8222237828
H	6.6648717463	-3.3110528385	1.9725827001
H	6.3844429520	0.9767856748	-2.3608251737
H	5.6160890474	3.2523830211	-2.1865150574
H	6.6664230952	3.3078522564	1.9725228630
H	7.3870236049	1.0032094320	1.8222366341
H	5.4339371993	5.4955651016	-1.8710911449
H	3.4444760697	6.9227138347	-1.8010815185
H	2.5871855044	5.5208265183	2.1628600086
H	4.5566934891	4.0940396838	2.0903666909
H	1.2203202980	6.2479030173	-1.9893994465
H	-1.2173366486	6.2485032496	-1.9894266747
H	-1.2244612398	7.3893156447	2.1468445141
H	1.2280073931	7.3887356618	2.1468673669
H	-3.4411274991	6.9243159631	-1.8011105453
H	-5.4313205352	5.4981682105	-1.8710914097
H	-4.5547948631	4.0962352957	2.0903712665
H	-2.5845583022	5.5219587330	2.1628470583
H	-5.6145166129	3.2550389799	-2.1865023377
H	-6.3838804843	0.9798326277	-2.3607911352
H	-7.3864930585	1.0067246265	1.8222496840
H	-6.6648631274	3.3110419088	1.9725423278

Cartesian coordinates (in Å) of [11]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-6.5768757131	3.8015098276	0.1609160577
C	-5.8525064174	4.1359036007	1.3127251767
C	-6.4686358557	4.6637581238	-0.9402718232
C	-4.9410880401	5.1815084670	1.3072440608
C	-5.5555547547	5.7094621818	-0.9461650374
C	-4.7111892544	5.9380575700	0.1504437167
C	-3.4658014060	6.7286245963	0.0451983989
C	-2.8619432383	7.3444801373	1.1513351529
C	-2.7209876404	6.6643362789	-1.1400246012
C	-1.5280234664	7.7288445617	1.1174530704
C	-1.3882894301	7.0460857639	-1.1730647755
C	-0.7390246758	7.5116360278	-0.0219584664
C	0.7390125594	7.5116397420	0.0219593355
C	1.3882776731	7.0460854874	1.1730640696
C	1.5280107378	7.7288465205	-1.1174528658
C	2.7209778293	6.6643428478	1.1400253957
C	2.8619316306	7.3444857665	-1.1513350455
C	3.4657893805	6.7286286773	-0.0451990841
C	4.7111797711	5.9380658068	-0.1504443458
C	5.5555450773	5.7094707062	0.9461646734
C	4.9410785086	5.1815151104	-1.3072436425
C	6.4686283470	4.6637686157	0.9402716732
C	5.8525005031	4.1359133381	-1.3127257294
C	6.5768683237	3.8015197674	-0.1609158544
C	7.1925053644	2.4607374966	-0.0582350727
C	7.0356629662	1.7352627704	1.1299092722
C	7.7166710325	1.7766468871	-1.1648265477
C	7.2375947531	0.3644386204	1.1659275830
C	7.9224514923	0.4036197727	-1.1273948231
C	7.6090408385	-0.3461159011	0.0163293044
C	7.4073882142	-1.8111167703	-0.0162120566
C	7.4895239832	-2.6036214180	1.1390722246
C	6.8719490534	-2.4071716478	-1.1661367910
C	6.9021440868	-3.8598739141	1.1892873965
C	6.2930127087	-3.6672758649	-1.1192131660
C	6.2168732057	-4.3825098758	0.0828663445
C	5.2275892449	-5.4733882150	0.2126469513
C	4.3830709144	-5.4744619918	1.3302088555
C	4.9212331323	-6.3637843208	-0.8261080081
C	3.2092231305	-6.2093675455	1.3400828092
C	3.7513051509	-7.1127698132	-0.8078058232
C	2.8251873805	-6.9903531045	0.2404239012
C	1.4171902904	-7.4321090511	0.1266462999
C	0.5846007179	-7.5382841480	1.2507160253
C	0.7965261701	-7.5207352026	-1.1280526810
C	-0.7965139829	-7.5207364930	1.1280527324
C	-0.5845885202	-7.5382851415	-1.2507163966
C	-1.4171779190	-7.4321116711	-0.1266465099
C	-2.8251752161	-6.9903564088	-0.2404234958
C	-3.7512938113	-7.1127760903	0.8078053054
C	-3.2092134104	-6.2093727254	-1.3400827842
C	-4.9212225137	-6.3637918099	0.8261086943
C	-4.3830624939	-5.4744691152	-1.3302091449
C	-5.2275803292	-5.4733969589	-0.2126470102
C	-6.2168675225	-4.3825214066	-0.0828659418
C	-6.2930047912	-3.6672849300	1.1192124068
C	-6.9021373584	-3.8598847492	-1.1892872396
C	-6.8719465703	-2.4071833017	1.1661373602
C	-7.4895203921	-2.6036337355	-1.1390721699
C	-7.4073836828	-1.8111285914	0.0162115994
C	-7.6090413364	-0.3461284913	-0.0163297085
C	-7.9224513749	0.4036068591	1.1273948944
C	-7.2375936653	0.3644268082	-1.1659270629
C	-7.7166744028	1.7766344840	1.1648265579
C	-7.0356673313	1.7352518500	-1.1299097350
C	-7.1925077601	2.4607252503	0.0582355586
H	-7.0732118133	4.4805120442	-1.8245505475
H	-5.4608090689	6.3274936289	-1.8350708547
H	-4.3049798162	5.3298958044	2.1749715065

H	-5.9082669461	3.4911281069	2.1849241303
H	-3.1542086891	6.1905204278	-2.0159765903
H	-0.8109345069	6.8606962857	-2.0740013606
H	-1.0770903615	8.1607247977	2.0068779886
H	-3.4314033934	7.4823904650	2.0666681222
H	1.0770773132	8.1607279389	-2.0068770336
H	3.4313909480	7.4823957439	-2.0666686084
H	3.1541990834	6.1905255458	2.0159766772
H	0.8109238829	6.8606972529	2.0740014369
H	4.3049706920	5.3299018018	-2.1749714061
H	5.9082608894	3.4911367969	-2.1849239985
H	7.0732038895	4.4805230781	1.8245507586
H	5.4607986281	6.3275022061	1.8350703412
H	7.9216296084	2.3202349254	-2.0833251078
H	8.2876398816	-0.1013990351	-2.0176387445
H	6.9800632996	-0.1791406026	2.0698821872
H	6.6269231036	2.2293772664	2.0062779690
H	6.7906177596	-1.8263528297	-2.0801885768
H	5.7750663820	-4.0445621921	-1.9964393948
H	6.9276980780	-4.4254197902	2.1170634966
H	7.9719222338	-2.2072195796	2.0284444839
H	5.5888546915	-6.4383434340	-1.6804932287
H	3.5323362398	-7.7671013956	-1.6469067533
H	2.5240189406	-6.0760057293	2.1706734843
H	4.5859593787	-4.7925147140	2.1506906496
H	1.3979428474	-7.4758522497	-2.0310003328
H	-1.0195870202	-7.5564682002	-2.2456140130
H	-1.3979307201	-7.4758541112	2.0310003886
H	1.0195991573	-7.5564665077	2.2456136501
H	-2.5240091044	-6.0760088184	-2.1706730563
H	-4.5859520680	-4.7925217466	-2.1506906085
H	-5.5888438315	-6.4383519917	1.6804940531
H	-3.5323233965	-7.7671065450	1.6469066642
H	-6.9276922123	-4.4254317480	-2.1170626223
H	-7.9719185798	-2.2072324257	-2.0284447248
H	-6.7906148479	-1.8263636849	2.0801887290
H	-5.7750608876	-4.0445718511	1.9964396448
H	-6.9800625053	-0.1791517882	-2.0698820029
H	-6.6269261781	2.2293667174	-2.0062777591
H	-7.9216325656	2.3202218134	2.0833255862
H	-8.2876396217	-0.1014124733	2.0176385474

Cartesian coordinates (in Å) of [12]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	6.8837231072	4.5857281582	-0.0575928184
C	7.5849843099	4.1030772502	1.0571391845
C	6.9011259605	3.8004953864	-1.2181653243
C	8.1447910811	2.8328047300	1.0574503423
C	7.4605067688	2.5316378522	-1.2178410265
C	8.0282462185	1.9894513536	-0.0573198337
C	8.2530624725	0.5304458375	0.0235944281
C	7.8860133906	-0.1542416784	1.1897631118
C	8.6060781527	-0.2418398311	-1.0927518977
C	7.7343766456	-1.5325098000	1.1955095348
C	8.4550559370	-1.6218894683	-1.0867033102
C	7.9435940579	-2.2899930956	0.0355690721
C	7.4092504654	-3.6668604064	-0.0349976810
C	7.3360763748	-4.5050764403	1.0870792640
C	6.7444432043	-4.0852139490	-1.1952350623
C	6.5168087497	-5.6261228239	1.0929941702
C	5.9268184585	-5.2052783930	-1.1895868784
C	5.7355123398	-5.9579748362	-0.0233984152
C	4.5857283101	-6.8837228361	0.0575928048
C	3.8004954503	-6.9011257672	1.2181652016
C	4.1030771322	-7.5849843428	-1.0571389929
C	2.5316378701	-7.4605064756	1.2178410421
C	2.8328045438	-8.1447908975	-1.0574502539
C	1.9894511411	-8.0282455775	0.0573198505
C	0.5304457803	-8.2530629386	-0.0235946029
C	-0.2418397244	-8.6060776980	1.0927519986
C	-0.1542418784	-7.8860130591	-1.1897630470
C	-1.6218894716	-8.4550563078	1.0867032615
C	-1.5325099681	-7.7343764546	-1.1955093852
C	-2.2899932652	-7.9435944912	-0.0355690163
C	-3.6668602240	-7.4092500487	0.0349974942
C	-4.0852139481	-6.7444434850	1.1952351233
C	-4.5050766727	-7.3360764515	-1.0870792813
C	-5.2052782430	-5.9268184685	1.1895869647
C	-5.6261227242	-6.5168084120	-1.0929941939
C	-5.9579745258	-5.7355120156	0.0233984994
C	-6.8837233318	-4.5857286070	-0.0575930025
C	-7.5849841613	-4.1030771772	1.0571390061
C	-6.9011256462	-3.8004952572	-1.2181651554
C	-8.1447910907	-2.8328047374	1.0574502525
C	-7.4605065258	-2.5316377716	-1.2178409606
C	-8.0282460140	-1.9894512732	-0.0573198084
C	-8.2530624115	-0.5304457967	0.0235944381
C	-7.8860133985	0.1542417260	1.1897631337
C	-8.6060781211	0.2418398435	-1.0927518970
C	-7.7343766928	1.5325098463	1.1955095521
C	-8.4550559642	1.6218894851	-1.0867033056
C	-7.9435940089	2.2899931043	0.0355690521
C	-7.4092504913	3.6668604408	-0.0349976884
C	-7.3360763927	4.5050764650	1.0870792583
C	-6.7444432112	4.0852139584	-1.1952350668
C	-6.5168087400	5.6261228254	1.0929941753
C	-5.9268184464	5.2052783896	-1.1895868783
C	-5.7355123573	5.9579748588	-0.0233984230
C	-4.5857283107	6.8837228318	0.0575928081
C	-3.8004954564	6.9011257648	1.2181652055
C	-4.1030771308	7.5849843385	-1.0571389933
C	-2.5316378786	7.4605064820	1.2178410570
C	-2.8328045537	8.1447909118	-1.0574502401
C	-1.9894511539	8.0282455666	0.0573198560
C	-0.5304457970	8.2530629089	-0.0235945761
C	0.2418397289	8.6060777134	1.0927519843
C	0.1542418591	7.8860131606	-1.1897630549
C	1.6218894573	8.4550561911	1.0867032757
C	1.5325099358	7.7343765320	-1.1955094163
C	2.2899932340	7.9435943616	-0.0355690073
C	3.6668602254	7.4092501255	0.0349975476
C	4.0852137009	6.7444432457	1.1952351144
C	4.5050765419	7.3360763675	-1.0870793136

C	5.2052780243	5.9268182844	1.1895867343
C	5.6261226717	6.5168084372	-1.0929940795
C	5.9579747936	5.7355120172	0.0233984987
H	7.6548707331	4.7156767674	1.9520682818
H	8.6448150057	2.4720662466	1.9523172940
H	7.3473408839	1.9060900957	-2.0984588954
H	6.3627580508	4.1382974804	-2.0988745625
H	7.5989190740	0.4108927445	2.0716176432
H	7.3321793204	-2.0142862529	2.0818454159
H	8.6978596228	-2.1879511233	-1.9820494832
H	8.9646356137	0.2497551439	-1.9931772945
H	7.8966053449	-4.2516597181	1.9829335764
H	6.4499624958	-6.2309939195	1.9933170019
H	5.3339562306	-5.4285141155	-2.0717274975
H	6.7720421179	-3.4585261319	-2.0817552073
H	4.1382974690	-6.3627579131	2.0988745017
H	1.9060901443	-7.3473408211	2.0984589291
H	2.4720661999	-8.6448144228	-1.9523175210
H	4.7156765559	-7.6548705684	-1.9520680582
H	0.2497551865	-8.9646361033	1.9931771131
H	-2.1879511568	-8.6978599088	1.9820493814
H	-2.0142864425	-7.3321798258	-2.0818456105
H	0.4108925438	-7.5989190303	-2.0716176137
H	-3.4585260540	-6.7720421096	2.0817552790
H	-5.4285138501	-5.3339559107	2.0717273470
H	-6.2309936464	-6.4499620346	-1.9933171914
H	-4.2516596738	-7.8966049682	-1.9829337367
H	-7.6548709494	-4.7156768530	1.9520679161
H	-8.6448149772	-2.4720664016	1.9523172687
H	-7.3473407382	-1.9060901534	-2.0984589348
H	-6.3627580680	-4.1382974292	-2.0988745085
H	-7.5989190562	-0.4108926901	2.0716176605
H	-7.3321793464	2.0142863070	2.0818454169
H	-8.6978596119	2.1879511226	-1.9820495002
H	-8.9646355361	-0.2497551540	-1.9931773027
H	-7.8966053616	4.2516597390	1.9829335693
H	-6.4499625006	6.2309939378	1.9933169983
H	-5.3339562285	5.4285141182	-2.0717275007
H	-6.7720421151	3.4585261426	-2.0817552142
H	-4.1382974861	6.3627579082	2.0988745024
H	-1.9060901570	7.3473408129	2.0984589451
H	-2.4720661941	8.6448144179	-1.9523175114
H	-4.7156765547	7.6548705667	-1.9520680590
H	-0.2497551544	8.9646360740	1.9931771334
H	2.1879511423	8.6978598030	1.9820493908
H	2.0142864232	7.3321799393	-2.0818456305
H	-0.4108925311	7.5989191112	-2.0716176335
H	3.4585258691	6.7720419831	2.0817552785
H	5.4285137810	5.3339561328	2.0717273563
H	6.2309936645	6.4499621699	-1.9933169833
H	4.2516597535	7.8966051121	-1.9829336931

