

Supplementary Information

for

Convergence in the Evolution of Nanodiamond Raman Spectra with Particle Size: A Theoretical Investigation

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Table S1. Cartesian coordinates of SCC-DFTB optimized compounds in [Å]. Names of model structures are given in the main text.

A	C	-0.734812	-1.272732	-0.519591	O2	C	-0.010855	1.818277	-1.818277
	C	-0.738708	-1.279480	1.044691		C	0.010855	-1.818277	-1.818277
	C	0.738708	-1.279480	-1.044691		C	1.818277	-0.010855	-1.818277
	C	0.000000	0.000000	1.558772		C	-1.818277	0.010855	-1.818277
	H	-1.777566	-1.286355	1.416193		C	0.901408	-0.901408	-2.728269
	H	-0.225233	-2.182595	1.416193		C	-0.901408	0.901408	-2.728269
	C	-0.738708	1.279480	1.044691		C	-0.901408	-0.901408	2.728269
	H	0.000000	0.000000	2.665288		C	0.901408	0.901408	2.728269
	C	1.477417	0.000000	1.044691		C	0.010855	1.818277	1.818277
	C	-0.734812	1.272732	-0.519591		C	-0.010855	-1.818277	1.818277
	H	-1.777566	1.286355	1.416193		C	1.818277	0.010855	1.818277
	H	-0.225233	2.182595	1.416193		C	-1.818277	-0.010855	1.818277
	C	-1.477417	0.000000	-1.044691		C	0.901408	2.728269	0.901408
	H	-1.256429	2.176199	-0.888429		C	-0.901408	-2.728269	0.901408
	C	0.738708	1.279480	-1.044691		C	-2.728269	-0.901408	0.901408
	H	-2.520244	0.000000	-0.684416		C	0.913877	-0.913877	0.913877
	H	-1.485355	0.000000	-2.147970		C	2.728269	0.901408	0.901408
	C	1.469624	0.000000	-0.519591		C	-0.913877	0.913877	0.913877
	H	2.512858	0.000000	-0.888430		C	1.818277	1.818277	0.010855
	H	-1.256429	-2.176199	-0.888429		C	-1.818277	1.818277	-0.010855
	H	0.742677	-1.286355	-2.147970		C	1.818277	-1.818277	-0.010855
	H	1.260122	-2.182595	-0.684416		C	-1.818277	-1.818277	0.010855
	H	0.742677	1.286355	-2.147970		C	0.000000	0.000000	0.000000
	H	1.260122	2.182595	-0.684416		C	-0.901408	2.728269	-0.901408
	H	2.002800	-0.896240	1.416193		C	0.901408	-2.728269	-0.901408
	H	2.002800	0.896240	1.416193		C	2.728269	-0.901408	-0.901408
						C	-0.913877	-0.913877	-0.913877
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						C	0.913877	0.913877	-0.913877
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						C	0.000000	0.000000	3.633736
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						C	0.000000	-3.633736	0.000000
						C	-3.633736	0.000000	0.000000
						C	3.633736	0.000000	0.000000
						H	0.620389	2.465066	-2.465066
						H	-0.620389	-2.465066	-2.465066
						H	2.465066	0.620389	-2.465066
						H	-2.465066	-0.620389	-2.465066
						H	1.537250	-1.537250	-3.377863
						H	-1.537250	1.537250	-3.377863
						H	-1.537250	-1.537250	3.377863
						H	1.537250	1.537250	3.377863
						H	-0.620389	2.465066	2.465066
						H	0.620389	-2.465066	2.465066
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						H	-2.465066	0.620389	2.465066
						H	1.537250	3.377863	1.537250
						H	-1.537250	-3.377863	1.537250
						H	-3.377863	-1.537250	1.537250

					H	3.377863	1.537250	1.537250	
					H	2.465066	2.465066	-0.620389	
					H	-2.465066	2.465066	0.620389	
					H	2.465066	-2.465066	0.620389	
					H	-2.465066	-2.465066	-0.620389	
					H	-1.537250	3.377863	-1.537250	
					H	1.537250	-3.377863	-1.537250	
					H	3.377863	-1.537250	-1.537250	
					H	-3.377863	1.537250	-1.537250	
					H	0.633747	0.633747	-4.277798	
					H	-0.633747	-0.633747	-4.277798	
					H	-0.633747	0.633747	4.277798	
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					H	0.633747	4.277798	-0.633747	
					H	0.633747	-4.277798	0.633747	
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					H	-4.277798	-0.633747	-0.633747	
					H	-4.277798	0.633747	0.633747	
					H	4.277798	0.633747	-0.633747	
					H	4.277798	-0.633747	0.633747	
O3	C	0.000000	0.000000	5.459411	O4	C	-3.419469	-3.992798	-3.832428
	C	-0.010768	1.817511	3.643013		C	-2.679335	-2.701126	-4.328291
	C	1.817511	-0.010768	3.643013		C	-3.002635	-1.507460	-3.349198
	C	-1.817511	0.010768	3.643013		C	-2.488619	-1.879930	-1.901421
	C	0.010768	-1.817511	3.643013		C	-3.217466	-3.191269	-1.403248
	C	-0.010768	3.643013	1.817511		C	-2.891898	-4.367166	-2.402877
	C	1.819475	1.819475	1.819475		C	-0.927246	-2.128592	-1.944212
	C	3.643013	-0.010768	1.817511		C	-0.412365	-2.500445	-0.495892
	C	-1.826208	1.826208	1.826208		C	-0.729434	-1.311804	0.497750
	C	0.000000	0.000000	1.826556		C	-2.290475	-1.062758	0.540782
	C	1.826208	-1.826208	1.826208		C	-2.805257	-0.690981	-0.907593
	C	-3.643013	0.010768	1.817511		C	-2.607626	0.125803	1.534635
	C	-1.819475	-1.819475	1.819475		C	-1.878073	1.437551	1.036561
	C	0.010768	-3.643013	1.817511		C	-0.317001	1.188692	0.993567
	C	0.000000	5.459411	0.000000		C	0.000001	-0.000001	0.000001
	C	1.817511	3.643013	-0.010768		C	-2.392754	1.809939	-0.411693
	C	3.643013	1.817511	-0.010768		C	-2.075655	0.620966	-1.405071
	C	5.459411	0.000000	0.000000		C	-0.514598	0.372046	-1.448248
	C	-1.817511	3.643013	0.010768		C	-0.214760	-1.683768	1.946018
	C	0.000000	1.826556	0.000000		C	-0.532021	-0.495174	2.939798
	C	1.826556	0.000000	0.000000		C	0.197641	0.816541	2.441798
	C	3.643013	-1.817511	0.010768		C	1.758837	0.567871	2.398890
	C	-3.643013	1.817511	0.010768		C	2.075538	-0.620983	1.405242
	C	-1.826556	0.000000	0.000000		C	1.561037	-0.248939	-0.043066
	C	0.000000	-1.826556	0.000000		C	0.214904	1.683872	-1.945909
	C	1.817511	-3.643013	0.010768		C	-0.102316	2.872789	-0.952501
	C	-5.459411	0.000000	0.000000		C	0.412486	2.500457	0.495724
	C	-3.643013	-1.817511	-0.010768		C	2.290383	1.062933	-0.540831
	C	-1.817511	-3.643013	-0.010768		C	1.973670	2.251698	0.452919
	C	0.000000	-5.459411	0.000000		C	-0.197545	-0.816721	-2.441745
	C	0.000000	0.000000	-5.459411		C	1.363613	-1.065548	-2.485120
	C	0.010768	1.817511	-3.643013		C	1.877934	-1.437660	-1.036667

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C	-1.817511	-0.010768	-3.643013	C	1.776040	1.434914	-1.989310
C	-0.010768	-1.817511	-3.643013	C	1.346334	-1.933049	1.902989
C	0.010768	3.643013	-1.817511	C	-2.093338	-0.246275	2.983296
C	1.826208	1.826208	-1.826208	C	-2.822275	-1.557989	3.480350
C	3.643013	0.010768	-1.817511	C	-4.377060	-1.294862	3.517627
C	-1.819475	1.819475	-1.819475	C	-4.680392	-0.123637	4.516785
C	0.000000	0.000000	-1.826556	C	-3.968990	1.179185	4.008199
C	1.819475	-1.819475	-1.819475	C	-2.409852	0.942446	3.976154
C	-3.643013	-0.010768	-1.817511	C	-4.167841	0.374828	1.576583
C	-1.826208	-1.826208	-1.826208	C	-4.468462	1.560784	2.570269
C	-0.010768	-3.643013	-1.817511	C	-2.298952	-1.916588	4.924484
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C	0.901163	-0.901163	4.553859	C	-1.890882	0.557459	5.415056
C	-0.903498	2.729546	2.729546	C	-0.016649	-0.867121	4.386896
C	0.913104	0.913104	2.739069	C	-0.339600	0.325516	5.365465
C	2.729546	-0.903498	2.729546	C	-2.193988	2.625250	2.029388
C	-2.729546	0.903498	2.729546	C	-1.678061	2.245059	3.470863
C	-0.913104	-0.913104	2.739069	C	-0.119415	2.004582	3.433851
C	0.903498	-2.729546	2.729546	C	-2.499732	-2.736564	2.483070
C	-0.901163	4.553859	0.901163	C	-0.943952	-2.994420	2.442612
C	0.913104	2.739069	0.913104	C	-0.752029	-2.174959	4.869652
C	2.739069	0.913104	0.913104	C	-3.018525	-2.373752	1.038148
C	4.553859	-0.901163	0.901163	C	-4.880891	-0.939691	2.074457
C	-2.729546	2.729546	0.903498	C	-1.663570	3.122175	-0.909567
C	-0.913222	0.913222	0.913222	C	-1.463209	3.929034	1.524721
C	0.913222	-0.913222	0.913222	C	0.095311	3.687572	1.488848
C	2.729546	-2.729546	0.903498	C	-3.752567	2.861829	2.062031
C	-4.553859	0.901163	0.901163	C	-3.953130	2.057701	-0.368286
C	-2.739069	-0.913104	0.913104	C	-4.671490	0.744961	0.128881
C	-0.913104	-2.739069	0.913104	C	-4.253666	3.244326	0.624628
C	0.901163	-4.553859	0.901163	C	-1.980183	4.310124	0.084183
C	-0.901163	-0.901163	-4.553859	C	2.093340	0.246273	-2.983294
C	0.901163	0.901163	-4.553859	C	1.578274	0.618254	-4.430824
C	-2.729546	-0.903498	-2.729546	C	0.021304	0.864331	-4.376705
C	-0.913104	0.913104	-2.739069	C	-0.299725	2.054930	-3.392840
C	0.903498	2.729546	-2.729546	C	3.849891	0.813453	-0.583594
C	-0.903498	-2.729546	-2.729546	C	4.156494	-0.372830	-1.577226
C	0.913104	-0.913104	-2.739069	C	3.653857	-0.002716	-3.025677
C	2.729546	0.903498	-2.729546	C	2.313596	1.927646	-4.913296
C	-4.553859	-0.901163	-0.901163	C	1.982646	3.104575	-3.929404
C	-2.739069	0.913104	-0.913104	C	2.504673	2.746594	-2.485930
C	-0.913104	2.739069	-0.913104	C	4.367275	1.313229	-3.522977
C	0.901163	4.553859	-0.901163	C	4.058263	2.483595	-2.524234
C	-2.729546	-2.729546	-0.903498	C	1.900672	-0.575830	-5.409703
C	-0.913222	-0.913222	-0.913222	C	3.452444	-0.803972	-5.454995
C	0.913222	0.913222	-0.913222	C	3.954351	-1.190247	-4.019385
C	2.729546	2.729546	-0.903498	C	1.679822	-2.254306	-3.477546
C	-0.901163	-4.553859	-0.901163	C	3.237850	-2.490405	-3.510515
C	0.913104	-2.739069	-0.913104	C	3.859544	1.664198	-4.965588
C	2.739069	-0.913104	-0.913104	C	3.437669	-1.685765	-1.079157
C	4.553859	0.901163	-0.901163	C	1.162233	-1.869425	-4.915685
H	0.633768	0.633768	6.103405	C	-0.711947	-0.444288	-3.888403
H	-0.633768	-0.633768	6.103405	C	0.435530	3.363558	-3.875640

H	0.621231	2.464104	4.289637	C	0.627726	4.183391	-1.449898
H	2.464104	0.621231	4.289637	C	2.182878	3.925647	-1.489544
H	-2.464104	-0.621231	4.289637	C	-1.856872	2.302069	-3.339995
H	-0.621231	-2.464104	4.289637	C	-2.589024	0.992609	-2.852300
H	0.621231	4.289637	2.464104	C	-2.177775	3.493498	-2.357571
H	2.462822	2.462822	2.462822	C	0.104954	4.541943	-2.892961
H	4.289637	0.621231	2.464104	C	-0.421394	-3.352883	3.886441
H	-4.289637	-0.621231	2.464104	C	1.860298	-2.303918	3.350864
H	-2.462822	-2.462822	2.462822	C	1.539969	-1.113376	4.333972
H	-0.621231	-4.289637	2.464104	C	1.663572	-3.122177	0.909568
H	0.633768	6.103405	0.633768	C	-0.621556	-4.174302	1.446360
H	-0.633768	6.103405	-0.633768	C	-1.141448	-3.810649	0.002045
H	2.464104	4.289637	0.621231	C	0.933774	-4.433233	1.407097
H	4.289637	2.464104	0.621231	C	1.125663	-3.612327	3.833209
H	6.103405	-0.633768	-0.633768	C	3.941642	-2.056805	0.368917
H	6.103405	0.633768	0.633768	C	3.635165	-0.869537	1.361410
H	-2.464104	4.289637	-0.621231	C	3.738435	-2.872508	-2.072829
H	4.289637	-2.464104	-0.621231	C	1.465111	-3.937179	-1.532677
H	-4.289637	2.464104	-0.621231	C	0.948648	-3.557237	-2.973306
H	2.464104	-4.289637	-0.621231	C	3.023053	-4.173946	-1.564874
H	-6.103405	0.633768	-0.633768	C	3.224188	-3.370394	0.866294
H	-6.103405	-0.633768	0.633768	C	-1.441712	4.802323	-2.840452
H	-4.289637	-2.464104	0.621231	C	-1.246206	5.610331	-0.424465
H	-2.464104	-4.289637	0.621231	C	0.302549	5.358582	-0.451166
H	-0.633768	-6.103405	0.633768	C	-3.539406	4.546199	0.116996
H	0.633768	-6.103405	-0.633768	C	-3.734912	3.738192	-2.298991
H	0.633768	-0.633768	-6.103405	C	-4.451261	2.427687	-1.817166
H	-0.633768	0.633768	-6.103405	C	-4.035837	4.928284	-1.321637
H	-0.621231	2.464104	-4.289637	C	-1.774978	5.977408	-1.855461
H	2.464104	-0.621231	-4.289637	C	1.456356	-4.791265	2.851640
H	-2.464104	0.621231	-4.289637	C	3.722599	-3.739643	2.316544
H	0.621231	-2.464104	-4.289637	C	3.416114	-2.549471	3.292398
H	-0.621231	4.289637	-2.464104	C	3.524767	-4.557262	-0.128181
H	4.289637	-0.621231	-2.464104	C	1.258524	-5.608884	0.406914
H	-2.462822	2.462822	-2.462822	C	0.732602	-5.236802	-1.024063
H	2.462822	-2.462822	-2.462822	C	2.807889	-5.855892	0.383426
H	-4.289637	0.621231	-2.464104	C	3.002931	-5.049804	2.793674
H	0.621231	-4.289637	-2.464104	C	0.612578	3.308002	2.930007
H	-1.537017	1.537017	5.203335	C	2.488621	1.879927	1.901423
H	1.537017	-1.537017	5.203335	C	2.702155	3.562766	-0.045532
H	-1.536607	3.375895	3.375895	C	4.563321	2.128610	-1.081170
H	3.375895	-1.536607	3.375895	C	0.398806	1.619826	4.872466
H	-3.375895	1.536607	3.375895	C	4.354105	0.443876	0.864771
H	1.536607	-3.375895	3.375895	C	2.272491	0.195127	3.846393
H	-1.537017	5.203335	1.537017	C	-2.269335	-0.198613	-3.835848
H	5.203335	-1.537017	1.537017	C	-4.365323	-0.441344	-0.863815
H	-3.375895	3.375895	1.536607	C	-4.572767	-2.110880	1.076006
H	3.375895	-3.375895	1.536607	C	-0.389356	-1.637561	-4.867299
H	-5.203335	1.537017	1.537017	C	-2.697343	-3.553270	0.041074
H	1.537017	-5.203335	1.537017	C	-0.609318	-3.316554	-2.937043
H	-1.537017	-1.537017	-5.203335	C	0.828489	4.987612	0.980371
H	1.537017	1.537017	-5.203335	C	4.133638	-1.239176	2.810925
H	-3.375895	-1.536607	-3.375895	C	-4.145525	1.237775	-2.793980
H	1.536607	3.375895	-3.375895	C	-0.816598	-4.986216	-0.997313

H	-1.536607	-3.375895	-3.375895	C	1.950449	1.388186	4.824748
H	3.375895	1.536607	-3.375895	C	2.171057	3.068161	2.894529
H	-5.203335	-1.537017	-1.537017	C	4.049048	1.630565	1.857921
H	1.537017	5.203335	-1.537017	C	4.255823	3.300091	-0.082866
H	-3.375895	-3.375895	-1.536607	C	-5.078452	-1.756186	-0.366910
H	3.375895	3.375895	-1.536607	C	-1.127817	-2.932094	-4.374968
H	-1.537017	-5.203335	-1.537017	C	2.377802	4.737710	0.953758
H	5.203335	1.537017	-1.537017	C	3.828471	-0.049434	3.788124
				C	-4.863618	-0.072350	-2.312892
				C	-1.342651	-4.615931	-2.428987
				C	2.904216	4.368612	2.385327
				C	4.762388	2.946188	1.359659
				C	2.689124	2.682755	4.333644
				C	4.547296	1.260330	3.307976
				C	-4.559610	-1.261781	-3.290422
				C	-4.772174	-2.927821	-1.365008
				C	4.240320	2.452233	4.281234
				C	4.452378	4.114315	2.360393
				C	-5.273226	-2.573752	-2.809196
				C	-3.317817	6.226852	-1.814036
				C	3.317819	-6.226854	1.814037
				H	-4.203546	2.013633	4.704102
				H	5.049927	-1.374271	-4.057428
				H	1.959035	2.198848	-5.931301
				H	-2.805412	-2.838213	5.284630
				H	-3.773992	5.380410	0.813172
				H	4.620373	-4.741049	-0.166498
				H	-1.796010	5.073323	-3.858603
				H	0.949633	-5.712689	3.211931
				H	-3.986456	3.696427	2.758378
				H	4.834384	-3.055897	-2.110522
				H	0.080563	3.634121	-4.893947
				H	-0.928487	-4.274655	4.246094
				H	4.375345	2.578726	-5.323340
				H	-2.280979	-0.996624	6.923533
				H	-5.775366	0.048822	4.557871
				H	3.681004	-1.630928	-6.158060
				H	-1.273144	6.902627	-2.205503
				H	3.367511	-5.320526	3.805696
				H	-5.129213	5.113266	-1.295024
				H	3.034851	-6.695371	-0.305167
				H	2.489601	4.026586	-4.288782
				H	-0.396689	-2.445584	5.887864
				H	-5.564454	1.744274	2.607588
				H	3.471547	-3.325281	-4.206667
				H	0.612409	5.463570	-3.252615
				H	1.480503	-3.882568	4.851697
				H	-5.349714	3.427366	0.662466
				H	3.256808	-5.008373	-2.261545
				H	-2.108529	1.386848	6.122406
				H	5.466211	1.149575	-3.556981
				H	1.542751	-0.324999	-6.431748
				H	-4.900429	-2.211429	3.866326
				H	-1.462133	6.453200	0.267306

H	4.819815	-3.916778	2.298120
H	-4.107869	4.000533	-3.312737
H	0.750191	-6.536960	0.747314
H	-1.901248	3.082836	4.170773
H	5.256432	-0.548300	-1.607256
H	-0.341593	1.126510	-5.397059
H	-3.013587	-3.661051	2.833545
H	-1.686442	4.766448	2.225050
H	5.041627	-2.231912	0.338467
H	-2.219364	2.563938	-4.360573
H	-1.135815	-5.098479	1.797059
H	4.580964	3.400894	-2.872951
H	0.018869	0.073862	6.387438
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H	1.380183	-2.699589	-5.622497
H	2.696867	4.849997	-1.840279
H	1.902576	-1.375536	5.354467
H	-5.771459	0.920373	0.159228
H	1.172021	-4.394839	-3.673413
H	0.811504	6.286404	-0.792295
H	3.788330	-2.811648	4.306782
H	-5.548809	2.604532	-1.797854
H	0.948980	-6.079292	-1.716630
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H	5.662393	1.964156	-1.115108
H	-0.747446	-1.385932	-5.889361
H	-5.095577	-3.027949	1.425019
H	0.388898	4.145550	3.630033
H	5.454001	0.268230	0.834214
H	-2.631739	0.063796	-4.856320
H	-3.211156	-4.477581	0.392076
H	0.611944	5.830258	1.672623
H	5.231083	-1.416381	2.791722
H	-4.517836	1.500289	-3.808192
H	-1.325187	-5.914171	-0.656150
H	4.778472	4.217172	-0.432235
H	2.308307	1.136248	5.846865
H	-6.177520	-1.591449	-0.332702
H	-0.909256	-3.761975	-5.081925
H	2.886203	5.665698	0.612254
H	4.200577	-0.312278	4.802376
H	-5.961056	0.105162	-2.293448
H	-1.125720	-5.458586	-3.121179
H	2.471155	3.511995	5.041070
H	5.861297	2.782419	1.325312
H	-3.036934	-2.450145	-5.350412
H	-5.295515	-3.844273	-1.015967
H	2.687997	5.211569	3.076900
H	5.644455	1.082845	3.289483
H	-4.932508	-0.999088	-4.304099
H	-3.399940	-5.295329	-2.062280
C	-4.963291	-3.749320	-3.792185
H	4.607966	2.200107	5.296943
H	-6.369669	-2.407367	-2.786270

