Supporting Information

Combined Experimental and Theoretical Studies on the Photophysical Properties of Cycloparaphenylenes

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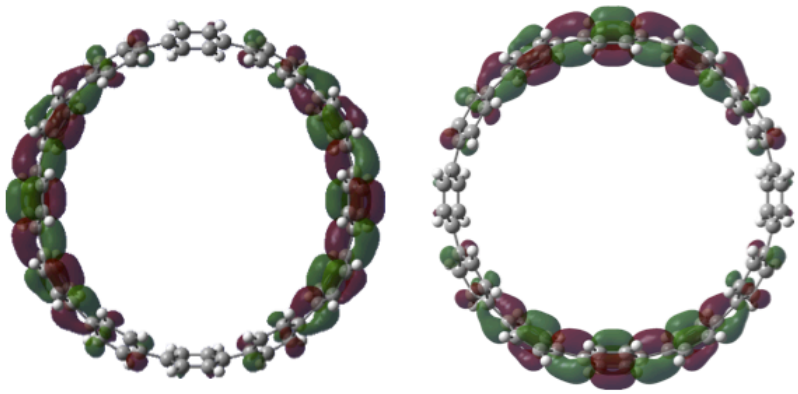
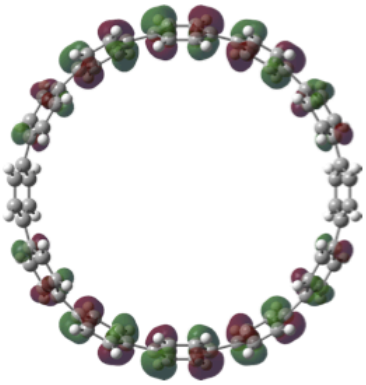
1. MOs of [12]CPP



LUMO+1, LUMO+2
(–1.39 eV)

HOMO
(–5.25 eV)

LUMO
(–1.64 eV)



HOMO–1, HOMO–2
(–5.49 eV)

2. Cartesian coordinates of optimized species

[6]CPP (θ = 31°)

C	-3.294290	-1.868889	1.265517	C	2.354602	-2.962622	1.265743	C	1.391199	3.519106	1.265617
C	-4.002733	-2.115846	-1.007294	C	3.835299	-2.406594	-1.006987	C	0.167643	4.520066	-1.007606
C	-3.748707	-0.555374	1.265773	H	2.801484	-4.051037	-1.910326	H	2.109191	4.451950	-1.910196
H	-2.776942	-2.233612	2.147652	C	3.267759	-1.914684	1.265592	C	0.026746	3.784035	1.265440
C	-4.459774	-0.798619	-1.006483	H	1.738242	-3.106889	2.147848	H	1.824852	3.058316	2.147938
H	-4.115277	-2.709635	-1.911122	C	3.913511	-1.513221	0.081182	C	-0.644377	4.139462	0.080490
C	-4.196763	0.058957	0.081500	H	4.405907	-2.208183	-1.910988	H	-0.290041	4.915473	-1.911139
H	-3.567937	0.050707	2.148264	H	3.326487	-1.284437	2.147711	H	-0.547832	3.519844	2.147972
H	-4.915025	-0.400796	-1.910191	C	4.196758	-0.058958	-0.081568	C	-2.045148	3.657060	-0.081302
C	-1.536608	-4.255775	1.007020	C	4.459803	0.798606	1.006415	C	-2.919742	3.458108	1.006674
C	-1.391200	-3.519136	-1.265582	C	3.748642	0.555379	-1.265814	C	-2.354592	2.962680	-1.265738
C	-0.167647	-4.520028	1.007677	C	4.002742	2.115825	1.007276	C	-3.835322	2.406580	1.006940
H	-2.109214	-4.451959	1.910231	H	4.915151	0.400787	1.910075	H	-2.801465	4.050935	1.910393
C	-0.026746	-3.784067	-1.265392	C	3.294285	1.868915	-1.265538	C	-3.267681	1.914682	-1.265617
H	-1.824840	-3.058346	-2.147907	H	3.567888	-0.050680	-2.148323	H	-1.738206	3.106969	-2.147822
C	0.644376	-4.139461	-0.080431	C	3.266246	2.627925	-0.080664	C	-3.913490	1.513218	-0.081238
H	0.290037	-4.915366	1.911241	H	4.115255	2.709578	1.911130	H	-4.406027	2.208201	1.910886
H	0.547838	-3.519846	-2.147911	H	2.776925	2.233660	-2.147658	H	-3.326404	1.284469	-2.147759
C	2.045150	-3.657049	0.081336	C	2.147092	3.598712	0.081119	C	-2.147105	-3.598732	-0.081090
C	2.919729	-3.458131	-1.006656	C	1.536597	4.255784	-1.006975	C	-3.266259	-2.627934	0.080664

[8]CPP (θ = 31°)

C	0.644845	5.147509	1.235356	C	5.399672	2.331836	1.056105	H	-2.021204	5.913113	1.962433
C	1.988718	4.791364	1.235655	H	4.684886	4.135314	1.963124	C	-3.932689	3.932689	-0.055841
C	2.754379	4.832107	0.056443	C	4.793024	1.981357	-1.235515	H	-3.459232	3.537550	-2.125311
C	2.169531	5.467505	-1.056199	H	3.537550	3.459232	-2.125311	H	-4.135314	4.684886	1.963124
C	0.823405	5.823745	-1.056670	C	5.363857	1.468932	-0.056521	C	5.561739	-0.000235	0.055833
C	0.000235	5.561739	0.055833	H	5.913113	2.021204	1.962433	C	5.823745	-0.823405	-1.056670
H	0.056095	4.948526	2.125701	H	4.755979	1.361263	-2.126000	C	5.147509	-0.644845	1.235356
H	2.401269	4.326838	2.126119	C	-1.468932	5.363857	-0.056521	C	5.467505	-2.169531	-1.056199
H	2.752133	5.610690	-1.962641	C	-1.981357	4.793024	-1.235515	H	6.236617	-0.388637	-1.963324
H	0.388637	6.236617	-1.963324	C	-2.331836	5.399672	1.056105	C	4.791364	-1.988718	1.235655
C	3.932689	3.932689	-0.055841	C	-3.183602	4.094889	-1.235182	H	4.948526	-0.056095	2.125701
C	4.700128	3.535835	1.056519	H	-1.361263	4.755979	-2.126000	C	4.832107	-2.754379	0.056443
C	4.094889	3.183602	-1.235182	C	-3.535835	4.700128	1.056519	H	5.610690	-2.752133	-1.962641

H	4.326838	-2.401269	2.126119	C	-2.169531	-5.467505	-1.056199	C	-5.363857	-1.468932	-0.056521
C	3.932689	-3.932689	-0.055841	H	-0.388637	-6.236617	-1.963324	H	-5.913113	-2.021204	1.962433
C	3.535835	-4.700128	1.056519	C	-1.988718	-4.791364	1.235655	H	-4.755979	-1.361263	-2.126000
C	3.183602	-4.094889	-1.235182	H	-0.056095	-4.948526	2.125701	C	-5.561739	0.000235	0.055833
C	2.331836	-5.399672	1.056105	C	-2.754379	-4.832107	0.056443	C	-5.823745	0.823405	-1.056670
H	4.135314	-4.684886	1.963124	H	-2.752133	-5.610690	-1.962641	C	-5.147509	0.644845	1.235356
C	1.981357	-4.793024	-1.235515	H	-2.401269	-4.326838	2.126119	C	-5.467505	2.169531	-1.056199
H	3.459232	-3.537550	-2.125311	C	-3.932689	-3.932689	-0.055841	H	-6.236617	0.388637	-1.963324
C	1.468932	-5.363857	-0.056521	C	-4.700128	-3.535835	1.056519	C	-4.791364	1.988718	1.235655
H	2.021204	-5.913113	1.962433	C	-4.094889	-3.183602	-1.235182	H	-4.948526	0.056095	2.125701
H	1.361263	-4.755979	-2.126000	C	-5.399672	-2.331836	1.056105	C	-4.832107	2.754379	0.056443
C	-0.000235	-5.561739	0.055833	H	-4.684886	-4.135314	1.963124	H	-5.610690	2.752133	-1.962641
C	-0.823405	-5.823745	-1.056670	C	-4.793024	-1.981357	-1.235515	H	-4.326838	2.401269	2.126119
C	-0.644845	-5.147509	1.235356	H	-3.537550	-3.459232	-2.125311				

[10]CPP (θ = 31°)