Cartesian coordinates (in Å) of [13]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-5.6670748308	-6.8725109618	0.4923663219
C	-5.7626455413	-5.9463028538	1.5407284636
C	-6.6419133283	-6.7977444061	-0.5145659952
C	-6.6981771339	-4.9238394724	1.5198131671
C	-7.5676870973	-5.7629345174	-0.5462579875
C	-7.5749886176	-4.7667576576	0.4393924537
C	-8.2835715386	-3.4801112635	0.2761191155
C	-8.8160087268	-2.7705691386	1.3611812529
C	-8.2386965527	-2.8292578705	-0.9630580453
C	-9.1622382860	-1.4316174233	1.2408617496
C	-8.5699705351	-1.4873802714	-1.0784721135
C	-8.9742107154	-0.7387597770	0.0353312662
C	-8.9742098311	0.7387646615	-0.0353312596
C	-8.5699691787	1.4873853952	1.0784718321
C	-9.1622381854	1.4316228599	-1.2408612990
C	-8.2386953449	2.8292630011	0.9630582534
C	-8.8160071009	2.7705742140	-1.3611815417
C	-8.2835698094	3.4801158720	-0.2761192368
C	-7.5749856202	4.7667615362	-0.4393926641
C	-7.5676833188	5.7629387436	0.5462575229
C	-6.6981735031	4.9238429318	-1.5198129013
C	-6.6419088537	6.7977479089	0.5145660545
C	-5.7626416535	5.9463061808	-1.5407288453
C	-5.6670706578	6.8725139984	-0.4923665915
C	-4.4613286047	7.7216210635	-0.3766368230
C	-3.9534976055	8.0658507202	0.8843911530
C	-3.6654840244	8.0356954137	-1.4879319089
C	-2.6658868623	8.5577186684	1.0347110925
C	-2.3672526559	8.5013874056	-1.3360233994
C	-1.8097924357	8.7042323939	-0.0657764950
C	-0.3482758896	8.8472869690	0.1067586724
C	0.2633389657	8.2760628114	1.2315255886
C	0.4952163276	9.3630824808	-0.8887994594
C	1.6377189124	8.1265949475	1.3069722316
C	1.8740545093	9.2035470728	-0.8187818036
C	2.4717096017	8.5320462233	0.2568540119
C	3.8703882425	8.0542118287	0.2443260419
C	4.6019159892	7.8936951950	1.4301723343
C	4.4241587008	7.5338229712	-0.9324415370
C	5.7497324973	7.1156210322	1.4632578249
C	5.5744013873	6.7566158219	-0.8997426036
C	6.2166723845	6.4670736021	0.3110110842
C	7.1759422451	5.3450225518	0.3856689743
C	7.0552707255	4.4312701153	1.4404970483
C	8.0702469346	5.0252678178	-0.6453967174
C	7.6955248980	3.2039240976	1.4035035693
C	8.7222746654	3.7985565490	-0.6753759774
C	8.4986327703	2.8312188979	0.3163015024
C	8.8874560089	1.4124405944	0.1625803429
C	8.9795360156	0.5521763120	1.2663491667
C	8.9648758340	0.8255370403	-1.1085502412
C	8.9648758031	-0.8255423236	1.1085503589
C	8.9795359344	-0.5521816007	-1.2663494310
C	8.8874553229	-1.41244454628	-0.1625804182
C	8.4986306276	-2.8312233927	-0.3163014125
C	8.7222718729	-3.7985614652	0.6753759401
C	7.6955222295	-3.2039285074	-1.4035030795
C	8.0702438745	-5.0252725393	0.6453970697
C	7.0552683807	-4.4312747309	-1.4404975354
C	7.1759394161	-5.3450266485	-0.3856690487
C	6.2166686539	-6.4670769215	-0.3110112334
C	5.5743968491	-6.7566186418	0.8997421998
C	5.7497286790	-7.1156249116	-1.4632575412
C	4.4241544092	-7.5338259869	0.9324416570
C	4.6019116394	-7.8936984400	-1.4301726235
C	3.8703843189	-8.0542148701	-0.2443261200
C	2.4717048670	-8.5320468527	-0.2568538383
C	1.8740490614	-9.2035480238	0.8187814974
C	1.6377141141	-8.1265955126	-1.3069719597

C	0.4952108570	-9.3630819461	0.8887999759
C	0.2633340473	-8.2760634232	-1.2315261593
C	-0.3482807549	-8.8472868120	-0.1067588770
C	-1.8097970102	-8.7042301609	0.0657766911
C	-2.3672576024	-8.5013851968	1.3360235007
C	-2.6658918360	-8.5577170174	-1.0347106647
C	-3.6654888420	-8.0356930036	1.4879322258
C	-3.9535023864	-8.0658483269	-0.8843910593
C	-4.4613334089	-7.7216190272	0.3766370145
H	-6.6553769366	-7.5378121972	-1.3099330715
H	-8.2766389090	-5.7078920864	-1.3684726917
H	-6.6709865079	-4.1658351747	2.2976430134
H	-5.0232760741	-5.9542817258	2.3354880497
H	-7.8264236213	-3.3504253411	-1.8224015447
H	-8.4043896028	-0.9880722365	-2.0282411733
H	-9.5482102407	-0.9056869330	2.1096402050
H	-8.9264526470	-3.2660887075	2.3221583193
H	-9.5482108313	0.9056927521	-2.1096396935
H	-8.9264505314	3.2660938044	-2.3221586562
H	-7.8264220316	3.3504303575	1.8224016104
H	-8.4043887601	0.9880774727	2.0282410371
H	-6.6709830400	4.1658386219	-2.2976427453
H	-5.0232716527	5.9542843439	-2.3354879194
H	-6.6553719378	7.5378156305	1.3099331508
H	-8.2766349971	5.7078968455	1.3684723949
H	-4.0417915117	7.8529451799	-2.4902231213
H	-1.7491676472	8.6251754729	-2.2204529280
H	-2.2996929238	8.7726511213	2.0343860221
H	-4.5411798841	7.8640039103	1.7747419333
H	0.0647313598	9.8705273952	-1.7476819927
H	2.4963560336	9.5827393418	-1.6250231701
H	2.0647424038	7.5866657739	2.1466958348
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H	3.8829978286	7.6386898988	-1.8685704229
H	5.9108968872	6.2696075705	-1.8106853595
H	6.2705518281	6.9721804790	2.4061676084
H	4.2400651575	8.3495291669	2.3478921116
H	8.2337273336	5.7360502585	-1.4511518584
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H	6.3590274030	4.6404064341	2.2472081427
H	8.9217027568	1.4528409195	-1.9939602422
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H	8.9964605194	0.9651576847	2.2707782060
H	7.4786493703	-2.4813954776	-2.1836111450
H	6.3590240296	-4.6404103820	-2.2472079654
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H	4.2400603374	-8.3495319341	-2.3478924585
H	3.8829934742	-7.6386927739	1.8685704868
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H	0.0647254721	-9.8705261387	1.7476827126
H	2.4963502212	-9.5827406688	1.6250229422
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Cartesian coordinates (in Å) of [14]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	9.4138891482	-2.0744099483	-0.0348178243
C	9.1591528007	-1.3286198889	-1.1931773544
C	9.8913406710	-1.3815945441	1.0870923758
C	9.2548235034	0.0549107176	-1.1919528276
C	9.9870703921	0.0032761886	1.0883656082
C	9.6097861772	0.7568593653	-0.0324813320
C	9.3819331834	2.2158647350	0.0342232254
C	9.5156015231	3.0490776504	-1.0858112120
C	8.8273159419	2.7762193438	1.1922824465
C	9.0011448731	4.3385953250	-1.0869305128
C	8.3137688957	4.0643264931	1.1912920115
C	8.3301574032	4.8518759928	0.0323314842
C	7.4904051170	6.0665186466	-0.0335718107
C	6.7490402087	6.3323593683	-1.1924344037
C	7.2468819202	6.8720337655	1.0879940119
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C	5.4001393643	7.9854868732	-0.0324168003
C	4.1177089523	8.7176697426	0.0337240714
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C	-2.2267697575	9.7354075051	1.0867802645
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C	-5.8120641221	7.2014236608	1.1914466228
C	-6.5839038285	7.0420929484	0.0331530752
C	-7.5812785770	5.9530105690	-0.0335080521
C	-7.6758321685	5.1713160150	-1.1924234882
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C	-8.9992828903	4.3298024903	1.0897798844
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C	-9.4154572207	2.0745782974	0.0345391530
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C	-9.1585527384	1.3287607954	1.1923707688
C	-9.9916938877	-0.0030544859	-1.0872468290
C	-9.2535708311	-0.0546759771	1.1911376271
C	-9.6101443419	-0.7566290890	0.0321875566
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C	-8.8277865395	-2.7765954013	-1.1930598851
C	-9.5107314559	-3.0471842957	1.0869581575
C	-8.3147545989	-4.0650556844	-1.1920779913
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C	-7.2504326438	-6.8758488433	-1.0868584547
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C	-5.4005642496	-7.9856719933	0.0321476279
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C	4.2473015703	-8.6522548466	-0.0325348223
C	4.6709495513	-7.9892862942	-1.1918530773
C	5.0875412671	-8.5936564141	1.0884497445
C	5.8130206141	-7.2022370578	-1.1922722510
C	6.2306598351	-7.8057600787	1.0880484933
C	6.5838700018	-7.0416635907	-0.0334617276
C	7.5826030772	-5.9538273954	0.0332388213
C	8.3159525449	-5.5380700603	-1.0874573284
C	7.6752748008	-5.1711906788	1.1916386336
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H	8.9447072284	0.6063623801	-2.0747374829
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H	10.1615136169	-1.9351889276	1.9823209481
H	10.0030545075	2.6695422273	-1.9798128027
H	9.0936677252	4.9479085569	-1.9820511539
H	7.7935247483	4.4253993874	2.0736848694
H	8.6981724213	2.1572514542	2.0753806170
H	6.9032981136	5.7196672742	-2.0759014849
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H	6.0403860526	8.3980477269	1.9841110414
H	7.8483491238	6.7384434078	1.9830853227
H	4.1491614578	9.4876984430	-1.9803119095
H	1.8002732424	10.1948192866	-1.9805909494
H	1.3993516538	8.8505450955	2.0742019188
H	3.7375819142	8.1457448129	2.0746845492
H	-0.1655278512	8.9634080707	-2.0761105825
H	-2.5797279829	8.5855705984	-2.0770896510
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H	-0.3775519835	10.3372878316	1.9831852883
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H	-6.8485679262	7.7640697577	-1.9815419442
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H	-8.7745646282	1.8306732554	2.0756435458
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H	-5.1015081791	-7.3696900198	2.0734614936
H	-6.9021877929	-5.7180873612	2.0744948883
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H	-1.3997242539	-8.8535584477	-2.0756514920
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H	-4.1466942589	-9.4793614779	1.9825515803
H	0.3789448346	-10.3458896185	-1.9809729180
H	2.8028858291	-9.9652361115	-1.9796812330
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H	6.8439962464	-7.7579912493	1.9837683558
H	4.8245302580	-9.1494359488	1.9844203586
H	8.3223934255	-6.1551813118	-1.9819060583
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Cartesian coordinates (in Å) of [15]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

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C -5.7322399440 -9.0272167924 0.9403052165
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C 1.4160393232 -9.8194373133 -1.1520870231
C 1.5049108603 -10.5313450846 1.1340028114
C 2.7725772307 -9.5331249507 -1.1156598291
C 2.8624590768 -10.2434742078 1.1709889349
C 3.5137900432 -9.6823564765 0.0636696184
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C 6.8574867176 -8.2144522626 -0.9220686651
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H	4.8406095696	7.8650194887	-2.1643951733
H	1.4089133355	10.2115718970	2.0255954935
H	-1.0164806259	10.2831658148	2.2488431028
H	-1.4089107792	10.2115722474	-2.0255955950
H	1.0164832317	10.2831654818	-2.2488429092
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H	-3.5054374846	10.7959288194	-1.5793311657
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H	-8.7129673671	4.0200175857	2.1640709453
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H	-10.8624922664	2.3120657958	-1.9416621602
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H	-11.0934362963	0.0167105639	1.9263978823
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H	-9.3814053936	-2.1424389916	-2.1746981253
H	-9.6499795817	0.2881679844	-2.1043426876
H	-8.9635763643	-3.7620156510	1.9423935356
H	-7.7348093215	-5.8728853185	1.9256998594
H	-8.8271053337	-6.4802440111	-2.1792929256
H	-10.0614031618	-4.3611033299	-2.1623511462

Cartesian coordinates (in Å) of [16]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

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C 3.7102071824 -10.6198306236 1.3944726999
C 3.3998742867 -10.0836719511 -0.9201767712
C 2.8655229473 -10.5794738129 0.2761878505
C 1.4186886568 -10.8677701652 0.3624835018
C 0.6936532278 -10.4730806775 1.4943611408
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C -0.6936544335 -10.4730809278 1.4943612751
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C 5.4803407576 9.4685429110 0.3007199147
C 6.7246703355 8.6899871730 0.1259698640
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C 7.1745037373 8.3283364232 -1.1512899911
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C	11.2091947555	0.6658595777	-1.5622778593
C	10.8088177278	-0.6524853096	0.8399604172
C	11.2155350880	-0.7211071297	-1.5201841617
C	10.9511516560	-1.4123778444	-0.3288729866
C	10.6470287331	-2.8589098432	-0.3165421232
C	10.8491815301	-3.6602536689	0.8162374354
C	9.9785865369	-3.4372353639	-1.4040446415
C	10.3117036029	-4.9380763876	0.8991768758
C	9.4493570109	-4.7162047756	-1.3250297243
C	9.5559015745	-5.4745971612	-0.1522382227
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C	8.4804281035	-7.5561682330	-1.0812314835
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C	7.4958600691	-8.5307113966	-0.9995215148
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H	1.2227091985	-10.0663222830	2.3514081133
H	-1.2227106618	-10.0663225108	2.3514080715
H	-1.2261262974	-11.7457944456	-1.5972474744
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H	-5.6168489188	-10.1215773975	2.2326729401
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H	-7.3052375873	-9.1686037712	-1.8581888900
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H	11.6619409679	3.4400859982	1.3348372161
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Cartesian coordinates (in Å) of [17]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

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C	3.9525977905	11.4668333310	1.0883917619
C	3.7117033367	10.4011406398	-1.0430614370
C	4.5189043765	10.6917809401	0.0655212509
C	5.8510519128	10.0611548091	0.1822103545
C	6.3591968775	9.6722495268	1.4293298075
C	6.5834842422	9.6825469112	-0.9516861671
C	7.4761186852	8.8555003338	1.5304666020
C	7.6851939728	8.8467895510	-0.8518276484
C	8.1273472645	8.3667756506	0.3888717539
C	9.1162247302	7.2696566695	0.4628642828
C	9.0358091380	6.3239271011	1.4945226145
C	10.0566632744	7.0371317877	-0.5519597583
C	9.7885820188	5.1600730497	1.4648294814
C	10.7968930366	5.8631806879	-0.5926926756
C	10.6441102404	4.8786934951	0.3923857034
C	11.2017889107	3.5174755321	0.2497092739
C	11.6769607133	2.7856690949	1.3457613410
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C	10.7968924589	-5.8631829031	0.5926920923
C	9.7885811731	-5.1600750351	-1.4648294575
C	10.0566620449	-7.0371336741	0.5519599094
C	9.0358081300	-6.3239289272	-1.4945229423
C	9.1162235643	-7.2696581066	-0.4628641712
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C	-11.6163511017	-1.4162079914	0.1265033325
C	-11.6857694065	-0.5840856731	1.2527686378
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C	-9.2700370871	7.5157297202	-1.4182710957
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C	-6.4554464202	9.7516133307	-0.2556454860
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C	-5.5890144407	9.6994335089	-1.355952627
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C	-4.3483069655	10.3150799016	-1.3226278705
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H	9.6411493344	-4.4089727539	-2.2354980758
H	8.1667037008	-8.5041542817	1.7628329366
H	6.2593145069	-10.0108025243	1.9349521530
H	5.8306283851	-9.9538739676	-2.3354733432
H	7.8204892245	-8.5564994863	-2.5162019364
H	4.1034277121	-9.7802535281	1.8426289419
H	1.7673917900	-10.4830330899	1.9285267542
H	2.2034956251	-12.4334502770	-1.8654853068
H	4.5618953855	-11.7608107129	-1.9385570285
H	0.1522408884	-12.1956968887	2.0975846873
H	-2.2938824127	-11.9975288226	2.1658106660
H	-2.3224139543	-10.9782078679	-2.0022551097
H	0.1168617108	-11.1933756596	-2.0726772412
H	-3.6671766615	-10.1752677746	2.1567908837
H	-5.8533505139	-9.0897524916	2.2144835668
H	-6.7288989331	-10.6344859213	-1.6918111537
H	-4.5305979500	-11.7227535585	-1.7511592720