					C	-4.174943	-0.491168	5.949870
					H	-4.400843	0.333298	6.647905
					H	-4.687141	-1.402468	6.303726
					C	4.174945	0.491166	-5.949868
					H	3.823574	0.750117	-6.963530
					H	5.264414	0.319049	-5.988098
					H	2.816116	-7.146188	2.162099
					H	4.406088	-6.408381	1.786682
					C	4.963292	3.749319	3.792188
					H	6.053865	3.581767	3.767604
					H	4.750190	4.579724	4.487201
					H	4.969649	5.034916	2.020802
					H	-5.327461	-3.496308	-4.802825
					H	-5.476594	-4.665184	-3.451975
					H	-3.207944	-4.827659	-4.531471
					H	-3.542516	7.060727	-1.126875
					H	-3.679681	6.493837	-2.821906
O5	C	0.000000	0.000000	9.110697	O6	C	0.000000	10.936259
	C	-0.010788	1.817467	7.294301		C	-0.010812	9.119905
	C	1.817467	-0.010788	7.294301		C	1.817510	9.119905
	C	-1.817467	0.010788	7.294301		C	-1.817510	9.119905
	C	0.010788	-1.817467	7.294301		C	0.010812	9.119905
	C	-0.010248	3.641340	5.466954		C	-0.010264	7.292416
	C	1.818810	1.818810	5.470659		C	1.818805	7.296304
	C	3.641340	-0.010248	5.466954		C	3.641319	7.292416
	C	-1.825820	1.825820	5.476330		C	-1.825837	7.301892
	C	0.000000	0.000000	5.478665		C	0.000000	7.304391
	C	1.825820	-1.825820	5.476330		C	1.825837	7.301892
	C	-3.641340	0.010248	5.466954		C	-3.641319	7.292416
	C	-1.818810	-1.818810	5.470659		C	-1.818805	7.296304
	C	0.010248	-3.641340	5.466954		C	0.010264	7.292416
	C	-0.010248	5.466954	3.641340		C	-0.010052	5.466395
	C	1.818624	3.644087	3.644087		C	1.818601	5.469470
	C	3.644087	1.818624	3.644087		C	3.643804	5.469470
	C	5.466954	-0.010248	3.641340		C	5.466395	5.466395
	C	-1.825697	3.650354	3.650354		C	-1.825555	5.475614
	C	-0.000088	1.825547	3.651783		C	-0.000072	5.477479
	C	1.825547	-0.000088	3.651783		C	1.825396	5.477479
	C	3.650354	-1.825697	3.650354		C	3.650073	5.475614
	C	-3.650354	1.825697	3.650354		C	-3.650073	5.475614
	C	-1.825547	0.000088	3.651783		C	-1.825396	5.477479
	C	0.000088	-1.825547	3.651783		C	0.000072	5.477479
	C	1.825697	-3.650354	3.650354		C	1.825555	5.475614
	C	-5.466954	0.010248	3.641340		C	-5.466395	5.466395
	C	-3.644087	-1.818624	3.644087		C	-3.643804	5.469470
	C	-1.818624	-3.644087	3.644087		C	-1.818601	5.469470
	C	0.010248	-5.466954	3.641340		C	0.010052	5.466395
	C	-0.010788	7.294301	1.817467		C	-0.010264	3.641319
	C	1.818810	5.470659	1.818810		C	1.818601	3.643804
	C	3.644087	3.644087	1.818624		C	3.643546	3.643546
	C	5.470659	1.818810	1.818810		C	5.469470	3.643804
	C	7.294301	-0.010788	1.817467		C	7.292416	3.641319
	C	-1.825820	5.476330	1.825820		C	-1.825555	3.650073

C	-0.000088	3.651783	1.825547	C	-0.000078	3.651148	3.651148
C	1.825595	1.825595	1.825595	C	1.825338	1.825338	3.651169
C	3.651783	-0.000088	1.825547	C	3.651148	-0.000078	3.651148
C	5.476330	-1.825820	1.825820	C	5.475614	-1.825555	3.650073
C	-3.650354	3.650354	1.825697	C	-3.649954	3.649954	3.649954
C	-1.825772	1.825772	1.825772	C	-1.825517	1.825517	3.651431
C	0.000000	0.000000	1.825906	C	0.000000	0.000000	3.651595
C	1.825772	-1.825772	1.825772	C	1.825517	-1.825517	3.651431
C	3.650354	-3.650354	1.825697	C	3.649954	-3.649954	3.649954
C	-5.476330	1.825820	1.825820	C	-5.475614	1.825555	3.650073
C	-3.651783	0.000088	1.825547	C	-3.651148	0.000078	3.651148
C	-1.825595	-1.825595	1.825595	C	-1.825338	-1.825338	3.651169
C	0.000088	-3.651783	1.825547	C	0.000078	-3.651148	3.651148
C	1.825820	-5.476330	1.825820	C	1.825555	-5.475614	3.650073
C	-7.294301	0.010788	1.817467	C	-7.292416	0.010264	3.641319
C	-5.470659	-1.818810	1.818810	C	-5.469470	-1.818601	3.643804
C	-3.644087	-3.644087	1.818624	C	-3.643546	-3.643546	3.643546
C	-1.818810	-5.470659	1.818810	C	-1.818601	-5.469470	3.643804
C	0.010788	-7.294301	1.817467	C	0.010264	-7.292416	3.641319
C	0.000000	9.110697	0.000000	C	-0.010812	9.119905	1.817510
C	1.817467	7.294301	-0.010788	C	1.818805	7.296304	1.818805
C	3.641340	5.466954	-0.010248	C	3.643804	5.469470	1.818601
C	5.466954	3.641340	-0.010248	C	5.469470	3.643804	1.818601
C	7.294301	1.817467	-0.010788	C	7.296304	1.818805	1.818805
C	9.110697	0.000000	0.000000	C	9.119905	-0.010812	1.817510
C	-1.817467	7.294301	0.010788	C	-1.825837	7.301892	1.825837
C	0.000000	5.478665	0.000000	C	-0.000072	5.477479	1.825396
C	1.825547	3.651783	-0.000088	C	1.825338	3.651169	1.825338
C	3.651783	1.825547	-0.000088	C	3.651169	1.825338	1.825338
C	5.478665	0.000000	0.000000	C	5.477479	-0.000072	1.825396
C	7.294301	-1.817467	0.010788	C	7.301892	-1.825837	1.825837
C	-3.641340	5.466954	0.010248	C	-3.650073	5.475614	1.825555
C	-1.825547	3.651783	0.000088	C	-1.825517	3.651431	1.825517
C	0.000000	1.825906	0.000000	C	0.000008	1.825660	1.825660
C	1.825906	0.000000	0.000000	C	1.825660	0.000008	1.825660
C	3.651783	-1.825547	0.000088	C	3.651431	-1.825517	1.825517
C	5.466954	-3.641340	0.010248	C	5.475614	-3.650073	1.825555
C	-5.466954	3.641340	0.010248	C	-5.475614	3.650073	1.825555
C	-3.651783	1.825547	0.000088	C	-3.651431	1.825517	1.825517
C	-1.825906	0.000000	0.000000	C	-1.825660	-0.000008	1.825660
C	0.000000	-1.825906	0.000000	C	-0.000008	-1.825660	1.825660
C	1.825547	-3.651783	0.000088	C	1.825517	-3.651431	1.825517
C	3.641340	-5.466954	0.010248	C	3.650073	-5.475614	1.825555
C	-7.294301	1.817467	0.010788	C	-7.301892	1.825837	1.825837
C	-5.478665	0.000000	0.000000	C	-5.477479	0.000072	1.825396
C	-3.651783	-1.825547	-0.000088	C	-3.651169	-1.825338	1.825338
C	-1.825547	-3.651783	-0.000088	C	-1.825338	-3.651169	1.825338
C	0.000000	-5.478665	0.000000	C	0.000072	-5.477479	1.825396
C	1.817467	-7.294301	0.010788	C	1.825837	-7.301892	1.825837
C	-9.110697	0.000000	0.000000	C	-9.119905	0.010812	1.817510
C	-7.294301	-1.817467	-0.010788	C	-7.296304	-1.818805	1.818805
C	-5.466954	-3.641340	-0.010248	C	-5.469470	-3.643804	1.818601
C	-3.641340	-5.466954	-0.010248	C	-3.643804	-5.469470	1.818601
C	-1.817467	-7.294301	-0.010788	C	-1.818805	-7.296304	1.818805

C	0.000000	-9.110697	0.000000	C	0.010812	-9.119905	1.817510
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C	0.010788	1.817467	-7.294301	C	1.817510	9.119905	-0.010812
C	1.817467	0.010788	-7.294301	C	3.641319	7.292416	-0.010264
C	-1.817467	-0.010788	-7.294301	C	5.466395	5.466395	-0.010052
C	-0.010788	-1.817467	-7.294301	C	7.292416	3.641319	-0.010264
C	0.010248	3.641340	-5.466954	C	9.119905	1.817510	-0.010812
C	1.825820	1.825820	-5.476330	C	10.936259	0.000000	0.000000
C	3.641340	0.010248	-5.466954	C	-1.817510	9.119905	0.010812
C	-1.818810	1.818810	-5.470659	C	0.000000	7.304391	0.000000
C	0.000000	0.000000	-5.478665	C	1.825396	5.477479	-0.000072
C	1.818810	-1.818810	-5.470659	C	3.651148	3.651148	-0.000078
C	-3.641340	-0.010248	-5.466954	C	5.477479	1.825396	-0.000072
C	-1.825820	-1.825820	-5.476330	C	7.304391	0.000000	0.000000
C	-0.010248	-3.641340	-5.466954	C	9.119905	-1.817510	0.010812
C	0.010248	5.466954	-3.641340	C	-3.641319	7.292416	0.010264
C	1.825697	3.650354	-3.650354	C	-1.825396	5.477479	0.000072
C	3.650354	1.825697	-3.650354	C	0.000000	3.651595	0.000000
C	5.466954	0.010248	-3.641340	C	1.825660	1.825660	0.000008
C	-1.818624	3.644087	-3.644087	C	3.651595	0.000000	0.000000
C	0.000088	1.825547	-3.651783	C	5.477479	-1.825396	0.000072
C	1.825547	0.000088	-3.651783	C	7.292416	-3.641319	0.010264
C	3.644087	-1.818624	-3.644087	C	-5.466395	5.466395	0.010052
C	-3.644087	1.818624	-3.644087	C	-3.651148	3.651148	0.000078
C	-1.825547	-0.000088	-3.651783	C	-1.825660	1.825660	-0.000008
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C	1.818624	-3.644087	-3.644087	C	1.825660	-1.825660	-0.000008
C	-5.466954	-0.010248	-3.641340	C	3.651148	-3.651148	0.000078
C	-3.650354	-1.825697	-3.650354	C	5.466395	-5.466395	0.010052
C	-1.825697	-3.650354	-3.650354	C	-7.292416	3.641319	0.010264
C	-0.010248	-5.466954	-3.641340	C	-5.477479	1.825396	0.000072
C	0.010788	7.294301	-1.817467	C	-3.651595	0.000000	0.000000
C	1.825820	5.476330	-1.825820	C	-1.825660	-1.825660	0.000008
C	3.650354	3.650354	-1.825697	C	0.000000	-3.651595	0.000000
C	5.476330	1.825820	-1.825820	C	1.825396	-5.477479	0.000072
C	7.294301	0.010788	-1.817467	C	3.641319	-7.292416	0.010264
C	-1.818810	5.470659	-1.818810	C	-9.119905	1.817510	0.010812
C	0.000088	3.651783	-1.825547	C	-7.304391	0.000000	0.000000
C	1.825772	1.825772	-1.825772	C	-5.477479	-1.825396	-0.000072
C	3.651783	0.000088	-1.825547	C	-3.651148	-3.651148	-0.000078
C	5.470659	-1.818810	-1.818810	C	-1.825396	-5.477479	-0.000072
C	-3.644087	3.644087	-1.818624	C	0.000000	-7.304391	0.000000
C	-1.825595	1.825595	-1.825595	C	1.817510	-9.119905	0.010812
C	0.000000	0.000000	-1.825906	C	-10.936259	0.000000	0.000000
C	1.825595	-1.825595	-1.825595	C	-9.119905	-1.817510	-0.010812
C	3.644087	-3.644087	-1.818624	C	-7.292416	-3.641319	-0.010264
C	-5.470659	1.818810	-1.818810	C	-5.466395	-5.466395	-0.010052
C	-3.651783	-0.000088	-1.825547	C	-3.641319	-7.292416	-0.010264
C	-1.825772	-1.825772	-1.825772	C	-1.817510	-9.119905	-0.010812
C	-0.000088	-3.651783	-1.825547	C	0.000000	-10.936259	0.000000
C	1.818810	-5.470659	-1.818810	C	0.000000	0.000000	-10.936259
C	-7.294301	-0.010788	-1.817467	C	0.010812	1.817510	-9.119905
C	-5.476330	-1.825820	-1.825820	C	1.817510	0.010812	-9.119905
C	-3.650354	-3.650354	-1.825697	C	-1.817510	-0.010812	-9.119905

C	-1.825820	-5.476330	-1.825820	C	-0.010812	-1.817510	-9.119905
C	-0.010788	-7.294301	-1.817467	C	0.010264	3.641319	-7.292416
C	-0.901228	0.901228	8.205196	C	1.825837	1.825837	-7.301892
C	0.901228	-0.901228	8.205196	C	3.641319	0.010264	-7.292416
C	-0.903115	2.729072	6.380209	C	-1.818805	1.818805	-7.296304
C	0.912974	0.912974	6.390701	C	0.000000	0.000000	-7.304391
C	2.729072	-0.903115	6.380209	C	1.818805	-1.818805	-7.296304
C	-2.729072	0.903115	6.380209	C	-3.641319	-0.010264	-7.292416
C	-0.912974	-0.912974	6.390701	C	-1.825837	-1.825837	-7.301892
C	0.903115	-2.729072	6.380209	C	-0.010264	-3.641319	-7.292416
C	-0.902711	4.554019	4.554019	C	0.010052	5.466395	-5.466395
C	0.912669	2.737334	4.563279	C	1.825555	3.650073	-5.475614
C	2.737334	0.912669	4.563279	C	3.650073	1.825555	-5.475614
C	4.554019	-0.902711	4.554019	C	5.466395	0.010052	-5.466395
C	-2.731809	2.731809	4.557270	C	-1.818601	3.643804	-5.469470
C	-0.912841	0.912841	4.565085	C	0.000072	1.825396	-5.477479
C	0.912841	-0.912841	4.565085	C	1.825396	0.000072	-5.477479
C	2.731809	-2.731809	4.557270	C	3.643804	-1.818601	-5.469470
C	-4.554019	0.902711	4.554019	C	-3.643804	1.818601	-5.469470
C	-2.737334	-0.912669	4.563279	C	-1.825396	-0.000072	-5.477479
C	-0.912669	-2.737334	4.563279	C	-0.000072	-1.825396	-5.477479
C	0.902711	-4.554019	4.554019	C	1.818601	-3.643804	-5.469470
C	-0.903115	6.380209	2.729072	C	-5.466395	-0.010052	-5.466395
C	0.912669	4.563279	2.737334	C	-3.650073	-1.825555	-5.475614
C	2.737247	2.737247	2.737247	C	-1.825555	-3.650073	-5.475614
C	4.563279	0.912669	2.737334	C	-0.010052	-5.466395	-5.466395
C	6.380209	-0.903115	2.729072	C	0.010264	7.292416	-3.641319
C	-2.731809	4.557270	2.731809	C	1.825555	5.475614	-3.650073
C	-0.912941	2.738639	2.738639	C	3.649954	3.649954	-3.649954
C	0.912757	0.912757	2.738813	C	5.475614	1.825555	-3.650073
C	2.738639	-0.912941	2.738639	C	7.292416	0.010264	-3.641319
C	4.557270	-2.731809	2.731809	C	-1.818601	5.469470	-3.643804
C	-4.557270	2.731809	2.731809	C	0.000078	3.651148	-3.651148
C	-2.738639	0.912941	2.738639	C	1.825517	1.825517	-3.651431
C	-0.912757	-0.912757	2.738813	C	3.651148	0.000078	-3.651148
C	0.912941	-2.738639	2.738639	C	5.469470	-1.818601	-3.643804
C	2.731809	-4.557270	2.731809	C	-3.643546	3.643546	-3.643546
C	-6.380209	0.903115	2.729072	C	-1.825338	1.825338	-3.651169
C	-4.563279	-0.912669	2.737334	C	0.000000	0.000000	-3.651595
C	-2.737247	-2.737247	2.737247	C	1.825338	-1.825338	-3.651169
C	-0.912669	-4.563279	2.737334	C	3.643546	-3.643546	-3.643546
C	0.903115	-6.380209	2.729072	C	-5.469470	1.818601	-3.643804
C	-0.901228	8.205196	0.901228	C	-3.651148	-0.000078	-3.651148
C	0.912974	6.390701	0.912974	C	-1.825517	-1.825517	-3.651431
C	2.737334	4.563279	0.912669	C	-0.000078	-3.651148	-3.651148
C	4.563279	2.737334	0.912669	C	1.818601	-5.469470	-3.643804
C	6.390701	0.912974	0.912974	C	-7.292416	-0.010264	-3.641319
C	8.205196	-0.901228	0.901228	C	-5.475614	-1.825555	-3.650073
C	-2.729072	6.380209	0.903115	C	-3.649954	-3.649954	-3.649954
C	-0.912841	4.565085	0.912841	C	-1.825555	-5.475614	-3.650073
C	0.912757	2.738813	0.912757	C	-0.010264	-7.292416	-3.641319
C	2.738813	0.912757	0.912757	C	0.010812	9.119905	-1.817510
C	4.565085	-0.912841	0.912841	C	1.825837	7.301892	-1.825837
C	6.380209	-2.729072	0.903115	C	3.650073	5.475614	-1.825555

C	-4.554019	4.554019	0.902711	C	5.475614	3.650073	-1.825555
C	-2.738639	2.738639	0.912941	C	7.301892	1.825837	-1.825837
C	-0.912941	0.912941	0.912941	C	9.119905	0.010812	-1.817510
C	0.912941	-0.912941	0.912941	C	-1.818805	7.296304	-1.818805
C	2.738639	-2.738639	0.912941	C	0.000072	5.477479	-1.825396
C	4.554019	-4.554019	0.902711	C	1.825517	3.651431	-1.825517
C	-6.380209	2.729072	0.903115	C	3.651431	1.825517	-1.825517
C	-4.565085	0.912841	0.912841	C	5.477479	0.000072	-1.825396
C	-2.738813	-0.912757	0.912757	C	7.296304	-1.818805	-1.818805
C	-0.912757	-2.738813	0.912757	C	-3.643804	5.469470	-1.818601
C	0.912841	-4.565085	0.912841	C	-1.825338	3.651169	-1.825338
C	2.729072	-6.380209	0.903115	C	-0.000008	1.825660	-1.825660
C	-8.205196	0.901228	0.901228	C	1.825660	-0.000008	-1.825660
C	-6.390701	-0.912974	0.912974	C	3.651169	-1.825338	-1.825338
C	-4.563279	-2.737334	0.912669	C	5.469470	-3.643804	-1.818601
C	-2.737334	-4.563279	0.912669	C	-5.469470	3.643804	-1.818601
C	-0.912974	-6.390701	0.912974	C	-3.651169	1.825338	-1.825338
C	0.901228	-8.205196	0.901228	C	-1.825660	0.000008	-1.825660
C	-0.901228	-0.901228	-8.205196	C	0.000008	-1.825660	-1.825660
C	0.901228	0.901228	-8.205196	C	1.825338	-3.651169	-1.825338
C	-2.729072	-0.903115	-6.380209	C	3.643804	-5.469470	-1.818601
C	-0.912974	0.912974	-6.390701	C	-7.296304	1.818805	-1.818805
C	0.903115	2.729072	-6.380209	C	-5.477479	-0.000072	-1.825396
C	-0.903115	-2.729072	-6.380209	C	-3.651431	-1.825517	-1.825517
C	0.912974	-0.912974	-6.390701	C	-1.825517	-3.651431	-1.825517
C	2.729072	0.903115	-6.380209	C	-0.000072	-5.477479	-1.825396
C	-4.554019	-0.902711	-4.554019	C	1.818805	-7.296304	-1.818805
C	-2.737334	0.912669	-4.563279	C	-9.119905	-0.010812	-1.817510
C	-0.912669	2.737334	-4.563279	C	-7.301892	-1.825837	-1.825837
C	0.902711	4.554019	-4.554019	C	-5.475614	-3.650073	-1.825555
C	-2.731809	-2.731809	-4.557270	C	-3.650073	-5.475614	-1.825555
C	-0.912841	-0.912841	-4.565085	C	-1.825837	-7.301892	-1.825837
C	0.912841	0.912841	-4.565085	C	-0.010812	-9.119905	-1.817510
C	2.731809	2.731809	-4.557270	C	-0.901253	0.901253	10.030788
C	-0.902711	-4.554019	-4.554019	C	0.901253	-0.901253	10.030788
C	0.912669	-2.737334	-4.563279	C	-0.903134	2.729111	8.205749
C	2.737334	-0.912669	-4.563279	C	0.912986	0.912986	8.216370
C	4.554019	0.902711	-4.554019	C	2.729111	-0.903134	8.205749
C	-6.380209	-0.903115	-2.729072	C	-2.729111	0.903134	8.205749
C	-4.563279	0.912669	-2.737334	C	-0.912986	-0.912986	8.216370
C	-2.737247	2.737247	-2.737247	C	0.903134	-2.729111	8.205749
C	-0.912669	4.563279	-2.737334	C	-0.902649	4.553843	6.379247
C	0.903115	6.380209	-2.729072	C	0.912690	2.737237	6.388871
C	-4.557270	-2.731809	-2.731809	C	2.737237	0.912690	6.388871
C	-2.738639	-0.912941	-2.738639	C	4.553843	-0.902649	6.379247
C	-0.912757	0.912757	-2.738813	C	-2.731751	2.731751	6.382618
C	0.912941	2.738639	-2.738639	C	-0.912800	0.912800	6.390798
C	2.731809	4.557270	-2.731809	C	0.912800	-0.912800	6.390798
C	-2.731809	-4.557270	-2.731809	C	2.731751	-2.731751	6.382618
C	-0.912941	-2.738639	-2.738639	C	-4.553843	0.902649	6.379247
C	0.912757	-0.912757	-2.738813	C	-2.737237	-0.912690	6.388871
C	2.738639	0.912941	-2.738639	C	-0.912690	-2.737237	6.388871
C	4.557270	2.731809	-2.731809	C	0.902649	-4.553843	6.379247
C	-0.903115	-6.380209	-2.729072	C	-0.902649	6.379247	4.553843