C	4.904134	-5.339247	1.080429	C	2.046362	-6.244964	1.218613	C	2.292843	6.874112	-1.081785
C	5.835834	-4.305224	1.080031	C	0.826649	-7.198776	-1.080402	H	4.162691	6.356791	-1.988128
C	6.004339	-3.474990	-0.044294	H	2.762332	-7.076595	-1.988198	C	1.451072	6.777058	0.042364
C	5.331072	-3.852178	-1.219735	C	0.686713	-6.534918	1.219287	H	1.409061	6.164367	2.112388
C	4.400629	-4.885170	-1.219440	H	2.486561	-5.813262	2.112356	H	1.926618	7.347485	-1.988958
C	4.095983	-5.593838	-0.043809	H	0.369997	-7.587013	-1.987018	C	-0.023452	6.930065	-0.044103
H	4.762882	-5.920938	1.987560	H	0.109709	-6.320132	2.113635	C	-0.686692	6.534809	-1.219270
H	6.399958	-4.103676	1.986876	C	6.592261	2.165122	-0.042466	C	-0.826654	7.198814	1.080376
H	5.433810	-3.244991	-2.114046	C	6.011387	2.672776	-1.218089	C	-2.046342	6.244872	-1.218601
H	3.807202	-5.050863	-2.113541	C	6.598283	3.012326	1.081788	H	-0.109665	6.319933	-2.113582
C	6.607089	-2.120632	0.042757	C	5.314000	3.875358	-1.218341	C	-2.187899	6.908423	1.081032
C	6.436466	-1.368625	1.218624	H	5.986575	2.057133	-2.112155	H	-0.370010	7.587065	1.986989
C	7.111087	-1.438989	-1.081103	C	5.900089	4.216493	1.081503	C	-2.812315	6.335343	-0.042995
C	6.580807	0.014050	1.219317	H	7.108659	2.699025	1.988695	H	-2.486532	5.813094	-2.112313
H	6.054592	-1.852046	2.112774	C	5.161765	4.631795	-0.042838	H	-2.762346	7.076697	1.988155
C	7.255545	-0.054589	-1.080457	H	4.767680	4.159488	-2.112654	C	-4.096000	5.593858	0.043798
H	7.339438	-1.992338	-1.988213	H	5.881355	4.815244	1.988336	C	-4.400707	4.885253	1.219453
C	6.902792	0.715569	0.043928	C	4.058126	5.621598	0.043272	C	-4.904110	5.339218	-1.080460
H	6.306853	0.565070	2.113991	C	3.289356	5.691419	1.218575	C	-5.331138	3.852246	1.219747
H	7.593398	0.440426	-1.987073	C	3.565430	6.310285	-1.081340	H	-3.807351	5.051009	2.113589
C	2.812316	-6.335345	0.042987	C	2.018404	6.254871	1.218217	C	-5.835800	4.305186	-1.080060
C	2.187893	-6.908374	-1.081061	H	3.630939	5.179371	2.113087	H	-4.762845	5.920901	-1.987596

C	-6.004337	3.474992	0.044288	H	-7.593493	-0.440400	1.987044	C	-3.289309	-5.691317	-1.218550
H	-5.433926	3.245116	2.114091	C	-6.592288	-2.165136	0.042472	C	-3.565448	-6.310313	1.081322
H	-6.399889	4.103596	-1.986918	C	-6.011491	-2.672830	1.218117	C	-2.018366	-6.254783	-1.218196
C	-6.607058	2.120625	-0.042761	C	-6.598256	-3.012316	-1.081802	H	-3.630858	-5.179186	-2.113028
C	-6.436351	1.368601	-1.218603	C	-5.314086	-3.875404	1.218367	C	-2.292864	-6.874149	1.081765
C	-7.111117	1.438999	1.081081	H	-5.986755	-2.057233	2.112217	H	-4.162710	-6.356835	1.988107
C	-6.580712	-0.014069	-1.219295	C	-5.900053	-4.216478	-1.081517	C	-1.451070	-6.777052	-0.042364
H	-6.054386	1.852011	-2.112721	H	-7.108621	-2.699005	-1.988712	H	-1.408987	-6.164214	-2.112337
C	-7.255587	0.054601	1.080439	C	-5.161772	-4.631798	0.042845	H	-1.926666	-7.347569	1.988925
H	-7.339483	1.992350	1.988184	H	-4.767832	-4.159563	2.112710	C	0.023456	-6.930088	0.044099
C	-6.902789	-0.715571	-0.043924	H	-5.881271	-4.815208	-1.988362				
H	-6.306687	-0.565107	-2.113936	C	-4.058116	-5.621575	-0.043269				

[12]CPP (θ = 31°)

C	-0.695133	7.929959	1.208463	C	7.215113	-3.362977	1.208463	C	-6.519980	-4.566982	1.208463
C	0.695133	7.929959	1.208463	C	6.519980	-4.566982	1.208463	C	-7.215113	-3.362977	1.208463
C	1.426345	8.186834	0.035518	C	6.376833	-5.328668	0.035518	C	-7.803179	-2.858166	0.035518
C	0.695745	8.596500	-1.095529	C	7.096915	-4.900783	-1.095529	C	-7.792660	-3.695717	-1.095529
C	-0.695745	8.596500	-1.095529	C	7.792660	-3.695717	-1.095529	C	-7.096915	-4.900783	-1.095529
C	2.858166	7.803179	-0.035518	C	5.328668	-6.376833	-0.035518	C	-8.186834	-1.426345	-0.035518
C	3.695717	7.792660	1.095529	C	4.900783	-7.096915	1.095529	C	-8.596500	-0.695745	1.095529
C	4.900783	7.096915	1.095529	C	3.695717	-7.792660	1.095529	C	-8.596500	0.695745	1.095529
C	5.328668	6.376833	-0.035518	C	2.858166	-7.803179	-0.035518	C	-8.186834	1.426345	-0.035518
C	4.566982	6.519980	-1.208463	C	3.362977	-7.215113	-1.208463	C	-7.929959	0.695133	-1.208463
C	3.362977	7.215113	-1.208463	C	4.566982	-6.519980	-1.208463	C	-7.929959	-0.695133	-1.208463
C	6.376833	5.328668	0.035518	C	1.426345	-8.186834	0.035518	C	-7.803179	2.858166	0.035518
C	6.519980	4.566982	1.208463	C	0.695133	-7.929959	1.208463	C	-7.215113	3.362977	1.208463
C	7.215113	3.362977	1.208463	C	-0.695133	-7.929959	1.208463	C	-6.519980	4.566982	1.208463
C	7.803179	2.858166	0.035518	C	-1.426345	-8.186834	0.035518	C	-6.376833	5.328668	0.035518
C	7.792660	3.695717	-1.095529	C	-0.695745	-8.596500	-1.095529	C	-7.096915	4.900783	-1.095529
C	7.096915	4.900783	-1.095529	C	0.695745	-8.596500	-1.095529	C	-7.792660	3.695717	-1.095529
C	8.186834	1.426345	-0.035518	C	-2.858166	-7.803179	-0.035518	C	-5.328668	6.376833	-0.035518
C	8.596500	0.695745	1.095529	C	-3.695717	-7.792660	1.095529	C	-4.900783	7.096915	1.095529
C	8.596500	-0.695745	1.095529	C	-4.900783	-7.096915	1.095529	C	-3.695717	7.792660	1.095529
C	8.186834	-1.426345	-0.035518	C	-5.328668	-6.376833	-0.035518	C	-3.362977	7.215113	-1.208463
C	7.929959	-0.695133	-1.208463	C	-4.566982	-6.519980	-1.208463	C	-4.566982	6.519980	-1.208463
C	7.929959	0.695133	-1.208463	C	-3.362977	-7.215113	-1.208463	H	-1.216154	7.608117	2.105193
C	7.803179	-2.858166	0.035518	C	-6.376833	-5.328668	0.035518	H	1.216154	7.608117	2.105193

H	1.223319	8.880528	-2.002051	H	7.079103	-5.499689	-2.002051	H	-8.302422	-3.380839	-2.002051
H	-1.223319	8.880528	-2.002051	H	8.302422	-3.380839	-2.002051	H	-7.079103	-5.499689	-2.002051
H	3.380839	8.302422	2.002051	H	5.499689	-7.079103	2.002051	H	-8.880528	-1.223319	2.002051
H	5.499689	7.079103	2.002051	H	3.380839	-8.302422	2.002051	H	-8.880528	1.223319	2.002051
H	4.857279	5.980746	-2.105193	H	2.750838	-7.196900	-2.105193	H	-7.608117	1.216154	-2.105193
H	2.750838	7.196900	-2.105193	H	4.857279	-5.980746	-2.105193	H	-7.608117	-1.216154	-2.105193
H	5.980746	4.857279	2.105193	H	1.216154	-7.608117	2.105193	H	-7.196900	2.750838	2.105193
H	7.196900	2.750838	2.105193	H	-1.216154	-7.608117	2.105193	H	-5.980746	4.857279	2.105193
H	8.302422	3.380839	-2.002051	H	-1.223319	-8.880528	-2.002051	H	-7.079103	5.499689	-2.002051
H	7.079103	5.499689	-2.002051	H	1.223319	-8.880528	-2.002051	H	-8.302422	3.380839	-2.002051
H	8.880528	1.223319	2.002051	H	-3.380839	-8.302422	2.002051	H	-5.499689	7.079103	2.002051
H	8.880528	-1.223319	2.002051	H	-5.499689	-7.079103	2.002051	H	-3.380839	8.302422	2.002051
H	7.608117	-1.216154	-2.105193	H	-4.857279	-5.980746	-2.105193	H	-2.750838	7.196900	-2.105193
H	7.608117	1.216154	-2.105193	H	-2.750838	-7.196900	-2.105193	H	-4.857279	5.980746	-2.105193
H	7.196900	-2.750838	2.105193	H	-5.980746	-4.857279	2.105193	C	-2.858166	7.803179	-0.035518
H	5.980746	-4.857279	2.105193	H	-7.196900	-2.750838	2.105193	C	-1.426345	8.186834	0.035518