H	-8.1213543067	-9.0789273502	2.3237929651
H	-9.7672701928	-7.2566477137	2.3491624882
H	-9.1600016243	-6.6512836258	-1.8531219179
H	-7.5024687429	-8.4545408803	-1.8761703537
H	-9.4017286534	-4.9156643425	2.1639244050
H	-10.2524298078	-2.6327913673	2.1059850977
H	-12.2935049021	-3.4854399621	-1.5756264324
H	-11.4053516926	-5.7673777167	-1.5326408083
H	-11.7033269868	-1.0238776258	2.2457392990
H	-11.6340052990	1.4041572792	2.0296743660
H	-11.7033262590	1.0238797410	-2.2457394602
H	-11.6340052561	-1.4041550918	-2.0296741953
H	-12.2935046692	3.4854423635	1.5756259586
H	-11.4053506068	5.7673798465	1.5326411019
H	-9.4017280517	4.9156663208	-2.1639247465
H	-10.2524290860	2.6327934328	-2.1059847912
H	-9.1600000385	6.6512851278	1.8531217900
H	-7.5024671128	8.4545424204	1.8761705836
H	-8.1213522563	9.0789285246	-2.3237932207
H	-9.7672686962	7.2566494588	-2.3491622932
H	-6.7288970461	10.6344875476	1.6918109102
H	-4.5305956637	11.7227544676	1.7511594736
H	-3.6671748824	10.1752687706	-2.1567910386
H	-5.8533487172	9.0897536733	-2.2144832976
H	-2.3224118296	10.9782080204	2.0022549670
H	0.1168638679	11.1933758363	2.0726772804
H	0.1522430893	12.1956964906	-2.0975848743
H	-2.2938802906	11.9975293243	-2.1658105387

Cartesian coordinates (in Å) of [18]-cycloparaphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	12.2987474806	-1.4189419283	0.0249974404
C	12.7138718747	-0.6940925655	-1.1009487825
C	11.9796948717	-0.6935048702	1.1801770968
C	12.7138832847	0.6938729346	-1.1009492336
C	11.9797070419	0.6932978404	1.1801770677
C	12.2987720434	1.4187293061	0.0249973168
C	12.0416855299	2.8728084559	-0.0267192378
C	11.4885166737	3.4434967270	-1.1802844803
C	12.1888107915	3.6976574567	1.0972845129
C	11.0149454669	4.7469596959	-1.1800742090
C	11.7141607876	5.0020572267	1.0977382805
C	11.0712579613	5.5396065072	-0.0259629476
C	10.3322997520	6.8179612784	0.0260723777
C	10.1884653218	7.6428308815	-1.0979278766
C	9.6175631776	7.1648864219	1.1800106298
C	9.2966674450	8.7066264116	-1.0985481215
C	8.7266870013	8.2278063042	1.1793746234
C	8.5091114677	8.9919666909	0.0255530570
C	7.3776144454	9.9409802190	-0.0258782250
C	6.5893144372	10.0278597364	-1.1807151242
C	6.9581360410	10.6621640407	1.1007914502
C	5.3888502699	10.7223285302	-1.1792269049
C	5.7564947808	11.3566131769	1.1024024017
C	4.9207606476	11.3605815688	-0.0232693396
C	3.5328739298	11.8651296935	0.0288649877
C	2.8928244938	12.4048262689	-1.0956276086
C	2.7613965146	11.6705068365	1.1819321675
C	1.5258500614	12.6452494364	-1.0965643421
C	1.3955183358	11.9112793901	1.1812157699
C	0.7384518023	12.3570733940	0.0268842044
C	-0.7382380305	12.3570865648	-0.0268843724
C	-1.3953125605	11.9113030389	-1.1812155117
C	-1.5256315151	12.6452762705	1.0965639541
C	-2.7611949728	11.6705548272	-1.1819324051
C	-2.8926100202	12.4048760734	1.0956278528
C	-3.5326686879	11.8651910151	-0.0288649810
C	-4.9205640505	11.3606667025	0.0232694048
C	-5.7562987364	11.3567128117	-1.1024021331
C	-5.3886649366	10.7224215269	1.1792267156
C	-6.9579514880	10.6622837870	-1.1007917308
C	-6.5891412380	10.0279737803	1.1807154760
C	-7.3774421574	9.9411074018	0.0258781786
C	-8.5089560616	8.9921140349	-0.0255529185
C	-8.7265447612	8.2279568355	-1.1793742402
C	-9.2965171558	8.7067872476	1.0985479820
C	-9.6174396959	7.1650528057	-1.1800106838
C	-10.1883331391	7.6430069326	1.0979283252
C	-10.3321820920	6.8181402244	-0.0260721452
C	-11.0711620086	5.5397979916	0.0259630160
C	-11.7140745820	5.0022597307	-1.0977380127
C	-11.0148631762	4.7471497537	1.1800739698
C	-12.1887464298	3.6978679807	-1.0972849522
C	-11.4884576172	3.4436952370	1.1802846431
C	-12.0416356248	2.8730166995	0.0267190782
C	-12.2987479489	1.4189421115	-0.0249974420
C	-11.9796945177	0.6935047625	-1.1801767349
C	-12.7138718162	0.6940926728	1.1009488653
C	-11.9797068648	-0.6932979172	-1.1801770085
C	-12.7138834304	-0.6938728712	1.1009491630
C	-12.2987720592	-1.4187293010	-0.0249972249
C	-12.0416851959	-2.8728083692	0.0267192570
C	-12.1888108269	-3.6976575532	-1.0972843708
C	-11.4885167234	-3.4434966249	1.1802846285
C	-11.7141603629	-5.0020571258	-1.0977384487
C	-11.0149457530	-4.7469597122	1.1800742944
C	-11.0712579235	-5.5396064903	0.0259630435
C	-10.3323001709	-6.8179615502	-0.0260723886
C	-9.6175631554	-7.1648865283	-1.1800104920
C	-10.1884653600	-7.6428308165	1.0979279963

C	-8.7266869314	-8.2278063228	-1.1793746205
C	-9.2966677268	-8.7066265988	1.0985479786
C	-8.5091114754	-8.9919666858	-0.0255529645
C	-7.3776141240	-9.9409797919	0.0258781764
C	-6.9581359740	-10.6621641138	-1.1007913256
C	-6.5893143893	-10.0278595337	1.1807151715
C	-5.7564946012	-11.3566129870	-1.1024025403
C	-5.3888503182	-10.7223285608	1.1792268713
C	-4.9207606428	-11.3605816160	0.0232694029
C	-3.5328740524	-11.8651301629	-0.0288649982
C	-2.7613964677	-11.6705069840	-1.1819320721
C	-2.8928245423	-12.4048261063	1.0956278077
C	-1.3955182792	-11.9112792621	-1.1812157535
C	-1.5258501313	-12.6452496396	1.0965642301
C	-0.7384518266	-12.3570735120	-0.0268841974
C	0.7382379872	-12.3570861922	0.0268843183
C	1.5256316269	-12.6452764573	-1.0965638173
C	1.3953124043	-11.9113029622	1.1812155687
C	2.8926099989	-12.4048756751	-1.0956280396
C	2.7611949143	-11.6705550939	1.1819324606
C	3.5326686611	-11.8651909504	0.0288650379
C	4.9205642202	-11.3606671010	-0.0232694093
C	5.3886650585	-10.7224214872	-1.1792265690
C	5.7562986396	-11.3567127987	1.1024022577
C	6.5891412701	-10.0279736684	-1.1807154484
C	6.9579516399	-10.6622841319	1.1007915900
C	7.3774421792	-9.9411074332	-0.0258780718
C	8.5089557123	-8.9921136495	0.0255528964
C	9.2965172983	-8.7067872409	-1.0985478156
C	8.7265445869	-8.2279567672	1.1793743138
C	10.1883329744	-7.6430067249	-1.0979284601
C	9.6174397399	-7.1650528733	1.1800106295
C	10.3321821742	-6.8181402143	0.0260722002
C	11.0711624720	-5.5397982148	-0.0259630660
C	11.0148635273	-4.7471499363	-1.1800740644
C	11.7140742861	-5.0022596915	1.0977382279
C	11.4884573491	-3.4436952254	-1.1802846509
C	12.1887467157	-3.6978681107	1.0972845930
C	12.0416354660	-2.8730165414	-0.0267191520
H	11.6367796992	-1.2228178879	2.0644405654
H	11.6368007856	1.2226170644	2.0644402456
H	13.0251261012	1.2268259999	-1.9953278745
H	13.0251047166	-1.2270512655	-1.9953275564
H	12.6681380789	3.3046928638	1.9898101944
H	11.8291700968	5.6109555189	1.9904493852
H	10.5080046046	5.1256901418	-2.0629641876
H	11.3429834424	2.8273192236	-2.0628760552
H	9.6925300797	6.5369552824	2.0630950837
H	8.1203774549	8.4113609021	2.0617064568
H	9.1969645942	9.3179720309	-1.9913215810
H	10.7735962439	7.4362843453	-1.9899190347
H	7.5763274549	10.6652671026	1.9944503245
H	5.4519142798	11.8928763137	1.9970850419
H	4.7584412528	10.6915043158	-2.0632311450
H	6.8756924316	9.4666058544	-2.0654504995
H	3.2228906624	11.2371814423	2.0645930250
H	0.8127111131	11.6621097508	2.0633508228
H	1.0559220727	13.0490798931	-1.9892557267
H	3.4737103972	12.6245434474	-1.9873232865
H	-1.0556966510	13.0490986985	1.9892553910
H	-3.4734922423	12.6246032534	1.9873234433
H	-3.2226966902	11.2372373990	-2.0645931816
H	-0.8125098044	11.6621234812	-2.0633507198
H	-4.7582563782	10.6915864891	2.0632309956
H	-6.8755287797	9.4667245110	2.0654506756
H	-7.5761429604	10.6653972694	-1.9944505176
H	-5.4517088998	11.8929703534	-1.9970849832
H	-9.1968037379	9.3181314206	1.9913213043
H	-10.7734679990	7.4364706116	1.9899192222
H	-9.6924178190	6.5371229949	-2.0630951066
H	-8.1202323965	8.4115011047	-2.0617063157
H	-10.5079156768	5.1258712932	2.0629640019
H	-11.3429351099	2.8275150848	2.0628761519

H	-12.6680805174	3.3049117308	-1.9898106105
H	-11.8290729616	5.6111599831	-1.9904492209
H	-13.0251052912	1.2270511115	1.9953275945
H	-13.0251261087	-1.2268261294	1.9953277105
H	-11.6368007066	-1.2226168345	-2.0644403919
H	-11.6367795661	1.2228179170	-2.0644401664
H	-11.3429836180	-2.8273194176	2.0628764622
H	-10.5080043497	-5.1256902299	2.0629639252
H	-11.8291698851	-5.6109552432	-1.9904496620
H	-12.6681376193	-3.3046925806	-1.9898101122
H	-10.7735964675	-7.4362847091	1.9899191743
H	-9.1969647584	-9.3179724813	1.9913212211
H	-8.1203778077	-8.4113608780	-2.0617067609
H	-9.6925303395	-6.5369552752	-2.0630948021
H	-6.8756920996	-9.4666056307	2.0654506569
H	-4.7584409856	-10.6915043378	2.0632308870
H	-5.4519143336	-11.8928759577	-1.9970853858
H	-7.5763274244	-10.6652667861	-1.9944501388
H	-3.4737103217	-12.6245437079	1.9873234957
H	-1.0559218727	-13.0490798992	1.9892555473
H	-0.8127113585	-11.6621096992	-2.0633510269
H	-3.2228908279	-11.2371816320	-2.0645928173
H	0.8125098631	-11.6621235644	2.0633509875
H	3.2226967888	-11.2372372140	2.0645929273
H	3.4734920979	-12.6246031814	-1.9873236561
H	1.0556964930	-13.0490982483	-1.9892553677
H	5.4517092149	-11.8929706942	1.9970850699
H	7.5761433115	-10.6653975076	1.9944502180
H	6.8755287726	-9.4667248745	-2.0654509672
H	4.7582562507	-10.6915865135	-2.0632306409
H	8.1202323107	-8.4115007434	2.0617065410
H	9.6924178151	-6.5371226852	2.0630947896
H	10.7734675582	-7.4364705635	-1.9899196001
H	9.1968034092	-9.3181312986	-1.9913211214
H	11.8290730071	-5.6111598085	1.9904495057
H	12.6680806999	-3.3049116323	1.9898101927
H	11.3429349610	-2.8275154080	-2.0628763894
H	10.5079159442	-5.1258716884	-2.0629639220

Cartesian coordinates (in Å) of [5]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	10.0210875954	0.0000557216	-0.0001826085
C	9.3194365380	1.1560225837	0.3313421951
C	9.3194703838	-1.1560592363	-0.3312657882
C	7.9293715554	1.1560433365	0.3302721419
C	7.9294000904	-1.1562461994	-0.3297799945
C	7.2098503625	-0.0000929442	0.0001908283
C	5.7314738499	-0.0000357129	0.0000185761
C	5.0070580149	0.7262752750	0.9537387285
C	5.0071758320	-0.7262867944	-0.9538430758
C	3.6195550192	0.7262762194	0.9538882804
C	3.6196646802	-0.7261611054	-0.9542768705
C	2.8954522372	0.0001735002	-0.0003239557
C	1.4182872274	0.0000732975	-0.0002034336
C	0.6940213647	-0.0101091566	1.1986898537
C	0.6938133789	0.0099808769	-1.1989637300
C	-0.6936178712	-0.0103671154	1.1988122311
C	-0.6938218116	0.0102346523	-1.1988044709
C	-1.4181560468	0.0000742437	0.0000616644
C	-2.8953691457	0.0000370229	0.0001152494
C	-3.6196760092	-0.7373134836	0.9455479335
C	-3.6196213690	0.7375520097	-0.9452591759
C	-5.0071607392	-0.7369120047	0.9455914933
C	-5.0071232770	0.7369168823	-0.9455741419
C	-5.7315377540	-0.0002356539	-0.0001899594
C	-7.2099499913	-0.0000392209	0.0000328533
C	-7.9294763367	-1.1603877423	0.3150009454
C	-7.9294322149	1.1603792280	-0.3147110710
C	-9.3195565038	-1.1602609498	0.3162681600
C	-9.3195072984	1.1603593940	-0.3158280464
C	-10.0211564071	-0.0000310164	-0.0001215982
H	5.5411570994	-1.2844472449	-1.7178260057
H	3.0852362761	-1.3127576041	-1.6962974461
H	3.0849998293	1.3129847733	1.6957203247
H	5.5409011776	1.2844166546	1.7178286765
H	7.3906341287	-2.0708476041	-0.5613304272
H	9.8571802172	-2.0658523606	-0.5828977082
H	11.1071465158	0.0000756066	-0.0001382629
H	9.8570863839	2.0658253570	0.5830516547
H	7.3905675251	2.0706366026	0.5617491715
H	1.2272022312	0.0360803086	-2.1450651813
H	1.2276113309	-0.0360856519	2.1446866917
H	-1.2273118684	-0.0003040541	-2.1451484641
H	-1.2268992195	-0.0000409133	2.1452743981
H	-3.0852903316	1.3324818837	-1.6806308835
H	-3.0853606930	-1.3321759012	1.6809838708
H	-5.5409977505	1.3040056969	-1.7029937278
H	-5.5411087815	-1.3040844718	1.7028939755
H	-7.3906589660	-2.0778678494	0.5347181126
H	-7.3905498174	2.0778989302	-0.5340989012
H	-9.8572581477	-2.0732246975	0.5561449579
H	-9.8571987835	2.0733777741	-0.5555131493
H	-11.1072235403	-0.0000371599	-0.0001751043