C	0.912669	-4.563279	-2.737334	C	0.912647	4.562592	4.562592
C	2.737247	-2.737247	-2.737247	C	2.736967	2.736967	4.562550
C	4.563279	-0.912669	-2.737334	C	4.562592	0.912647	4.562592
C	6.380209	0.903115	-2.729072	C	6.379247	-0.902649	4.553843
C	-8.205196	-0.901228	-0.901228	C	-2.731447	4.556715	4.556715
C	-6.390701	0.912974	-0.912974	C	-0.912841	2.738295	4.564229
C	-4.563279	2.737334	-0.912669	C	0.912656	0.912656	4.564512
C	-2.737334	4.563279	-0.912669	C	2.738295	-0.912841	4.564229
C	-0.912974	6.390701	-0.912974	C	4.556715	-2.731447	4.556715
C	0.901228	8.205196	-0.901228	C	-4.556715	2.731447	4.556715
C	-6.380209	-2.729072	-0.903115	C	-2.738295	0.912841	4.564229
C	-4.565085	-0.912841	-0.912841	C	-0.912656	-0.912656	4.564512
C	-2.738813	0.912757	-0.912757	C	0.912841	-2.738295	4.564229
C	-0.912757	2.738813	-0.912757	C	2.731447	-4.556715	4.556715
C	0.912841	4.565085	-0.912841	C	-6.379247	0.902649	4.553843
C	2.729072	6.380209	-0.903115	C	-4.562592	-0.912647	4.562592
C	-4.554019	-4.554019	-0.902711	C	-2.736967	-2.736967	4.562550
C	-2.738639	-2.738639	-0.912941	C	-0.912647	-4.562592	4.562592
C	-0.912941	-0.912941	-0.912941	C	0.902649	-6.379247	4.553843
C	0.912941	0.912941	-0.912941	C	-0.903134	8.205749	2.729111
C	2.738639	2.738639	-0.912941	C	0.912690	6.388871	2.737237
C	4.554019	4.554019	-0.902711	C	2.736967	4.562550	2.736967
C	-2.729072	-6.380209	-0.903115	C	4.562550	2.736967	2.736967
C	-0.912841	-4.565085	-0.912841	C	6.388871	0.912690	2.737237
C	0.912757	-2.738813	-0.912757	C	8.205749	-0.903134	2.729111
C	2.738813	-0.912757	-0.912757	C	-2.731751	6.382618	2.731751
C	4.565085	0.912841	-0.912841	C	-0.912841	4.564229	2.738295
C	6.380209	2.729072	-0.903115	C	0.912550	2.738371	2.738371
C	-0.901228	-8.205196	-0.901228	C	2.738371	0.912550	2.738371
C	0.912974	-6.390701	-0.912974	C	4.564229	-0.912841	2.738295
C	2.737334	-4.563279	-0.912669	C	6.382618	-2.731751	2.731751
C	4.563279	-2.737334	-0.912669	C	-4.556715	4.556715	2.731447
C	6.390701	-0.912974	-0.912974	C	-2.738313	2.738313	2.738313
C	8.205196	0.901228	-0.901228	C	-0.912855	0.912855	2.738570
H	0.633768	0.633768	9.754665	C	0.912855	-0.912855	2.738570
H	-0.633768	-0.633768	9.754665	C	2.738313	-2.738313	2.738313
H	0.621044	2.464315	7.940799	C	4.556715	-4.556715	2.731447
H	2.464315	0.621044	7.940799	C	-6.382618	2.731751	2.731751
H	-2.464315	-0.621044	7.940799	C	-4.564229	0.912841	2.738295
H	-0.621044	-2.464315	7.940799	C	-2.738371	-0.912550	2.738371
H	0.622371	4.288038	6.113266	C	-0.912550	-2.738371	2.738371
H	2.462332	2.462332	6.113533	C	0.912841	-4.564229	2.738295
H	4.288038	0.622371	6.113266	C	2.731751	-6.382618	2.731751
H	-4.288038	-0.622371	6.113266	C	-8.205749	0.903134	2.729111
H	-2.462332	-2.462332	6.113533	C	-6.388871	-0.912690	2.737237
H	-0.622371	-4.288038	6.113266	C	-4.562550	-2.736967	2.736967
H	0.622371	6.113266	4.288038	C	-2.736967	-4.562550	2.736967
H	2.461845	4.287409	4.287409	C	-0.912690	-6.388871	2.737237
H	4.287409	2.461845	4.287409	C	0.903134	-8.205749	2.729111
H	6.113266	0.622371	4.288038	C	-0.901253	10.030788	0.901253
H	-6.113266	-0.622371	4.288038	C	0.912986	8.216370	0.912986
H	-4.287409	-2.461845	4.287409	C	2.737237	6.388871	0.912690
H	-2.461845	-4.287409	4.287409	C	4.562592	4.562592	0.912647
H	-0.622371	-6.113266	4.288038	C	6.388871	2.737237	0.912690

H	0.621044	7.940799	2.464315	C	8.216370	0.912986	0.912986
H	2.462332	6.113533	2.462332	C	10.030788	-0.901253	0.901253
H	4.287409	4.287409	2.461845	C	-2.729111	8.205749	0.903134
H	6.113533	2.462332	2.462332	C	-0.912800	6.390798	0.912800
H	7.940799	0.621044	2.464315	C	0.912656	4.564512	0.912656
H	-7.940799	-0.621044	2.464315	C	2.738371	2.738371	0.912550
H	-6.113533	-2.462332	2.462332	C	4.564512	0.912656	0.912656
H	-4.287409	-4.287409	2.461845	C	6.390798	-0.912800	0.912800
H	-2.462332	-6.113533	2.462332	C	8.205749	-2.729111	0.903134
H	-0.621044	-7.940799	2.464315	C	-4.553843	6.379247	0.902649
H	0.633768	9.754665	0.633768	C	-2.738295	4.564229	0.912841
H	-0.633768	9.754665	-0.633768	C	-0.912855	2.738570	0.912855
H	2.464315	7.940799	0.621044	C	0.912790	0.912790	0.912790
H	4.288038	6.113266	0.622371	C	2.738570	-0.912855	0.912855
H	6.113266	4.288038	0.622371	C	4.564229	-2.738295	0.912841
H	7.940799	2.464315	0.621044	C	6.379247	-4.553843	0.902649
H	9.754665	-0.633768	-0.633768	C	-6.379247	4.553843	0.902649
H	9.754665	0.633768	0.633768	C	-4.564229	2.738295	0.912841
H	-2.464315	7.940799	-0.621044	C	-2.738570	0.912855	0.912855
H	7.940799	-2.464315	-0.621044	C	-0.912790	-0.912790	0.912790
H	-4.288038	6.113266	-0.622371	C	0.912855	-2.738570	0.912855
H	6.113266	-4.288038	-0.622371	C	2.738295	-4.564229	0.912841
H	-6.113266	4.288038	-0.622371	C	4.553843	-6.379247	0.902649
H	4.288038	-6.113266	-0.622371	C	-8.205749	2.729111	0.903134
H	-7.940799	2.464315	-0.621044	C	-6.390798	0.912800	0.912800
H	2.464315	-7.940799	-0.621044	C	-4.564512	-0.912656	0.912656
H	-9.754665	0.633768	-0.633768	C	-2.738371	-2.738371	0.912550
H	-9.754665	-0.633768	0.633768	C	-0.912656	-4.564512	0.912656
H	-7.940799	-2.464315	0.621044	C	0.912800	-6.390798	0.912800
H	-6.113266	-4.288038	0.622371	C	2.729111	-8.205749	0.903134
H	-4.288038	-6.113266	0.622371	C	-10.030788	0.901253	0.901253
H	-2.464315	-7.940799	0.621044	C	-8.216370	-0.912986	0.912986
H	-0.633768	-9.754665	0.633768	C	-6.388871	-2.737237	0.912690
H	0.633768	-9.754665	-0.633768	C	-4.562592	-4.562592	0.912647
H	0.633768	-0.633768	-9.754665	C	-2.737237	-6.388871	0.912690
H	-0.633768	0.633768	-9.754665	C	-0.912986	-8.216370	0.912986
H	-0.621044	2.464315	-7.940799	C	0.901253	-10.030788	0.901253
H	2.464315	-0.621044	-7.940799	C	-0.901253	-0.901253	-10.030788
H	-2.464315	0.621044	-7.940799	C	0.901253	0.901253	-10.030788
H	0.621044	-2.464315	-7.940799	C	-2.729111	-0.903134	-8.205749
H	-0.622371	4.288038	-6.113266	C	-0.912986	0.912986	-8.216370
H	4.288038	-0.622371	-6.113266	C	0.903134	2.729111	-8.205749
H	-2.462332	2.462332	-6.113533	C	-0.903134	-2.729111	-8.205749
H	2.462332	-2.462332	-6.113533	C	0.912986	-0.912986	-8.216370
H	-4.288038	0.622371	-6.113266	C	2.729111	0.903134	-8.205749
H	0.622371	-4.288038	-6.113266	C	-4.553843	-0.902649	-6.379247
H	-0.622371	6.113266	-4.288038	C	-2.737237	0.912690	-6.388871
H	6.113266	-0.622371	-4.288038	C	-0.912690	2.737237	-6.388871
H	-2.461845	4.287409	-4.287409	C	0.902649	4.553843	-6.379247
H	4.287409	-2.461845	-4.287409	C	-2.731751	-2.731751	-6.382618
H	-4.287409	2.461845	-4.287409	C	-0.912800	-0.912800	-6.390798
H	2.461845	-4.287409	-4.287409	C	0.912800	0.912800	-6.390798
H	-6.113266	0.622371	-4.288038	C	2.731751	2.731751	-6.382618
H	0.622371	-6.113266	-4.288038	C	-0.902649	-4.553843	-6.379247

H	-0.621044	7.940799	-2.464315	C	0.912690	-2.737237	-6.388871
H	7.940799	-0.621044	-2.464315	C	2.737237	-0.912690	-6.388871
H	-2.462332	6.113533	-2.462332	C	4.553843	0.902649	-6.379247
H	6.113533	-2.462332	-2.462332	C	-6.379247	-0.902649	-4.553843
H	-4.287409	4.287409	-2.461845	C	-4.562592	0.912647	-4.562592
H	4.287409	-4.287409	-2.461845	C	-2.736967	2.736967	-4.562550
H	-6.113533	2.462332	-2.462332	C	-0.912647	4.562592	-4.562592
H	2.462332	-6.113533	-2.462332	C	0.902649	6.379247	-4.553843
H	-7.940799	0.621044	-2.464315	C	-4.556715	-2.731447	-4.556715
H	0.621044	-7.940799	-2.464315	C	-2.738295	-0.912841	-4.564229
H	-1.537064	1.537064	8.854663	C	-0.912656	0.912656	-4.564512
H	1.537064	-1.537064	8.854663	C	0.912841	2.738295	-4.564229
H	-1.535948	3.375901	7.026244	C	2.731447	4.556715	-4.556715
H	3.375901	-1.535948	7.026244	C	-2.731447	-4.556715	-4.556715
H	-3.375901	1.535948	7.026244	C	-0.912841	-2.738295	-4.564229
H	1.535948	-3.375901	7.026244	C	0.912656	-0.912656	-4.564512
H	-1.535231	5.200584	5.200584	C	2.738295	0.912841	-4.564229
H	5.200584	-1.535231	5.200584	C	4.556715	2.731447	-4.556715
H	-3.375086	3.375086	5.200638	C	-0.902649	-6.379247	-4.553843
H	3.375086	-3.375086	5.200638	C	0.912647	-4.562592	-4.562592
H	-5.200584	1.535231	5.200584	C	2.736967	-2.736967	-4.562550
H	1.535231	-5.200584	5.200584	C	4.562592	-0.912647	-4.562592
H	-1.535948	7.026244	3.375901	C	6.379247	0.902649	-4.553843
H	7.026244	-1.535948	3.375901	C	-8.205749	-0.903134	-2.729111
H	-3.375086	5.200638	3.375086	C	-6.388871	0.912690	-2.737237
H	5.200638	-3.375086	3.375086	C	-4.562550	2.736967	-2.736967
H	-5.200638	3.375086	3.375086	C	-2.736967	4.562550	-2.736967
H	3.375086	-5.200638	3.375086	C	-0.912690	6.388871	-2.737237
H	-7.026244	1.535948	3.375901	C	0.903134	8.205749	-2.729111
H	1.535948	-7.026244	3.375901	C	-6.382618	-2.731751	-2.731751
H	-1.537064	8.854663	1.537064	C	-4.564229	-0.912841	-2.738295
H	8.854663	-1.537064	1.537064	C	-2.738371	0.912550	-2.738371
H	-3.375901	7.026244	1.535948	C	-0.912550	2.738371	-2.738371
H	7.026244	-3.375901	1.535948	C	0.912841	4.564229	-2.738295
H	-5.200584	5.200584	1.535231	C	2.731751	6.382618	-2.731751
H	5.200584	-5.200584	1.535231	C	-4.556715	-4.556715	-2.731447
H	-7.026244	3.375901	1.535948	C	-2.738313	-2.738313	-2.738313
H	3.375901	-7.026244	1.535948	C	-0.912855	-0.912855	-2.738570
H	-8.854663	1.537064	1.537064	C	0.912855	0.912855	-2.738570
H	1.537064	-8.854663	1.537064	C	2.738313	2.738313	-2.738313
H	-1.537064	-1.537064	-8.854663	C	4.556715	4.556715	-2.731447
H	1.537064	1.537064	-8.854663	C	-2.731751	-6.382618	-2.731751
H	-3.375901	-1.535948	-7.026244	C	-0.912841	-4.564229	-2.738295
H	1.535948	3.375901	-7.026244	C	0.912550	-2.738371	-2.738371
H	-1.535948	-3.375901	-7.026244	C	2.738371	-0.912550	-2.738371
H	3.375901	1.535948	-7.026244	C	4.564229	0.912841	-2.738295
H	-5.200584	-1.535231	-5.200584	C	6.382618	2.731751	-2.731751
H	1.535231	5.200584	-5.200584	C	-0.903134	-8.205749	-2.729111
H	-3.375086	-3.375086	-5.200638	C	0.912690	-6.388871	-2.737237
H	3.375086	3.375086	-5.200638	C	2.736967	-4.562550	-2.736967
H	-1.535231	-5.200584	-5.200584	C	4.562550	-2.736967	-2.736967
H	5.200584	1.535231	-5.200584	C	6.388871	-0.912690	-2.737237
H	-7.026244	-1.535948	-3.375901	C	8.205749	0.903134	-2.729111
H	1.535948	7.026244	-3.375901	C	-10.030788	-0.901253	-0.901253

H	-5.200638	-3.375086	-3.375086	C	-8.216370	0.912986	-0.912986
H	3.375086	5.200638	-3.375086	C	-6.388871	2.737237	-0.912690
H	-3.375086	-5.200638	-3.375086	C	-4.562592	4.562592	-0.912647
H	5.200638	3.375086	-3.375086	C	-2.737237	6.388871	-0.912690
H	-1.535948	-7.026244	-3.375901	C	-0.912986	8.216370	-0.912986
H	7.026244	1.535948	-3.375901	C	0.901253	10.030788	-0.901253
H	-8.854663	-1.537064	-1.537064	C	-8.205749	-2.729111	-0.903134
H	1.537064	8.854663	-1.537064	C	-6.390798	-0.912800	-0.912800
H	-7.026244	-3.375901	-1.535948	C	-4.564512	0.912656	-0.912656
H	3.375901	7.026244	-1.535948	C	-2.738371	2.738371	-0.912550
H	-5.200584	-5.200584	-1.535231	C	-0.912656	4.564512	-0.912656
H	5.200584	5.200584	-1.535231	C	0.912800	6.390798	-0.912800
H	-3.375901	-7.026244	-1.535948	C	2.729111	8.205749	-0.903134
H	7.026244	3.375901	-1.535948	C	-6.379247	-4.553843	-0.902649
H	-1.537064	-8.854663	-1.537064	C	-4.564229	-2.738295	-0.912841
H	8.854663	1.537064	-1.537064	C	-2.738570	-0.912855	-0.912855
				C	-0.912790	0.912790	-0.912790
				C	0.912855	2.738570	-0.912855
				C	2.738295	4.564229	-0.912841
				C	4.553843	6.379247	-0.902649
				C	-4.553843	-6.379247	-0.902649
				C	-2.738295	-4.564229	-0.912841
				C	-0.912855	-2.738570	-0.912855
				C	0.912790	-0.912790	-0.912790
				C	2.738570	0.912855	-0.912855
				C	4.564229	2.738295	-0.912841
				C	6.379247	4.553843	-0.902649
				C	-2.729111	-8.205749	-0.903134
				C	-0.912800	-6.390798	-0.912800
				C	0.912656	-4.564512	-0.912656
				C	2.738371	-2.738371	-0.912550
				C	4.564512	-0.912656	-0.912656
				C	6.390798	0.912800	-0.912800
				C	8.205749	2.729111	-0.903134
				C	-0.901253	-10.030788	-0.901253
				C	0.912986	-8.216370	-0.912986
				C	2.737237	-6.388871	-0.912690
				C	4.562592	-4.562592	-0.912647
				C	6.388871	-2.737237	-0.912690
				C	8.216370	-0.912986	-0.912986
				C	10.030788	0.901253	-0.901253
				H	-0.633768	-0.633768	11.580221
				H	0.633768	0.633768	11.580221
				H	0.620984	2.464384	9.766403
				H	2.464384	0.620984	9.766403
				H	-2.464384	-0.620984	9.766403
				H	-0.620984	-2.464384	9.766403
				H	0.622305	4.288121	7.938662
				H	2.462339	2.462339	7.939143
				H	4.288121	0.622305	7.938662
				H	-4.288121	-0.622305	7.938662
				H	-2.462339	-2.462339	7.939143
				H	-0.622305	-4.288121	7.938662
				H	0.622551	6.112904	6.112904

H	2.461874	4.287244	6.112606
H	4.287244	2.461874	6.112606
H	6.112904	0.622551	6.112904
H	-6.112904	-0.622551	6.112904
H	-4.287244	-2.461874	6.112606
H	-2.461874	-4.287244	6.112606
H	-0.622551	-6.112904	6.112904
H	0.622305	7.938662	4.288121
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H	4.286814	4.286814	4.286814
H	6.112606	2.461874	4.287244
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H	-7.938662	-0.622305	4.288121
H	-6.112606	-2.461874	4.287244
H	-4.286814	-4.286814	4.286814
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H	-0.622305	-7.938662	4.288121
H	0.620984	9.766403	2.464384
H	2.462339	7.939143	2.462339
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H	6.112606	4.287244	2.461874
H	7.939143	2.462339	2.462339
H	9.766403	0.620984	2.464384
H	-9.766403	-0.620984	2.464384
H	-7.939143	-2.462339	2.462339
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H	-0.620984	-9.766403	2.464384
H	0.633768	11.580221	0.633768
H	-0.633768	11.580221	-0.633768
H	2.464384	9.766403	0.620984
H	4.288121	7.938662	0.622305
H	6.112904	6.112904	0.622551
H	7.938662	4.288121	0.622305
H	9.766403	2.464384	0.620984
H	11.580221	-0.633768	-0.633768
H	11.580221	0.633768	0.633768
H	-2.464384	9.766403	-0.620984
H	9.766403	-2.464384	-0.620984
H	-4.288121	7.938662	-0.622305
H	7.938662	-4.288121	-0.622305
H	-6.112904	6.112904	-0.622551
H	6.112904	-6.112904	-0.622551
H	-7.938662	4.288121	-0.622305
H	4.288121	-7.938662	-0.622305
H	-9.766403	2.464384	-0.620984
H	2.464384	-9.766403	-0.620984
H	-11.580221	0.633768	-0.633768
H	-11.580221	-0.633768	0.633768
H	-9.766403	-2.464384	0.620984
H	-7.938662	-4.288121	0.622305
H	-6.112904	-6.112904	0.622551
H	-4.288121	-7.938662	0.622305