[14]CPP (θ = 31°)

C	-4.220327	-9.064668	1.105326	C	-8.702489	-4.256147	-0.028954	C	3.626680	-8.976893	-0.030681
C	-4.761739	-8.433913	-0.029936	C	-8.672394	-3.479308	-1.200007	C	4.124030	-8.378679	-1.201604
C	-3.984118	-8.448493	-1.201030	C	-9.300776	-3.679008	1.106401	C	4.456766	-8.947838	1.104944
C	-2.685574	-8.945428	-1.201167	C	-9.093076	-2.154196	-1.200365	C	5.323103	-7.674828	-1.201359
C	-2.096972	-9.454004	-0.030332	H	-8.212295	-3.881527	-2.097630	H	3.513513	-8.369888	-2.099623
C	-2.921009	-9.562042	1.105077	C	-9.722359	-2.353127	1.105963	C	5.656761	-8.243810	1.105152
H	-4.814178	-9.141195	2.012188	H	-9.411661	-4.267366	2.013262	H	4.145438	-9.460081	2.011234
H	-4.358413	-7.965305	-2.098633	C	-9.567043	-1.537014	-0.029603	C	6.087493	-7.532858	-0.030101
H	-2.084334	-8.835648	-2.098824	H	-8.948650	-1.560587	-2.098207	H	5.613006	-7.136794	-2.099038
H	-2.529967	-10.015587	2.011793	H	-10.152844	-1.936147	2.012504	H	6.255484	-8.222208	2.011682
C	-5.993142	-7.609296	0.030265	C	-0.629582	-9.662417	0.029383	C	7.166905	-6.517367	0.030315
C	-6.302636	-6.895945	1.201450	C	0.131732	-9.995358	-1.106189	C	7.903162	-6.130801	-1.104694
C	-6.782509	-7.348781	-1.104962	C	0.077606	-9.338170	1.200291	C	7.354851	-5.762940	1.201552
C	-7.256337	-5.884235	1.201591	C	1.518191	-9.879674	-1.106393	C	8.678594	-4.975644	-1.104255
H	-5.713489	-7.058412	2.099094	H	-0.370174	-10.322290	-2.012854	H	7.845416	-6.727243	-2.011207
C	-7.737086	-6.336634	-1.104748	C	1.463022	-9.222014	1.200005	C	8.129626	-4.608615	1.202003
H	-6.627428	-7.927386	-2.011652	H	-0.469017	-9.065794	2.098255	H	6.800569	-6.020043	2.099358
C	-7.950681	-5.533433	0.030724	C	2.213920	-9.424807	0.028873	C	8.757098	-4.148384	0.031193
H	-7.383706	-5.286465	2.099210	H	2.067356	-10.119141	-2.013033	H	9.208989	-4.696010	-2.010566
H	-8.305832	-6.148184	-2.011373	H	1.956960	-8.862281	2.097835	H	8.157226	-3.998509	2.099996

C	9.287824	-2.764612	-0.028953	C	5.993082	7.609232	-0.030264	C	-9.129480	2.003672	1.200287
C	9.129341	-2.003637	-1.200205	H	5.713261	7.058228	-2.098980	H	-9.085297	0.066010	2.098863
C	9.782160	-2.096221	1.106222	H	6.627324	7.927334	2.011648	C	-9.287824	2.764608	0.028969
C	9.325449	-0.627227	-1.200785	C	4.761719	8.433880	0.029909	H	-9.989042	2.658180	-2.012940
H	8.741336	-2.476214	-2.097633	C	4.220313	9.064596	-1.105376	H	-8.741646	2.476283	2.097775
C	9.978469	-0.718814	1.105619	C	3.984130	8.448578	1.201044	C	-8.757039	4.148336	-0.031190
H	9.988994	-2.658198	2.012963	C	2.921016	9.562031	-1.105146	C	-8.129501	4.608480	-1.201955
C	9.690238	0.060169	-0.030060	H	4.814228	9.141217	-2.012201	C	-8.678591	4.975660	1.104226
H	9.084963	-0.065901	-2.098692	C	2.685623	8.945574	1.201173	C	-7.354743	5.762828	-1.201532
H	10.334033	-0.236167	2.011956	H	4.358463	7.965550	2.098722	H	-8.156987	3.998247	-2.099874
C	9.567021	1.537013	0.029658	C	2.096996	9.454078	0.030275	C	-7.903206	6.130848	1.104637
C	9.722311	2.353111	-1.105921	H	2.530034	10.015649	-2.011864	H	-9.208952	4.696000	2.010538
C	9.093176	2.154238	1.200468	H	2.084453	8.835943	2.098886	H	-6.800312	6.019814	-2.099274
C	9.300810	3.679017	-1.106364	C	0.629581	9.662456	-0.029463	H	-7.845403	6.727275	2.011148
H	10.152885	1.936142	-2.012438	C	-0.077597	9.338086	-1.200320	C	-2.213912	9.424755	-0.028949
C	8.672542	3.479353	1.200104	C	-0.131739	9.995459	1.106089	C	-7.166897	6.517351	-0.030361
H	8.948897	1.560690	2.098378	C	-1.463020	9.221867	-1.200025	C	-6.087505	7.532895	0.030041
C	8.702574	4.256180	0.028995	H	0.469050	9.065524	-2.098208	C	-5.323156	7.674982	1.201356
H	9.411768	4.267367	-2.013233	C	-1.518193	9.879727	1.106289	C	-5.656737	8.243760	-1.105243
H	8.212589	3.881596	2.097782	H	0.370170	10.322299	2.012774	C	-4.124068	8.378786	1.201583
C	7.950706	5.533452	-0.030704	H	-1.956966	8.861960	-2.097790	H	-5.613128	7.137119	2.099106
C	7.256283	5.884165	-1.201529	H	-2.067365	10.119114	2.012933	C	-4.456721	8.947752	-1.105043
C	7.737122	6.336680	1.104752	C	-9.690334	-0.060156	0.030117	H	-6.255480	8.222206	-2.011774
C	6.302531	6.895846	-1.201392	C	-9.978511	0.718802	-1.105582	C	-3.626662	8.976878	0.030600
H	7.383551	5.286277	-2.099080	C	-9.325629	0.627279	1.200889	H	-3.513652	8.370171	2.099677
C	6.782492	7.348775	1.104956	C	-9.782121	2.096197	-1.106211	H	-4.145438	9.460059	-2.011323
H	8.305775	6.148170	2.011410	H	-10.334145	0.236173	-2.011913				

[16]CPP (θ = 31°)

C	3.454050	10.155070	1.195839	H	3.324096	11.221017	-2.019823	H	9.098308	7.368837	2.018100
C	4.738581	9.623066	1.195776	C	6.749799	8.767822	-0.026124	H	8.205088	6.482426	-2.093362
C	5.517482	9.591571	0.025920	C	7.540000	8.523693	1.111920	C	1.426964	10.972412	-0.025858
C	4.988329	10.225490	-1.113040	C	7.074547	8.057588	-1.195072	C	0.695134	10.699801	-1.194795
C	3.703094	10.757789	-1.112977	C	8.523693	7.540003	1.111929	C	0.695582	11.358450	1.112228
C	2.880829	10.683598	0.026088	H	7.368815	9.098306	2.018089	C	-0.695140	10.699813	-1.194793
H	2.851526	10.066931	2.094962	C	8.057613	7.074521	-1.195062	H	1.218099	10.385368	-2.093067
H	5.102403	9.134650	2.094843	H	6.482473	8.205062	-2.093387	C	-0.695580	11.358447	1.112235
H	5.583794	10.285153	-2.019924	C	8.767841	6.749797	-0.026106	H	1.222935	11.643675	2.018422