Cartesian coordinates (in Å) of [6]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	0.0000001743	-0.0000057790	-12.1808226455
C	1.2014783946	0.0504366984	-11.4792667831
C	-1.2014788388	-0.0504265496	-11.4792666619
C	1.2011677003	0.0517536638	-10.0888906068
C	-1.2011670093	-0.0517604356	-10.0888905963
C	0.0000002077	0.0000021150	-9.3695111909
C	-0.0000003484	-0.0000006404	-7.8908033264
C	0.9812812043	-0.6883520628	-7.1662043774
C	-0.9812803040	0.6883531570	-7.1662042277
C	0.9814813222	-0.6883492141	-5.7786277097
C	-0.9814818770	0.6883483013	-5.7786273839
C	0.0000001957	0.0000002100	-5.0537871455
C	0.00000021725	0.0000009557	-3.5766229470
C	0.3761828163	-1.1380868207	-2.8512016237
C	-0.3761899399	1.1380848754	-2.8512013969
C	0.3768683048	-1.1378872780	-1.4638497098
C	-0.3768610701	1.1378901498	-1.4638494631
C	-0.0000024817	-0.0000005793	-0.7385807623
C	-0.0000010266	0.0000000913	0.7385811432
C	-0.3768620892	-1.1378900336	1.4638495802
C	0.3768664648	1.1378879376	1.4638496110
C	-0.3761905949	-1.1380846385	2.8512013960
C	0.3761831982	1.1380870283	2.8512016151
C	0.0000030704	-0.0000010601	3.5766230807
C	-0.0000010271	0.0000018485	5.0537871859
C	-0.9814804236	-0.6883499824	5.7786278476
C	0.9814831625	0.6883468727	5.7786276583
C	-0.9812813436	-0.6883522348	7.1662045267
C	0.9812805114	0.6883530827	7.1662044836
C	-0.0000000834	0.0000000824	7.8908033599
C	0.0000001206	-0.0000027912	9.3695112129
C	-1.2011670325	0.0517615541	10.0888906016
C	1.2011676908	-0.0517525952	10.0888906467
C	-1.2014789563	0.0504248871	11.4792666796
C	1.2014782691	-0.0504379843	11.4792668169
C	0.0000001502	0.00000066545	12.1808226819
H	0.6551747006	2.0429068212	3.3839070282
H	0.6925265941	2.0305403711	0.9311766251
H	-0.6925258883	-2.0305413635	0.9311767782
H	-0.6551735413	-2.0429066475	3.3839074415
H	1.7669063663	1.2172946636	5.2459823690
H	1.7457472023	1.2459696358	7.7000884005
H	-1.7457482258	-1.2459690626	7.7000880164
H	-1.7669060952	-1.2172934917	5.2459821085
H	-0.6925274372	2.0305406322	-0.9311768517
H	0.6925262554	-2.0305407035	-0.9311773875
H	-0.6551736123	2.0429066950	-3.3839074307
H	0.6551738744	-2.0429064231	-3.3839074631
H	-1.7669063988	1.2172943690	-5.2459823506
H	1.7669058598	-1.2172946360	-5.2459822873
H	-1.7457478122	1.2459685877	-7.7000881890
H	1.7457473742	-1.2459692355	-7.7000883874
H	2.1422574625	0.1208023706	-9.5504775715
H	-2.1422571410	-0.1208012593	-9.5504774642
H	2.1442909406	0.0993106400	-12.0166301282
H	-2.1442909183	-0.0993115140	-12.0166298342
H	-0.0000001240	0.0000005116	-13.2669089380
H	2.1422572944	-0.1208024773	9.5504774724
H	-2.1422572789	0.1208010051	9.5504775422
H	2.1442909376	-0.0993104913	12.0166300755
H	-2.1442909122	0.0993118920	12.0166298846
H	-0.0000001598	-0.0000003728	13.2669089718

Cartesian coordinates (in Å) of [7]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	14.3375653559	0.0000014078	0.0000036941
C	13.6359620055	-1.1180077600	0.4431794932
C	13.6359620363	1.1180051836	-0.4431859383
C	12.2458053581	-1.1175835449	0.4436346225
C	12.2458052650	1.1175857730	-0.4436297496
C	11.5265093836	-0.0000005214	-0.0000018787
C	10.0479087653	-0.0000002285	0.0000009775
C	9.3232671242	-1.1514567870	-0.3330393411
C	9.3232672614	1.1514573590	0.3330375288
C	7.9357682321	-1.1517533268	-0.3325375567
C	7.9357685180	1.1517529190	0.3325390631
C	7.2107202426	0.0000001840	-0.0000005158
C	5.7334346867	0.0000008669	-0.0000006779
C	5.0085294841	-0.7221224472	-0.9569812765
C	5.0085296740	0.7221197868	0.9569832472
C	3.6210804821	-0.7221876576	-0.9569512202
C	3.6210807515	0.7221906968	0.9569488563
C	2.8962243756	-0.0000015753	0.0000011292
C	1.4188262056	0.0000015676	-0.0000000803
C	0.6938336054	0.0001314575	-1.1986639157
C	0.6938337075	-0.0001338155	1.1986639798
C	-0.6938335940	-0.0001318008	-1.1986640086
C	-0.6938334052	0.0001333642	1.1986637238
C	-1.4188263444	-0.0000004546	-0.0000001813
C	-2.8962244117	0.0000013151	0.0000004958
C	-3.6210807228	0.7221877894	-0.9569514385
C	-3.6210809501	-0.7221908367	0.9569482471
C	-5.0085297140	0.7221232772	-0.9569810582
C	-5.0085298672	-0.7221190091	0.9569839089
C	-5.7334346706	-0.0000019709	-0.0000018090
C	-7.2107202303	0.0000000522	0.0000008471
C	-7.9357682751	1.1517528830	-0.3325383545
C	-7.9357684713	-1.1517533622	0.3325382604
C	-9.3232671531	1.1514567301	-0.3330387050
C	-9.3232672315	-1.1514574022	0.3330381889
C	-10.0479087679	-0.0000001578	0.0000004220
C	-11.5265093853	-0.0000002467	0.0000010391
C	-12.2458052147	1.1175855225	0.4436303837
C	-12.2458054050	-1.1175838127	-0.4436339575
C	-13.6359619931	1.1180053475	0.4431855791
C	-13.6359620439	-1.1180076117	-0.4431798126
C	-14.3375653521	0.0000013483	-0.0000034308
H	-1.2266131740	-0.01916663206	-2.1451921312
H	1.2266136934	0.01916667424	-2.1451916908
H	1.2266133147	-0.0191659825	2.1451921048
H	-1.2266134163	0.0191659304	2.1451915982
H	-3.0873941613	1.3061074455	-1.7014987192
H	-5.5416285838	1.2777516137	-1.7233557326
H	-5.5416279308	-1.2777522767	1.7233555982
H	-3.0873940847	-1.3061063501	1.7014984333
H	3.0873940426	-1.3061076170	-1.7014983321
H	3.0873942836	1.3061065189	1.7014989879
H	5.5416282461	-1.2777517551	-1.7233553441
H	5.5416283715	1.2777519575	1.7233552405
H	7.4025548176	-2.0661933233	-0.5769470793
H	7.4025548447	2.0661930390	0.5769472021
H	9.8572186994	-2.0552234694	-0.6129756469
H	9.8572188559	2.0552233058	0.6129761059
H	11.7074731596	1.9837100601	-0.8181681326
H	11.7074731099	-1.9837100799	0.8181671948
H	14.1735171182	1.9921399743	-0.7995063193
H	14.1735169693	-1.9921397507	0.7995069258
H	15.4235773110	-0.0000001886	-0.0000003472
H	-7.4025548292	2.0661932212	-0.5769465301
H	-7.4025548072	-2.0661930837	0.5769478324
H	-9.8572186237	2.0552231820	-0.6129759610
H	-9.8572188823	-2.0552236469	0.6129756949
H	-11.7074731196	1.9837101858	0.8181679041
H	-11.7074731527	-1.9837099870	-0.8181673651
H	-14.1735170639	1.9921400253	0.7995062584

H -14.1735170172 -1.9921397325 -0.7995069090
H -15.4235773080 -0.0000001284 0.0000003784

Cartesian coordinates (in Å) of [8]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	16.4899939821	0.0000091721	-0.0001079360
C	15.7888114763	0.8957354763	-0.8030430505
C	15.7888605895	-0.8957331562	0.8028508067
C	14.3986469866	0.8957420891	-0.8028143322
C	14.3986895805	-0.8956815693	0.8027594484
C	13.6803585244	-0.0000322891	-0.0000847791
C	12.2016920027	0.0000133400	0.0000161607
C	11.4780252899	1.1973857841	-0.0593856950
C	11.4780507096	-1.1973986832	0.0593801671
C	10.0902583678	1.1974828093	-0.0588186272
C	10.0902939918	-1.1975641074	0.0586908971
C	9.3659939993	-0.0000514301	0.0001156643
C	7.8888857771	-0.0000254010	0.0000048592
C	7.1643456360	0.9878300581	0.6793215775
C	7.1643198997	-0.9878720671	-0.6792884604
C	5.7769301853	0.9876582897	0.6796494828
C	5.7769104559	-0.9877235719	-0.6795833299
C	5.0523262043	-0.0000073057	-0.0000049679
C	3.5754920051	-0.0000668625	0.0000807224
C	2.8504879368	0.3847168217	1.1354767558
C	2.8504793735	-0.3846076230	-1.1353763799
C	1.4631680951	0.3846994211	1.1355384819
C	1.4631707781	-0.3847967581	-1.1353737678
C	0.7384680869	0.0001756739	0.0000079646
C	-0.7384676917	-0.0001493249	-0.0000035495
C	-1.4631869919	-0.3846773837	1.1355135076
C	-1.4631515990	0.3848269753	-1.1353956375
C	-2.8505039869	-0.3846298230	1.1354660648
C	-2.8504630723	0.3847012609	-1.1353847045
C	-3.5754918975	0.0000108922	0.0000163089
C	-5.0523261680	0.0000447261	0.0000499216
C	-5.7769399758	-0.9876264715	0.6797200363
C	-5.7769007256	0.9877579489	-0.6795090860
C	-7.1643606202	-0.9878640804	0.6792882430
C	-7.1643049176	0.9878412357	-0.6793175732
C	-7.8888859699	0.0001217360	0.0001641959
C	-9.3659940426	-0.0000182263	0.0000568237
C	-10.0902980918	-1.1975344643	-0.0587976029
C	-10.0902542851	1.1975123475	0.0587156449
C	-11.4780607267	-1.1974141119	-0.0592894285
C	-11.4780152608	1.1973702682	0.0594801016
C	-12.2016920842	-0.0000115146	-0.0001382711
C	-13.6803586293	-0.0000707187	-0.0000565816
C	-14.3986775766	-0.8957699412	-0.8028796694
C	-14.3986590833	0.8956505833	0.8026977413
C	-15.7888525471	-0.8957487717	-0.8030803744
C	-15.7888196308	0.8957169786	0.8028167657
C	-16.4899940405	-0.0000137835	-0.0001203742
H	0.9298604399	-0.7060480932	-2.0256912418
H	3.3836423911	-0.6708092871	-2.0376973922
H	3.3836635447	0.6708057584	2.0378336248
H	0.9298346057	0.7060773059	2.0258026194
H	-0.9298319780	0.7060899119	-2.0257013894
H	-3.3836345058	0.6708483451	-2.0377187006
H	-3.3836709898	-0.6707793615	2.0378081248
H	-0.9298629172	-0.7060493011	2.0257872903
H	5.2438351110	-1.7777987409	-1.2011547958
H	5.2438786273	1.7777386328	1.2012322229
H	7.6980958127	-1.7577319603	-1.2295522446
H	7.6981310246	1.7576768797	1.2296121933
H	9.5566979322	-2.1416828758	0.1238032966
H	9.5566521432	2.1415851606	-0.1237712987
H	12.0126698679	-2.1427619991	0.0888563567
H	12.0126319687	2.1427498210	-0.0888681274
H	13.8576354260	1.5790029955	-1.4513580161
H	13.8577227732	-1.5789981943	1.4512689133
H	16.3273073761	1.5923720580	-1.4392187243
H	16.3273940127	-1.5923569788	1.4390070251
H	17.5760493619	0.0000110134	-0.0001407216
H	-5.2438201365	1.7777901417	-1.2011420731

H	-5.2438940571	-1.7777520855	1.2012380890
H	-7.6980655490	1.7577402246	-1.2295398171
H	-7.6981611688	-1.7576743488	1.2296172255
H	-9.5566456176	2.1416189396	0.1238129592
H	-9.5567044894	-2.1416488735	-0.1237679504
H	-12.0126144971	2.1427419015	0.0888188493
H	-12.0126873301	-2.1427696628	-0.0889127769
H	-13.8576894995	-1.5790486647	-1.4514159991
H	-13.8576687234	1.5789468264	1.4512172684
H	-16.3273722847	-1.5923817070	-1.4392448512
H	-16.3273290894	1.5923421179	1.4389865472
H	-17.5760494106	0.0000108414	-0.0001322395

Cartesian coordinates (in Å) of [9]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	0.0000003574	0.0000005740	-18.6524505387
C	1.0228583739	-0.6325544241	-17.9509239842
C	-1.0228589372	0.6325535374	-17.9509241036
C	1.0229514204	-0.6319307391	-16.5606790131
C	-1.0229510728	0.6319311432	-16.5606792566
C	-0.0000001131	-0.0000002319	-15.8415830828
C	0.0000003110	0.0000001972	-14.3631509658
C	0.4199740510	-1.1225991863	-13.6383145843
C	-0.4199753457	1.1225988068	-13.6383144377
C	0.4204927408	-1.1225796138	-12.2507940005
C	-0.4204918677	1.1225801087	-12.2507937657
C	-0.0000002486	-0.0000000251	-11.5258443956
C	-0.0000003555	-0.0000000758	-10.0486003223
C	-0.3377632953	-1.1501493878	-9.3234331417
C	0.3377637879	1.1501489193	-9.3234330851
C	-0.3371879059	-1.1503170830	-7.9360727556
C	0.3371879455	1.1503167918	-7.9360726118
C	-0.0000005924	0.0000000639	-7.2107594928
C	0.0000011318	-0.0000011973	-5.7335874344
C	-0.9582167089	-0.7204650112	-5.0086056159
C	0.9582151034	0.7204674465	-5.0086054977
C	-0.9581404178	-0.7205679364	-3.6211745867
C	0.9581419817	0.7205666323	-3.6211743950
C	-0.0000000906	0.0000005345	-2.8962463014
C	0.0000001240	0.0000001006	-1.4188714772
C	-1.1986471472	0.0001607684	-0.6938262607
C	1.1986473420	-0.0001605045	-0.6938264078
C	-1.1986474273	-0.0001609760	0.6938265198
C	1.1986473435	0.0001599583	0.6938264329
C	0.0000000406	0.0000009473	1.4188712088
C	-0.0000008034	-0.0000011355	2.8962461089
C	-0.9581401952	0.7205684653	3.6211744310
C	0.9581419486	-0.7205662073	3.6211742273
C	-0.9582164935	0.7204651041	5.0086054820
C	0.9582151025	-0.7204670000	5.0086053409
C	0.0000005026	0.0000006424	5.7335874803
C	0.0000004476	0.0000001631	7.2107595185
C	-0.3371886857	1.1503167410	7.9360727957
C	0.3371873481	-1.1503170780	7.9360725967
C	-0.3377627373	1.1501494413	9.3234331641
C	0.3377644048	-1.1501488546	9.3234330836
C	-0.0000009365	-0.0000002009	10.0486003283
C	0.0000009606	-0.0000002742	11.5258444019
C	0.4204911430	1.1225803552	12.2507938054
C	-0.4204934055	-1.1225793886	12.2507939690
C	0.4199755941	1.1225986801	13.6383144613
C	-0.4199737401	-1.1225993378	13.6383145688
C	-0.0000008915	0.0000003516	14.3631509704
C	-0.000001663	0.0000001850	15.8415830859
C	1.0229514449	0.6319305619	16.5606789892
C	-1.0229510225	-0.6319313617	16.5606792841
C	1.0228580557	0.6325548546	17.9509239659
C	-1.0228592162	-0.6325531726	17.9509241248
C	0.0000005373	-0.0000009302	18.6524505392
H	1.7037341000	1.3032500398	-3.0875873361
H	1.7257764262	1.2745902291	-5.5415724609
H	-1.7257763005	-1.2745907516	-5.5415720003
H	-1.7037337213	-1.3032494823	-3.0875872523
H	2.1452185054	-0.0193124807	-1.2265288549
H	2.1452183053	0.0193125240	1.2265292241
H	-2.1452186334	-0.0193120717	1.2265289788
H	-2.1452180920	0.0193122959	-1.2265290447
H	0.5853196948	2.0638596917	-7.4030403425
H	-0.5853204990	-2.0638595804	-7.4030403526
H	0.6222205389	2.0529479146	-9.8565691684
H	-0.6222204032	-2.0529481875	-9.8565693386
H	-0.7704097277	2.0023421657	-11.7181056580
H	0.7704096419	-2.0023418819	-11.7181057819
H	-0.7344234001	2.0153213469	-14.1717477306
H	0.7344232717	-2.0153213124	-14.1717478700