H	-2.464384	-9.766403	0.620984
H	-0.633768	-11.580221	0.633768
H	0.633768	-11.580221	-0.633768
H	0.633768	-0.633768	-11.580221
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H	-0.620984	2.464384	-9.766403
H	2.464384	-0.620984	-9.766403
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H	0.620984	-2.464384	-9.766403
H	-0.622305	4.288121	-7.938662
H	4.288121	-0.622305	-7.938662
H	-2.462339	2.462339	-7.939143
H	2.462339	-2.462339	-7.939143
H	-4.288121	0.622305	-7.938662
H	0.622305	-4.288121	-7.938662
H	-0.622551	6.112904	-6.112904
H	6.112904	-0.622551	-6.112904
H	-2.461874	4.287244	-6.112606
H	4.287244	-2.461874	-6.112606
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H	-6.112904	0.622551	-6.112904
H	0.622551	-6.112904	-6.112904
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H	7.938662	-0.622305	-4.288121
H	-2.461874	6.112606	-4.287244
H	6.112606	-2.461874	-4.287244
H	-4.286814	4.286814	-4.286814
H	4.286814	-4.286814	-4.286814
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H	2.461874	-6.112606	-4.287244
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H	0.622305	-7.938662	-4.288121
H	-0.620984	9.766403	-2.464384
H	9.766403	-0.620984	-2.464384
H	-2.462339	7.939143	-2.462339
H	7.939143	-2.462339	-2.462339
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H	-1.537072	1.537072	10.680281
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H	-1.535948	3.375982	8.851750
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H	-3.375982	1.535948	8.851750
H	1.535948	-3.375982	8.851750
H	-1.535163	5.200594	7.025612
H	5.200594	-1.535163	7.025612
H	-3.375094	3.375094	7.025835

H	3.375094	-3.375094	7.025835
H	-5.200594	1.535163	7.025612
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H	5.200053	-3.374632	5.200053
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H	-7.025612	1.535163	5.200594
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H	-1.535948	8.851750	3.375982
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H	-3.375094	7.025835	3.375094
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H	8.851750	-3.375982	1.535948
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H	-10.680281	1.537072	1.537072
H	1.537072	-10.680281	1.537072
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H	-3.375982	-1.535948	-8.851750
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H	1.535163	5.200594	-7.025612
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H	3.375094	3.375094	-7.025835
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H	-3.374632	-5.200053	-5.200053
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H	7.025612	1.535163	-5.200594
H	-8.851750	-1.535948	-3.375982

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					H	-5.200053	-5.200053	-3.374632	
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					H	7.025835	3.375094	-3.375094	
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					H	8.851750	1.535948	-3.375982	
					H	-10.680281	-1.537072	-1.537072	
					H	1.537072	10.680281	-1.537072	
					H	-8.851750	-3.375982	-1.535948	
					H	3.375982	8.851750	-1.535948	
					H	-7.025612	-5.200594	-1.535163	
					H	5.200594	7.025612	-1.535163	
					H	-5.200594	-7.025612	-1.535163	
					H	7.025612	5.200594	-1.535163	
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					H	8.851750	3.375982	-1.535948	
					H	-1.537072	-10.680281	-1.537072	
					H	10.680281	1.537072	-1.537072	
O7	C	0.000000	0.000000	12.761774	O8	C	0.000000	0.000000	14.587246
	C	-0.010825	1.817537	10.945444		C	-0.010832	1.817553	12.770929
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	C	-1.817537	0.010825	10.945444		C	-1.817553	0.010832	12.770929
	C	0.010825	-1.817537	10.945444		C	0.010832	-1.817553	12.770929
	C	-0.010285	3.641344	9.117897		C	-0.010299	3.641371	10.943357
	C	1.818812	1.818812	9.121877		C	1.818819	1.818819	10.947384
	C	3.641344	-0.010285	9.117897		C	3.641371	-0.010299	10.943357
	C	-1.825861	1.825861	9.127424		C	-1.825879	1.825879	10.952911
	C	0.000000	0.000000	9.129996		C	0.000000	0.000000	10.955516
	C	1.825861	-1.825861	9.127424		C	1.825879	-1.825879	10.952911
	C	-3.641344	0.010285	9.117897		C	-3.641371	0.010299	10.943357
	C	-1.818812	-1.818812	9.121877		C	-1.818819	-1.818819	10.947384
	C	0.010285	-3.641344	9.117897		C	0.010299	-3.641371	10.943357
	C	-0.010038	5.466263	7.291692		C	-0.010046	5.466235	9.117053
	C	1.818610	3.643731	7.294957		C	1.818616	3.643715	9.120429
	C	3.643731	1.818610	7.294957		C	3.643715	1.818616	9.120429
	C	5.466263	-0.010038	7.291692		C	5.466235	-0.010046	9.117053
	C	-1.825558	3.650021	7.301036		C	-1.825574	3.650016	9.126474
	C	-0.000069	1.825350	7.303090		C	-0.000070	1.825338	9.128622
	C	1.825350	-0.000069	7.303090		C	1.825338	-0.000070	9.128622
	C	3.650021	-1.825558	7.301036		C	3.650016	-1.825574	9.126474
	C	-3.650021	1.825558	7.301036		C	-3.650016	1.825574	9.126474
	C	-1.825350	0.000069	7.303090		C	-1.825338	0.000070	9.128622
	C	0.000069	-1.825350	7.303090		C	0.000070	-1.825338	9.128622
	C	1.825558	-3.650021	7.301036		C	1.825574	-3.650016	9.126474
	C	-5.466263	0.010038	7.291692		C	-5.466235	0.010046	9.117053
	C	-3.643731	-1.818610	7.294957		C	-3.643715	-1.818616	9.120429
	C	-1.818610	-3.643731	7.294957		C	-1.818616	-3.643715	9.120429
	C	0.010038	-5.466263	7.291692		C	0.010046	-5.466235	9.117053
	C	-0.010038	7.291692	5.466263		C	-0.010003	7.291451	7.291451
	C	1.818631	5.469024	5.469024		C	1.818663	5.468861	7.294383

C	3.643383	3.643383	5.468755	C	3.643338	3.643338	7.294123
C	5.469024	1.818631	5.469024	C	5.468861	1.818663	7.294383
C	7.291692	-0.010038	5.466263	C	7.291451	-0.010003	7.291451
C	-1.825396	5.475188	5.475188	C	-1.825390	5.475050	7.300494
C	-0.000049	3.650859	5.476678	C	-0.000040	3.650743	7.302173
C	1.825230	1.825230	5.476738	C	1.825188	1.825188	7.302262
C	3.650859	-0.000049	5.476678	C	3.650743	-0.000040	7.302173
C	5.475188	-1.825396	5.475188	C	5.475050	-1.825390	7.300494
C	-3.649707	3.649707	5.475085	C	-3.649659	3.649659	7.300412
C	-1.825386	1.825386	5.476995	C	-1.825337	1.825337	7.302514
C	0.000000	0.000000	5.477214	C	0.000000	0.000000	7.302767
C	1.825386	-1.825386	5.476995	C	1.825337	-1.825337	7.302514
C	3.649707	-3.649707	5.475085	C	3.649659	-3.649659	7.300412
C	-5.475188	1.825396	5.475188	C	-5.475050	1.825390	7.300494
C	-3.650859	0.000049	5.476678	C	-3.650743	0.000040	7.302173
C	-1.825230	-1.825230	5.476738	C	-1.825188	-1.825188	7.302262
C	0.000049	-3.650859	5.476678	C	0.000040	-3.650743	7.302173
C	1.825396	-5.475188	5.475188	C	1.825390	-5.475050	7.300494
C	-7.291692	0.010038	5.466263	C	-7.291451	0.010003	7.291451
C	-5.469024	-1.818631	5.469024	C	-5.468861	-1.818663	7.294383
C	-3.643383	-3.643383	5.468755	C	-3.643338	-3.643338	7.294123
C	-1.818631	-5.469024	5.469024	C	-1.818663	-5.468861	7.294383
C	0.010038	-7.291692	5.466263	C	0.010003	-7.291451	7.291451
C	-0.010285	9.117897	3.641344	C	-0.010046	9.117053	5.466235
C	1.818610	7.294957	3.643731	C	1.818663	7.294383	5.468861
C	3.643383	5.468755	3.643383	C	3.643292	5.468467	5.468467
C	5.468755	3.643383	3.643383	C	5.468467	3.643292	5.468467
C	7.294957	1.818610	3.643731	C	7.294383	1.818663	5.468861
C	9.117897	-0.010285	3.641344	C	9.117053	-0.010046	5.466235
C	-1.825558	7.301036	3.650021	C	-1.825390	7.300494	5.475050
C	-0.000049	5.476678	3.650859	C	-0.000010	5.476273	5.476273
C	1.825143	3.650750	3.650750	C	1.825071	3.650534	5.476196
C	3.650750	1.825143	3.650750	C	3.650534	1.825071	5.476196
C	5.476678	-0.000049	3.650859	C	5.476273	-0.000010	5.476273
C	7.301036	-1.825558	3.650021	C	7.300494	-1.825390	5.475050
C	-3.649707	5.475085	3.649707	C	-3.649475	5.474733	5.474733
C	-1.825328	3.651008	3.651008	C	-1.825219	3.650775	5.476451
C	-0.000009	1.825483	3.651208	C	-0.000004	1.825377	5.476722
C	1.825483	-0.000009	3.651208	C	1.825377	-0.000004	5.476722
C	3.651008	-1.825328	3.651008	C	3.650775	-1.825219	5.476451
C	5.475085	-3.649707	3.649707	C	5.474733	-3.649475	5.474733
C	-5.475085	3.649707	3.649707	C	-5.474733	3.649475	5.474733
C	-3.651008	1.825328	3.651008	C	-3.650775	1.825219	5.476451
C	-1.825483	0.000009	3.651208	C	-1.825377	0.000004	5.476722
C	0.000009	-1.825483	3.651208	C	0.000004	-1.825377	5.476722
C	1.825328	-3.651008	3.651008	C	1.825219	-3.650775	5.476451
C	3.649707	-5.475085	3.649707	C	3.649475	-5.474733	5.474733
C	-7.301036	1.825558	3.650021	C	-7.300494	1.825390	5.475050
C	-5.476678	0.000049	3.650859	C	-5.476273	0.000010	5.476273
C	-3.650750	-1.825143	3.650750	C	-3.650534	-1.825071	5.476196
C	-1.825143	-3.650750	3.650750	C	-1.825071	-3.650534	5.476196
C	0.000049	-5.476678	3.650859	C	0.000010	-5.476273	5.476273
C	1.825558	-7.301036	3.650021	C	1.825390	-7.300494	5.475050
C	-9.117897	0.010285	3.641344	C	-9.117053	0.010046	5.466235

C	-7.294957	-1.818610	3.643731	C	-7.294383	-1.818663	5.468861
C	-5.468755	-3.643383	3.643383	C	-5.468467	-3.643292	5.468467
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C	-1.818610	-7.294957	3.643731	C	-1.818663	-7.294383	5.468861
C	0.010285	-9.117897	3.641344	C	0.010046	-9.117053	5.466235
C	-0.010825	10.945444	1.817537	C	-0.010299	10.943357	3.641371
C	1.818812	9.121877	1.818812	C	1.818616	9.120429	3.643715
C	3.643731	7.294957	1.818610	C	3.643338	7.294123	3.643338
C	5.469024	5.469024	1.818631	C	5.468467	5.468467	3.643292
C	7.294957	3.643731	1.818610	C	7.294123	3.643338	3.643338
C	9.121877	1.818812	1.818812	C	9.120429	1.818616	3.643715
C	10.945444	-0.010825	1.817537	C	10.943357	-0.010299	3.641371
C	-1.825861	9.127424	1.825861	C	-1.825574	9.126474	3.650016
C	-0.000069	7.303090	1.825350	C	-0.000040	7.302173	3.650743
C	1.825230	5.476738	1.825230	C	1.825071	5.476196	3.650534
C	3.650750	3.650750	1.825143	C	3.650435	3.650435	3.650435
C	5.476738	1.825230	1.825230	C	5.476196	1.825071	3.650534
C	7.303090	-0.000069	1.825350	C	7.302173	-0.000040	3.650743
C	9.127424	-1.825861	1.825861	C	9.126474	-1.825574	3.650016
C	-3.650021	7.301036	1.825558	C	-3.649659	7.300412	3.649659
C	-1.825386	5.476995	1.825386	C	-1.825219	5.476451	3.650775
C	-0.000009	3.651208	1.825483	C	-0.000029	3.650908	3.650908
C	1.825488	1.825488	1.825488	C	1.825345	1.825345	3.650942
C	3.651208	-0.000009	1.825483	C	3.650908	-0.000029	3.650908
C	5.476995	-1.825386	1.825386	C	5.476451	-1.825219	3.650775
C	7.301036	-3.650021	1.825558	C	7.300412	-3.649659	3.649659
C	-5.475188	5.475188	1.825396	C	-5.474733	5.474733	3.649475
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C	-1.825519	1.825519	1.825519	C	-1.825402	1.825402	3.650961
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C	1.825519	-1.825519	1.825519	C	1.825402	-1.825402	3.650961
C	3.651008	-3.651008	1.825328	C	3.650695	-3.650695	3.650695
C	5.475188	-5.475188	1.825396	C	5.474733	-5.474733	3.649475
C	-7.301036	3.650021	1.825558	C	-7.300412	3.649659	3.649659
C	-5.476995	1.825386	1.825386	C	-5.476451	1.825219	3.650775
C	-3.651208	0.000009	1.825483	C	-3.650908	0.000029	3.650908
C	-1.825488	-1.825488	1.825488	C	-1.825345	-1.825345	3.650942
C	0.000009	-3.651208	1.825483	C	0.000029	-3.650908	3.650908
C	1.825386	-5.476995	1.825386	C	1.825219	-5.476451	3.650775
C	3.650021	-7.301036	1.825558	C	3.649659	-7.300412	3.649659
C	-9.127424	1.825861	1.825861	C	-9.126474	1.825574	3.650016
C	-7.303090	0.000069	1.825350	C	-7.302173	0.000040	3.650743
C	-5.476738	-1.825230	1.825230	C	-5.476196	-1.825071	3.650534
C	-3.650750	-3.650750	1.825143	C	-3.650435	-3.650435	3.650435
C	-1.825230	-5.476738	1.825230	C	-1.825071	-5.476196	3.650534
C	0.000069	-7.303090	1.825350	C	0.000040	-7.302173	3.650743
C	1.825861	-9.127424	1.825861	C	1.825574	-9.126474	3.650016
C	-10.945444	0.010825	1.817537	C	-10.943357	0.010299	3.641371
C	-9.121877	-1.818812	1.818812	C	-9.120429	-1.818616	3.643715
C	-7.294957	-3.643731	1.818610	C	-7.294123	-3.643338	3.643338
C	-5.469024	-5.469024	1.818631	C	-5.468467	-5.468467	3.643292
C	-3.643731	-7.294957	1.818610	C	-3.643338	-7.294123	3.643338
C	-1.818812	-9.121877	1.818812	C	-1.818616	-9.120429	3.643715
C	0.010825	-10.945444	1.817537	C	0.010299	-10.943357	3.641371

C	0.000000	12.761774	0.000000	C	-0.010832	12.770929	1.817553
C	1.817537	10.945444	-0.010825	C	1.818819	10.947384	1.818819
C	3.641344	9.117897	-0.010285	C	3.643715	9.120429	1.818616
C	5.466263	7.291692	-0.010038	C	5.468861	7.294383	1.818663
C	7.291692	5.466263	-0.010038	C	7.294383	5.468861	1.818663
C	9.117897	3.641344	-0.010285	C	9.120429	3.643715	1.818616
C	10.945444	1.817537	-0.010825	C	10.947384	1.818819	1.818819
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C	-1.817537	10.945444	0.010825	C	-1.825879	10.952911	1.825879
C	0.000000	9.129996	0.000000	C	-0.000070	9.128622	1.825338
C	1.825350	7.303090	-0.000069	C	1.825188	7.302262	1.825188
C	3.650859	5.476678	-0.000049	C	3.650534	5.476196	1.825071
C	5.476678	3.650859	-0.000049	C	5.476196	3.650534	1.825071
C	7.303090	1.825350	-0.000069	C	7.302262	1.825188	1.825188
C	9.129996	0.000000	0.000000	C	9.128622	-0.000070	1.825338
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C	-3.641344	9.117897	0.010285	C	-3.650016	9.126474	1.825574
C	-1.825350	7.303090	0.000069	C	-1.825337	7.302514	1.825337
C	0.000000	5.477214	0.000000	C	-0.000004	5.476722	1.825377
C	1.825483	3.651208	-0.000009	C	1.825345	3.650942	1.825345
C	3.651208	1.825483	-0.000009	C	3.650942	1.825345	1.825345
C	5.477214	0.000000	0.000000	C	5.476722	-0.000004	1.825377
C	7.303090	-1.825350	0.000069	C	7.302514	-1.825337	1.825337
C	9.117897	-3.641344	0.010285	C	9.126474	-3.650016	1.825574
C	-5.466263	7.291692	0.010038	C	-5.475050	7.300494	1.825390
C	-3.650859	5.476678	0.000049	C	-3.650775	5.476451	1.825219
C	-1.825483	3.651208	0.000009	C	-1.825402	3.650961	1.825402
C	0.000000	1.825562	0.000000	C	-0.000031	1.825452	1.825452
C	1.825562	0.000000	0.000000	C	1.825452	-0.000031	1.825452
C	3.651208	-1.825483	0.000009	C	3.650961	-1.825402	1.825402
C	5.476678	-3.650859	0.000049	C	5.476451	-3.650775	1.825219
C	7.291692	-5.466263	0.010038	C	7.300494	-5.475050	1.825390
C	-7.291692	5.466263	0.010038	C	-7.300494	5.475050	1.825390
C	-5.476678	3.650859	0.000049	C	-5.476451	3.650775	1.825219
C	-3.651208	1.825483	0.000009	C	-3.650961	1.825402	1.825402
C	-1.825562	0.000000	0.000000	C	-1.825452	0.000031	1.825452
C	0.000000	-1.825562	0.000000	C	0.000031	-1.825452	1.825452
C	1.825483	-3.651208	0.000009	C	1.825402	-3.650961	1.825402
C	3.650859	-5.476678	0.000049	C	3.650775	-5.476451	1.825219
C	5.466263	-7.291692	0.010038	C	5.475050	-7.300494	1.825390
C	-9.117897	3.641344	0.010285	C	-9.126474	3.650016	1.825574
C	-7.303090	1.825350	0.000069	C	-7.302514	1.825337	1.825337
C	-5.477214	0.000000	0.000000	C	-5.476722	0.000004	1.825377
C	-3.651208	-1.825483	-0.000009	C	-3.650942	-1.825345	1.825345
C	-1.825483	-3.651208	-0.000009	C	-1.825345	-3.650942	1.825345
C	0.000000	-5.477214	0.000000	C	0.000004	-5.476722	1.825377
C	1.825350	-7.303090	0.000069	C	1.825337	-7.302514	1.825337
C	3.641344	-9.117897	0.010285	C	3.650016	-9.126474	1.825574
C	-10.945444	1.817537	0.010825	C	-10.952911	1.825879	1.825879
C	-9.129996	0.000000	0.000000	C	-9.128622	0.000070	1.825338
C	-7.303090	-1.825350	-0.000069	C	-7.302262	-1.825188	1.825188
C	-5.476678	-3.650859	-0.000049	C	-5.476196	-3.650534	1.825071
C	-3.650859	-5.476678	-0.000049	C	-3.650534	-5.476196	1.825071
C	-1.825350	-7.303090	-0.000069	C	-1.825188	-7.302262	1.825188

C	0.000000	-9.129996	0.000000	C	0.000070	-9.128622	1.825338
C	1.817537	-10.945444	0.010825	C	1.825879	-10.952911	1.825879
C	-12.761774	0.000000	0.000000	C	-12.770929	0.010832	1.817553
C	-10.945444	-1.817537	-0.010825	C	-10.947384	-1.818819	1.818819
C	-9.117897	-3.641344	-0.010285	C	-9.120429	-3.643715	1.818616
C	-7.291692	-5.466263	-0.010038	C	-7.294383	-5.468861	1.818663
C	-5.466263	-7.291692	-0.010038	C	-5.468861	-7.294383	1.818663
C	-3.641344	-9.117897	-0.010285	C	-3.643715	-9.120429	1.818616
C	-1.817537	-10.945444	-0.010825	C	-1.818819	-10.947384	1.818819
C	0.000000	-12.761774	0.000000	C	0.010832	-12.770929	1.817553
C	0.000000	0.000000	-12.761774	C	0.000000	14.587246	0.000000
C	0.010825	1.817537	-10.945444	C	1.817553	12.770929	-0.010832
C	1.817537	0.010825	-10.945444	C	3.641371	10.943357	-0.010299
C	-1.817537	-0.010825	-10.945444	C	5.466235	9.117053	-0.010046
C	-0.010825	-1.817537	-10.945444	C	7.291451	7.291451	-0.010003
C	0.010285	3.641344	-9.117897	C	9.117053	5.466235	-0.010046
C	1.825861	1.825861	-9.127424	C	10.943357	3.641371	-0.010299
C	3.641344	0.010285	-9.117897	C	12.770929	1.817553	-0.010832
C	-1.818812	1.818812	-9.121877	C	14.587246	0.000000	0.000000
C	0.000000	0.000000	-9.129996	C	-1.817553	12.770929	0.010832
C	1.818812	-1.818812	-9.121877	C	0.000000	10.955516	0.000000
C	-3.641344	-0.010285	-9.117897	C	1.825338	9.128622	-0.000070
C	-1.825861	-1.825861	-9.127424	C	3.650743	7.302173	-0.000040
C	-0.010285	-3.641344	-9.117897	C	5.476273	5.476273	-0.000010
C	0.010038	5.466263	-7.291692	C	7.302173	3.650743	-0.000040
C	1.825558	3.650021	-7.301036	C	9.128622	1.825338	-0.000070
C	3.650021	1.825558	-7.301036	C	10.955516	0.000000	0.000000
C	5.466263	0.010038	-7.291692	C	12.770929	-1.817553	0.010832
C	-1.818610	3.643731	-7.294957	C	-3.641371	10.943357	0.010299
C	0.000069	1.825350	-7.303090	C	-1.825338	9.128622	0.000070
C	1.825350	0.000069	-7.303090	C	0.000000	7.302767	0.000000
C	3.643731	-1.818610	-7.294957	C	1.825377	5.476722	-0.000004
C	-3.643731	1.818610	-7.294957	C	3.650908	3.650908	-0.000029
C	-1.825350	-0.000069	-7.303090	C	5.476722	1.825377	-0.000004
C	-0.000069	-1.825350	-7.303090	C	7.302767	0.000000	0.000000
C	1.818610	-3.643731	-7.294957	C	9.128622	-1.825338	0.000070
C	-5.466263	-0.010038	-7.291692	C	10.943357	-3.641371	0.010299
C	-3.650021	-1.825558	-7.301036	C	-5.466235	9.117053	0.010046
C	-1.825558	-3.650021	-7.301036	C	-3.650743	7.302173	0.000040
C	-0.010038	-5.466263	-7.291692	C	-1.825377	5.476722	0.000004
C	0.010038	7.291692	-5.466263	C	0.000000	3.651049	0.000000
C	1.825396	5.475188	-5.475188	C	1.825452	1.825452	-0.000031
C	3.649707	3.649707	-5.475085	C	3.651049	0.000000	0.000000
C	5.475188	1.825396	-5.475188	C	5.476722	-1.825377	0.000004
C	7.291692	0.010038	-5.466263	C	7.302173	-3.650743	0.000040
C	-1.818631	5.469024	-5.469024	C	9.117053	-5.466235	0.010046
C	0.000049	3.650859	-5.476678	C	-7.291451	7.291451	0.010003
C	1.825386	1.825386	-5.476995	C	-5.476273	5.476273	0.000010
C	3.650859	0.000049	-5.476678	C	-3.650908	3.650908	0.000029
C	5.469024	-1.818631	-5.469024	C	-1.825452	1.825452	0.000031
C	-3.643383	3.643383	-5.468755	C	0.000000	0.000000	0.000000
C	-1.825230	1.825230	-5.476738	C	1.825452	-1.825452	0.000031
C	0.000000	0.000000	-5.477214	C	3.650908	-3.650908	0.000029
C	1.825230	-1.825230	-5.476738	C	5.476273	-5.476273	0.000010