C	-1.426966	10.972431	-0.025855
H	-1.218114	10.385410	-2.093073
H	-1.222925	11.643654	2.018439
C	9.591588	5.517481	0.025949
C	10.225499	4.988333	-1.113018
C	9.623070	4.738564	1.195795
C	10.757795	3.703097	-1.112968
H	10.285136	5.583797	-2.019905
C	10.155073	3.454032	1.195845
H	9.134660	5.102379	2.094868
C	10.683615	2.880828	0.026093
H	11.221011	3.324099	-2.019820
H	10.066880	2.851477	2.094942
C	10.972431	1.426966	-0.025855
C	11.358447	0.695580	1.112235
C	10.699813	0.695140	-1.194793
C	11.358450	-0.695582	1.112228
H	11.643654	1.222925	2.018439
C	10.699801	-0.695134	-1.194795
H	10.385410	1.218114	-2.093073
C	10.972412	-1.426964	-0.025858
H	11.643675	-1.222935	2.018422
H	10.385368	-1.218099	-2.093067
C	10.683598	-2.880829	0.026088
C	10.757789	-3.703094	-1.112977
C	10.155070	-3.454050	1.195839
C	10.225490	-4.988329	-1.113040
H	11.221017	-3.324096	-2.019823
C	9.623066	-4.738581	1.195776
H	10.066931	-2.851526	2.094962
C	9.591571	-5.517482	0.025920
H	10.285153	-5.583794	-2.019924
H	9.134650	-5.102403	2.094843
C	8.767822	-6.749799	-0.026124
C	8.057588	-7.074547	-1.195072
C	8.523693	-7.540000	1.111920
C	7.074521	-8.057613	-1.195062
H	8.205062	-6.482473	-2.093387
C	7.540003	-8.523693	1.111929
H	9.098306	-7.368815	2.018089
C	6.749797	-8.767841	-0.026106
H	6.482426	-8.205088	-2.093362
H	7.368837	-9.098308	2.018100
C	5.517481	-9.591588	0.025949
C	4.738564	-9.623070	1.195795
C	4.988333	-10.225499	-1.113018
C	3.454032	-10.155073	1.195845
H	5.102379	-9.134660	2.094868
C	3.703097	-10.757795	-1.112968
H	5.583797	-10.285136	-2.019905
C	2.880828	-10.683615	0.026093
H	2.851477	-10.066880	2.094942
H	3.324099	-11.221011	-2.019820
C	1.426966	-10.972431	-0.025855
C	0.695140	-10.699813	-1.194793
C	0.695580	-11.358447	1.112235
C	-0.695134	-10.699801	-1.194795
H	1.218114	-10.385410	-2.093073
C	-0.695582	-11.358450	1.112228
H	1.222925	-11.643654	2.018439
C	-1.426964	-10.972412	-0.025858
H	-1.218099	-10.385368	-2.093067
H	-1.222935	-11.643675	2.018422
C	-2.880829	-10.683598	0.026088
C	-3.454050	-10.155070	1.195839
C	-3.703094	-10.757789	-1.112977
C	-4.738581	-9.623066	1.195776
H	-2.851526	-10.066931	2.094962
C	-4.988329	-10.225490	-1.113040
H	-3.324096	-11.221017	-2.019823
C	-5.517482	-9.591571	0.025920
H	-5.102403	-9.134650	2.094843
H	-5.583794	-10.285153	-2.019924
C	-6.749799	-8.767822	-0.026124
C	-7.540000	-8.523693	1.111920
C	-7.074547	-8.057588	-1.195072
C	-8.523693	-7.540003	1.111929
H	-7.368815	-9.098306	2.018089
C	-8.057613	-7.074521	-1.195062
H	-6.482473	-8.205062	-2.093387
C	-8.767841	-6.749797	-0.026106
H	-9.098308	-7.368837	2.018100
H	-8.205088	-6.482426	-2.093362
C	-9.591588	-5.517481	0.025949
C	-10.225499	-4.988333	-1.113018
C	-9.623070	-4.738564	1.195795
C	-10.757795	-3.703097	-1.112968
H	-10.285136	-5.583797	-2.019905
C	-10.155073	-3.454032	1.195845
H	-9.134660	-5.102379	2.094868
C	-10.683615	-2.880828	0.026093
H	-11.221011	-3.324099	-2.019820
H	-10.066880	-2.851477	2.094942
C	-10.972431	-1.426966	-0.025855
C	-11.358447	-0.695580	1.112235
C	-10.699813	-0.695140	-1.194793
C	-11.358450	0.695582	1.112228
H	-11.643654	-1.222925	2.018439
C	-10.699801	0.695134	-1.194795
H	-10.385410	-1.218114	-2.093073
C	-10.972412	1.426964	-0.025858
H	-11.643675	1.222935	2.018422
H	-10.385368	1.218099	-2.093067
C	-10.683598	2.880829	0.026088
C	-10.757789	3.703094	-1.112977
C	-10.155070	3.454050	1.195839
C	-10.225490	4.988329	-1.113040
H	-11.221017	3.324096	-2.019823
C	-9.623066	4.738581	1.195776
H	-10.066931	2.851526	2.094962
C	-9.591571	5.517482	0.025920

H	-10.285153	5.583794	-2.019924	H	-9.098306	7.368815	2.018089	H	-5.583797	10.285136	-2.019905
H	-9.134650	5.102403	2.094843	C	-6.749797	8.767841	-0.026106	C	-3.454032	10.155073	1.195845
C	-8.767822	6.749799	-0.026124	H	-6.482426	8.205088	-2.093362	H	-5.102379	9.134660	2.094868
C	-8.057588	7.074547	-1.195072	H	-7.368837	9.098308	2.018100	C	-2.880828	10.683615	0.026093
C	-8.523693	7.540000	1.111920	C	-5.517481	9.591588	0.025949	H	-3.324099	11.221011	-2.019820
C	-7.074521	8.057613	-1.195062	C	-4.988333	10.225499	-1.113018	H	-2.851477	10.066880	2.094942
H	-8.205062	6.482473	-2.093387	C	-4.738564	9.623070	1.195795				
C	-7.540003	8.523693	1.111929	C	-3.703097	10.757795	-1.112968				

[18]CPP (θ = 31°)

C	-6.553581	-10.177100	1.189588	H	-2.086954	-11.649364	-2.090839	H	-11.114952	4.079306	2.091358
C	-7.677448	-9.358661	1.189357	H	-2.429121	-12.849912	2.023568	C	-10.479155	6.712807	0.023079
C	-8.431588	-9.150921	0.021408	C	-11.655833	-4.361618	0.023185	H	-11.163688	6.819998	-2.023724
C	-8.061832	-9.885910	-1.119572	C	-12.198384	-3.742251	-1.117300	H	-10.043676	6.268263	2.090713
C	-6.937045	-10.704321	-1.119576	C	-11.564487	-3.585208	1.191549	C	-9.606175	7.910651	-0.023434
C	-6.124009	-10.830588	0.021443	C	-12.534113	-2.392338	-1.116813	C	-8.888390	8.219666	-1.191954
H	-5.947723	-10.234283	2.089014	H	-12.347129	-4.322651	-2.023688	C	-9.340065	8.689544	1.117198
H	-7.917974	-8.799406	2.088588	C	-11.899784	-2.235978	1.191956	C	-7.886944	9.184106	-1.192559
H	-8.655451	-9.805200	-2.026017	H	-11.136788	-4.018482	2.090832	H	-9.050359	7.632741	-2.091168
H	-6.677612	-11.244175	-2.026166	C	-12.344452	-1.591819	0.024273	C	-8.338006	9.654316	1.116695
C	-9.460490	-8.083915	-0.024262	H	-12.937496	-1.948810	-2.022976	H	-9.916975	8.528444	2.023644
C	-10.181386	-7.687786	1.116925	H	-11.724336	-1.653267	2.091347	C	-7.550244	9.890302	-0.024627
C	-9.640952	-7.322616	-1.192164	C	-12.446314	-0.113060	-0.021541	H	-7.294979	9.323565	-2.092214
C	-10.957972	-6.533733	1.117403	C	-12.742946	0.654165	1.119592	H	-8.154739	10.224830	2.023049
H	-10.122513	-8.284204	2.023210	C	-12.095087	0.585627	-1.189643	C	-6.319967	10.716970	0.021164
C	-10.417240	-6.169244	-1.191690	C	-12.595737	2.037395	1.119570	C	-5.538808	10.760960	1.189005
H	-9.091461	-7.583455	-2.091782	H	-13.080624	0.159650	2.026237	C	-5.803872	11.357919	-1.119750
C	-11.054143	-5.716225	-0.023248	C	-11.948111	1.968128	-1.189730	C	-4.267815	11.324494	1.189154
H	-11.488258	-6.254913	2.023772	H	-11.841955	0.032199	-2.088994	H	-5.891422	10.264528	2.088151
H	-10.451932	-5.561394	-2.090925	C	-12.144416	2.725046	-0.021569	C	-4.532127	11.921477	-1.119722
C	-4.792406	-11.481623	-0.024315	H	-12.821852	2.592014	2.026143	H	-6.401277	11.404156	-2.026140
C	-4.012365	-11.419000	-1.192111	H	-11.584289	2.455852	-2.089198	H	-3.663394	11.252774	2.088520
C	-4.193911	-12.046103	1.116712	C	-11.734106	4.149370	0.024184	H	-4.165133	12.395091	-2.026154
C	-2.676138	-11.803014	-1.191571	C	-11.751552	4.971939	-1.116824	C	6.553581	10.177100	-1.189588
H	-4.429233	-10.975783	-2.091538	C	-11.164119	4.685760	1.191895	C	6.937045	10.704321	1.119576
C	-2.857106	-12.430624	1.117186	C	-11.139926	6.221294	-1.117354	C	7.677449	9.358661	-1.189357
H	-4.779733	-12.173759	2.022818	H	-12.239293	4.623047	-2.022846	H	5.947723	10.234283	-2.089014
C	-2.049367	-12.270280	-0.023237	C	-10.552805	5.934437	1.191396	C	8.061832	9.885910	1.119572