H	1.8401618842	-1.1037896405	-16.0222129399
H	-1.8401615462	1.1037895990	-16.0222129831
H	1.8308467105	-1.1210477191	-18.4881792244
H	-1.8308466683	1.1210478402	-18.4881793028
H	0.0000000020	-0.0000000422	-19.7384477723
H	1.7037335538	-1.3032503257	3.0875873325
H	-1.7037339776	1.3032495796	3.0875875109
H	1.7257761176	-1.2745903587	5.5415721601
H	-1.7257760560	1.2745904820	5.5415722487
H	0.5853201329	-2.0638597190	7.4030403693
H	-0.5853202098	2.0638595378	7.4030403788
H	0.6222204334	-2.0529480478	9.8565692123
H	-0.6222207480	2.0529479733	9.8565693415
H	0.7704099090	2.0023420550	11.7181056925
H	-0.7704093458	-2.0023420385	11.7181057587
H	0.7344233178	2.0153213106	14.1717478058
H	-0.7344232497	-2.0153213868	14.1717478074
H	1.8401618134	1.1037896502	16.0222129479
H	-1.8401615664	-1.1037896723	16.0222129765
H	1.8308467040	1.1210476497	18.4881791931
H	-1.8308466236	-1.1210479964	18.4881793322
H	-0.0000000098	0.0000000533	19.7384477731

Cartesian coordinates (in Å) of [10]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	20.8065566135	0.0000364246	-0.0001358910
C	20.1050132385	1.1711265701	0.2734808787
C	20.1050123809	-1.1711589289	-0.2732778885
C	18.7148892769	1.1711721093	0.2722997280
C	18.7148947113	-1.1711335305	-0.2724794029
C	17.9956260066	-0.0000523542	0.0001625654
C	16.5171304240	0.0000435422	-0.0000354287
C	15.7928406758	0.7667101100	0.9216947950
C	15.7928397436	-0.7667783687	-0.9216425612
C	14.4053392993	0.7671680178	0.9215500515
C	14.4053348343	-0.7671557690	-0.9215949960
C	13.6811565722	-0.0000722429	0.0000437195
C	12.2038435244	-0.0000511075	-0.0000051391
C	11.4793572532	0.0453686686	1.1979336980
C	11.4793512689	-0.0453127843	-1.1979663757
C	10.0917540129	0.0452487480	1.1979121437
C	10.0917294894	-0.0453046644	-1.1979387299
C	9.3669840141	0.0000960466	0.0000036789
C	7.8898957674	-0.0000744158	-0.0000455381
C	7.1650949428	-0.6841801975	0.9844074319
C	7.1650927102	0.6842788202	-0.9843375229
C	5.7776870015	-0.6842929115	0.9843721781
C	5.7776907162	0.6844005164	-0.9842935009
C	5.0528796381	-0.0000842150	-0.0000744232
C	3.5759690573	0.0000610173	0.0001338801
C	2.8507740616	-1.1362614807	0.3819460921
C	2.8507656776	1.1361967075	-0.3821388880
C	1.4634383101	-1.1361890301	0.3823173367
C	1.4634419185	1.1362091994	-0.3822683517
C	0.7385123995	-0.0000019622	-0.0000279470
C	-0.7385121915	-0.0000075889	0.0000089758
C	-1.4634437747	-1.1361878290	-0.3823237675
C	-1.4634366881	1.1362117504	0.3822572312
C	-2.8507693303	-1.1362170016	-0.3820596408
C	-2.8507706536	1.1362430231	0.3820199422
C	-3.5759688483	-0.0000246424	0.0000552876
C	-5.0528794007	0.0000871334	-0.0000602563
C	-5.7776910200	-0.6843692418	-0.9843043428
C	-5.7776863992	0.6843295501	0.9843574007
C	-7.1650921881	-0.6842597042	-0.9843469839
C	-7.1650951905	0.6842053265	0.9843933180
C	-7.8898957986	0.0000073275	-0.0000066143
C	-9.3669840370	-0.0000027003	0.0000091217
C	-10.0917374569	0.0453144773	-1.1979251453
C	-10.0917460241	-0.0452308745	1.1979260120
C	-11.4793576914	0.0452469598	-1.1979612193
C	-11.4793507808	-0.0454266544	1.1979392486
C	-12.2038435214	0.0000567855	0.0000021110
C	-13.6811566623	-0.0000454926	-0.0000124014
C	-14.4053426308	0.7672366870	-0.9214946822
C	-14.4053314740	-0.7670808677	0.9216555567
C	-15.7928468438	0.7666918003	-0.9217115077
C	-15.7928335763	-0.7667903141	0.9216310154
C	-16.5171304075	-0.0000919934	-0.0000869540
C	-17.9956261040	-0.0000211090	-0.0000136611
C	-18.7148767590	1.1711694097	-0.2723388520
C	-18.7149075419	-1.1711345349	0.2724481536
C	-20.1050035989	1.1711649523	-0.2733729783
C	-20.1050220087	-1.1711187770	0.2733936296
C	-20.8065565256	0.0000074757	-0.0000595167
H	5.2447922754	1.2096223150	-1.7720534621
H	7.6985687562	1.2384899210	-1.7515507212
H	7.6986010496	-1.2384905035	1.7515321106
H	5.2448105289	-1.2096562533	1.7720494695
H	3.3837608411	2.0393608367	-0.6659709399
H	0.9303632192	2.0272573173	-0.7018649163
H	0.9303484060	-2.0272477636	0.7018727368
H	3.3837555966	-2.0393584180	0.6660076681
H	9.5586410517	-0.0999270219	-2.1429754189
H	9.5586865958	0.0999474046	2.1429520177

H	12.0127349292	-0.0626572050	-2.1442663575
H	12.0127424930	0.0626649674	2.1442222360
H	13.8707210887	-1.3853082209	-1.6372783863
H	13.8707350704	1.3852933813	1.6372623705
H	16.3272379965	-1.3567160381	-1.6609907188
H	16.3272471890	1.3567099847	1.6609771224
H	18.1756892804	2.0958310114	0.4583821375
H	18.1756948161	-2.0958205397	-0.4584010337
H	20.6428373245	2.0923205767	0.4792215584
H	20.6428177538	-2.0923006899	-0.4792628888
H	21.8926274617	-0.0000068256	0.0000247978
H	-0.9303471855	2.0272512292	0.7018713290
H	-0.9303649029	-2.0272569887	-0.7018568540
H	-3.3837492082	2.0393752502	0.6659855408
H	-3.3837678111	-2.0393469726	-0.6659834381
H	-5.2448056677	1.2096655402	1.7720529533
H	-5.2447974889	-1.2096235971	-1.7720428150
H	-7.6985916834	1.2385163767	1.7515264038
H	-7.6985781333	-1.2384738607	-1.7515487953
H	-9.5586613784	0.0999384341	-2.1429675639
H	-9.5586663754	-0.0999219683	2.1429606182
H	-12.0127459714	0.0626979136	-2.1442455131
H	-12.0127313660	-0.0626103675	2.1442435459
H	-13.8707517846	1.3852900769	-1.6372779703
H	-13.8707044070	-1.3853004247	1.6372722011
H	-16.3272548173	1.3567180685	-1.6609705784
H	-16.3272302659	-1.3566964939	1.6610065339
H	-18.1756706019	2.0958305824	-0.4584302139
H	-18.1757138667	-2.0958177770	0.4583676333
H	-20.6428324283	2.0923230834	-0.4792638114
H	-20.6428225765	-2.0922948169	0.4792352852
H	-21.8926273318	0.0000158183	0.0000085580

Cartesian coordinates (in Å) of [11]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-22.9664709398	0.0000237811	-0.0000472627
C	-22.2649230335	1.2005969090	0.0683350113
C	-22.2649348195	-1.2005670385	-0.0682443784
C	-20.8746046789	1.2003025637	0.0692756071
C	-20.8746231897	-1.2002787578	-0.0694489018
C	-20.1553216607	-0.0000134059	0.0001132962
C	-18.6768544935	-0.0000445698	-0.0000597663
C	-17.9522487318	0.9934226319	-0.6705545243
C	-17.9522480763	-0.9934463857	0.6706153236
C	-16.5647455966	0.9938244283	-0.6703254163
C	-16.5647213554	-0.9939069987	0.6702982295
C	-15.8399399016	0.0000053966	0.0000321266
C	-14.3629861344	0.0000001775	-0.0000011630
C	-13.6376151687	0.4014160852	-1.1293934435
C	-13.6375937023	-0.4013030129	1.1294368466
C	-12.2503073702	0.4021162023	-1.1292339335
C	-12.2502776938	-0.4021787515	1.1291913323
C	-11.5251416174	0.0000059064	-0.0000163143
C	-10.0481346034	0.0000095916	-0.0000190369
C	-9.3229152067	-0.3533697342	-1.1454115634
C	-9.3229348547	0.3533693579	1.1454104148
C	-7.9356312319	-0.3525136775	-1.1456195987
C	-7.9356393998	0.3525177854	1.1456437747
C	-7.2102136198	-0.0000608685	0.0000318656
C	-5.7332496320	0.0000445354	-0.0000128076
C	-5.0082184676	-0.9595875971	-0.7185528231
C	-5.0081948371	0.9596450801	0.7185438335
C	-3.6208524466	-0.9594183645	-0.7187921919
C	-3.6208215657	0.9594319731	0.7187878611
C	-2.8959459327	-0.0000152376	0.0000054702
C	-1.4187538719	-0.0000103836	-0.0000208815
C	-0.6937925471	-1.1986811091	0.0002074643
C	-0.6938001274	1.1986597209	-0.0002010149
C	0.6938001332	-1.1986715071	-0.0001843360
C	0.6937924411	1.1986692906	0.0002239160
C	1.4187536846	-0.0000017770	0.0000019475
C	2.8959457642	0.0000263936	0.0000149324
C	3.6208292765	-0.9594309385	0.7187665334
C	3.6208449737	0.9594189963	-0.7188136767
C	5.0081966042	-0.9596270850	0.7185373226
C	5.0082169349	0.9596054696	-0.7185597004
C	5.7332494586	-0.0000249483	-0.0000130233
C	7.2102134815	0.0000302550	0.0000148038
C	7.9356329139	-0.3525287893	1.1456384032
C	7.9356374847	0.3525027892	-1.1456248049
C	9.3229281625	-0.3533696639	1.1454173959
C	9.3229216627	0.3533701882	-1.1454040525
C	10.0481346530	-0.0000014676	-0.0000047976
C	11.5251416493	-0.0000164982	-0.0000015075
C	12.2502834993	0.4021860829	1.1291954267
C	12.2503016014	-0.4021076942	-1.1292302770
C	13.6375974732	0.4013278266	1.1294263347
C	13.6376114367	-0.4013900949	-1.1294043809
C	14.3629861663	0.0000057048	-0.0000030401
C	15.8399399124	0.0000002368	0.0000136682
C	16.5647237125	0.9938870501	0.6703069625
C	16.5647432380	-0.9938437432	-0.6703175915
C	17.9522480569	0.9934258628	0.6706269609
C	17.9522487594	-0.9934425626	-0.6705437552
C	18.6768545214	0.0000439405	-0.0000714872
C	20.1553217142	0.0000054621	0.0000086033
C	20.8746204225	1.2002885444	-0.0693321648
C	20.8746072980	-1.2002927538	0.0693913088
C	22.2649331067	1.2005631893	-0.0683868706
C	22.2649246284	-1.2006012194	0.0681914854
C	22.9664711623	-0.0000085990	0.0001164599
H	-7.4028190451	0.6128906384	2.0559289937
H	-9.8558561318	0.6504557403	2.0442953789
H	-9.8558358113	-0.6504790438	-2.0442821844
H	-7.4028070276	-0.6128543158	-2.0559045098

H	-5.5410815780	1.7287918895	1.2705865005
H	-3.0872345093	1.7064593624	1.2997066053
H	-3.0872855252	-1.7064679223	-1.2996991891
H	-5.5411146261	-1.7287658727	-1.2705363798
H	-11.7176771010	-0.7377095126	2.0146265543
H	-11.7177019321	0.7377373103	-2.0146366418
H	-14.1703071260	-0.7005129321	2.0277761138
H	-14.1703415593	0.7005344451	-2.0277596520
H	-16.0321006389	-1.7892583555	1.1842654912
H	-16.0321216586	1.7892253180	-1.1841869317
H	-18.4860266252	-1.7680962929	1.2141547084
H	-18.4860194474	1.7680539158	-1.2141158666
H	-20.3360327743	2.1401416107	0.1527133720
H	-20.3360615939	-2.1401315309	-0.1526677805
H	-22.8022827360	2.1426108216	0.1312649457
H	-22.8022891044	-2.1425732524	-0.1312727998
H	-24.0525525484	0.0000216233	-0.0000110229
H	-1.2265348595	2.1452557386	-0.0193868932
H	-1.2265207332	-2.1452800746	0.0193879947
H	1.2265157858	2.1452709820	0.0193865053
H	1.2265403183	-2.1452645034	-0.0193884196
H	3.0872755508	1.7064883029	-1.2996969449
H	3.0872451415	-1.7064388386	1.2997089539
H	5.5411170068	1.7287771496	-1.2705534946
H	5.5410799375	-1.7287803550	1.2705695215
H	7.4028092076	-0.6128878607	2.0559252008
H	7.4028171197	0.6128578731	-2.0559081351
H	9.8558494363	-0.6504616534	2.0443009107
H	9.8558423870	0.6504738185	-2.0442760477
H	11.7176863696	0.7377142274	2.0146327653
H	11.7176927499	-0.7377307218	-2.0146311831
H	14.1703179111	0.7005078299	2.0277710474
H	14.1703308070	-0.7005374653	-2.0277654658
H	16.0320984607	1.7892532689	1.1842430314
H	16.0321238093	-1.7892293550	-1.1842109327
H	18.4860180882	1.7681020272	1.2141346025
H	18.4860279757	-1.7680471549	-1.2141374446
H	20.3360348463	-2.1401392054	0.1526974107
H	20.3360595002	2.1401340087	-0.1526820411
H	22.8022842289	-2.1426048797	0.1312829767
H	22.8022877827	2.1425797005	-0.1312530632
H	24.0525529303	-0.0000171359	-0.0000445279