C	3.643383	-3.643383	-5.468755	C	7.291451	-7.291451	0.010003
C	-5.469024	1.818631	-5.469024	C	-9.117053	5.466235	0.010046
C	-3.650859	-0.000049	-5.476678	C	-7.302173	3.650743	0.000040
C	-1.825386	-1.825386	-5.476995	C	-5.476722	1.825377	0.000004
C	-0.000049	-3.650859	-5.476678	C	-3.651049	0.000000	0.000000
C	1.818631	-5.469024	-5.469024	C	-1.825452	-1.825452	-0.000031
C	-7.291692	-0.010038	-5.466263	C	0.000000	-3.651049	0.000000
C	-5.475188	-1.825396	-5.475188	C	1.825377	-5.476722	0.000004
C	-3.649707	-3.649707	-5.475085	C	3.650743	-7.302173	0.000040
C	-1.825396	-5.475188	-5.475188	C	5.466235	-9.117053	0.010046
C	-0.010038	-7.291692	-5.466263	C	-10.943357	3.641371	0.010299
C	0.010285	9.117897	-3.641344	C	-9.128622	1.825338	0.000070
C	1.825558	7.301036	-3.650021	C	-7.302767	0.000000	0.000000
C	3.649707	5.475085	-3.649707	C	-5.476722	-1.825377	-0.000004
C	5.475085	3.649707	-3.649707	C	-3.650908	-3.650908	-0.000029
C	7.301036	1.825558	-3.650021	C	-1.825377	-5.476722	-0.000004
C	9.117897	0.010285	-3.641344	C	0.000000	-7.302767	0.000000
C	-1.818610	7.294957	-3.643731	C	1.825338	-9.128622	0.000070
C	0.000049	5.476678	-3.650859	C	3.641371	-10.943357	0.010299
C	1.825328	3.651008	-3.651008	C	-12.770929	1.817553	0.010832
C	3.651008	1.825328	-3.651008	C	-10.955516	0.000000	0.000000
C	5.476678	0.000049	-3.650859	C	-9.128622	-1.825338	-0.000070
C	7.294957	-1.818610	-3.643731	C	-7.302173	-3.650743	-0.000040
C	-3.643383	5.468755	-3.643383	C	-5.476273	-5.476273	-0.000010
C	-1.825143	3.650750	-3.650750	C	-3.650743	-7.302173	-0.000040
C	0.000009	1.825483	-3.651208	C	-1.825338	-9.128622	-0.000070
C	1.825483	0.000009	-3.651208	C	0.000000	-10.955516	0.000000
C	3.650750	-1.825143	-3.650750	C	1.817553	-12.770929	0.010832
C	5.468755	-3.643383	-3.643383	C	-14.587246	0.000000	0.000000
C	-5.468755	3.643383	-3.643383	C	-12.770929	-1.817553	-0.010832
C	-3.650750	1.825143	-3.650750	C	-10.943357	-3.641371	-0.010299
C	-1.825483	-0.000009	-3.651208	C	-9.117053	-5.466235	-0.010046
C	-0.000009	-1.825483	-3.651208	C	-7.291451	-7.291451	-0.010003
C	1.825143	-3.650750	-3.650750	C	-5.466235	-9.117053	-0.010046
C	3.643383	-5.468755	-3.643383	C	-3.641371	-10.943357	-0.010299
C	-7.294957	1.818610	-3.643731	C	-1.817553	-12.770929	-0.010832
C	-5.476678	-0.000049	-3.650859	C	0.000000	-14.587246	0.000000
C	-3.651008	-1.825328	-3.651008	C	0.000000	0.000000	-14.587246
C	-1.825328	-3.651008	-3.651008	C	0.010832	1.817553	-12.770929
C	-0.000049	-5.476678	-3.650859	C	1.817553	0.010832	-12.770929
C	1.818610	-7.294957	-3.643731	C	-1.817553	-0.010832	-12.770929
C	-9.117897	-0.010285	-3.641344	C	-0.010832	-1.817553	-12.770929
C	-7.301036	-1.825558	-3.650021	C	0.010299	3.641371	-10.943357
C	-5.475085	-3.649707	-3.649707	C	1.825879	1.825879	-10.952911
C	-3.649707	-5.475085	-3.649707	C	3.641371	0.010299	-10.943357
C	-1.825558	-7.301036	-3.650021	C	-1.818819	1.818819	-10.947384
C	-0.010285	-9.117897	-3.641344	C	0.000000	0.000000	-10.955516
C	0.010825	10.945444	-1.817537	C	1.818819	-1.818819	-10.947384
C	1.825861	9.127424	-1.825861	C	-3.641371	-0.010299	-10.943357
C	3.650021	7.301036	-1.825558	C	-1.825879	-1.825879	-10.952911
C	5.475188	5.475188	-1.825396	C	-0.010299	-3.641371	-10.943357
C	7.301036	3.650021	-1.825558	C	0.010046	5.466235	-9.117053
C	9.127424	1.825861	-1.825861	C	1.825574	3.650016	-9.126474
C	10.945444	0.010825	-1.817537	C	3.650016	1.825574	-9.126474

C	-1.818812	9.121877	-1.818812	C	5.466235	0.010046	-9.117053
C	0.000069	7.303090	-1.825350	C	-1.818616	3.643715	-9.120429
C	1.825386	5.476995	-1.825386	C	0.000070	1.825338	-9.128622
C	3.651008	3.651008	-1.825328	C	1.825338	0.000070	-9.128622
C	5.476995	1.825386	-1.825386	C	3.643715	-1.818616	-9.120429
C	7.303090	0.000069	-1.825350	C	-3.643715	1.818616	-9.120429
C	9.121877	-1.818812	-1.818812	C	-1.825338	-0.000070	-9.128622
C	-3.643731	7.294957	-1.818610	C	-0.000070	-1.825338	-9.128622
C	-1.825230	5.476738	-1.825230	C	1.818616	-3.643715	-9.120429
C	0.000009	3.651208	-1.825483	C	-5.466235	-0.010046	-9.117053
C	1.825519	1.825519	-1.825519	C	-3.650016	-1.825574	-9.126474
C	3.651208	0.000009	-1.825483	C	-1.825574	-3.650016	-9.126474
C	5.476738	-1.825230	-1.825230	C	-0.010046	-5.466235	-9.117053
C	7.294957	-3.643731	-1.818610	C	0.010003	7.291451	-7.291451
C	-5.469024	5.469024	-1.818631	C	1.825390	5.475050	-7.300494
C	-3.650750	3.650750	-1.825143	C	3.649659	3.649659	-7.300412
C	-1.825488	1.825488	-1.825488	C	5.475050	1.825390	-7.300494
C	0.000000	0.000000	-1.825562	C	7.291451	0.010003	-7.291451
C	1.825488	-1.825488	-1.825488	C	-1.818663	5.468861	-7.294383
C	3.650750	-3.650750	-1.825143	C	0.000040	3.650743	-7.302173
C	5.469024	-5.469024	-1.818631	C	1.825337	1.825337	-7.302514
C	-7.294957	3.643731	-1.818610	C	3.650743	0.000040	-7.302173
C	-5.476738	1.825230	-1.825230	C	5.468861	-1.818663	-7.294383
C	-3.651208	-0.000009	-1.825483	C	-3.643338	3.643338	-7.294123
C	-1.825519	-1.825519	-1.825519	C	-1.825188	1.825188	-7.302262
C	-0.000009	-3.651208	-1.825483	C	0.000000	0.000000	-7.302767
C	1.825230	-5.476738	-1.825230	C	1.825188	-1.825188	-7.302262
C	3.643731	-7.294957	-1.818610	C	3.643338	-3.643338	-7.294123
C	-9.121877	1.818812	-1.818812	C	-5.468861	1.818663	-7.294383
C	-7.303090	-0.000069	-1.825350	C	-3.650743	-0.000040	-7.302173
C	-5.476995	-1.825386	-1.825386	C	-1.825337	-1.825337	-7.302514
C	-3.651008	-3.651008	-1.825328	C	-0.000040	-3.650743	-7.302173
C	-1.825386	-5.476995	-1.825386	C	1.818663	-5.468861	-7.294383
C	-0.000069	-7.303090	-1.825350	C	-7.291451	-0.010003	-7.291451
C	1.818812	-9.121877	-1.818812	C	-5.475050	-1.825390	-7.300494
C	-10.945444	-0.010825	-1.817537	C	-3.649659	-3.649659	-7.300412
C	-9.127424	-1.825861	-1.825861	C	-1.825390	-5.475050	-7.300494
C	-7.301036	-3.650021	-1.825558	C	-0.010003	-7.291451	-7.291451
C	-5.475188	-5.475188	-1.825396	C	0.010046	9.117053	-5.466235
C	-3.650021	-7.301036	-1.825558	C	1.825390	7.300494	-5.475050
C	-1.825861	-9.127424	-1.825861	C	3.649475	5.474733	-5.474733
C	-0.010825	-10.945444	-1.817537	C	5.474733	3.649475	-5.474733
C	-0.901267	0.901267	11.856319	C	7.300494	1.825390	-5.475050
C	0.901267	-0.901267	11.856319	C	9.117053	0.010046	-5.466235
C	-0.903151	2.729146	10.031265	C	-1.818663	7.294383	-5.468861
C	0.912994	0.912994	10.041944	C	0.000010	5.476273	-5.476273
C	2.729146	-0.903151	10.031265	C	1.825219	3.650775	-5.476451
C	-2.729146	0.903151	10.031265	C	3.650775	1.825219	-5.476451
C	-0.912994	-0.912994	10.041944	C	5.476273	0.000010	-5.476273
C	0.903151	-2.729146	10.031265	C	7.294383	-1.818663	-5.468861
C	-0.902654	4.553823	8.204633	C	-3.643292	5.468467	-5.468467
C	0.912702	2.737222	8.214425	C	-1.825071	3.650534	-5.476196
C	2.737222	0.912702	8.214425	C	0.000004	1.825377	-5.476722
C	4.553823	-0.902654	8.204633	C	1.825377	0.000004	-5.476722

C	-2.731764	2.731764	8.208076	C	3.650534	-1.825071	-5.476196
C	-0.912793	0.912793	8.216406	C	5.468467	-3.643292	-5.468467
C	0.912793	-0.912793	8.216406	C	-5.468467	3.643292	-5.468467
C	2.731764	-2.731764	8.208076	C	-3.650534	1.825071	-5.476196
C	-4.553823	0.902654	8.204633	C	-1.825377	-0.000004	-5.476722
C	-2.737222	-0.912702	8.214425	C	-0.000004	-1.825377	-5.476722
C	-0.912702	-2.737222	8.214425	C	1.825071	-3.650534	-5.476196
C	0.902654	-4.553823	8.204633	C	3.643292	-5.468467	-5.468467
C	-0.902569	6.378927	6.378927	C	-7.294383	1.818663	-5.468861
C	0.912687	4.562373	6.388013	C	-5.476273	-0.000010	-5.476273
C	2.736906	2.736906	6.388007	C	-3.650775	-1.825219	-5.476451
C	4.562373	0.912687	6.388013	C	-1.825219	-3.650775	-5.476451
C	6.378927	-0.902569	6.378927	C	-0.000010	-5.476273	-5.476273
C	-2.731385	4.556554	6.381912	C	1.818663	-7.294383	-5.468861
C	-0.912801	2.738165	6.389795	C	-9.117053	-0.010046	-5.466235
C	0.912620	0.912620	6.390134	C	-7.300494	-1.825390	-5.475050
C	2.738165	-0.912801	6.389795	C	-5.474733	-3.649475	-5.474733
C	4.556554	-2.731385	6.381912	C	-3.649475	-5.474733	-5.474733
C	-4.556554	2.731385	6.381912	C	-1.825390	-7.300494	-5.475050
C	-2.738165	0.912801	6.389795	C	-0.010046	-9.117053	-5.466235
C	-0.912620	-0.912620	6.390134	C	0.010299	10.943357	-3.641371
C	0.912801	-2.738165	6.389795	C	1.825574	9.126474	-3.650016
C	2.731385	-4.556554	6.381912	C	3.649659	7.300412	-3.649659
C	-6.378927	0.902569	6.378927	C	5.474733	5.474733	-3.649475
C	-4.562373	-0.912687	6.388013	C	7.300412	3.649659	-3.649659
C	-2.736906	-2.736906	6.388007	C	9.126474	1.825574	-3.650016
C	-0.912687	-4.562373	6.388013	C	10.943357	0.010299	-3.641371
C	0.902569	-6.378927	6.378927	C	-1.818616	9.120429	-3.643715
C	-0.902654	8.204633	4.553823	C	0.000040	7.302173	-3.650743
C	0.912687	6.388013	4.562373	C	1.825219	5.476451	-3.650775
C	2.736774	4.562099	4.562099	C	3.650695	3.650695	-3.650695
C	4.562099	2.736774	4.562099	C	5.476451	1.825219	-3.650775
C	6.388013	0.912687	4.562373	C	7.302173	0.000040	-3.650743
C	8.204633	-0.902654	4.553823	C	9.120429	-1.818616	-3.643715
C	-2.731385	6.381912	4.556554	C	-3.643338	7.294123	-3.643338
C	-0.912756	4.563723	4.563723	C	-1.825071	5.476196	-3.650534
C	0.912474	2.738112	4.563913	C	0.000029	3.650908	-3.650908
C	2.738112	0.912474	4.563913	C	1.825402	1.825402	-3.650961
C	4.563723	-0.912756	4.563723	C	3.650908	0.000029	-3.650908
C	6.381912	-2.731385	4.556554	C	5.476196	-1.825071	-3.650534
C	-4.556226	4.556226	4.556226	C	7.294123	-3.643338	-3.643338
C	-2.738064	2.738064	4.563748	C	-5.468467	5.468467	-3.643292
C	-0.912778	0.912778	4.564156	C	-3.650435	3.650435	-3.650435
C	0.912778	-0.912778	4.564156	C	-1.825345	1.825345	-3.650942
C	2.738064	-2.738064	4.563748	C	0.000000	0.000000	-3.651049
C	4.556226	-4.556226	4.556226	C	1.825345	-1.825345	-3.650942
C	-6.381912	2.731385	4.556554	C	3.650435	-3.650435	-3.650435
C	-4.563723	0.912756	4.563723	C	5.468467	-5.468467	-3.643292
C	-2.738112	-0.912474	4.563913	C	-7.294123	3.643338	-3.643338
C	-0.912474	-2.738112	4.563913	C	-5.476196	1.825071	-3.650534
C	0.912756	-4.563723	4.563723	C	-3.650908	-0.000029	-3.650908
C	2.731385	-6.381912	4.556554	C	-1.825402	-1.825402	-3.650961
C	-8.204633	0.902654	4.553823	C	-0.000029	-3.650908	-3.650908
C	-6.388013	-0.912687	4.562373	C	1.825071	-5.476196	-3.650534

C	-4.562099	-2.736774	4.562099	C	3.643338	-7.294123	-3.643338
C	-2.736774	-4.562099	4.562099	C	-9.120429	1.818616	-3.643715
C	-0.912687	-6.388013	4.562373	C	-7.302173	-0.000040	-3.650743
C	0.902654	-8.204633	4.553823	C	-5.476451	-1.825219	-3.650775
C	-0.903151	10.031265	2.729146	C	-3.650695	-3.650695	-3.650695
C	0.912702	8.214425	2.737222	C	-1.825219	-5.476451	-3.650775
C	2.736906	6.388007	2.736906	C	-0.000040	-7.302173	-3.650743
C	4.562099	4.562099	2.736774	C	1.818616	-9.120429	-3.643715
C	6.388007	2.736906	2.736906	C	-10.943357	-0.010299	-3.641371
C	8.214425	0.912702	2.737222	C	-9.126474	-1.825574	-3.650016
C	10.031265	-0.903151	2.729146	C	-7.300412	-3.649659	-3.649659
C	-2.731764	8.208076	2.731764	C	-5.474733	-5.474733	-3.649475
C	-0.912801	6.389795	2.738165	C	-3.649659	-7.300412	-3.649659
C	0.912474	4.563913	2.738112	C	-1.825574	-9.126474	-3.650016
C	2.738030	2.738030	2.738030	C	-0.010299	-10.943357	-3.641371
C	4.563913	0.912474	2.738112	C	0.010832	12.770929	-1.817553
C	6.389795	-0.912801	2.738165	C	1.825879	10.952911	-1.825879
C	8.208076	-2.731764	2.731764	C	3.650016	9.126474	-1.825574
C	-4.556554	6.381912	2.731385	C	5.475050	7.300494	-1.825390
C	-2.738064	4.563748	2.738064	C	7.300494	5.475050	-1.825390
C	-0.912818	2.738320	2.738320	C	9.126474	3.650016	-1.825574
C	0.912696	0.912696	2.738336	C	10.952911	1.825879	-1.825879
C	2.738320	-0.912818	2.738320	C	12.770929	0.010832	-1.817553
C	4.563748	-2.738064	2.738064	C	-1.818819	10.947384	-1.818819
C	6.381912	-4.556554	2.731385	C	0.000070	9.128622	-1.825338
C	-6.381912	4.556554	2.731385	C	1.825337	7.302514	-1.825337
C	-4.563748	2.738064	2.738064	C	3.650775	5.476451	-1.825219
C	-2.738320	0.912818	2.738320	C	5.476451	3.650775	-1.825219
C	-0.912696	-0.912696	2.738336	C	7.302514	1.825337	-1.825337
C	0.912818	-2.738320	2.738320	C	9.128622	0.000070	-1.825338
C	2.738064	-4.563748	2.738064	C	10.947384	-1.818819	-1.818819
C	4.556554	-6.381912	2.731385	C	-3.643715	9.120429	-1.818616
C	-8.208076	2.731764	2.731764	C	-1.825188	7.302262	-1.825188
C	-6.389795	0.912801	2.738165	C	0.000004	5.476722	-1.825377
C	-4.563913	-0.912474	2.738112	C	1.825402	3.650961	-1.825402
C	-2.738030	-2.738030	2.738030	C	3.650961	1.825402	-1.825402
C	-0.912474	-4.563913	2.738112	C	5.476722	0.000004	-1.825377
C	0.912801	-6.389795	2.738165	C	7.302262	-1.825188	-1.825188
C	2.731764	-8.208076	2.731764	C	9.120429	-3.643715	-1.818616
C	-10.031265	0.903151	2.729146	C	-5.468861	7.294383	-1.818663
C	-8.214425	-0.912702	2.737222	C	-3.650534	5.476196	-1.825071
C	-6.388007	-2.736906	2.736906	C	-1.825345	3.650942	-1.825345
C	-4.562099	-4.562099	2.736774	C	0.000031	1.825452	-1.825452
C	-2.736906	-6.388007	2.736906	C	1.825452	0.000031	-1.825452
C	-0.912702	-8.214425	2.737222	C	3.650942	-1.825345	-1.825345
C	0.903151	-10.031265	2.729146	C	5.476196	-3.650534	-1.825071
C	-0.901267	11.856319	0.901267	C	7.294383	-5.468861	-1.818663
C	0.912994	10.041944	0.912994	C	-7.294383	5.468861	-1.818663
C	2.737222	8.214425	0.912702	C	-5.476196	3.650534	-1.825071
C	4.562373	6.388013	0.912687	C	-3.650942	1.825345	-1.825345
C	6.388013	4.562373	0.912687	C	-1.825452	-0.000031	-1.825452
C	8.214425	2.737222	0.912702	C	-0.000031	-1.825452	-1.825452
C	10.041944	0.912994	0.912994	C	1.825345	-3.650942	-1.825345
C	11.856319	-0.901267	0.901267	C	3.650534	-5.476196	-1.825071