H	6.677612	11.244176	2.026166	H	12.821852	-2.592014	-2.026143	C	2.271986	-12.230361	0.024410
C	8.431588	9.150921	-0.021408	H	11.584289	-2.455852	2.089198	C	1.568477	-12.656240	-1.116864
H	7.917974	8.799406	-2.088588	C	11.734106	-4.149370	-0.024184	C	1.522389	-12.006086	1.192298
H	8.655451	9.805200	2.026017	C	11.751552	-4.971939	1.116824	C	0.180781	-12.751891	-1.117389
C	9.460490	8.083915	0.024262	C	11.164119	-4.685760	-1.191895	H	2.114574	-12.903604	-2.022999
C	9.640952	7.322616	1.192164	C	11.139926	-6.221294	1.117354	C	0.135324	-12.101487	1.191705
C	10.181386	7.687786	-1.116925	H	12.239293	-4.623047	2.022846	H	2.022927	-11.660547	2.091922
C	10.417240	6.169244	1.191690	C	10.552805	-5.934437	-1.191396	C	-0.575418	-12.426441	0.023208
H	9.091461	7.583455	2.091782	H	11.114952	-4.079306	-2.091358	H	-0.325562	-13.071809	-2.023858
C	10.957972	6.533733	-1.117403	C	10.479155	-6.712807	-0.023079	H	-0.408581	-11.828066	2.091019
H	10.122513	8.284204	-2.023210	H	11.163688	-6.819998	2.023724	C	6.124009	10.830588	-0.021443
C	11.054143	5.716225	0.023248	H	10.043675	-6.268263	-2.090713	C	-3.710596	11.873499	0.021145
H	10.451932	5.561394	2.090926	C	9.606175	-7.910651	0.023434	C	4.792406	11.481624	0.024315
H	11.488258	6.254913	-2.023772	C	9.340065	-8.689544	-1.117198	C	4.193911	12.046103	-1.116712
C	11.655833	4.361618	-0.023185	C	8.888390	-8.219666	1.191954	C	4.012365	11.419000	1.192111
C	12.198384	3.742251	1.117300	C	8.338006	-9.654316	-1.116695	C	2.857106	12.430624	-1.117186
C	11.564487	3.585208	-1.191549	H	9.916975	-8.528444	-2.023644	H	4.779733	12.173759	-2.022818
C	12.534113	2.392338	1.116813	C	7.886944	-9.184106	1.192559	C	2.676138	11.803014	1.191571
H	12.347129	4.322651	2.023688	H	9.050359	-7.632741	2.091168	H	4.429233	10.975784	2.091538
C	11.899784	2.235978	-1.191956	C	7.550244	-9.890302	0.024627	C	2.049367	12.270280	0.023237
H	11.136788	4.018482	-2.090832	H	8.154739	-10.224830	-2.023049	H	2.429122	12.849912	-2.023568
C	12.344452	1.591819	-0.024273	H	7.294979	-9.323565	2.092214	H	2.086955	11.649364	2.090839
H	12.937496	1.948810	2.022976	C	6.319967	-10.716970	-0.021164	C	-2.271986	12.230361	-0.024411
H	11.724336	1.653267	-2.091347	C	5.538808	-10.760960	-1.189005	C	-1.568477	12.656240	1.116864
C	12.446314	0.113060	0.021541	C	5.803872	-11.357919	1.119750	C	-1.522389	12.006086	-1.192298
C	12.742946	-0.654165	-1.119592	C	4.267815	-11.324494	-1.189154	C	-0.180781	12.751891	1.117389
C	12.095087	-0.585627	1.189643	H	5.891422	-10.264528	-2.088151	H	-2.114574	12.903604	2.022999
C	12.595737	-2.037395	-1.119570	C	4.532127	-11.921477	1.119722	C	-0.135324	12.101487	-1.191706
H	13.080624	-0.159650	-2.026236	H	6.401277	-11.404156	2.026140	H	-2.022927	11.660547	-2.091922
C	11.948111	-1.968128	1.189730	C	3.710596	-11.873499	-0.021145	C	0.575418	12.426441	-0.023208
H	11.841955	-0.032199	2.088994	H	3.663394	-11.252774	-2.088520	H	0.325562	13.071809	2.023857
C	12.144416	-2.725046	0.021569	H	4.165133	-12.395091	2.026154	H	0.408581	11.828066	-2.091019

[20]CPP (θ = 31°)

C	-8.860652	11.012391	-1.123413	C	-8.476793	10.488240	1.186569	H	-6.746672	11.365059	2.084805
C	-7.735882	11.830631	-1.124499	C	-9.233911	10.283110	0.020009	H	-8.718422	9.931048	2.086814
C	-6.925641	11.962127	0.017695	H	-9.455251	10.932044	-2.029203	C	-5.605475	12.636033	-0.024431
C	-7.352396	11.306000	1.185395	H	-7.477417	12.370837	-2.030985	C	-4.823240	12.596262	-1.191790

C	-5.024225	13.215731	1.117745
C	-3.501105	13.026255	-1.192183
H	-5.226087	12.140362	-2.091397
C	-3.701555	13.646057	1.117282
H	-5.613848	13.323951	2.023872
C	-2.891185	13.518958	-0.025428
H	-2.907645	12.894185	-2.091953
H	-3.287952	14.080724	2.023047
C	-10.281764	9.234756	-0.019937
C	-11.011114	8.861407	1.123393
C	-10.486262	8.477315	-1.186361
C	-11.828743	7.736167	1.124570
H	-10.931239	9.456256	2.029071
C	-11.303405	7.352446	-1.185105
H	-9.929027	8.719068	-2.086544
C	-11.959464	6.925535	-0.017474
H	-12.369104	7.477668	2.030986
H	-11.361942	6.746503	-2.084391
C	-1.427088	13.750624	0.015625
C	-0.695131	13.471352	1.182838
C	-0.695269	14.120575	-1.127236
C	0.695128	13.470862	1.182799
H	-1.218984	13.163579	2.082892
C	0.695698	14.120090	-1.127268
H	-1.222712	14.405045	-2.033545
C	1.427254	13.749570	0.015554
H	1.218797	13.162616	2.082857
H	1.223358	14.404184	-2.033562
C	2.891185	13.516891	-0.025448
C	3.500840	13.023846	-1.192221
C	3.701542	13.643490	1.117258
C	4.822838	12.593368	-1.191824
H	2.907346	12.892007	-2.092021
C	5.024051	13.212717	1.117740
H	3.288037	14.078174	2.023018
C	5.605173	12.633035	-0.024526
H	5.225579	12.137509	-2.091480
H	5.613690	13.320745	2.023872
C	6.925584	11.959654	0.017459
C	7.352747	11.303954	1.185204
C	7.736057	11.828711	-1.124669
C	8.477630	10.486830	1.186474
H	6.747022	11.362804	2.084617
C	8.861289	11.011069	-1.123488
H	7.477439	12.368908	-2.031148
C	9.234803	10.281959	0.019939
H	8.719585	9.929887	2.086784
H	9.456026	10.931023	-2.029225
C	10.283023	9.233972	-0.020009
C	11.012515	8.860843	1.123324
C	10.487777	8.476591	-1.186461
C	11.830730	7.736057	1.124403
H	10.932336	9.455541	2.029065
C	11.305480	7.352152	-1.185282
H	9.930285	8.718011	-2.086575
C	11.961965	6.925640	-0.017698
H	12.371082	7.477692	2.030829
H	11.364230	6.746215	-2.084569
C	12.635989	5.605534	0.024426
C	13.215421	5.024202	-1.117840
C	12.596624	4.823434	1.191891
C	13.645721	3.701523	-1.117387
H	13.323466	5.613777	-2.024020
C	13.026636	3.501305	1.192289
H	12.141091	5.226404	2.091629
H	14.080203	3.287858	-2.023211
H	12.894901	2.907955	2.092180
C	5.024225	-13.215731	1.117745
C	4.823240	-12.596262	-1.191790
C	3.701555	-13.646057	1.117282
H	5.613848	-13.323951	2.023872
C	3.501105	-13.026255	-1.192183
H	5.226087	-12.140362	-2.091397
C	2.891185	-13.518958	-0.025428
H	3.287952	-14.080724	2.023047
H	2.907645	-12.894185	-2.091953
C	1.427088	-13.750624	0.015625
C	0.695269	-14.120575	-1.127236
C	0.695131	-13.471352	1.182838
C	-0.695698	-14.120090	-1.127268
H	1.222712	-14.405045	-2.033545
C	-0.695128	-13.470862	1.182799
H	1.218984	-13.163579	2.082892
C	-1.427254	-13.749570	0.015554
H	-1.223358	-14.404184	-2.033562
H	-1.218797	-13.162616	2.082857
C	-2.891185	-13.516891	-0.025448
C	-3.500840	-13.023846	-1.192221
C	-3.701542	-13.643490	1.117258
C	-4.822838	-12.593368	-1.191824
H	-2.907346	-12.892007	-2.092021
C	-5.024051	-13.212717	1.117740
H	-3.288037	-14.078174	2.023018
C	-5.605173	-12.633035	-0.024526
H	-5.225579	-12.137509	-2.091480
H	-5.613690	-13.320745	2.023872
C	-6.925584	-11.959654	0.017459
C	-7.352747	-11.303954	1.185204
C	-7.736057	-11.828711	-1.124669
C	-8.477630	-10.486830	1.186474
H	-6.747022	-11.362804	2.084617
C	-8.861289	-11.011069	-1.123488
H	-7.477439	-12.368908	-2.031148
C	-9.234803	-10.281959	0.019939
H	-8.719585	-9.929887	2.086784
H	-9.456026	-10.931023	-2.029225
C	-10.283023	-9.233972	-0.020009
C	-10.487777	-8.476591	-1.186461
C	-11.012515	-8.860843	1.123324
C	-11.305480	-7.352152	-1.185282
H	-9.930285	-8.718011	-2.086575