Cartesian coordinates (in Å) of [12]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	25.1253590780	-0.0000004886	-0.0000012092
C	24.4237536728	-1.1075011313	0.4688029766
C	24.4237537035	1.1075020392	-0.4688008855
C	23.0336048754	-1.1070172113	0.4693039458
C	23.0336049945	1.1070163834	-0.4693056525
C	22.3142372798	0.0000002084	0.0000006712
C	20.8356683417	0.0000001123	-0.0000004351
C	20.1109601873	-1.1595039009	-0.3037136014
C	20.1109600963	1.1595037016	0.3037143617
C	18.7234677280	-1.1598452767	-0.3030003459
C	18.7234675501	1.1598454638	0.3029996558
C	17.9984143007	-0.0000000848	0.0000002794
C	16.5210626005	-0.0000002571	0.0000001499
C	15.7960713423	-0.7495440730	-0.9356772023
C	15.7960712398	0.7495446185	0.9356766744
C	14.4086731392	-0.7499409222	-0.9354013366
C	14.4086729803	0.7499399300	0.9354020646
C	13.6838212863	0.0000005780	-0.0000004772
C	12.2063533476	-0.0000011905	0.0000001226
C	11.4813471792	-0.0357616572	-1.1981033381
C	11.4813471141	0.0357640175	1.1981033170
C	10.0937186122	-0.0361514741	-1.1980793595
C	10.0937184985	0.0361492109	1.1980796598
C	9.3685775429	0.0000008694	0.0000001185
C	7.8912693599	-0.0000007620	-0.0000003253
C	7.1662020551	0.6879092315	-0.9817303516
C	7.1662022032	-0.6879076738	0.9817317966
C	5.7787637265	0.6876478697	-0.9819220482
C	5.7787638163	-0.6876496725	0.9819208877
C	5.0537392669	0.0000008987	0.0000007509
C	3.5766479704	-0.0000000327	-0.0000003593
C	2.8512270791	1.1379722406	-0.3765809295
C	2.8512272076	-1.1379720402	0.3765809301
C	1.4638872379	1.1377727712	-0.3771888319
C	1.4638872981	-1.1377724291	0.3771892175
C	0.7385956290	0.0000000470	-0.0000002205
C	-0.7385954292	-0.0000000140	-0.0000000684
C	-1.4638872370	1.1377725353	0.3771892280
C	-1.4638870525	-1.1377727378	-0.3771889167
C	-2.8512270792	1.1379721959	0.3765806170
C	-2.8512269634	-1.1379720173	-0.3765813208
C	-3.5766477359	-0.0000001311	0.0000002652
C	-5.0537390331	0.0000001579	-0.0000001018
C	-5.7787636906	0.6876485432	0.9819215461
C	-5.7787638077	-0.6876489656	-0.9819212284
C	-7.1662020962	0.6879085232	0.9817309653
C	-7.1662021323	-0.6879080661	-0.9817313772
C	-7.8912691713	-0.0000002134	0.0000000760
C	-9.3685774044	0.0000001587	0.0000000099
C	-10.0937183796	-0.0361503634	1.1980794686
C	-10.0937185200	0.0361502777	-1.1980794475
C	-11.4813470237	-0.0357629327	1.1981031920
C	-11.4813470977	0.0357628098	-1.1981032235
C	-12.2063533769	0.0000002721	-0.0000000080
C	-13.6838213046	-0.0000001204	-0.0000000790
C	-14.4086729844	-0.7499402671	0.9354018485
C	-14.4086731568	0.7499404769	-0.9354016289
C	-15.7960712542	-0.7495444409	0.9356768304
C	-15.7960713440	0.7495442151	-0.9356770806
C	-16.5210626089	0.0000000166	-0.0000000179
C	-17.9984143100	-0.0000000111	-0.0000001378
C	-18.7234677183	-1.1598452956	0.3030001589
C	-18.7234675732	1.1598454382	-0.3029998743
C	-20.1109601837	-1.1595038377	0.3037137617
C	-20.1109601111	1.1595037553	-0.3037142348
C	-20.8356683485	0.0000001064	0.0000003587
C	-22.3142372869	0.0000002092	-0.0000006769
C	-23.0336048804	-1.1070172257	-0.4693039127
C	-23.0336050013	1.1070163824	0.4693056545
C	-24.4237536764	-1.1075011319	-0.4688029746

C	-24.4237537112	1.1075020524	0.4688008559
C	-25.1253590829	-0.0000004916	0.0000012110
H	9.5610547707	0.0839299411	2.1436545463
H	12.0141127423	0.0451506759	2.1447816342
H	12.0141125271	-0.0451510038	-2.1447817871
H	9.5610547319	-0.0839296104	-2.1436542590
H	7.6993784646	-1.2453979728	1.7467094948
H	5.2460581164	-1.2154705360	1.7680277347
H	5.2460584061	1.2154708410	-1.7680277477
H	7.6993784873	1.2453973880	-1.7467094267
H	13.8748939799	1.3552053406	1.6625493890
H	13.8748940508	-1.3552048268	-1.6625497332
H	16.3293458867	1.3259865029	1.6863238250
H	16.3293459814	-1.3259865523	-1.6863238698
H	18.1901992275	2.0802123792	0.5238574638
H	18.1901992799	-2.0802122212	-0.5238574954
H	20.6449396430	2.0700494818	0.5607453409
H	20.6449397448	-2.0700494054	-0.5607454988
H	22.4954498856	-1.9643365955	0.8638425424
H	22.4954498832	1.9643365719	-0.8638421271
H	24.9612473055	-1.9733341255	0.8449088982
H	24.9612472893	1.9733340616	-0.8449090890
H	26.2113685648	0.0000000457	0.0000001020
H	3.3839922737	-2.0426265784	0.6559069548
H	3.3839922410	2.0426264782	-0.6559074915
H	0.9312117964	-2.0303407838	0.6929877279
H	0.9312116707	2.0303409463	-0.6929876971
H	-0.9312118490	-2.0303410496	-0.6929879962
H	-0.9312119424	2.0303408376	0.6929879795
H	-3.3839924290	-2.0426264575	-0.6559069581
H	-3.3839925377	2.0426264315	0.6559069061
H	-5.2460584737	1.2154707743	1.7680277692
H	-5.2460584593	-1.2154707701	-1.7680275483
H	-7.6993786314	1.2453974999	1.7467094479
H	-7.6993786919	-1.2453975476	-1.7467094577
H	-9.5610548285	-0.0839300511	2.1436544601
H	-9.5610548622	0.0839300105	-2.1436543220
H	-12.0141125810	-0.0451507226	2.1447815257
H	-12.0141126164	0.0451507205	-2.1447815756
H	-13.8748939934	-1.3552051069	1.6625496523
H	-13.8748940557	1.3552049961	-1.6625495184
H	-16.3293458910	-1.3259865113	1.6863238387
H	-16.3293460084	1.3259864512	-1.6863239242
H	-18.1901992413	2.0802124110	-0.5238574474
H	-18.1901992786	-2.0802121841	0.5238575543
H	-20.6449396702	2.0700494827	-0.5607453779
H	-20.6449397282	-2.0700493951	0.5607454983
H	-22.4954498836	-1.9643366051	-0.8638425142
H	-22.4954498970	1.9643365834	0.8638421139
H	-24.9612473080	-1.9733341313	-0.8449088798
H	-24.9612472968	1.9733340723	0.8449090666
H	-26.2113685688	0.0000000489	-0.0000001025

Cartesian coordinates (in Å) of [13]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	27.2803786915	-0.0000047087	-0.0000049716
C	26.5791115889	0.8914257859	-0.8075987416
C	26.5791092379	-0.8914131603	0.8076114646
C	25.1889788641	0.8909802147	-0.8078524981
C	25.1889785758	-0.8909950400	0.8078309166
C	24.4702883645	0.0000156701	0.0000153459
C	22.9915770784	-0.0000083484	0.0000016505
C	22.2674789127	1.1958901051	-0.0816949880
C	22.2674736315	-1.1958991514	0.0816800856
C	20.8797611363	1.1959891392	-0.0818277935
C	20.8797556875	-1.1959920737	0.0818791501
C	20.1550425175	-0.0000016091	-0.0000457880
C	18.6778906654	-0.0000184471	0.0000297458
C	17.9528808564	1.0060680163	0.6516422683
C	17.9528855584	-1.0060529906	-0.6516797714
C	16.5654320653	1.0061403628	0.6516408571
C	16.5654359331	-1.0061463719	-0.6516441036
C	15.8404747825	-0.0000150296	0.0000070644
C	14.3635039976	0.0000852660	-0.0000296452
C	13.6381359752	0.4154071954	1.1243478992
C	13.6381315803	-0.4155203687	-1.1242928152
C	12.2507620507	0.4159996483	1.1241751460
C	12.2507638093	-0.4158821979	-1.1242041005
C	11.5255507216	-0.0000703206	0.0000312866
C	10.0484064247	-0.0000178686	-0.0000149832
C	9.3232017067	-0.3416331346	1.1489863944
C	9.3231996956	0.3416844028	-1.1489838355
C	7.9358463277	-0.3412126577	1.1490799820
C	7.9358413348	0.3411367018	-1.1491150517
C	7.2105314779	0.0000602175	0.0000162925
C	5.7334468271	-0.0000166155	-0.0000149188
C	5.0084890164	-0.9576642993	0.7211936521
C	5.0084928142	0.9576753116	-0.7211805114
C	3.6210570004	-0.9576831202	0.7211377186
C	3.6210608142	0.9576968788	-0.7211198698
C	2.8961730405	-0.0000113875	-0.0000220636
C	1.4188490905	0.0000010687	0.0000548052
C	0.6938239169	-1.1986386507	-0.0001598570
C	0.6938218585	1.1986339311	0.0000848247
C	-0.6938238262	-1.1986383987	0.0001561802
C	-0.6938218936	1.1986341670	-0.0000884058
C	-1.4188489556	0.0000006451	-0.0000495503
C	-2.8961729070	-0.0000093941	0.0000204820
C	-3.6210583446	-0.9576813274	-0.7211369704
C	-3.6210596512	0.9576984275	0.7211206486
C	-5.0084909657	-0.9576751583	-0.7211770695
C	-5.0084910585	0.9576645093	0.7211971884
C	-5.7334466811	0.0000158579	-0.0000143218
C	-7.2105313566	-0.0000408928	0.0000121971
C	-7.9358424495	-0.3411486839	-1.1491079456
C	-7.9358450207	0.3412006977	1.1490869578
C	-9.3232005248	-0.3416839163	-1.1489806455
C	-9.3232006810	0.3416342206	1.1489891552
C	-10.0484064619	0.0000297135	-0.0000116794
C	-11.5255507606	0.0000100702	0.0000076994
C	-12.2507628467	0.4159273879	-1.1241917266
C	-12.2507630580	-0.4159537874	1.1241877250
C	-13.6381328789	0.4154795748	-1.1243116966
C	-13.6381346665	-0.4154473888	1.1243291737
C	-14.3635039932	-0.0000241163	-0.0000075137
C	-15.8404747819	0.0000009814	-0.0000036078
C	-16.5654346673	1.0061473037	-0.6516387258
C	-16.5654333559	-1.0061391545	0.6516466603
C	-17.9528843685	1.0060526366	-0.6516764365
C	-17.9528820701	-1.0060680880	0.6516460358
C	-18.6778906783	0.0000147798	0.0000259322
C	-20.1550425287	0.0000020960	-0.0000428928
C	-20.8797557462	1.1959923840	0.0818779685
C	-20.8797610992	-1.1959888601	-0.0818284674
C	-22.2674736565	1.1958994358	0.0816803004

C	-22.2674789080	-1.1958898537	-0.0816942661
C	-22.9915770915	0.0000085523	0.0000024691
C	-24.4702883778	-0.0000152772	0.0000154316
C	-25.1889785542	0.8909953422	0.8078312053
C	-25.1889789079	-0.8909802535	-0.8078518424
C	-26.5791092216	0.8914136263	0.8076116019
C	-26.5791116247	-0.8914256588	-0.8075982343
C	-27.2803786986	0.0000049546	-0.0000045686
H	7.4026768099	-0.5925840713	2.0617194404
H	9.8562474273	-0.6292241453	2.0509011982
H	9.8562507911	0.6292132591	-2.0509146920
H	7.4026736717	0.5926015815	-2.0617267734
H	5.5417143525	-1.7252727800	1.2750972243
H	3.0873883305	-1.7036069959	1.3034216314
H	3.0873882335	1.7036064945	-1.3034211858
H	5.5417133126	1.7252755682	-1.2750976519
H	11.7182163357	0.7622197007	2.0055222519
H	11.7182198134	-0.7622354741	-2.0055024055
H	14.1708474053	0.7259007797	2.0188969298
H	14.1708432464	-0.7258762316	-2.0188923936
H	16.0328346652	1.8107756869	1.1509873655
H	16.0328311845	-1.8107735541	-1.1509974926
H	18.4860129869	1.7907715929	1.1812473019
H	18.4860135118	-1.7907803873	-1.1812494301
H	20.3465135748	-2.1388482446	0.1655084052
H	20.3465138463	2.1388395113	-0.1655166431
H	22.8016400604	-2.1407814991	0.1284484711
H	22.8016394693	2.1407762785	-0.1284441950
H	1.2265628357	-2.1452558775	-0.0191414011
H	1.2265627295	2.1452498140	0.0191526378
H	-1.2265640975	-2.1452550065	0.0191426992
H	-1.2265618920	2.1452504087	-0.0191517848
H	-3.0873890551	-1.7036054959	-1.3034213327
H	-3.0873880365	1.7036082585	1.3034211517
H	-5.5417128217	-1.7252735487	-1.2750968419
H	-5.5417154551	1.7252747476	1.2750978566
H	-7.4026765102	0.5925882979	2.0617216919
H	-7.4026741740	-0.5925979398	-2.0617243841
H	-9.8562487053	0.6292228509	2.0509035365
H	-9.8562494292	-0.6292150482	-2.0509118683
H	-11.7182171981	-0.7622250244	2.0055156552
H	-11.7182190412	0.7622291479	-2.0055093448
H	-14.1708461096	-0.7258924561	2.0188958645
H	-14.1708445333	0.7258835417	-2.0188937659
H	-16.0328340242	-1.8107748783	1.1509908106
H	-16.0328318372	1.8107738798	-1.1509947829
H	-18.4860139980	-1.7907728117	1.1812486288
H	-18.4860125207	1.7907786794	-1.1812488486
H	-20.3465131921	2.1388482586	0.1655081598
H	-20.3465142553	-2.1388395647	-0.1655159988
H	-22.8016399378	2.1407818082	0.1284484156
H	-22.8016396177	-2.1407760171	-0.1284433647
H	-24.6486290675	-1.5706339139	-1.4606318716
H	-24.6486233318	1.5706264843	1.4606317664
H	-27.1176133612	-1.5850682121	-1.4470858705
H	-27.1176071966	1.5850761570	1.4470807715
H	-28.3664122636	0.0000065686	-0.0000029131
H	24.6486290567	1.5706338839	-1.4606325381
H	24.6486233267	-1.5706259155	1.4606317409
H	27.1176133235	1.5850681576	-1.4470865887
H	27.1176072209	-1.5850756170	1.4470806991
H	28.3664122559	-0.0000063376	-0.0000033622

Cartesian coordinates (in Å) of [14]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	29.4406727245	0.0000000292	0.0000000116
C	28.7390691812	-0.6061216098	1.0386128561
C	28.7390692420	0.6061218317	-1.0386127328
C	27.3487779715	-0.6059634599	1.0384944561
C	27.3487781053	0.6059631699	-1.0384945658
C	26.6295370610	0.0000000046	0.0000000273
C	25.1508654841	0.0000000109	-0.0000000072
C	24.4258748270	-1.1140791069	0.4420633828
C	24.4258747439	1.1140788969	-0.4420639616
C	23.0383453099	-1.1139372936	0.4426929526
C	23.0383451707	1.1139374460	-0.4426926298
C	22.3134609449	0.0000000004	-0.0000000028
C	20.8364927524	-0.0000000070	0.0000000255
C	20.1113911328	-1.1575479228	-0.3111100061
C	20.1113911731	1.1575479459	0.3111098633
C	18.7240120085	-1.1578693492	-0.3102198348
C	18.7240121046	1.1578692364	0.3102199645
C	17.9985968985	-0.0000000463	0.0000000362
C	16.5212017724	-0.0000002776	0.0000002673
C	15.7960322610	-0.7447548279	-0.9394582333
C	15.7960321594	0.7447556492	0.9394576432
C	14.4085616033	-0.7449283789	-0.9392801083
C	14.4085614468	0.7449280626	0.9392804611
C	13.6836538155	0.0000000447	-0.0000000057
C	12.2062338495	0.0000005233	-0.0000001125
C	11.4812096782	-0.0288480679	-1.1982899270
C	11.4812096503	0.0288471338	1.1982897952
C	10.0935769639	-0.0290545141	-1.1982539679
C	10.0935768864	0.0290550699	1.1982538947
C	9.3684398293	-0.0000002158	-0.0000000349
C	7.8912121026	0.0000006418	0.0000004429
C	7.1661392203	0.6930209830	-0.9781040064
C	7.1661392108	-0.6930221816	0.9781030929
C	5.7787305385	0.6926739819	-0.9783944683
C	5.7787304512	-0.6926735474	0.9783949352
C	5.0536873184	-0.0000000702	0.0000000472
C	3.5767141735	-0.0000002051	-0.0000002119
C	2.8512306454	1.1387095555	-0.3741688202
C	2.8512307904	-1.1387095303	0.3741696843
C	1.4639388788	1.1384575286	-0.3750277637
C	1.4639389961	-1.1384584435	0.3750255160
C	0.7385476339	0.0000003298	0.0000015149
C	-0.7385474617	0.0000001044	0.0000000434
C	-1.4639390366	1.1384581862	0.3750261743
C	-1.4639388793	-1.1384575314	-0.3750274495
C	-2.8512307775	1.1387093194	0.3741704118
C	-2.8512307046	-1.1387098193	-0.3741682116
C	-3.5767139880	0.0000004168	-0.0000008760
C	-5.0536871738	-0.0000001044	0.0000000520
C	-5.7787304475	0.6926735552	0.9783947362
C	-5.7787303212	-0.6926736652	-0.9783947574
C	-7.1661391486	0.6930216555	0.9781033449
C	-7.1661390857	-0.6930215988	-0.9781033957
C	-7.8912121236	0.0000000120	-0.0000000139
C	-9.3684398414	-0.0000000007	-0.0000000108
C	-10.0935768750	-0.0290547118	1.1982539266
C	-10.0935769718	0.0290547441	-1.1982539480
C	-11.4812096411	-0.0288476185	1.1982898267
C	-11.4812096874	0.0288475102	-1.1982899037
C	-12.2062338451	0.0000000040	-0.0000000509
C	-13.6836538139	-0.0000000118	-0.0000000113
C	-14.4085614652	-0.7449280836	0.9392803931
C	-14.4085615739	0.7449282997	-0.9392802255
C	-15.7960321819	-0.7447551707	0.9394579588
C	-15.7960322244	0.7447553181	-0.9394579020
C	-16.5212017698	0.0000000525	-0.0000000082
C	-17.9985968986	-0.0000000160	-0.0000000066
C	-18.7240119978	-1.1578693007	0.3102199458
C	-18.7240121191	1.1578692543	-0.3102199675
C	-20.1113911273	-1.1575479402	0.3111099327