C	-2.729146	10.031265	0.903151	C	5.468861	-7.294383	-1.818663
C	-0.912793	8.216406	0.912793	C	-9.120429	3.643715	-1.818616
C	0.912620	6.390134	0.912620	C	-7.302262	1.825188	-1.825188
C	2.738112	4.563913	0.912474	C	-5.476722	-0.000004	-1.825377
C	4.563913	2.738112	0.912474	C	-3.650961	-1.825402	-1.825402
C	6.390134	0.912620	0.912620	C	-1.825402	-3.650961	-1.825402
C	8.216406	-0.912793	0.912793	C	-0.000004	-5.476722	-1.825377
C	10.031265	-2.729146	0.903151	C	1.825188	-7.302262	-1.825188
C	-4.553823	8.204633	0.902654	C	3.643715	-9.120429	-1.818616
C	-2.738165	6.389795	0.912801	C	-10.947384	1.818819	-1.818819
C	-0.912778	4.564156	0.912778	C	-9.128622	-0.000070	-1.825338
C	0.912696	2.738336	0.912696	C	-7.302514	-1.825337	-1.825337
C	2.738336	0.912696	0.912696	C	-5.476451	-3.650775	-1.825219
C	4.564156	-0.912778	0.912778	C	-3.650775	-5.476451	-1.825219
C	6.389795	-2.738165	0.912801	C	-1.825337	-7.302514	-1.825337
C	8.204633	-4.553823	0.902654	C	-0.000070	-9.128622	-1.825338
C	-6.378927	6.378927	0.902569	C	1.818819	-10.947384	-1.818819
C	-4.563723	4.563723	0.912756	C	-12.770929	-0.010832	-1.817553
C	-2.738320	2.738320	0.912818	C	-10.952911	-1.825879	-1.825879
C	-0.912774	0.912774	0.912774	C	-9.126474	-3.650016	-1.825574
C	0.912774	-0.912774	0.912774	C	-7.300494	-5.475050	-1.825390
C	2.738320	-2.738320	0.912818	C	-5.475050	-7.300494	-1.825390
C	4.563723	-4.563723	0.912756	C	-3.650016	-9.126474	-1.825574
C	6.378927	-6.378927	0.902569	C	-1.825879	-10.952911	-1.825879
C	-8.204633	4.553823	0.902654	C	-0.010832	-12.770929	-1.817553
C	-6.389795	2.738165	0.912801	C	-0.901275	0.901275	13.681800
C	-4.564156	0.912778	0.912778	C	0.901275	-0.901275	13.681800
C	-2.738336	-0.912696	0.912696	C	-0.903163	2.729170	11.856741
C	-0.912696	-2.738336	0.912696	C	0.912999	0.912999	11.867448
C	0.912778	-4.564156	0.912778	C	2.729170	-0.903163	11.856741
C	2.738165	-6.389795	0.912801	C	-2.729170	0.903163	11.856741
C	4.553823	-8.204633	0.902654	C	-0.912999	-0.912999	11.867448
C	-10.031265	2.729146	0.903151	C	0.903163	-2.729170	11.856741
C	-8.216406	0.912793	0.912793	C	-0.902663	4.553837	10.030046
C	-6.390134	-0.912620	0.912620	C	0.912707	2.737227	10.039925
C	-4.563913	-2.738112	0.912474	C	2.737227	0.912707	10.039925
C	-2.738112	-4.563913	0.912474	C	4.553837	-0.902663	10.030046
C	-0.912620	-6.390134	0.912620	C	-2.731781	2.731781	10.033532
C	0.912793	-8.216406	0.912793	C	-0.912794	0.912794	10.041932
C	2.729146	-10.031265	0.903151	C	0.912794	-0.912794	10.041932
C	-11.856319	0.901267	0.901267	C	2.731781	-2.731781	10.033532
C	-10.041944	-0.912994	0.912994	C	-4.553837	0.902663	10.030046
C	-8.214425	-2.737222	0.912702	C	-2.737227	-0.912707	10.039925
C	-6.388013	-4.562373	0.912687	C	-0.912707	-2.737227	10.039925
C	-4.562373	-6.388013	0.912687	C	0.902663	-4.553837	10.030046
C	-2.737222	-8.214425	0.912702	C	-0.902564	6.378827	8.204194
C	-0.912994	-10.041944	0.912994	C	0.912705	4.562297	8.213447
C	0.901267	-11.856319	0.901267	C	2.736892	2.736892	8.213473
C	-0.901267	-0.901267	-11.856319	C	4.562297	0.912705	8.213447
C	0.901267	0.901267	-11.856319	C	6.378827	-0.902564	8.204194
C	-2.729146	-0.903151	-10.031265	C	-2.731391	4.556517	8.207260
C	-0.912994	0.912994	-10.041944	C	-0.912790	2.738120	8.215306
C	0.903151	2.729146	-10.031265	C	0.912608	0.912608	8.215680
C	-0.903151	-2.729146	-10.031265	C	2.738120	-0.912790	8.215306

C	0.912994	-0.912994	-10.041944	C	4.556517	-2.731391	8.207260
C	2.729146	0.903151	-10.031265	C	-4.556517	2.731391	8.207260
C	-4.553823	-0.902654	-8.204633	C	-2.738120	0.912790	8.215306
C	-2.737222	0.912702	-8.214425	C	-0.912608	-0.912608	8.215680
C	-0.912702	2.737222	-8.214425	C	0.912790	-2.738120	8.215306
C	0.902654	4.553823	-8.204633	C	2.731391	-4.556517	8.207260
C	-2.731764	-2.731764	-8.208076	C	-6.378827	0.902564	8.204194
C	-0.912793	-0.912793	-8.216406	C	-4.562297	-0.912705	8.213447
C	0.912793	0.912793	-8.216406	C	-2.736892	-2.736892	8.213473
C	2.731764	2.731764	-8.208076	C	-0.912705	-4.562297	8.213447
C	-0.902654	-4.553823	-8.204633	C	0.902564	-6.378827	8.204194
C	0.912702	-2.737222	-8.214425	C	-0.902564	8.204194	6.378827
C	2.737222	-0.912702	-8.214425	C	0.912739	6.387680	6.387680
C	4.553823	0.902654	-8.204633	C	2.736747	4.561943	6.387427
C	-6.378927	-0.902569	-6.378927	C	4.561943	2.736747	6.387427
C	-4.562373	0.912687	-6.388013	C	6.387680	0.912739	6.387680
C	-2.736906	2.736906	-6.388007	C	8.204194	-0.902564	6.378827
C	-0.912687	4.562373	-6.388013	C	-2.731323	6.381645	6.381645
C	0.902569	6.378927	-6.378927	C	-0.912718	4.563497	6.389167
C	-4.556554	-2.731385	-6.381912	C	0.912449	2.737994	6.389423
C	-2.738165	-0.912801	-6.389795	C	2.737994	0.912449	6.389423
C	-0.912620	0.912620	-6.390134	C	4.563497	-0.912718	6.389167
C	0.912801	2.738165	-6.389795	C	6.381645	-2.731323	6.381645
C	2.731385	4.556554	-6.381912	C	-4.556089	4.556089	6.381314
C	-2.731385	-4.556554	-6.381912	C	-2.737955	2.737955	6.389206
C	-0.912801	-2.738165	-6.389795	C	-0.912740	0.912740	6.389693
C	0.912620	-0.912620	-6.390134	C	0.912740	-0.912740	6.389693
C	2.738165	0.912801	-6.389795	C	2.737955	-2.737955	6.389206
C	4.556554	2.731385	-6.381912	C	4.556089	-4.556089	6.381314
C	-0.902569	-6.378927	-6.378927	C	-6.381645	2.731323	6.381645
C	0.912687	-4.562373	-6.388013	C	-4.563497	0.912718	6.389167
C	2.736906	-2.736906	-6.388007	C	-2.737994	-0.912449	6.389423
C	4.562373	-0.912687	-6.388013	C	-0.912449	-2.737994	6.389423
C	6.378927	0.902569	-6.378927	C	0.912718	-4.563497	6.389167
C	-8.204633	-0.902654	-4.553823	C	2.731323	-6.381645	6.381645
C	-6.388013	0.912687	-4.562373	C	-8.204194	0.902564	6.378827
C	-4.562099	2.736774	-4.562099	C	-6.387680	-0.912739	6.387680
C	-2.736774	4.562099	-4.562099	C	-4.561943	-2.736747	6.387427
C	-0.912687	6.388013	-4.562373	C	-2.736747	-4.561943	6.387427
C	0.902654	8.204633	-4.553823	C	-0.912739	-6.387680	6.387680
C	-6.381912	-2.731385	-4.556554	C	0.902564	-8.204194	6.378827
C	-4.563723	-0.912756	-4.563723	C	-0.902663	10.030046	4.553837
C	-2.738112	0.912474	-4.563913	C	0.912705	8.213447	4.562297
C	-0.912474	2.738112	-4.563913	C	2.736747	6.387427	4.561943
C	0.912756	4.563723	-4.563723	C	4.561774	4.561774	4.561774
C	2.731385	6.381912	-4.556554	C	6.387427	2.736747	4.561943
C	-4.556226	-4.556226	-4.556226	C	8.213447	0.912705	4.562297
C	-2.738064	-2.738064	-4.563748	C	10.030046	-0.902663	4.553837
C	-0.912778	-0.912778	-4.564156	C	-2.731391	8.207260	4.556517
C	0.912778	0.912778	-4.564156	C	-0.912718	6.389167	4.563497
C	2.738064	2.738064	-4.563748	C	0.912415	4.563531	4.563531
C	4.556226	4.556226	-4.556226	C	2.737836	2.737836	4.563459
C	-2.731385	-6.381912	-4.556554	C	4.563531	0.912415	4.563531
C	-0.912756	-4.563723	-4.563723	C	6.389167	-0.912718	4.563497

C	0.912474	-2.738112	-4.563913	C	8.207260	-2.731391	4.556517
C	2.738112	-0.912474	-4.563913	C	-4.556089	6.381314	4.556089
C	4.563723	0.912756	-4.563723	C	-2.737863	4.563377	4.563377
C	6.381912	2.731385	-4.556554	C	-0.912765	2.738123	4.563788
C	-0.902654	-8.204633	-4.553823	C	0.912632	0.912632	4.563836
C	0.912687	-6.388013	-4.562373	C	2.738123	-0.912765	4.563788
C	2.736774	-4.562099	-4.562099	C	4.563377	-2.737863	4.563377
C	4.562099	-2.736774	-4.562099	C	6.381314	-4.556089	4.556089
C	6.388013	-0.912687	-4.562373	C	-6.381314	4.556089	4.556089
C	8.204633	0.902654	-4.553823	C	-4.563377	2.737863	4.563377
C	-10.031265	-0.903151	-2.729146	C	-2.738123	0.912765	4.563788
C	-8.214425	0.912702	-2.737222	C	-0.912632	-0.912632	4.563836
C	-6.388007	2.736906	-2.736906	C	0.912765	-2.738123	4.563788
C	-4.562099	4.562099	-2.736774	C	2.737863	-4.563377	4.563377
C	-2.736906	6.388007	-2.736906	C	4.556089	-6.381314	4.556089
C	-0.912702	8.214425	-2.737222	C	-8.207260	2.731391	4.556517
C	0.903151	10.031265	-2.729146	C	-6.389167	0.912718	4.563497
C	-8.208076	-2.731764	-2.731764	C	-4.563531	-0.912415	4.563531
C	-6.389795	-0.912801	-2.738165	C	-2.737836	-2.737836	4.563459
C	-4.563913	0.912474	-2.738112	C	-0.912415	-4.563531	4.563531
C	-2.738030	2.738030	-2.738030	C	0.912718	-6.389167	4.563497
C	-0.912474	4.563913	-2.738112	C	2.731391	-8.207260	4.556517
C	0.912801	6.389795	-2.738165	C	-10.030046	0.902663	4.553837
C	2.731764	8.208076	-2.731764	C	-8.213447	-0.912705	4.562297
C	-6.381912	-4.556554	-2.731385	C	-6.387427	-2.736747	4.561943
C	-4.563748	-2.738064	-2.738064	C	-4.561774	-4.561774	4.561774
C	-2.738320	-0.912818	-2.738320	C	-2.736747	-6.387427	4.561943
C	-0.912696	0.912696	-2.738336	C	-0.912705	-8.213447	4.562297
C	0.912818	2.738320	-2.738320	C	0.902663	-10.030046	4.553837
C	2.738064	4.563748	-2.738064	C	-0.903163	11.856741	2.729170
C	4.556554	6.381912	-2.731385	C	0.912707	10.039925	2.737227
C	-4.556554	-6.381912	-2.731385	C	2.736892	8.213473	2.736892
C	-2.738064	-4.563748	-2.738064	C	4.561943	6.387427	2.736747
C	-0.912818	-2.738320	-2.738320	C	6.387427	4.561943	2.736747
C	0.912696	-0.912696	-2.738336	C	8.213473	2.736892	2.736892
C	2.738320	0.912818	-2.738320	C	10.039925	0.912707	2.737227
C	4.563748	2.738064	-2.738064	C	11.856741	-0.903163	2.729170
C	6.381912	4.556554	-2.731385	C	-2.731781	10.033532	2.731781
C	-2.731764	-8.208076	-2.731764	C	-0.912790	8.215306	2.738120
C	-0.912801	-6.389795	-2.738165	C	0.912449	6.389423	2.737994
C	0.912474	-4.563913	-2.738112	C	2.737836	4.563459	2.737836
C	2.738030	-2.738030	-2.738030	C	4.563459	2.737836	2.737836
C	4.563913	-0.912474	-2.738112	C	6.389423	0.912449	2.737994
C	6.389795	0.912801	-2.738165	C	8.215306	-0.912790	2.738120
C	8.208076	2.731764	-2.731764	C	10.033532	-2.731781	2.731781
C	-0.903151	-10.031265	-2.729146	C	-4.556517	8.207260	2.731391
C	0.912702	-8.214425	-2.737222	C	-2.737955	6.389206	2.737955
C	2.736906	-6.388007	-2.736906	C	-0.912765	4.563788	2.738123
C	4.562099	-4.562099	-2.736774	C	0.912613	2.738123	2.738123
C	6.388007	-2.736906	-2.736906	C	2.738123	0.912613	2.738123
C	8.214425	-0.912702	-2.737222	C	4.563788	-0.912765	2.738123
C	10.031265	0.903151	-2.729146	C	6.389206	-2.737955	2.737955
C	-11.856319	-0.901267	-0.901267	C	8.207260	-4.556517	2.731391
C	-10.041944	0.912994	-0.912994	C	-6.381645	6.381645	2.731323

C	-8.214425	2.737222	-0.912702	C	-4.563377	4.563377	2.737863
C	-6.388013	4.562373	-0.912687	C	-2.738164	2.738164	2.738164
C	-4.562373	6.388013	-0.912687	C	-0.912721	0.912721	2.738236
C	-2.737222	8.214425	-0.912702	C	0.912721	-0.912721	2.738236
C	-0.912994	10.041944	-0.912994	C	2.738164	-2.738164	2.738164
C	0.901267	11.856319	-0.901267	C	4.563377	-4.563377	2.737863
C	-10.031265	-2.729146	-0.903151	C	6.381645	-6.381645	2.731323
C	-8.216406	-0.912793	-0.912793	C	-8.207260	4.556517	2.731391
C	-6.390134	0.912620	-0.912620	C	-6.389206	2.737955	2.737955
C	-4.563913	2.738112	-0.912474	C	-4.563788	0.912765	2.738123
C	-2.738112	4.563913	-0.912474	C	-2.738123	-0.912613	2.738123
C	-0.912620	6.390134	-0.912620	C	-0.912613	-2.738123	2.738123
C	0.912793	8.216406	-0.912793	C	0.912765	-4.563788	2.738123
C	2.729146	10.031265	-0.903151	C	2.737955	-6.389206	2.737955
C	-8.204633	-4.553823	-0.902654	C	4.556517	-8.207260	2.731391
C	-6.389795	-2.738165	-0.912801	C	-10.033532	2.731781	2.731781
C	-4.564156	-0.912778	-0.912778	C	-8.215306	0.912790	2.738120
C	-2.738336	0.912696	-0.912696	C	-6.389423	-0.912449	2.737994
C	-0.912696	2.738336	-0.912696	C	-4.563459	-2.737836	2.737836
C	0.912778	4.564156	-0.912778	C	-2.737836	-4.563459	2.737836
C	2.738165	6.389795	-0.912801	C	-0.912449	-6.389423	2.737994
C	4.553823	8.204633	-0.902654	C	0.912790	-8.215306	2.738120
C	-6.378927	-6.378927	-0.902569	C	2.731781	-10.033532	2.731781
C	-4.563723	-4.563723	-0.912756	C	-11.856741	0.903163	2.729170
C	-2.738320	-2.738320	-0.912818	C	-10.039925	-0.912707	2.737227
C	-0.912774	-0.912774	-0.912774	C	-8.213473	-2.736892	2.736892
C	0.912774	0.912774	-0.912774	C	-6.387427	-4.561943	2.736747
C	2.738320	2.738320	-0.912818	C	-4.561943	-6.387427	2.736747
C	4.563723	4.563723	-0.912756	C	-2.736892	-8.213473	2.736892
C	6.378927	6.378927	-0.902569	C	-0.912707	-10.039925	2.737227
C	-4.553823	-8.204633	-0.902654	C	0.903163	-11.856741	2.729170
C	-2.738165	-6.389795	-0.912801	C	-0.901275	13.681800	0.901275
C	-0.912778	-4.564156	-0.912778	C	0.912999	11.867448	0.912999
C	0.912696	-2.738336	-0.912696	C	2.737227	10.039925	0.912707
C	2.738336	-0.912696	-0.912696	C	4.562297	8.213447	0.912705
C	4.564156	0.912778	-0.912778	C	6.387680	6.387680	0.912739
C	6.389795	2.738165	-0.912801	C	8.213447	4.562297	0.912705
C	8.204633	4.553823	-0.902654	C	10.039925	2.737227	0.912707
C	-2.729146	-10.031265	-0.903151	C	11.867448	0.912999	0.912999
C	-0.912793	-8.216406	-0.912793	C	13.681800	-0.901275	0.901275
C	0.912620	-6.390134	-0.912620	C	-2.729170	11.856741	0.903163
C	2.738112	-4.563913	-0.912474	C	-0.912794	10.041932	0.912794
C	4.563913	-2.738112	-0.912474	C	0.912608	8.215680	0.912608
C	6.390134	-0.912620	-0.912620	C	2.737994	6.389423	0.912449
C	8.216406	0.912793	-0.912793	C	4.563531	4.563531	0.912415
C	10.031265	2.729146	-0.903151	C	6.389423	2.737994	0.912449
C	-0.901267	-11.856319	-0.901267	C	8.215680	0.912608	0.912608
C	0.912994	-10.041944	-0.912994	C	10.041932	-0.912794	0.912794
C	2.737222	-8.214425	-0.912702	C	11.856741	-2.729170	0.903163
C	4.562373	-6.388013	-0.912687	C	-4.553837	10.030046	0.902663
C	6.388013	-4.562373	-0.912687	C	-2.738120	8.215306	0.912790
C	8.214425	-2.737222	-0.912702	C	-0.912740	6.389693	0.912740
C	10.041944	-0.912994	-0.912994	C	0.912632	4.563836	0.912632
C	11.856319	0.901267	-0.901267	C	2.738123	2.738123	0.912613