C	-11.830730	-7.736057	1.124403	C	-13.024164	3.500989	1.192308	H	14.405270	1.222714	2.033385
H	-10.932336	-9.455541	2.029065	C	-13.643128	3.701458	-1.117371	H	13.161509	-1.218756	-2.082639
C	-11.961965	-6.925640	-0.017698	C	-12.593739	4.823003	1.191923	H	14.404413	-1.223346	2.033378
H	-11.364230	-6.746215	-2.084569	H	-12.892677	2.907607	2.092235	C	13.749275	-1.427231	-0.015574
H	-12.371082	-7.477692	2.030829	C	-13.212369	5.023972	-1.117853	C	9.233911	-10.283110	0.020009
C	-12.635989	-5.605534	0.024426	H	-14.077614	3.287880	-2.023192	C	13.516772	-2.891190	0.025422
C	-12.596624	-4.823434	1.191891	C	-12.632981	5.605192	0.024509	C	13.024164	-3.500989	1.192308
C	-13.215421	-5.024202	-1.117840	H	-12.138225	5.225861	2.091702	C	13.643128	-3.701458	-1.117371
C	-13.026636	-3.501305	1.192289	H	-13.320206	5.613551	-2.024047	C	12.593739	-4.823003	1.191923
H	-12.141091	-5.226404	2.091629	C	5.605475	-12.636033	-0.024431	H	12.892677	-2.907607	2.092235
C	-13.645721	-3.701523	-1.117387	C	13.518891	2.891243	0.025416	C	13.212369	-5.023972	-1.117853
H	-13.323466	-5.613777	-2.024020	C	6.925641	-11.962127	0.017695	H	14.077614	-3.287880	-2.023192
C	-13.518891	-2.891243	0.025416	C	7.352396	-11.306000	1.185395	C	12.632981	-5.605192	0.024509
H	-12.894901	-2.907955	2.092180	C	7.735882	-11.830631	-1.124499	H	12.138225	-5.225861	2.091702
H	-14.080203	-3.287858	-2.023211	C	8.476793	-10.488240	1.186569	H	13.320206	-5.613551	-2.024047
C	-13.750372	-1.427116	-0.015638	H	6.746672	-11.365059	2.084805	C	10.281764	-9.234756	-0.019937
C	-14.120588	-0.695285	1.127134	C	8.860652	-11.012391	-1.123413	C	10.486262	-8.477315	-1.186361
C	-13.470653	-0.695164	-1.182743	H	7.477417	-12.370837	-2.030985	C	11.011114	-8.861407	1.123393
C	-14.120101	0.695681	1.127155	H	8.718422	-9.931048	2.086814	C	11.303405	-7.352446	-1.185105
H	-14.405270	-1.222714	2.033385	H	9.455251	-10.932044	-2.029203	H	9.929027	-8.719068	-2.086544
C	-13.470113	0.695095	-1.182701	C	13.750372	1.427116	-0.015638	C	11.828743	-7.736167	1.124570
H	-13.162508	-1.219020	-2.082668	C	13.470653	0.695164	-1.182743	H	10.931239	-9.456256	2.029071
C	-13.749275	1.427231	-0.015574	C	14.120588	0.695285	1.127134	C	11.959464	-6.925535	-0.017474
H	-14.404413	1.223346	2.033378	C	13.470113	-0.695095	-1.182701	H	11.361942	-6.746503	-2.084391
H	-13.161509	1.218756	-2.082639	H	13.162508	1.219020	-2.082668	H	12.369104	-7.477668	2.030986
C	-13.516772	2.891190	0.025422	C	14.120101	-0.695681	1.127155				

[12]CPP (θ = 27°)

C	-0.695184	7.983878	1.211439	C	3.389892	7.261834	-1.211439	C	8.195562	-1.428519	-0.030952
C	0.695184	7.983878	1.211439	C	6.383305	5.334914	0.030952	C	7.983878	-0.695184	-1.211439
C	1.428519	8.195562	0.030952	C	6.566649	4.593987	1.211439	C	7.983878	0.695184	-1.211439
C	0.695329	8.565585	-1.113089	C	7.261834	3.389892	1.211439	C	7.811824	-2.860647	0.030952
C	-0.695329	8.565585	-1.113089	C	7.811824	2.860647	0.030952	C	7.261834	-3.389892	1.211439
C	2.860647	7.811824	-0.030952	C	7.765679	3.680620	-1.113089	C	6.566649	-4.593987	1.211439
C	3.680620	7.765679	1.113089	C	7.070350	4.884965	-1.113089	C	6.383305	-5.334914	0.030952
C	4.884965	7.070350	1.113089	C	8.195562	1.428519	-0.030952	C	7.070350	-4.884965	-1.113089
C	5.334914	6.383305	-0.030952	C	8.565585	0.695329	1.113089	C	7.765679	-3.680620	-1.113089
C	4.593987	6.566649	-1.211439	C	8.565585	-0.695329	1.113089	C	5.334914	-6.383305	-0.030952

C	4.884965	-7.070350	1.113089	C	-7.261834	3.389892	1.211439	H	5.467713	-7.029737	2.029063
C	3.680620	-7.765679	1.113089	C	-6.566649	4.593987	1.211439	H	3.354075	-8.250046	2.029063
C	2.860647	-7.811824	-0.030952	C	-6.383305	5.334914	0.030952	H	2.798150	-7.270461	-2.121639
C	3.389892	-7.261834	-1.211439	C	-7.070350	4.884965	-1.113089	H	4.897329	-6.058499	-2.121639
C	4.593987	-6.566649	-1.211439	C	-7.765679	3.680620	-1.113089	H	1.211962	-7.695479	2.121639
C	1.428519	-8.195562	0.030952	C	-5.334914	6.383305	-0.030952	H	-1.211962	-7.695479	2.121639
C	0.695184	-7.983878	1.211439	C	-4.884965	7.070350	1.113089	H	-1.220309	-8.821787	-2.029063
C	-0.695184	-7.983878	1.211439	C	-3.680620	7.765679	1.113089	H	1.220309	-8.821787	-2.029063
C	-1.428519	-8.195562	0.030952	C	-3.389892	7.261834	-1.211439	H	-3.354075	-8.250046	2.029063
C	-0.695329	-8.565585	-1.113089	C	-4.593987	6.566649	-1.211439	H	-5.467713	-7.029737	2.029063
C	0.695329	-8.565585	-1.113089	H	-1.211962	7.695479	2.121639	H	-4.897329	-6.058499	-2.121639
C	-2.860647	-7.811824	-0.030952	H	1.211962	7.695479	2.121639	H	-2.798150	-7.270461	-2.121639
C	-3.680620	-7.765679	1.113089	H	1.220309	8.821787	-2.029063	H	-6.058499	-4.897329	2.121639
C	-4.884965	-7.070350	1.113089	H	-1.220309	8.821787	-2.029063	H	-7.270461	-2.798150	2.121639
C	-5.334914	-6.383305	-0.030952	H	3.354075	8.250046	2.029063	H	-8.250046	-3.354075	-2.029063
C	-4.593987	-6.566649	-1.211439	H	5.467713	7.029737	2.029063	H	-7.029737	-5.467713	-2.029063
C	-3.389892	-7.261834	-1.211439	H	4.897329	6.058499	-2.121639	H	-8.821787	-1.220309	2.029063
C	-6.383305	-5.334914	0.030952	H	2.798150	7.270461	-2.121639	H	-8.821787	1.220309	2.029063
C	-6.566649	-4.593987	1.211439	H	6.058499	4.897329	2.121639	H	-7.695479	1.211962	-2.121639
C	-7.261834	-3.389892	1.211439	H	7.270461	2.798150	2.121639	H	-7.695479	-1.211962	-2.121639
C	-7.811824	-2.860647	0.030952	H	8.250046	3.354075	-2.029063	H	-7.270461	2.798150	2.121639
C	-7.765679	-3.680620	-1.113089	H	7.029737	5.467713	-2.029063	H	-6.058499	4.897329	2.121639
C	-7.070350	-4.884965	-1.113089	H	8.821787	1.220309	2.029063	H	-7.029737	5.467713	-2.029063
C	-8.195562	-1.428519	-0.030952	H	8.821787	-1.220309	2.029063	H	-8.250046	3.354075	-2.029063
C	-8.565585	-0.695329	1.113089	H	7.695479	-1.211962	-2.121639	H	-5.467713	7.029737	2.029063
C	-8.565585	0.695329	1.113089	H	7.695479	1.211962	-2.121639	H	-3.354075	8.250046	2.029063
C	-8.195562	1.428519	-0.030952	H	7.270461	-2.798150	2.121639	H	-2.798150	7.270461	-2.121639
C	-7.983878	0.695184	-1.211439	H	6.058499	-4.897329	2.121639	H	-4.897329	6.058499	-2.121639
C	-7.983878	-0.695184	-1.211439	H	7.029737	-5.467713	-2.029063	C	-2.860647	7.811824	-0.030952
C	-7.811824	2.860647	0.030952	H	8.250046	-3.354075	-2.029063	C	-1.428519	8.195562	0.030952