C	-20.1113911836	1.1575479430	-0.3111098938
C	-20.8364927505	-0.0000000104	-0.0000000251
C	-22.3134609426	0.0000000021	0.0000000058
C	-23.0383453114	-1.1139373802	-0.4426927230
C	-23.0383451723	1.1139373666	0.4426928371
C	-24.4258748235	-1.1140789240	-0.4420638439
C	-24.4258747501	1.1140790832	0.4420634919
C	-25.1508654855	-0.0000000935	0.0000002748
C	-26.6295370618	0.0000000102	-0.0000000208
C	-27.3487779649	-0.6059632814	-1.0384945516
C	-27.3487781120	0.6059633508	1.0384944698
C	-28.7390691791	-0.6061218879	-1.0386126994
C	-28.7390692463	0.6061215883	1.0386128683
C	-29.4406727259	0.0000001330	-0.0000000891
H	5.2461201489	-1.2241263199	1.7621611723
H	7.6992351977	-1.2543982923	1.7403280084
H	7.6992349900	1.2543985832	-1.7403280084
H	5.2461200051	1.2241262785	-1.7621608353
H	3.3837695087	-2.0441236969	0.6516267755
H	0.9316489337	-2.0318433433	0.6892999963
H	0.9316492113	2.0318435712	-0.6892996861
H	3.3837695016	2.0441233494	-0.6516267433
H	9.5609138708	0.0711026636	2.1441572291
H	9.5609138404	-0.0711026206	-2.1441571665
H	12.0138903441	0.0330756497	2.1451040163
H	12.0138904157	-0.0330755124	-2.1451041327
H	13.8747112054	1.3459618193	1.6699754726
H	13.8747112510	-1.3459617196	-1.6699752896
H	16.3291040940	1.3172772421	1.6933399187
H	16.3291041951	-1.3172772975	-1.6933398384
H	18.1910757487	-2.0770873225	-0.5367759612
H	18.1910757657	2.0770871326	0.5367759682
H	20.6449514679	-2.0664467486	-0.5747944123
H	20.6449514893	2.0664467413	0.5747944107
H	-0.9316492216	-2.0318433814	-0.6892998941
H	-0.9316492238	2.0318434738	0.6892998083
H	-3.3837696230	-2.0441233494	-0.6516269441
H	-3.3837697348	2.0441236188	0.6516265873
H	-5.2461201345	-1.2241263614	-1.7621610826
H	-5.2461202107	1.2241262461	1.7621609524
H	-7.6992350300	-1.2543982885	-1.7403279222
H	-7.6992351177	1.2543982718	1.7403279009
H	-9.5609138855	-0.0711027003	2.1441572620
H	-9.5609138644	0.0711025658	-2.1441571722
H	-12.0138903850	-0.0330755689	2.1451040243
H	-12.0138903849	0.0330755176	-2.1451041262
H	-13.8747112195	-1.3459618629	1.6699753841
H	-13.8747112225	1.3459616685	-1.6699753815
H	-16.3291041233	-1.3172772561	1.6933398540
H	-16.3291041444	1.3172772537	-1.6933399219
H	-18.1910757306	-2.0770872993	0.5367759440
H	-18.1910757874	2.0770871542	-0.5367759819
H	-20.6449514357	-2.0664467543	0.5747944448
H	-20.6449515227	2.0664467276	-0.5747944176
H	-22.5057080115	1.9865822753	0.8102430635
H	-22.5057080489	-1.9865821673	-0.8102429403
H	-24.9587184433	2.0008140932	0.7741742089
H	-24.9587185410	-2.0008141307	-0.7741740096
H	-26.8103551504	-1.0576600660	-1.8670676174
H	-26.8103551312	1.0576600788	1.8670673903
H	-29.2766238140	-1.0741426665	-1.8584660266
H	-29.2766238226	1.0741427044	1.8584660271
H	-30.5267388300	-0.0000000048	-0.0000000060
H	22.5057080131	1.9865822651	-0.8102430776
H	22.5057080446	-1.9865821673	0.8102429560
H	24.9587184586	2.0008141110	-0.7741741161
H	24.9587185239	-2.0008141002	0.7741741336
H	26.8103551419	-1.0576600419	1.8670676268
H	26.8103551380	1.0576600756	-1.8670673947
H	29.2766238276	-1.0741426959	1.8584659951
H	29.2766238137	1.0741426540	-1.8584660669
H	30.5267388276	0.0000000019	0.0000000087

Cartesian coordinates (in Å) of [15]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-31.5855403659	-0.4390291215	-0.0667740266
C	-30.9272705716	0.7652251669	-0.3010140509
C	-30.8419454584	-1.5891383159	0.1840018429
C	-29.5381174254	0.8191256063	-0.2844857803
C	-29.4530091555	-1.5351647578	0.1989284361
C	-28.7770021153	-0.3304525906	-0.0347553208
C	-27.2995018009	-0.2769674691	-0.0211636861
C	-26.5946943232	0.5319991835	-0.9213830956
C	-26.5564571801	-1.0380171203	0.8903982371
C	-25.2078877201	0.5770131170	-0.9118391589
C	-25.1696512635	-0.9940800055	0.8994720990
C	-24.4646990275	-0.1860472837	-0.0019090023
C	-22.9879835700	-0.1416376223	0.0050894365
C	-22.2606451384	-0.0447434980	-1.1881693500
C	-22.2665233238	-0.1965181727	1.2044864264
C	-20.8736088343	-0.0060716475	-1.1823790146
C	-20.8794121689	-0.1582174692	1.2101801706
C	-20.1517624961	-0.0627384845	0.0168565538
C	-18.6751220159	-0.0251360653	0.0224273072
C	-17.9304245401	-0.6631588232	-0.9780552334
C	-17.9700978773	0.6487975171	1.0280923885
C	-16.5434585009	-0.6298468154	-0.9725420257
C	-16.5829438517	0.6820515139	1.0337384421
C	-15.8383927426	0.0430991107	0.0338746696
C	-14.3617354415	0.0757206527	0.0396109982
C	-13.6111394712	-1.0345525229	-0.3689038632
C	-13.6619455208	1.2169749377	0.4526776033
C	-12.2241565573	-1.0045314154	-0.3653931053
C	-12.2747772999	1.2467234958	0.4571334057
C	-11.5244100224	0.1366646378	0.0478733255
C	-10.0475885837	0.1674163236	0.0509850959
C	-9.3000357603	-0.9661537197	0.3959831433
C	-9.3449562681	1.3295609480	-0.2932928867
C	-7.9130454711	-0.9390072649	0.3952828872
C	-7.9577093389	1.3569812270	-0.2929290192
C	-7.2101561648	0.2227640117	0.0502011110
C	-5.7332834909	0.2478208028	0.0456791588
C	-4.9933820577	-0.4600324275	1.0018479859
C	-5.0232887690	0.9763766695	-0.9176321295
C	-3.6061022809	-0.4433166878	0.9927199106
C	-3.6359256401	0.9931740628	-0.9266312691
C	-2.8960660674	0.2825686836	0.0275074968
C	-1.4188629209	0.2925670285	0.0137027660
C	-0.6821230463	0.2952312101	1.2052756059
C	-0.7054512754	0.2948318877	-1.1918500354
C	0.7054514304	0.2948324989	1.1918502541
C	0.6821231582	0.2952306217	-1.2052756628
C	1.4188627420	0.2925668219	-0.0137026342
C	2.8960659273	0.2825688422	-0.0275075413
C	3.6359254542	0.9931745259	0.9266309114
C	3.6061022467	-0.4433171403	-0.9927194728
C	5.0232886457	0.9763768560	0.9176316764
C	4.9933819711	-0.4600326718	-1.0018478022
C	5.7332835197	0.2478205832	-0.0456791412
C	7.2101561817	0.2227639382	-0.0502012985
C	7.9577092210	1.3569812504	0.2929285939
C	7.9130456150	-0.9390073774	-0.3952828707
C	9.3449561979	1.3295609387	0.2932925933
C	9.3000358519	-0.9661538852	-0.3959829413
C	10.0475885906	0.1674162823	-0.0509852094
C	11.5244100297	0.1366646155	-0.0478734767
C	12.2747772801	1.2467234234	-0.4571337106
C	12.2241565875	-1.0045312907	0.3653933441
C	13.6619454992	1.2169748379	-0.4526780774
C	13.6111395019	-1.0345524250	0.3689039391
C	14.3617354468	0.0757207086	-0.0396110924
C	15.8383927472	0.0430991440	-0.0338746639
C	16.5829439741	0.6820512630	-1.0337385975
C	16.5434583736	-0.6298465617	0.9725422077
C	17.9700979456	0.6487972729	-1.0280925644

C	17.9304244715	-0.6631585814	0.9780553705
C	18.6751220156	-0.0251360464	-0.0224273089
C	20.1517624928	-0.0627384775	-0.0168564984
C	20.8794121636	-0.1582178072	-1.2101800984
C	20.8736088356	-0.0060713814	1.1823790464
C	22.2665233180	-0.1965184912	-1.2044863505
C	22.2606451411	-0.0447432136	1.1881693863
C	22.9879835681	-0.1416376454	-0.0050893786
C	24.4646990250	-0.1860473049	0.0019090771
C	25.1696512648	-0.9940802116	-0.8994718514
C	25.2078877191	0.5770133628	0.9118390125
C	26.5564571794	-1.0380173402	-0.8903979615
C	26.5946943230	0.5319994173	0.9213829774
C	27.2995018008	-0.2769674315	0.0211637431
C	28.7770021134	-0.3304525766	0.0347554035
C	29.4530091520	-1.5351647991	-0.1989280601
C	29.5381174230	0.8191256849	0.2844855672
C	30.8419454546	-1.5891383567	-0.1840014493
C	30.9272705689	0.7652252478	0.3010138551
C	31.5855403622	-0.4390291015	0.0667741434
H	-3.0606374412	-1.0180230530	1.7359733178
H	-5.5146047684	-1.0188718949	1.7741163248
H	-5.5680116368	1.5212238053	-1.6836607611
H	-3.1145140407	1.5795231381	-1.6780212062
H	-1.2054564929	0.3137442897	2.1571194705
H	1.2473642564	0.2750007463	2.1332275179
H	1.2054565575	0.3137434857	-2.1571195633
H	-1.2473640499	0.2750000683	-2.1332273106
H	-7.3624714392	-1.8408530270	0.6480598853
H	-7.4423518213	2.2788539961	-0.5476645898
H	-9.8151526241	-1.8775666981	0.6862293228
H	-9.8955954239	2.2201343058	-0.5831539000
H	-11.6716917193	-1.8756242097	-0.7062875159
H	-11.7622636808	2.1406436090	0.8014330020
H	-14.1239480883	-1.9412521374	-0.6775061566
H	-14.2144158165	2.1014462133	0.7575049888
H	-16.0660134198	1.1977205192	1.8383177423
H	-15.9955147942	-1.1197817724	-1.7726116356
H	-18.5187298278	1.1694724231	1.8080882301
H	-18.4475406279	-1.2086661174	-1.7625306561
H	3.1145142468	1.5795240659	1.6780207536
H	3.0606373684	-1.0180235276	-1.7359726924
H	5.5680117614	1.5212242712	1.6836599103
H	5.5146045498	-1.0188725676	-1.7741159181
H	7.4423517909	2.2788542161	0.5476638326
H	7.3624714998	-1.8408530896	-0.6480596838
H	9.8955953372	2.2201343798	0.5831533947
H	9.8151527318	-1.8775669082	-0.6862289331
H	11.6716917674	-1.8756240067	0.7062879840
H	11.7622636316	2.1406434263	-0.8014335571
H	14.1239481667	-1.9412518872	0.6775065817
H	14.2144157544	2.1014460948	-0.7575056008
H	15.9955147695	-1.1197812790	1.7726121102
H	16.0660134545	1.1977201259	-1.8383178663
H	18.4475405393	-1.2086656564	1.7625309637
H	18.5187299305	1.1694720105	-1.8080884896
H	20.3389877558	0.0877868569	2.1234875157
H	20.3483800277	-0.2223671604	-2.1557837083
H	22.7908476185	-0.0182888114	2.1360170537
H	22.8024196443	-0.2529074991	-2.1478615548
H	24.6197030603	-1.6102176199	-1.6052139377
H	24.6898503630	1.2269427143	1.6113607105
H	27.0761838737	-1.6600677468	-1.6137329778
H	27.1434212879	1.1190234747	1.6525261200
H	29.0332553880	1.7683977507	0.4404567077
H	28.8803833115	-2.4431844869	-0.3662054643
H	31.4983525111	1.6701614567	0.4886052859
H	31.3455258180	-2.5356534463	-0.3589977664
H	32.6707467780	-0.4807357948	0.0790577457
H	-20.3389877630	0.0877863687	-2.1234875111
H	-20.3483800222	-0.2223665662	2.1557837907
H	-22.7908476167	-0.0182893416	-2.1360170261
H	-22.8024196466	-0.2529069463	2.1478616444

H	-24.6197030591	-1.6102172118	1.6052143607
H	-24.6898503627	1.2269423115	-1.6113610044
H	-27.0761838756	-1.6600673581	1.6137333983
H	-27.1434212842	1.1190230409	-1.6525264019
H	-29.0332553906	1.7683976337	-0.4404571614
H	-28.8803833167	-2.4431844024	0.3662060800
H	-31.4983525101	1.6701613316	-0.4886057081
H	-31.3455258248	-2.5356533588	0.3589984110
H	-32.6707467816	-0.4807358154	-0.0790576231