H	-0.633768	-0.633768	13.405733	C	4.563836	0.912632	0.912632
H	0.633768	0.633768	13.405733	C	6.389693	-0.912740	0.912740
H	0.620954	2.464421	11.591945	C	8.215306	-2.738120	0.912790
H	2.464421	0.620954	11.591945	C	10.030046	-4.553837	0.902663
H	-2.464421	-0.620954	11.591945	C	-6.378827	8.204194	0.902564
H	-0.620954	-2.464421	11.591945	C	-4.563497	6.389167	0.912718
H	0.622254	4.288196	9.764117	C	-2.738123	4.563788	0.912765
H	2.462348	2.462348	9.764708	C	-0.912721	2.738236	0.912721
H	4.288196	0.622254	9.764117	C	0.912720	0.912720	0.912720
H	-4.288196	-0.622254	9.764117	C	2.738236	-0.912721	0.912721
H	-2.462348	-2.462348	9.764708	C	4.563788	-2.738123	0.912765
H	-0.622254	-4.288196	9.764117	C	6.389167	-4.563497	0.912718
H	0.622530	6.112883	7.938115	C	8.204194	-6.378827	0.902564
H	2.461892	4.287213	7.938033	C	-8.204194	6.378827	0.902564
H	4.287213	2.461892	7.938033	C	-6.389167	4.563497	0.912718
H	6.112883	0.622530	7.938115	C	-4.563788	2.738123	0.912765
H	-6.112883	-0.622530	7.938115	C	-2.738236	0.912721	0.912721
H	-4.287213	-2.461892	7.938033	C	-0.912720	-0.912720	0.912720
H	-2.461892	-4.287213	7.938033	C	0.912721	-2.738236	0.912721
H	-0.622530	-6.112883	7.938115	C	2.738123	-4.563788	0.912765
H	0.622530	7.938115	6.112883	C	4.563497	-6.389167	0.912718
H	2.461949	6.112282	6.112282	C	6.378827	-8.204194	0.902564
H	4.286732	4.286732	6.111847	C	-10.030046	4.553837	0.902663
H	6.112282	2.461949	6.112282	C	-8.215306	2.738120	0.912790
H	7.938115	0.622530	6.112883	C	-6.389693	0.912740	0.912740
H	-7.938115	-0.622530	6.112883	C	-4.563836	-0.912632	0.912632
H	-6.112282	-2.461949	6.112282	C	-2.738123	-2.738123	0.912613
H	-4.286732	-4.286732	6.111847	C	-0.912632	-4.563836	0.912632
H	-2.461949	-6.112282	6.112282	C	0.912740	-6.389693	0.912740
H	-0.622530	-7.938115	6.112883	C	2.738120	-8.215306	0.912790
H	0.622254	9.764117	4.288196	C	4.553837	-10.030046	0.902663
H	2.461892	7.938033	4.287213	C	-11.856741	2.729170	0.903163
H	4.286732	6.111847	4.286732	C	-10.041932	0.912794	0.912794
H	6.111847	4.286732	4.286732	C	-8.215680	-0.912608	0.912608
H	7.938033	2.461892	4.287213	C	-6.389423	-2.737994	0.912449
H	9.764117	0.622254	4.288196	C	-4.563531	-4.563531	0.912415
H	-9.764117	-0.622254	4.288196	C	-2.737994	-6.389423	0.912449
H	-7.938033	-2.461892	4.287213	C	-0.912608	-8.215680	0.912608
H	-6.111847	-4.286732	4.286732	C	0.912794	-10.041932	0.912794
H	-4.286732	-6.111847	4.286732	C	2.729170	-11.856741	0.903163
H	-2.461892	-7.938033	4.287213	C	-13.681800	0.901275	0.901275
H	-0.622254	-9.764117	4.288196	C	-11.867448	-0.912999	0.912999
H	0.620954	11.591945	2.464421	C	-10.039925	-2.737227	0.912707
H	2.462348	9.764708	2.462348	C	-8.213447	-4.562297	0.912705
H	4.287213	7.938033	2.461892	C	-6.387680	-6.387680	0.912739
H	6.112282	6.112282	2.461949	C	-4.562297	-8.213447	0.912705
H	7.938033	4.287213	2.461892	C	-2.737227	-10.039925	0.912707
H	9.764708	2.462348	2.462348	C	-0.912999	-11.867448	0.912999
H	11.591945	0.620954	2.464421	C	0.901275	-13.681800	0.901275
H	-11.591945	-0.620954	2.464421	C	-0.901275	-0.901275	-13.681800
H	-9.764708	-2.462348	2.462348	C	0.901275	0.901275	-13.681800
H	-7.938033	-4.287213	2.461892	C	-2.729170	-0.903163	-11.856741
H	-6.112282	-6.112282	2.461949	C	-0.912999	0.912999	-11.867448
H	-4.287213	-7.938033	2.461892	C	0.903163	2.729170	-11.856741

H	-2.462348	-9.764708	2.462348	C	-0.903163	-2.729170	-11.856741
H	-0.620954	-11.591945	2.464421	C	0.912999	-0.912999	-11.867448
H	0.633768	13.405733	0.633768	C	2.729170	0.903163	-11.856741
H	-0.633768	13.405733	-0.633768	C	-4.553837	-0.902663	-10.030046
H	2.464421	11.591945	0.620954	C	-2.737227	0.912707	-10.039925
H	4.288196	9.764117	0.622254	C	-0.912707	2.737227	-10.039925
H	6.112883	7.938115	0.622530	C	0.902663	4.553837	-10.030046
H	7.938115	6.112883	0.622530	C	-2.731781	-2.731781	-10.033532
H	9.764117	4.288196	0.622254	C	-0.912794	-0.912794	-10.041932
H	11.591945	2.464421	0.620954	C	0.912794	0.912794	-10.041932
H	13.405733	-0.633768	-0.633768	C	2.731781	2.731781	-10.033532
H	13.405733	0.633768	0.633768	C	-0.902663	-4.553837	-10.030046
H	-2.464421	11.591945	-0.620954	C	0.912707	-2.737227	-10.039925
H	11.591945	-2.464421	-0.620954	C	2.737227	-0.912707	-10.039925
H	-4.288196	9.764117	-0.622254	C	4.553837	0.902663	-10.030046
H	9.764117	-4.288196	-0.622254	C	-6.378827	-0.902564	-8.204194
H	-6.112883	7.938115	-0.622530	C	-4.562297	0.912705	-8.213447
H	7.938115	-6.112883	-0.622530	C	-2.736892	2.736892	-8.213473
H	-7.938115	6.112883	-0.622530	C	-0.912705	4.562297	-8.213447
H	6.112883	-7.938115	-0.622530	C	0.902564	6.378827	-8.204194
H	-9.764117	4.288196	-0.622254	C	-4.556517	-2.731391	-8.207260
H	4.288196	-9.764117	-0.622254	C	-2.738120	-0.912790	-8.215306
H	-11.591945	2.464421	-0.620954	C	-0.912608	0.912608	-8.215680
H	2.464421	-11.591945	-0.620954	C	0.912790	2.738120	-8.215306
H	-13.405733	0.633768	-0.633768	C	2.731391	4.556517	-8.207260
H	-13.405733	-0.633768	0.633768	C	-2.731391	-4.556517	-8.207260
H	-11.591945	-2.464421	0.620954	C	-0.912790	-2.738120	-8.215306
H	-9.764117	-4.288196	0.622254	C	0.912608	-0.912608	-8.215680
H	-7.938115	-6.112883	0.622530	C	2.738120	0.912790	-8.215306
H	-6.112883	-7.938115	0.622530	C	4.556517	2.731391	-8.207260
H	-4.288196	-9.764117	0.622254	C	-0.902564	-6.378827	-8.204194
H	-2.464421	-11.591945	0.620954	C	0.912705	-4.562297	-8.213447
H	-0.633768	-13.405733	0.633768	C	2.736892	-2.736892	-8.213473
H	0.633768	-13.405733	-0.633768	C	4.562297	-0.912705	-8.213447
H	0.633768	-0.633768	-13.405733	C	6.378827	0.902564	-8.204194
H	-0.633768	0.633768	-13.405733	C	-8.204194	-0.902564	-6.378827
H	-0.620954	2.464421	-11.591945	C	-6.387680	0.912739	-6.387680
H	2.464421	-0.620954	-11.591945	C	-4.561943	2.736747	-6.387427
H	-2.464421	0.620954	-11.591945	C	-2.736747	4.561943	-6.387427
H	0.620954	-2.464421	-11.591945	C	-0.912739	6.387680	-6.387680
H	-0.622254	4.288196	-9.764117	C	0.902564	8.204194	-6.378827
H	4.288196	-0.622254	-9.764117	C	-6.381645	-2.731323	-6.381645
H	-2.462348	2.462348	-9.764708	C	-4.563497	-0.912718	-6.389167
H	2.462348	-2.462348	-9.764708	C	-2.737994	0.912449	-6.389423
H	-4.288196	0.622254	-9.764117	C	-0.912449	2.737994	-6.389423
H	0.622254	-4.288196	-9.764117	C	0.912718	4.563497	-6.389167
H	-0.622530	6.112883	-7.938115	C	2.731323	6.381645	-6.381645
H	6.112883	-0.622530	-7.938115	C	-4.556089	-4.556089	-6.381314
H	-2.461892	4.287213	-7.938033	C	-2.737955	-2.737955	-6.389206
H	4.287213	-2.461892	-7.938033	C	-0.912740	-0.912740	-6.389693
H	-4.287213	2.461892	-7.938033	C	0.912740	0.912740	-6.389693
H	2.461892	-4.287213	-7.938033	C	2.737955	2.737955	-6.389206
H	-6.112883	0.622530	-7.938115	C	4.556089	4.556089	-6.381314
H	0.622530	-6.112883	-7.938115	C	-2.731323	-6.381645	-6.381645

H	-0.622530	7.938115	-6.112883	C	-0.912718	-4.563497	-6.389167
H	7.938115	-0.622530	-6.112883	C	0.912449	-2.737994	-6.389423
H	-2.461949	6.112282	-6.112282	C	2.737994	-0.912449	-6.389423
H	6.112282	-2.461949	-6.112282	C	4.563497	0.912718	-6.389167
H	-4.286732	4.286732	-6.111847	C	6.381645	2.731323	-6.381645
H	4.286732	-4.286732	-6.111847	C	-0.902564	-8.204194	-6.378827
H	-6.112282	2.461949	-6.112282	C	0.912739	-6.387680	-6.387680
H	2.461949	-6.112282	-6.112282	C	2.736747	-4.561943	-6.387427
H	-7.938115	0.622530	-6.112883	C	4.561943	-2.736747	-6.387427
H	0.622530	-7.938115	-6.112883	C	6.387680	-0.912739	-6.387680
H	-0.622254	9.764117	-4.288196	C	8.204194	0.902564	-6.378827
H	9.764117	-0.622254	-4.288196	C	-10.030046	-0.902663	-4.553837
H	-2.461892	7.938033	-4.287213	C	-8.213447	0.912705	-4.562297
H	7.938033	-2.461892	-4.287213	C	-6.387427	2.736747	-4.561943
H	-4.286732	6.111847	-4.286732	C	-4.561774	4.561774	-4.561774
H	6.111847	-4.286732	-4.286732	C	-2.736747	6.387427	-4.561943
H	-6.111847	4.286732	-4.286732	C	-0.912705	8.213447	-4.562297
H	4.286732	-6.111847	-4.286732	C	0.902663	10.030046	-4.553837
H	-7.938033	2.461892	-4.287213	C	-8.207260	-2.731391	-4.556517
H	2.461892	-7.938033	-4.287213	C	-6.389167	-0.912718	-4.563497
H	-9.764117	0.622254	-4.288196	C	-4.563531	0.912415	-4.563531
H	0.622254	-9.764117	-4.288196	C	-2.737836	2.737836	-4.563459
H	-0.620954	11.591945	-2.464421	C	-0.912415	4.563531	-4.563531
H	11.591945	-0.620954	-2.464421	C	0.912718	6.389167	-4.563497
H	-2.462348	9.764708	-2.462348	C	2.731391	8.207260	-4.556517
H	9.764708	-2.462348	-2.462348	C	-6.381314	-4.556089	-4.556089
H	-4.287213	7.938033	-2.461892	C	-4.563377	-2.737863	-4.563377
H	7.938033	-4.287213	-2.461892	C	-2.738123	-0.912765	-4.563788
H	-6.112282	6.112282	-2.461949	C	-0.912632	0.912632	-4.563836
H	6.112282	-6.112282	-2.461949	C	0.912765	2.738123	-4.563788
H	-7.938033	4.287213	-2.461892	C	2.737863	4.563377	-4.563377
H	4.287213	-7.938033	-2.461892	C	4.556089	6.381314	-4.556089
H	-9.764708	2.462348	-2.462348	C	-4.556089	-6.381314	-4.556089
H	2.462348	-9.764708	-2.462348	C	-2.737863	-4.563377	-4.563377
H	-11.591945	0.620954	-2.464421	C	-0.912765	-2.738123	-4.563788
H	0.620954	-11.591945	-2.464421	C	0.912632	-0.912632	-4.563836
H	-1.537076	1.537076	12.505826	C	2.738123	0.912765	-4.563788
H	1.537076	-1.537076	12.505826	C	4.563377	2.737863	-4.563377
H	-1.535952	3.376029	10.677262	C	6.381314	4.556089	-4.556089
H	3.376029	-1.535952	10.677262	C	-2.731391	-8.207260	-4.556517
H	-3.376029	1.535952	10.677262	C	-0.912718	-6.389167	-4.563497
H	1.535952	-3.376029	10.677262	C	0.912415	-4.563531	-4.563531
H	-1.535153	5.200647	8.850932	C	2.737836	-2.737836	-4.563459
H	5.200647	-1.535153	8.850932	C	4.563531	-0.912415	-4.563531
H	-3.375124	3.375124	8.851250	C	6.389167	0.912718	-4.563497
H	3.375124	-3.375124	8.851250	C	8.207260	2.731391	-4.556517
H	-5.200647	1.535153	8.850932	C	-0.902663	-10.030046	-4.553837
H	1.535153	-5.200647	8.850932	C	0.912705	-8.213447	-4.562297
H	-1.535085	7.025476	7.025476	C	2.736747	-6.387427	-4.561943
H	7.025476	-1.535085	7.025476	C	4.561774	-4.561774	-4.561774
H	-3.374626	5.199981	7.025089	C	6.387427	-2.736747	-4.561943
H	5.199981	-3.374626	7.025089	C	8.213447	-0.912705	-4.562297
H	-5.199981	3.374626	7.025089	C	10.030046	0.902663	-4.553837
H	3.374626	-5.199981	7.025089	C	-11.856741	-0.903163	-2.729170

H	-7.025476	1.535085	7.025476	C	-10.039925	0.912707	-2.737227
H	1.535085	-7.025476	7.025476	C	-8.213473	2.736892	-2.736892
H	-1.535153	8.850932	5.200647	C	-6.387427	4.561943	-2.736747
H	8.850932	-1.535153	5.200647	C	-4.561943	6.387427	-2.736747
H	-3.374626	7.025089	5.199981	C	-2.736892	8.213473	-2.736892
H	7.025089	-3.374626	5.199981	C	-0.912707	10.039925	-2.737227
H	-5.199494	5.199494	5.199494	C	0.903163	11.856741	-2.729170
H	5.199494	-5.199494	5.199494	C	-10.033532	-2.731781	-2.731781
H	-7.025089	3.374626	5.199981	C	-8.215306	-0.912790	-2.738120
H	3.374626	-7.025089	5.199981	C	-6.389423	0.912449	-2.737994
H	-8.850932	1.535153	5.200647	C	-4.563459	2.737836	-2.737836
H	1.535153	-8.850932	5.200647	C	-2.737836	4.563459	-2.737836
H	-1.535952	10.677262	3.376029	C	-0.912449	6.389423	-2.737994
H	10.677262	-1.535952	3.376029	C	0.912790	8.215306	-2.738120
H	-3.375124	8.851250	3.375124	C	2.731781	10.033532	-2.731781
H	8.851250	-3.375124	3.375124	C	-8.207260	-4.556517	-2.731391
H	-5.199981	7.025089	3.374626	C	-6.389206	-2.737955	-2.737955
H	7.025089	-5.199981	3.374626	C	-4.563788	-0.912765	-2.738123
H	-7.025089	5.199981	3.374626	C	-2.738123	0.912613	-2.738123
H	5.199981	-7.025089	3.374626	C	-0.912613	2.738123	-2.738123
H	-8.851250	3.375124	3.375124	C	0.912765	4.563788	-2.738123
H	3.375124	-8.851250	3.375124	C	2.737955	6.389206	-2.737955
H	-10.677262	1.535952	3.376029	C	4.556517	8.207260	-2.731391
H	1.535952	-10.677262	3.376029	C	-6.381645	-6.381645	-2.731323
H	-1.537076	12.505826	1.537076	C	-4.563377	-4.563377	-2.737863
H	12.505826	-1.537076	1.537076	C	-2.738164	-2.738164	-2.738164
H	-3.376029	10.677262	1.535952	C	-0.912721	-0.912721	-2.738236
H	10.677262	-3.376029	1.535952	C	0.912721	0.912721	-2.738236
H	-5.200647	8.850932	1.535153	C	2.738164	2.738164	-2.738164
H	8.850932	-5.200647	1.535153	C	4.563377	4.563377	-2.737863
H	-7.025476	7.025476	1.535085	C	6.381645	6.381645	-2.731323
H	7.025476	-7.025476	1.535085	C	-4.556517	-8.207260	-2.731391
H	-8.850932	5.200647	1.535153	C	-2.737955	-6.389206	-2.737955
H	5.200647	-8.850932	1.535153	C	-0.912765	-4.563788	-2.738123
H	-10.677262	3.376029	1.535952	C	0.912613	-2.738123	-2.738123
H	3.376029	-10.677262	1.535952	C	2.738123	-0.912613	-2.738123
H	-12.505826	1.537076	1.537076	C	4.563788	0.912765	-2.738123
H	1.537076	-12.505826	1.537076	C	6.389206	2.737955	-2.737955
H	-1.537076	-1.537076	-12.505826	C	8.207260	4.556517	-2.731391
H	1.537076	1.537076	-12.505826	C	-2.731781	-10.033532	-2.731781
H	-3.376029	-1.535952	-10.677262	C	-0.912790	-8.215306	-2.738120
H	1.535952	3.376029	-10.677262	C	0.912449	-6.389423	-2.737994
H	-1.535952	-3.376029	-10.677262	C	2.737836	-4.563459	-2.737836
H	3.376029	1.535952	-10.677262	C	4.563459	-2.737836	-2.737836
H	-5.200647	-1.535153	-8.850932	C	6.389423	-0.912449	-2.737994
H	1.535153	5.200647	-8.850932	C	8.215306	0.912790	-2.738120
H	-3.375124	-3.375124	-8.851250	C	10.033532	2.731781	-2.731781
H	3.375124	3.375124	-8.851250	C	-0.903163	-11.856741	-2.729170
H	-1.535153	-5.200647	-8.850932	C	0.912707	-10.039925	-2.737227
H	5.200647	1.535153	-8.850932	C	2.736892	-8.213473	-2.736892
H	-7.025476	-1.535085	-7.025476	C	4.561943	-6.387427	-2.736747
H	1.535085	7.025476	-7.025476	C	6.387427	-4.561943	-2.736747
H	-5.199981	-3.374626	-7.025089	C	8.213473	-2.736892	-2.736892
H	3.374626	5.199981	-7.025089	C	10.039925	-0.912707	-2.737227

H	-3.374626	-5.199981	-7.025089	C	11.856741	0.903163	-2.729170
H	5.199981	3.374626	-7.025089	C	-13.681800	-0.901275	-0.901275
H	-1.535085	-7.025476	-7.025476	C	-11.867448	0.912999	-0.912999
H	7.025476	1.535085	-7.025476	C	-10.039925	2.737227	-0.912707
H	-8.850932	-1.535153	-5.200647	C	-8.213447	4.562297	-0.912705
H	1.535153	8.850932	-5.200647	C	-6.387680	6.387680	-0.912739
H	-7.025089	-3.374626	-5.199981	C	-4.562297	8.213447	-0.912705
H	3.374626	7.025089	-5.199981	C	-2.737227	10.039925	-0.912707
H	-5.199494	-5.199494	-5.199494	C	-0.912999	11.867448	-0.912999
H	5.199494	5.199494	-5.199494	C	0.901275	13.681800	-0.901275
H	-3.374626	-7.025089	-5.199981	C	-11.856741	-2.729170	-0.903163
H	7.025089	3.374626	-5.199981	C	-10.041932	-0.912794	-0.912794
H	-1.535153	-8.850932	-5.200647	C	-8.215680	0.912608	-0.912608
H	8.850932	1.535153	-5.200647	C	-6.389423	2.737994	-0.912449
H	-10.677262	-1.535952	-3.376029	C	-4.563531	4.563531	-0.912415
H	1.535952	10.677262	-3.376029	C	-2.737994	6.389423	-0.912449
H	-8.851250	-3.375124	-3.375124	C	-0.912608	8.215680	-0.912608
H	3.375124	8.851250	-3.375124	C	0.912794	10.041932	-0.912794
H	-7.025089	-5.199981	-3.374626	C	2.729170	11.856741	-0.903163
H	5.199981	7.025089	-3.374626	C	-10.030046	-4.553837	-0.902663
H	-5.199981	-7.025089	-3.374626	C	-8.215306	-2.738120	-0.912790
H	7.025089	5.199981	-3.374626	C	-6.389693	-0.912740	-0.912740
H	-3.375124	-8.851250	-3.375124	C	-4.563836	0.912632	-0.912632
H	8.851250	3.375124	-3.375124	C	-2.738123	2.738123	-0.912613
H	-1.535952	-10.677262	-3.376029	C	-0.912632	4.563836	-0.912632
H	10.677262	1.535952	-3.376029	C	0.912740	6.389693	-0.912740
H	-12.505826	-1.537076	-1.537076	C	2.738120	8.215306	-0.912790
H	1.537076	12.505826	-1.537076	C	4.553837	10.030046	-0.902663
H	-10.677262	-3.376029	-1.535952	C	-8.204194	-6.378827	-0.902564
H	3.376029	10.677262	-1.535952	C	-6.389167	-4.563497	-0.912718
H	-8.850932	-5.200647	-1.535153	C	-4.563788	-2.738123	-0.912765
H	5.200647	8.850932	-1.535153	C	-2.738236	-0.912721	-0.912721
H	-7.025476	-7.025476	-1.535085	C	-0.912720	0.912720	-0.912720
H	7.025476	7.025476	-1.535085	C	0.912721	2.738236	-0.912721
H	-5.200647	-8.850932	-1.535153	C	2.738123	4.563788	-0.912765
H	8.850932	5.200647	-1.535153	C	4.563497	6.389167	-0.912718
H	-3.376029	-10.677262	-1.535952	C	6.378827	8.204194	-0.902564
H	10.677262	3.376029	-1.535952	C	-6.378827	-8.204194	-0.902564
H	-1.537076	-12.505826	-1.537076	C	-4.563497	-6.389167	-0.912718
H	12.505826	1.537076	-1.537076	C	-2.738123	-4.563788	-0.912765
				C	-0.912721	-2.738236	-0.912721
				C	0.912720	-0.912720	-0.912720
				C	2.738236	0.912721	-0.912721
				C	4.563788	2.738123	-0.912765
				C	6.389167	4.563497	-0.912718
				C	8.204194	6.378827	-0.902564
				C	-4.553837	-10.030046	-0.902663
				C	-2.738120	-8.215306	-0.912790
				C	-0.912740	-6.389693	-0.912740
				C	0.912632	-4.563836	-0.912632
				C	2.738123	-2.738123	-0.912613
				C	4.563836	-0.912632	-0.912632
				C	6.389693	0.912740	-0.912740
				C	8.215306	2.738120	-0.912790