[12]CPP (θ = 29°)

C	-0.695141	7.957017	1.213320	C	3.688493	7.778512	1.106437	C	6.543532	4.579685	1.209404
C	0.695141	7.957017	1.213320	C	4.893221	7.082907	1.105397	C	7.238334	3.375494	1.208227
C	1.427406	8.191285	0.036103	C	5.331655	6.380051	-0.032706	C	7.807244	2.859291	0.030688
C	0.695542	8.581588	-1.101242	C	4.579685	6.543532	-1.209404	C	7.778512	3.688493	-1.106437
C	-0.695542	8.581588	-1.101242	C	3.375494	7.238334	-1.208227	C	7.082907	4.893221	-1.105397
C	2.859291	7.807244	-0.030688	C	6.380051	5.331655	0.032706	C	8.191285	1.427406	-0.036103

C	8.581588	0.695542	1.101242	C	-7.082907	-4.893221	-1.105397	H	7.233090	-2.772106	2.110876
C	8.581588	-0.695542	1.101242	C	-8.191285	-1.427406	-0.036103	H	6.019580	-4.875975	2.113054
C	8.191285	-1.427406	-0.036103	C	-8.581588	-0.695542	1.101242	H	7.052854	-5.484168	-2.016707
C	7.957017	-0.695141	-1.213320	C	-8.581588	0.695542	1.101242	H	8.275021	-3.368359	-2.018305
C	7.957017	0.695141	-1.213320	C	-8.191285	1.427406	-0.036103	H	5.484168	-7.052854	2.016707
C	7.807244	-2.859291	0.030689	C	-7.957017	0.695141	-1.213320	H	3.368359	-8.275020	2.018305
C	7.238334	-3.375494	1.208227	C	-7.957017	-0.695141	-1.213320	H	2.772106	-7.233090	-2.110876
C	6.543532	-4.579685	1.209404	C	-7.807244	2.859291	0.030688	H	4.875975	-6.019580	-2.113054
C	6.380051	-5.331655	0.032706	C	-7.238334	3.375494	1.208227	H	1.214450	-7.652019	2.116838
C	7.082907	-4.893221	-1.105397	C	-6.543532	4.579685	1.209404	H	-1.214450	-7.652019	2.116838
C	7.778512	-3.688493	-1.106437	C	-6.380051	5.331655	0.032706	H	-1.221477	-8.851653	-2.012865
C	5.331655	-6.380051	-0.032706	C	-7.082907	4.893221	-1.105397	H	1.221477	-8.851653	-2.012865
C	4.893221	-7.082907	1.105397	C	-7.778512	3.688493	-1.106437	H	-3.368359	-8.275020	2.018305
C	3.688493	-7.778512	1.106437	C	-5.331655	6.380051	-0.032706	H	-5.484168	-7.052854	2.016707
C	2.859291	-7.807244	-0.030688	C	-4.893221	7.082907	1.105397	H	-4.875975	-6.019580	-2.113054
C	3.375494	-7.238334	-1.208227	C	-3.688493	7.778512	1.106437	H	-2.772106	-7.233090	-2.110876
C	4.579685	-6.543532	-1.209404	C	-3.375494	7.238334	-1.208227	H	-6.019580	-4.875975	2.113054
C	1.427406	-8.191285	0.036103	C	-4.579685	6.543532	-1.209404	H	-7.233090	-2.772106	2.110876
C	0.695141	-7.957017	1.213320	H	-1.214450	7.652019	2.116838	H	-8.275021	-3.368359	-2.018305
C	-0.695141	-7.957017	1.213320	H	1.214450	7.652019	2.116838	H	-7.052854	-5.484168	-2.016707
C	-1.427406	-8.191285	0.036103	H	1.221477	8.851653	-2.012865	H	-8.851653	-1.221477	2.012865
C	-0.695542	-8.581588	-1.101242	H	-1.221477	8.851653	-2.012865	H	-8.851653	1.221477	2.012865
C	0.695542	-8.581588	-1.101242	H	3.368359	8.275020	2.018305	H	-7.652019	1.214450	-2.116838
C	-2.859291	-7.807244	-0.030688	H	5.484168	7.052854	2.016707	H	-7.652019	-1.214450	-2.116838
C	-3.688493	-7.778512	1.106437	H	4.875975	6.019580	-2.113054	H	-7.233090	2.772106	2.110876
C	-4.893221	-7.082907	1.105397	H	2.772106	7.233090	-2.110876	H	-6.019580	4.875975	2.113054
C	-5.331655	-6.380051	-0.032706	H	6.019580	4.875975	2.113054	H	-7.052854	5.484168	-2.016707
C	-4.579685	-6.543532	-1.209404	H	7.233090	2.772106	2.110876	H	-8.275021	3.368359	-2.018305
C	-3.375494	-7.238334	-1.208227	H	8.275021	3.368359	-2.018305	H	-5.484168	7.052854	2.016707
C	-6.380051	-5.331655	0.032706	H	7.052854	5.484168	-2.016707	H	-3.368359	8.275020	2.018305
C	-6.543532	-4.579685	1.209404	H	8.851653	1.221477	2.012865	H	-2.772106	7.233090	-2.110876
C	-7.238334	-3.375494	1.208227	H	8.851653	-1.221477	2.012865	H	-4.875975	6.019580	-2.113054
C	-7.807244	-2.859291	0.030688	H	7.652019	-1.214450	-2.116838	C	-2.859291	7.807244	-0.030688
C	-7.778512	-3.688493	-1.106437	H	7.652019	1.214450	-2.116838	C	-1.427406	8.191285	0.036103

[12]CPP (θ = 33°)

C	-2.717410	7.454222	1.205741	C	-0.741133	8.272505	0.038087	C	-2.900962	8.138723	-1.086674
C	-1.373989	7.813838	1.205768	C	-1.556879	8.498407	-1.086698	C	0.741133	8.272505	-0.038087