Cartesian coordinates (in Å) of [16]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	-33.7338768853	-0.5898571387	-0.2355268262
C	-32.9823600626	-1.7294703806	0.0384672845
C	-33.0845136478	0.6181037924	-0.4754782555
C	-31.5943641022	-1.6614677444	0.0703941452
C	-31.6962930798	0.6860582013	-0.4418213860
C	-30.9272296997	-0.4529361662	-0.1689556803
C	-29.4506070478	-0.3851764999	-0.1382417854
C	-28.7114691589	-1.1297403054	0.7898991152
C	-28.7426693016	0.4203276268	-1.0391405991
C	-27.3253622217	-1.0731921074	0.8144613400
C	-27.3565110289	0.4777883447	-1.0142843089
C	-26.6172303017	-0.2688652658	-0.0877830802
C	-25.1411488378	-0.2115902978	-0.0640570502
C	-24.4337715101	-0.2470358036	1.1443892313
C	-24.4003061708	-0.1222523898	-1.2496240428
C	-23.0472183166	-0.1972609516	1.1662108579
C	-23.0138268101	-0.0720922352	-1.2277244065
C	-22.3060853910	-0.1093059329	-0.0194207638
C	-20.8299230197	-0.0599896734	0.0029665993
C	-20.1417603856	0.6302305316	1.0092605879
C	-20.0689217807	-0.7021165808	-0.9825108780
C	-18.7550314138	0.6747740735	1.0300593243
C	-18.6824938163	-0.6573516776	-0.9619464461
C	-17.9942011910	0.0317700639	0.0452246852
C	-16.5179537099	0.0759843109	0.0663607540
C	-15.8311898731	1.2266467307	0.4750303718
C	-15.7549175792	-1.0322961698	-0.3241881240
C	-14.4443941313	1.2674375146	0.4921802784
C	-14.3683440450	-0.9912373911	-0.3079556297
C	-13.6815527517	0.1595199329	0.1006179027
C	-12.2050746252	0.2019695411	0.1157146195
C	-11.5087555964	1.3661920178	-0.2343005362
C	-11.4515361515	-0.9224485256	0.4771975905
C	-10.1217826923	1.4040385686	-0.2247548369
C	-10.0648257220	-0.8849301773	0.4855143569
C	-9.3681983270	0.2786936446	0.1340162029
C	-7.8915066692	0.3133166782	0.1361902587
C	-7.1819446254	1.0379210264	-0.8304320337
C	-7.1511945143	-0.3830018736	1.1004511991
C	-5.7946858004	1.0612356514	-0.8353253699
C	-5.7639831714	-0.3598045100	1.0954261919
C	-5.0543864401	0.3611250052	0.1261870372
C	-3.5771875365	0.3753469763	0.1147804231
C	-2.8624605541	0.3693751320	-1.0899973401
C	-2.8417261474	0.3884520662	1.3070413960
C	-1.4749272738	0.3720386987	-1.1019378118
C	-1.4541010420	0.3901952574	1.2951179197
C	-0.7394303366	0.3798048525	0.0903431807
C	0.7378360793	0.3708886402	0.0776879383
C	1.4485672359	-0.3614977201	-0.8821048100
C	1.4770291524	1.0888821088	1.0267993532
C	2.8357797523	-0.3769360159	-0.8911659909
C	2.8644364141	1.0731199251	1.0180187823
C	3.5751233440	0.3386115249	0.0597282402
C	5.0520341343	0.3150721982	0.0539629563
C	5.7555370226	-0.8475178826	-0.2871997304
C	5.7991161439	1.4513529423	0.3912014412
C	7.1425003408	-0.8728145646	-0.2918772504
C	7.1863941291	1.4256983006	0.3879225207
C	7.8896325799	0.2631891947	0.0460260162
C	9.3665142928	0.2346479513	0.0419253823
C	10.0701602246	-0.9049661421	0.4530239062
C	10.1132234018	1.3446340230	-0.3741583001
C	11.4571419956	-0.9340665129	0.4463923478
C	11.5003791993	1.3159756274	-0.3793808396
C	12.2040713441	0.1757296856	0.0299014332
C	13.6807121332	0.1428426639	0.0218409662
C	14.3957822287	-0.5325238980	1.0195240492
C	14.4155096614	0.7831842590	-0.9844093496
C	15.7826861542	-0.5679844226	1.0100033846

C	15.8025232593	0.7481592355	-0.9935528626
C	16.5175601955	0.0707293596	0.0027162961
C	17.9940516486	0.0288249348	-0.0098628050
C	18.7316177317	0.0742953399	1.1803309682
C	18.7061514087	-0.0602058713	-1.2130048322
C	20.1184649104	0.0305618712	1.1680520856
C	20.0930141222	-0.1027933832	-1.2254298954
C	20.8302539104	-0.0597439727	-0.0350738177
C	22.3066698935	-0.1097624207	-0.0475432278
C	23.0648426045	0.6378584630	0.8629890704
C	22.9972358383	-0.9082074060	-0.9684727876
C	24.4513445833	0.5880637588	0.8537824438
C	24.3837331651	-0.9570197870	-0.9784173184
C	25.1420006116	-0.2107287062	-0.0667393892
C	26.6180374734	-0.2678090939	-0.0749652335
C	27.3907189759	0.8686421034	0.1972155397
C	27.2938258605	-1.4627664505	-0.3540806014
C	28.7771342893	0.8118468536	0.1902966373
C	28.6800981395	-1.5188816503	-0.3624441357
C	29.4525288181	-0.3824058528	-0.0911276684
C	30.9297846842	-0.4406181989	-0.1014522043
C	31.6876347319	0.6268476429	-0.6007924474
C	31.6093707569	-1.5638870864	0.3878984287
C	33.0767577715	0.5737575250	-0.6092778397
C	32.9984702668	-1.6180442138	0.3780074763
C	33.7386684789	-0.5492145636	-0.1200486436
H	-0.9132910186	0.3786357983	2.2372481374
H	-3.3662117531	0.4134726322	2.2581086548
H	-3.4032149303	0.3411519150	-2.0317975680
H	-0.9505756122	0.3841531020	-2.0533115531
H	0.9550453987	1.6801614546	1.7738970061
H	3.4086074608	1.6239794607	1.7800909992
H	3.3575041738	-0.9402716229	-1.6597742781
H	0.9036517105	-0.9419392966	-1.6212593742
H	-5.2183017883	-0.9262719919	1.8448456051
H	-5.2737478264	1.6440415036	-1.5897959705
H	-7.6720326080	-0.9382330489	1.8755683830
H	-7.7267012497	1.5743067123	-1.6023578431
H	-9.5095163414	-1.7803365405	0.7504250947
H	-9.6116274030	2.3273007749	-0.4848162272
H	-11.9617745311	-1.8349047677	0.7726577814
H	-12.0638738487	2.2498246152	-0.5365129961
H	-13.9420828755	2.1686263957	0.8324860140
H	-13.8056668763	-1.8610976794	-0.6349673456
H	-16.3934687409	2.1096441526	0.7658158900
H	-16.2579773469	-1.9456767950	-0.6290052231
H	5.2833573747	2.3737398233	0.6432001642
H	5.2054965661	-1.7510761481	-0.5348473672
H	7.7366022234	2.3182018699	0.6725788988
H	7.6578748645	-1.7847093629	-0.5800710284
H	9.5977094845	2.2374766398	-0.7166916184
H	9.5210293573	-1.7758961874	0.7996087185
H	12.0498554200	2.2003384815	-0.6898045839
H	11.9725363095	-1.8401361885	0.7524900348
H	13.8560317376	-1.0234673812	1.8245169805
H	13.8908374362	1.3008949313	-1.7826165742
H	16.3071351767	-1.1162364792	1.7876555775
H	16.3433366787	1.2695681735	-1.7784797928
H	18.2096935154	0.1629419134	2.1290124320
H	18.1630806107	-0.1160531420	-2.1522426460
H	20.6606414860	0.0478069670	2.1092927008
H	20.6161502093	-0.1533200689	-2.1762346935
H	22.5592081937	1.2802014326	1.5784383016
H	22.4363316175	-1.5129726023	-1.6754356515
H	25.0105370098	1.1636364904	1.5860411564
H	24.8907301642	-1.5706050640	-1.7178156120
H	26.7225566594	-2.3659558588	-0.5496035435
H	26.8961769577	1.8144286407	0.4000096427
H	29.1752366782	-2.4559580967	-0.6012892496
H	29.3493764404	1.7056453783	0.4228172514
H	31.1795950786	1.4949048710	-1.0116821000
H	31.0416981165	-2.3907528900	0.8054442412
H	33.6443265166	1.4096421994	-1.0083836722

H	33.5051354774	-2.4953187119	0.7702169513
H	34.8238575139	-0.5914847282	-0.1275134597
H	-18.1214576158	-1.1508290760	-1.7506301998
H	-18.2512946498	1.2028357009	1.8349449371
H	-20.5728355599	-1.2597229245	-1.7670088118
H	-20.7033318045	1.1547826768	1.7773405004
H	-22.5272087862	-0.2462412944	2.1187978309
H	-22.4687277341	0.0157645634	-2.1633646352
H	-24.9806495237	-0.2972073188	2.0817891131
H	-24.9190888527	-0.1108811492	-2.2040556550
H	-26.8360277798	1.1243609213	-1.7150872558
H	-26.7783335486	-1.6764516605	1.5334711159
H	-29.2879397314	0.9946347576	-1.7828495446
H	-29.2340584629	-1.7485390740	1.5139495858
H	-31.0151578111	-2.5617755843	0.2555855035
H	-31.1988873237	1.6384102104	-0.6027390477
H	-33.4787375118	-2.6788624254	0.2183317140
H	-33.6619464858	1.5150484781	-0.6810458506
H	-34.8183295514	-0.6425831476	-0.2612059663

Cartesian coordinates (in Å) of [17]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	35.9014753765	-0.4908260875	0.0290119367
C	35.1625185158	-1.5685939873	0.5093859983
C	35.2379909090	0.6329117799	-0.4563280343
C	33.7731169310	-1.5223873581	0.5058014479
C	33.8485663435	0.6780836532	-0.4612345050
C	33.0919322436	-0.3983922143	0.0203228908
C	31.6142955964	-0.3490522041	0.0159222706
C	30.8515825529	-1.4876027803	-0.2735881735
C	30.9287041842	0.8383908007	0.3015990930
C	29.4649533639	-1.4401289199	-0.2784166022
C	29.5419756386	0.8865445709	0.2953308374
C	28.7789983243	-0.2520052147	0.0050742974
C	27.3026022209	-0.2036448097	-0.0000650121
C	26.5568881731	-0.9461789390	-0.9250291758
C	26.5991264034	0.5836623454	0.9207468474
C	25.1701165953	-0.9045066434	-0.9278463070
C	25.2123669686	0.6261676855	0.9173222191
C	24.4667498098	-0.1177648143	-0.0064441837
C	22.9900091252	-0.0749881796	-0.0080859998
C	22.2648626442	-0.1105367132	-1.2060531761
C	22.2658206943	0.0008531201	1.1886694655
C	20.8777484972	-0.0740297131	-1.2071092247
C	20.8787163054	0.0383694923	1.1874851393
C	20.1532883128	0.0008371402	-0.0103728713
C	18.6765474312	0.0374085702	-0.0116210261
C	17.9685756376	0.7226264265	-1.0075906107
C	17.9345198123	-0.6135600569	0.9825265865
C	16.5814359289	0.7542546520	-1.0101274301
C	16.5475090442	-0.5815951732	0.9803080534
C	15.8395231812	0.1023891421	-0.0166025540
C	14.3627985887	0.1329873753	-0.0199201415
C	13.6608435029	1.2765499877	-0.4228774371
C	13.6141098058	-0.9816311366	0.3802519701
C	12.2736751270	1.3040341106	-0.4265996402
C	12.2270891559	-0.9537191982	0.3779105146
C	11.5251798229	0.1894467876	-0.0262874776
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C	9.3431736784	1.3766395131	0.3196043763
C	9.3029241490	-0.9155464605	-0.3813229368
C	7.9559218950	1.4017889105	0.3174760531
C	7.9159032040	-0.8907904068	-0.3819924413
C	7.2105722669	0.2682385129	-0.0325874498
C	5.7336518007	0.2913512673	-0.0308923999
C	5.0205601758	1.0166502879	0.9326161698
C	4.9966524405	-0.4154061606	-0.9901150669
C	3.6331780639	1.0323624516	0.9381058293
C	3.6093749698	-0.3999902824	-0.9843544165
C	2.8962410481	0.3231767296	-0.0193567291
C	1.4189608450	0.3324819980	-0.0097465900
C	0.7020998803	0.3342262314	1.1937966386
C	0.6854948115	0.3348218892	-1.2033017133
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C	-4.9966525560	-0.4154061536	0.9901152766
C	-5.0205602696	1.0166503356	-0.9326161704
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C	-16.5475090661	-0.5815951907	-0.9803080097
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C	-18.6765474348	0.0374085649	0.0116211014
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C	-30.9287042081	0.8383906962	-0.3015991528
C	-30.8515825196	-1.4876028858	0.2735881063
C	-31.6142955898	-0.3490523212	-0.0159222994
C	-33.0919322410	-0.3983922122	-0.0203228712
C	-33.8485661897	0.6780837395	0.4612344259
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H	11.6763121535	-1.8284790400	0.7120451819
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H	-20.3470394482	0.1161027774	-2.1316894617
H	-20.3443462346	-0.1233816617	2.1522313456
H	-22.7983495220	0.0117500299	-2.1355040329
H	-22.7976954118	-0.1501185625	2.1519907710
H	-24.6962667654	1.2592296718	-1.6335360608
H	-24.6190863717	-1.5058243187	1.6454197138
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H	20.3470394782	0.1161026245	2.1316893649
H	22.7976953525	-0.1501186558	-2.1519907662
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H	31.4929497471	1.7335828852	0.5478884501
H	33.2059931820	-2.3564521397	0.9095704055
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H	36.9869353852	-0.5268874599	0.0319826355

Cartesian coordinates (in Å) of [18]-paraphenylene optimized at the PBE0/6-31G(d,p) level of theory:

C	38.0579507178	0.3261899353	-0.3320583621
C	37.3257045393	1.4395025287	-0.7355128388
C	37.3876789711	-0.8148469936	0.1007208806
C	35.9362343872	1.4119070570	-0.7061546618
C	35.9981364179	-0.8417702911	0.1308234183
C	35.2482810280	0.2709265200	-0.2726027961
C	33.7703505622	0.2427816104	-0.2402023127
C	33.0321370332	1.3724153714	0.1349612696
C	33.0601047720	-0.9144282596	-0.5837004591
C	31.6452897971	1.3457644186	0.1659332558
C	31.6732357975	-0.9416395693	-0.5519240648
C	30.9346355372	0.1880117647	-0.1763631005
C	29.4581352567	0.1601061835	-0.1435622723
C	28.7416399551	0.8495206886	0.8433888156
C	28.7254763756	-0.5558311135	-1.0991359845
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C	27.3386638546	-0.5800151586	-1.0699529188
C	26.6220258820	0.1107415154	-0.0841301986
C	25.1451935816	0.0871481407	-0.0566331176
C	24.4415605664	0.0569240150	1.1542195669
C	24.3991019330	0.0948179063	-1.2423634276
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C	23.0119986028	0.0723644633	-1.2186912369
C	22.3083788937	0.0420181816	-0.0078746895
C	20.8314421168	0.0185109955	0.0170566726
C	20.1340854965	-0.7279409773	0.9757278366
C	20.0794202512	0.7418177205	-0.9178420482
C	18.7470229431	-0.7494735520	0.9990103498
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C	17.9949337930	-0.0257933286	0.0644095808
C	16.5181969903	-0.0492579172	0.0887091345
C	15.8172125982	-1.2150641836	0.4239309835
C	15.7690126050	1.0927000846	-0.2237633472
C	14.4303050231	-1.2381381131	0.4461182285
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C	13.6811333664	-0.0964495912	0.1328328800
C	12.2043431816	-0.1205875649	0.1528832324
C	11.4916135717	-1.2508521985	-0.2681121144
C	11.4667465361	0.9872079808	0.5904351680
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H	29.2816406438	1.3985593874	1.6097298836
H	31.1008761769	2.2441997798	0.4428809557
H	31.1517062106	-1.8602228740	-0.8057709522
H	33.5553556210	2.2797031275	0.4235492510
H	33.6042558341	-1.8012130004	-0.8963552849
H	35.3730005323	2.2753903938	-1.0487330771
H	35.4845367496	-1.7261481659	0.4973342600
H	37.8386856871	2.3316088585	-1.0833722201
H	37.9494730139	-1.6858516512	0.4260178388
H	39.1434831972	0.3475849682	-0.3549226945
H	-35.4318416117	1.1788742418	1.7572915705
H	-35.4219265146	-0.4517793140	-2.2126193722
H	-37.8950071720	1.2815397476	1.7094120438
H	-37.8865865723	-0.3885032934	-2.2455417338
H	-39.1400754895	0.4893743199	-0.2890198612