C	1.556879	8.498407	1.086698
C	2.900962	8.138723	1.086674
C	3.494900	7.535591	-0.038179
C	2.717410	7.454222	-1.205741
C	1.373989	7.813838	-1.205768
C	4.778563	6.794467	0.038179
C	5.096840	6.080457	1.205741
C	6.079988	5.096828	1.205768
C	6.793633	4.778092	0.038087
C	6.581397	5.597500	-1.086698
C	5.597860	6.581669	-1.086674
C	7.534766	3.494413	-0.038087
C	8.138276	2.900907	1.086698
C	8.498822	1.557055	1.086674
C	8.273463	0.741123	-0.038179
C	7.814250	1.373765	-1.205741
C	7.453976	2.717010	-1.205768
C	8.273463	-0.741123	0.038179
C	7.814250	-1.373765	1.205741
C	7.453976	-2.717010	1.205768
C	7.534766	-3.494413	0.038087
C	8.138276	-2.900907	-1.086698
C	8.498822	-1.557055	-1.086674
C	6.793633	-4.778092	-0.038087
C	6.581397	-5.597500	1.086698
C	5.597860	-6.581669	1.086674
C	4.778563	-6.794467	-0.038179
C	5.096840	-6.080457	-1.205741
C	6.079988	-5.096828	-1.205768
C	3.494900	-7.535591	0.038179
C	2.717410	-7.454222	1.205741
C	1.373989	-7.813838	1.205768
C	0.741133	-8.272505	0.038087
C	1.556879	-8.498407	-1.086698
C	2.900962	-8.138723	-1.086674
C	-0.741133	-8.272505	-0.038087
C	-1.556879	-8.498407	1.086698
C	-2.900962	-8.138723	1.086674
C	-3.494900	-7.535591	-0.038179
C	-2.717410	-7.454222	-1.205741
C	-1.373989	-7.813838	-1.205768
C	-4.778563	-6.794467	0.038179
C	-5.096840	-6.080457	1.205741
C	-6.079988	-5.096828	1.205768
C	-6.793633	-4.778092	0.038087
C	-6.581397	-5.597500	-1.086698
C	-5.597860	-6.581669	-1.086674
C	-7.534766	-3.494413	-0.038087
C	-8.138276	-2.900907	1.086698
C	-8.498822	-1.557055	1.086674
C	-8.273463	-0.741123	-0.038179
C	-7.814250	-1.373765	-1.205741
C	-7.453976	-2.717010	-1.205768
C	-8.273463	0.741123	0.038179
C	-7.814250	1.373765	1.205741
C	-7.453976	2.717010	1.205768
C	-7.534766	3.494413	0.038087
C	-8.138276	2.900907	-1.086698
C	-8.498822	1.557055	-1.086674
C	-6.793633	4.778092	-0.038087
C	-6.581397	5.597500	1.086698
C	-5.597860	6.581669	1.086674
C	-5.096840	6.080457	-1.205741
C	-6.079988	5.096828	-1.205768
H	-3.134300	6.991867	2.095536
H	-0.781806	7.621831	2.095600
H	-1.122035	8.922807	-1.987800
H	-3.489445	8.289107	-1.987886
H	1.122035	8.922807	1.987800
H	3.489445	8.289107	1.987886
H	3.134300	6.991867	-2.095536
H	0.781806	7.621831	-2.095600
H	4.487984	6.210317	2.095536
H	6.209796	4.487979	2.095600
H	7.166360	5.433115	-1.987800
H	5.433855	7.166501	-1.987886
H	8.288395	3.489693	1.987800
H	8.923300	1.122606	1.987886
H	7.622285	0.781550	-2.095536
H	6.991602	3.133852	-2.095600
H	7.622285	-0.781550	2.095536
H	6.991602	-3.133852	2.095600
H	8.288395	-3.489693	-1.987800
H	8.923300	-1.122606	-1.987886
H	7.166360	-5.433115	1.987800
H	5.433855	-7.166501	1.987886
H	4.487984	-6.210317	-2.095536
H	6.209796	-4.487979	-2.095600
H	3.134300	-6.991867	2.095536
H	0.781806	-7.621831	2.095600
H	1.122035	-8.922807	-1.987800
H	3.489445	-8.289107	-1.987886
H	-1.122035	-8.922807	1.987800
H	-3.489445	-8.289107	1.987886
H	-3.134300	-6.991867	-2.095536
H	-0.781806	-7.621831	-2.095600
H	-4.487984	-6.210317	2.095536
H	-6.209796	-4.487979	2.095600
H	-7.166360	-5.433115	-1.987800
H	-5.433855	-7.166501	-1.987886
H	-8.288395	-3.489693	1.987800
H	-8.923300	-1.122606	1.987886
H	-7.622285	-0.781550	-2.095536
H	-6.991602	-3.133852	-2.095600
H	-7.622285	0.781550	2.095536
H	-6.991602	3.133852	2.095600
H	-8.288395	3.489693	-1.987800
H	-8.923300	1.122606	-1.987886
H	-7.166360	5.433115	1.987800
H	-5.433855	7.166501	1.987886
H	-4.487984	6.210317	-2.095536

H	-6.209796	4.487979	-2.095600	C	-4.778563	6.794467	-0.038179	C	-3.494900	7.535591	0.038179

[12]CPP (θ = 35°)

C	-0.694995	7.877433	1.203515	C	1.424427	-8.179501	0.040020	H	-1.220221	7.524114	2.086052
C	0.694995	7.877433	1.203515	C	0.694995	-7.877433	1.203515	H	1.220221	7.524114	2.086052
C	1.424427	8.179501	0.040020	C	-0.694995	-7.877433	1.203515	H	1.225983	8.938971	-1.973226
C	0.696274	8.628038	-1.076555	C	-1.424427	-8.179501	0.040020	H	-1.225983	8.938971	-1.973226
C	-0.696274	8.628038	-1.076555	C	-0.696274	-8.628038	-1.076555	H	3.407753	8.354368	1.973226
C	2.856160	7.795869	-0.040020	C	0.696274	-8.628038	-1.076555	H	5.531218	7.128385	1.973226
C	3.711028	7.820237	1.076555	C	-2.856160	-7.795869	-0.040020	H	4.818800	5.905963	-2.086052
C	4.917010	7.123963	1.076555	C	-3.711028	-7.820237	1.076555	H	2.705314	7.126185	-2.086052
C	5.323341	6.371442	-0.040020	C	-4.917010	-7.123963	1.076555	H	5.905963	4.818800	2.086052
C	4.540600	6.474560	-1.203515	C	-5.323341	-6.371442	-0.040020	H	7.126185	2.705314	2.086052
C	3.336833	7.169555	-1.203515	C	-4.540600	-6.474560	-1.203515	H	8.354368	3.407753	-1.973226
C	6.371442	5.323341	0.040020	C	-3.336833	-7.169555	-1.203515	H	7.128385	5.531218	-1.973226
C	6.474560	4.540600	1.203515	C	-6.371442	-5.323341	0.040020	H	8.938971	1.225983	1.973226
C	7.169555	3.336833	1.203515	C	-6.474560	-4.540600	1.203515	H	8.938971	-1.225983	1.973226
C	7.795869	2.856160	0.040020	C	-7.169555	-3.336833	1.203515	H	7.524114	-1.220221	-2.086052
C	7.820237	3.711028	-1.076555	C	-7.795869	-2.856160	0.040020	H	7.524114	1.220221	-2.086052
C	7.123963	4.917010	-1.076555	C	-7.820237	-3.711028	-1.076555	H	7.126185	-2.705314	2.086052
C	8.179501	1.424427	-0.040020	C	-7.123963	-4.917010	-1.076555	H	5.905963	-4.818800	2.086052
C	8.628038	0.696274	1.076555	C	-8.179501	-1.424427	-0.040020	H	7.128385	-5.531218	-1.973226
C	8.628038	-0.696274	1.076555	C	-8.628038	-0.696274	1.076555	H	8.354368	-3.407753	-1.973226
C	8.179501	-1.424427	-0.040020	C	-8.628038	0.696274	1.076555	H	5.531218	-7.128385	1.973226
C	7.877433	-0.694995	-1.203515	C	-8.179501	1.424427	-0.040020	H	3.407753	-8.354368	1.973226
C	7.877433	0.694995	-1.203515	C	-7.877433	0.694995	-1.203515	H	2.705314	-7.126185	-2.086052
C	7.795869	-2.856160	0.040020	C	-7.877433	-0.694995	-1.203515	H	4.818800	-5.905963	-2.086052
C	7.169555	-3.336833	1.203515	C	-7.795869	2.856160	0.040020	H	1.220221	-7.524114	2.086052
C	6.474560	-4.540600	1.203515	C	-7.169555	3.336833	1.203515	H	-1.220221	-7.524114	2.086052
C	6.371442	-5.323341	0.040020	C	-6.474560	4.540600	1.203515	H	-1.225983	-8.938971	-1.973226
C	7.123963	-4.917010	-1.076555	C	-6.371442	5.323341	0.040020	H	1.225983	-8.938971	-1.973226
C	7.820237	-3.711028	-1.076555	C	-7.123963	4.917010	-1.076555	H	-3.407753	-8.354368	1.973226
C	5.323341	-6.371442	-0.040020	C	-7.820237	3.711028	-1.076555	H	-5.531218	-7.128385	1.973226
C	4.917010	-7.123963	1.076555	C	-5.323341	6.371442	-0.040020	H	-4.818800	-5.905963	-2.086052
C	3.711028	-7.820237	1.076555	C	-4.917010	7.123963	1.076555	H	-2.705314	-7.126185	-2.086052
C	2.856160	-7.795869	-0.040020	C	-3.711028	7.820237	1.076555	H	-5.905963	-4.818800	2.086052
C	3.336833	-7.169555	-1.203515	C	-3.336833	7.169555	-1.203515	H	-7.126185	-2.705314	2.086052
C	4.540600	-6.474560	-1.203515	C	-4.540600	6.474560	-1.203515	H	-8.354368	-3.407753	-1.973226

H	-7.128385	-5.531218	-1.973226
H	-8.938971	-1.225983	1.973226
H	-8.938971	1.225983	1.973226
H	-7.524114	1.220221	-2.086052
H	-7.524114	-1.220221	-2.086052
H	-7.126185	2.705314	2.086052
H	-5.905963	4.818800	2.086052
H	-7.128385	5.531218	-1.973226
H	-8.354368	3.407753	-1.973226
H	-5.531218	7.128385	1.973226
H	-3.407753	8.354368	1.973226
H	-2.705314	7.126185	-2.086052
H	-4.818800	5.905963	-2.086052
C	-2.856160	7.795869	-0.040020
C	-1.424427	8.179501	0.040020

3. Full Reference of ref. 25

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