C	10.030046	4.553837	-0.902663
C	-2.729170	-11.856741	-0.903163
C	-0.912794	-10.041932	-0.912794
C	0.912608	-8.215680	-0.912608
C	2.737994	-6.389423	-0.912449
C	4.563531	-4.563531	-0.912415
C	6.389423	-2.737994	-0.912449
C	8.215680	-0.912608	-0.912608
C	10.041932	0.912794	-0.912794
C	11.856741	2.729170	-0.903163
C	-0.901275	-13.681800	-0.901275
C	0.912999	-11.867448	-0.912999
C	2.737227	-10.039925	-0.912707
C	4.562297	-8.213447	-0.912705
C	6.387680	-6.387680	-0.912739
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C	10.039925	-2.737227	-0.912707
C	11.867448	-0.912999	-0.912999
C	13.681800	0.901275	-0.901275
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H	-0.620939	-2.464440	13.417432
H	0.622222	4.288246	11.589568
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H	-4.288246	-0.622222	11.589568
H	-2.462354	-2.462354	11.590214
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H	-4.287218	-2.461896	9.763483
H	-2.461896	-4.287218	9.763483
H	-0.622499	-6.112914	9.763436
H	0.622539	7.937982	7.937982
H	2.461992	6.112167	7.937574
H	4.286717	4.286717	7.937152
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H	7.937982	0.622539	7.937982
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H	-6.112167	-2.461992	7.937574
H	-4.286717	-4.286717	7.937152
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H	-0.622539	-7.937982	7.937982
H	0.622499	9.763436	6.112914
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H	4.286709	6.111647	6.111647
H	6.111647	4.286709	6.111647
H	7.937574	2.461992	6.112167

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H	-9.763436	-0.622499	6.112914
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H	-6.111647	-4.286709	6.111647
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H	0.622222	11.589568	4.288246
H	2.461896	9.763483	4.287218
H	4.286717	7.937152	4.286717
H	6.111647	6.111647	4.286709
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H	9.763483	2.461896	4.287218
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H	-11.589568	-0.622222	4.288246
H	-9.763483	-2.461896	4.287218
H	-7.937152	-4.286717	4.286717
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H	-2.461896	-9.763483	4.287218
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H	0.620939	13.417432	2.464440
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	C	-0.906319	0.906319	0.906319		C	-0.008284	1.819599
	C	0.000000	1.826755	0.000000		C	-0.914049	0.914049
	C	0.917673	2.728571	0.917673		C	-1.831905	1.831905
	C	-1.826755	0.000000	0.000000		C	-1.819599	1.819599
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	C	-1.812596	1.812596	-1.812596		C	0.000000	0.000000
	C	-0.917673	2.728571	-0.917673		C	0.911566	0.911566
	C	-0.906319	-0.906319	-0.906319		C	0.008284	1.819599
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	C	2.728571	-0.917673	-0.917673		C	-0.914049	-0.914049
	H	-3.373793	0.293617	-1.562225		C	-1.819599	-0.008284
	H	-3.373793	1.562225	-0.293617		C	-1.819599	-1.819599
	H	-2.451843	2.451843	-2.451843		C	-2.739093	-0.914049
	H	-1.562225	0.293617	-3.373793		C	-2.739093	0.914049
	H	-0.293617	1.562225	-3.373793		C	0.914049	-2.739093
	H	-1.549093	-1.549093	-1.549093		C	-0.914049	-2.739093
	H	-1.549093	1.549093	1.549093		C	0.000000	3.646134
	H	1.549093	1.549093	-1.549093		C	3.646134	0.000000

H	-1.562225	3.373793	-0.293617	C	0.000000	0.000000	-3.646134
H	-0.293617	3.373793	-1.562225	C	1.831905	1.831905	3.641980
H	-3.373793	-0.293617	1.562225	C	2.726763	2.726763	2.726763
H	-3.373793	-1.562225	0.293617	C	1.831905	3.641980	1.831905
H	0.293617	-1.562225	-3.373793	C	0.000000	0.000000	3.646134
H	1.562225	-0.293617	-3.373793	C	3.641980	1.831905	1.831905
H	2.451843	-2.451843	-2.451843	C	1.831905	-3.641980	-1.831905
H	-2.451843	-2.451843	2.451843	C	2.726763	-2.726763	-2.726763
H	1.562225	3.373793	0.293617	C	1.831905	-1.831905	-3.641980
H	0.293617	3.373793	1.562225	C	0.000000	-3.646134	0.000000
H	2.451843	2.451843	2.451843	C	3.641980	-1.831905	-1.831905
H	3.373793	-1.562225	-0.293617	C	-3.646134	0.000000	0.000000
H	3.373793	-0.293617	-1.562225	C	-3.641980	-1.831905	1.831905
H	3.373793	0.293617	1.562225	C	-2.726763	-2.726763	2.726763
H	3.373793	1.562225	0.293617	C	-1.831905	-1.831905	3.641980
H	-0.293617	-3.373793	1.562225	C	-1.831905	-3.641980	1.831905
H	-1.562225	-3.373793	0.293617	C	-3.641980	1.831905	-1.831905
H	1.562225	-3.373793	-0.293617	H	-3.366012	3.366012	-3.366012
H	0.293617	-3.373793	-1.562225	H	-2.476092	4.287047	-1.207406
H	1.562225	0.293617	3.373793	H	-1.207406	4.287047	-2.476092
H	0.293617	1.562225	3.373793	H	0.635388	2.462157	-2.462157
H	-0.293617	-1.562225	3.373793	H	-1.207406	2.476092	-4.287047
H	-1.562225	-0.293617	3.373793	H	-2.476092	1.207406	-4.287047
H	1.549093	-1.549093	1.549093	H	-2.462157	2.462157	0.635388
				H	-0.635388	2.462157	2.462157
				H	2.462157	2.462157	-0.635388
				H	2.462157	-0.635388	2.462157
				H	2.462157	0.635388	-2.462157
				H	-0.635388	-2.462157	-2.462157
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				H	-2.462157	-0.635388	-2.462157
				H	0.635388	-2.462157	2.462157
				H	-2.462157	0.635388	2.462157
				H	-2.462157	-2.462157	-0.635388
				H	0.634946	4.293570	-0.634946
				H	-0.634946	4.293570	0.634946
				H	4.293570	0.634946	-0.634946
				H	4.293570	-0.634946	0.634946
				H	-0.634946	-0.634946	-4.293570
				H	0.634946	0.634946	-4.293570
				H	1.207406	2.476092	4.287047
				H	2.476092	1.207406	4.287047
				H	3.366012	3.366012	3.366012
				H	2.476092	4.287047	1.207406
				H	1.207406	4.287047	2.476092
				H	-0.634946	0.634946	4.293570
				H	0.634946	-0.634946	4.293570
				H	4.287047	1.207406	2.476092
				H	4.287047	2.476092	1.207406
				H	2.476092	-4.287047	-1.207406
				H	1.207406	-4.287047	-2.476092
				H	3.366012	-3.366012	-3.366012
				H	1.207406	-2.476092	-4.287047
				H	2.476092	-1.207406	-4.287047

					H	0.634946	-4.293570	0.634946	
					H	-0.634946	-4.293570	-0.634946	
					H	4.287047	-1.207406	-2.476092	
					H	4.287047	-2.476092	-1.207406	
					H	-4.293570	-0.634946	-0.634946	
					H	-4.293570	0.634946	0.634946	
					H	-4.287047	-2.476092	1.207406	
					H	-4.287047	-1.207406	2.476092	
					H	-3.366012	-3.366012	3.366012	
					H	-2.476092	-1.207406	4.287047	
					H	-1.207406	-2.476092	4.287047	
					H	-1.207406	-4.287047	2.476092	
					H	-2.476092	-4.287047	1.207406	
					H	-4.287047	1.207406	-2.476092	
					H	-4.287047	2.476092	-1.207406	
T4	C	-4.555760	2.745770	2.745770	T5	C	1.818114	1.818114	-1.818114
	C	-3.640680	3.640680	3.640680		C	-4.554330	-4.554330	4.554330
	C	-2.745770	2.745770	4.555760		C	-1.826778	-1.826778	1.826778
	C	-1.828024	1.828024	3.652594		C	-0.913213	-0.913213	0.913213
	C	-2.733282	0.922328	2.733282		C	1.818949	3.644877	0.008550
	C	-3.652594	1.828024	1.828024		C	-1.818949	-0.008550	3.644877
	C	-0.922328	2.733282	2.733282		C	-0.911154	0.911154	2.737592
	C	-1.828024	3.652594	1.828024		C	1.818949	-0.008550	-3.644877
	C	-2.745770	4.555760	2.745770		C	-1.818949	-3.644877	0.008550
	C	-2.733282	2.733282	0.922328		C	-0.911154	-2.737592	-0.911154
	C	-0.002519	1.825019	1.825019		C	1.827714	5.471815	1.827714
	C	0.905286	0.905286	2.731879		C	1.827714	-1.827714	-5.471815
	C	0.000000	0.000000	3.650217		C	0.911154	2.737592	-0.911154
	C	-0.914093	0.914093	4.558564		C	-3.646848	-1.835995	3.646848
	C	-1.825019	0.002519	1.825019		C	-2.738491	-0.916237	2.738491
	C	-0.913267	0.913267	0.913267		C	0.000000	1.825692	0.000000
	C	-0.905286	-0.905286	2.731879		C	0.911154	0.911154	-2.737592
	C	0.905286	2.731879	0.905286		C	-3.646848	-3.646848	1.835995
	C	0.000000	3.650217	0.000000		C	-2.738491	-2.738491	0.916237
	C	-0.914093	4.558564	0.914093		C	0.000000	0.000000	-1.825692
	C	-1.825019	1.825019	0.002519		C	-3.659407	-3.659407	5.469384
	C	-0.905286	2.731879	-0.905286		C	-2.741694	-2.741694	4.566169
	C	0.002519	-1.825019	1.825019		C	0.000000	0.000000	1.825692
	C	0.913267	-0.913267	0.913267		C	0.913213	0.913213	0.913213
	C	1.825019	-0.002519	1.825019		C	-3.659407	-5.469384	3.659407
	C	2.733282	-0.922328	2.733282		C	-2.741694	-4.566169	2.741694
	C	1.828024	-1.828024	3.652594		C	0.000000	-1.825692	0.000000
	C	0.914093	-0.914093	4.558564		C	0.913213	-0.913213	-0.913213
	C	0.922328	-2.733282	2.733282		C	0.913856	4.562982	0.913856
	C	0.000000	0.000000	0.000000		C	0.008550	3.644877	1.818949
	C	2.731879	0.905286	0.905286		C	0.913856	-0.913856	-4.562982
	C	1.825019	1.825019	-0.002519		C	0.008550	-1.818949	-3.644877
	C	0.913267	0.913267	-0.913267		C	0.008550	1.818949	3.644877
	C	-2.731879	-0.905286	0.905286		C	0.916237	2.738491	2.738491
	C	-1.825019	-1.825019	-0.002519		C	0.008550	-3.644877	-1.818949
	C	-0.913267	-0.913267	-0.913267		C	0.916237	-2.738491	-2.738491
	C	-2.731879	0.905286	-0.905286		C	-5.469384	-3.659407	3.659407
	C	-1.825019	-0.002519	-1.825019		C	-4.566169	-2.741694	2.741694

C	0.002519	1.825019	-1.825019	C	-1.825692	0.000000	0.000000
C	-3.650217	0.000000	0.000000	C	-0.913213	0.913213	-0.913213
C	-0.905286	-2.731879	0.905286	C	-1.835995	-3.646848	3.646848
C	-0.002519	-1.825019	-1.825019	C	-0.916237	-2.738491	2.738491
C	0.905286	-2.731879	-0.905286	C	-1.818114	1.818114	1.818114
C	1.825019	-1.825019	0.002519	C	-0.911154	2.737592	0.911154
C	1.825019	0.002519	-1.825019	C	-1.818114	-1.818114	-1.818114
C	2.731879	-0.905286	-0.905286	C	-0.911154	-0.911154	-2.737592
C	0.905286	-0.905286	-2.731879	C	-1.827714	-1.827714	5.471815
C	-0.905286	0.905286	-2.731879	C	-0.913856	-0.913856	4.562982
C	3.650217	0.000000	0.000000	C	-1.827714	-5.471815	1.827714
C	2.733282	-2.733282	0.922328	C	-0.913856	-4.562982	0.913856
C	3.652594	-1.828024	1.828024	C	2.737592	0.911154	-0.911154
C	0.000000	-3.650217	0.000000	C	1.825692	0.000000	0.000000
C	1.828024	-3.652594	1.828024	C	2.738491	2.738491	0.916237
C	4.558564	-0.914093	0.914093	C	1.826778	1.826778	1.826778
C	0.914093	-4.558564	0.914093	C	2.738491	-0.916237	-2.738491
C	-0.914093	-4.558564	-0.914093	C	1.826778	-1.826778	-1.826778
C	-1.828024	-3.652594	-1.828024	C	2.741694	4.566169	2.741694
C	-2.733282	-2.733282	-0.922328	C	1.835995	3.646848	3.646848
C	-0.922328	-2.733282	-2.733282	C	2.741694	-2.741694	-4.566169
C	-3.652594	-1.828024	-1.828024	C	1.835995	-3.646848	-3.646848
C	-2.733282	-0.922328	-2.733282	C	-0.008550	3.644877	-1.818949
C	-4.558564	-0.914093	-0.914093	C	-3.644877	-0.008550	1.818949
C	0.000000	0.000000	-3.650217	C	-2.737592	0.911154	0.911154
C	-1.828024	-1.828024	-3.652594	C	-0.008550	1.818949	-3.644877
C	-0.914093	-0.914093	-4.558564	C	-3.644877	-1.818949	0.008550
C	2.733282	0.922328	-2.733282	C	-2.737592	-0.911154	-0.911154
C	1.828024	1.828024	-3.652594	C	3.644877	1.818949	0.008550
C	0.922328	2.733282	-2.733282	C	-0.008550	-1.818949	3.644877
C	2.733282	2.733282	-0.922328	C	0.911154	-0.911154	2.737592
C	1.828024	3.652594	-1.828024	C	3.644877	-0.008550	-1.818949
C	3.652594	1.828024	-1.828024	C	-0.008550	-3.644877	1.818949
C	0.914093	0.914093	-4.558564	C	0.911154	-2.737592	0.911154
C	0.914093	4.558564	-0.914093	C	0.000000	5.470278	0.000000
C	4.558564	0.914093	-0.914093	C	0.000000	0.000000	-5.470278
C	-4.558564	0.914093	0.914093	C	3.646848	3.646848	1.835995
C	-2.745770	-2.745770	-4.555760	C	0.000000	0.000000	5.470278
C	-3.640680	-3.640680	-3.640680	C	0.913856	0.913856	4.562982
C	-2.745770	-4.555760	-2.745770	C	3.646848	-1.835995	-3.646848
C	-4.555760	-2.745770	-2.745770	C	0.000000	-5.470278	0.000000
C	2.745770	-2.745770	4.555760	C	0.913856	-4.562982	-0.913856
C	3.640680	-3.640680	3.640680	C	3.659407	5.469384	3.659407
C	2.745770	-4.555760	2.745770	C	3.659407	-3.659407	-5.469384
C	4.555760	-2.745770	2.745770	C	-0.916237	2.738491	-2.738491
C	2.745770	4.555760	-2.745770	C	-5.471815	-1.827714	1.827714
C	3.640680	3.640680	-3.640680	C	-4.562982	-0.913856	0.913856
C	2.745770	2.745770	-4.555760	C	-1.826778	1.826778	-1.826778
C	4.555760	2.745770	-2.745770	C	1.818114	-1.818114	1.818114
H	-5.200802	3.389860	2.121164	C	2.737592	-0.911154	0.911154
H	-5.200802	2.121164	3.389860	C	-0.913856	4.562982	-0.913856
H	-4.279923	4.279923	4.279923	C	-1.818949	3.644877	-0.008550
H	-3.389860	2.121164	5.200802	C	-0.913856	0.913856	-4.562982
H	-2.121164	3.389860	5.200802	C	-1.818949	0.008550	-3.644877

H	-3.375613	0.278247	3.375613	C	1.818949	0.008550	3.644877
H	-0.278247	3.375613	3.375613	C	2.738491	0.916237	2.738491
H	-3.389860	5.200802	2.121164	C	1.818949	-3.644877	-0.008550
H	-2.121164	5.200802	3.389860	C	2.738491	-2.738491	-0.916237
H	-3.375613	3.375613	0.278247	C	1.827714	1.827714	5.471815
H	1.548736	1.548736	3.374264	C	2.741694	2.741694	4.566169
H	-1.548601	0.278637	5.205867	C	1.827714	-5.471815	-1.827714
H	-0.278637	1.548601	5.205867	C	2.741694	-4.566169	-2.741694
H	-1.548736	-1.548736	3.374264	C	-3.644877	1.818949	-0.008550
H	1.548736	3.374264	1.548736	C	-2.738491	2.738491	-0.916237
H	-1.548601	5.205867	0.278637	C	-3.644877	0.008550	-1.818949
H	-0.278637	5.205867	1.548601	C	-2.738491	0.916237	-2.738491
H	-1.548736	3.374264	-1.548736	C	4.562982	0.913856	0.913856
H	3.375613	-0.278247	3.375613	C	3.644877	0.008550	1.818949
H	0.278637	-1.548601	5.205867	C	4.562982	-0.913856	-0.913856
H	1.548601	-0.278637	5.205867	C	3.644877	-1.818949	-0.008550
H	0.278247	-3.375613	3.375613	C	4.566169	2.741694	2.741694
H	3.374264	1.548736	1.548736	C	3.646848	1.835995	3.646848
H	-3.374264	-1.548736	1.548736	C	4.566169	-2.741694	-2.741694
H	-3.374264	1.548736	-1.548736	C	3.646848	-3.646848	-1.835995
H	-1.548736	-3.374264	1.548736	C	4.554330	4.554330	4.554330
H	1.548736	-3.374264	-1.548736	C	3.659407	3.659407	5.469384
H	3.374264	-1.548736	-1.548736	C	4.554330	-4.554330	-4.554330
H	1.548736	-1.548736	-3.374264	C	3.659407	-5.469384	-3.659407
H	-1.548736	1.548736	-3.374264	C	-1.835995	3.646848	-3.646848
H	3.375613	-3.375613	0.278247	C	-5.470278	0.000000	0.000000
H	5.205867	-0.278637	1.548601	C	-4.562982	0.913856	-0.913856
H	5.205867	-1.548601	0.278637	C	5.470278	0.000000	0.000000
H	0.278637	-5.205867	1.548601	C	-1.827714	5.471815	-1.827714
H	1.548601	-5.205867	0.278637	C	-1.827714	1.827714	-5.471815
H	-1.548601	-5.205867	-0.278637	C	5.471815	1.827714	1.827714
H	-0.278637	-5.205867	-1.548601	C	5.471815	-1.827714	-1.827714
H	-3.375613	-3.375613	-0.278247	C	5.469384	3.659407	3.659407
H	-0.278247	-3.375613	-3.375613	C	5.469384	-3.659407	-3.659407
H	-3.375613	-0.278247	-3.375613	C	-2.741694	4.566169	-2.741694
H	-5.205867	-1.548601	-0.278637	C	-3.646848	3.646848	-1.835995
H	-5.205867	-0.278637	-1.548601	C	-2.741694	2.741694	-4.566169
H	-0.278637	-1.548601	-5.205867	C	-3.646848	1.835995	-3.646848
H	-1.548601	-0.278637	-5.205867	C	-5.471815	1.827714	-1.827714
H	3.375613	0.278247	-3.375613	C	-4.566169	2.741694	-2.741694
H	0.278247	3.375613	-3.375613	C	-3.659407	5.469384	-3.659407
H	3.375613	3.375613	-0.278247	C	-3.659407	3.659407	-5.469384
H	1.548601	0.278637	-5.205867	C	-4.554330	4.554330	-4.554330
H	0.278637	1.548601	-5.205867	C	-5.469384	3.659407	-3.659407
H	0.278637	5.205867	-1.548601	H	2.461377	2.461377	-2.461377
H	1.548601	5.205867	-0.278637	H	-5.193570	-5.193570	5.193570
H	5.205867	1.548601	-0.278637	H	2.462077	4.287165	-0.635291
H	5.205867	0.278637	-1.548601	H	-2.462077	0.635291	4.287165
H	-5.205867	1.548601	0.278637	H	2.462077	0.635291	-4.287165
H	-5.205867	0.278637	1.548601	H	-2.462077	-4.287165	-0.635291
H	-2.121164	-3.389860	-5.200802	H	2.462049	6.119099	1.192076
H	-3.389860	-2.121164	-5.200802	H	1.192076	6.119099	2.462049
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H	-2.121164	-5.200802	-3.389860	H	2.462049	-1.192076	-6.119099

H	-3.389860	-5.200802	-2.121164	H	-4.289107	-1.191785	4.289107
H	-5.200802	-3.389860	-2.121164	H	-4.289107	-4.289107	1.191785
H	-5.200802	-2.121164	-3.389860	H	-4.303474	-3.034775	6.114419
H	2.121164	-3.389860	5.200802	H	-3.034775	-4.303474	6.114419
H	3.389860	-2.121164	5.200802	H	-3.034775	-6.114419	4.303474
H	4.279923	-4.279923	4.279923	H	-4.303474	-6.114419	3.034775
H	3.389860	-5.200802	2.121164	H	-0.635291	4.287165	2.462077
H	2.121164	-5.200802	3.389860	H	-0.635291	-2.462077	-4.287165
H	5.200802	-2.121164	3.389860	H	-0.635291	2.462077	4.287165
H	5.200802	-3.389860	2.121164	H	-0.635291	-4.287165	-2.462077
H	2.121164	5.200802	-3.389860	H	-6.114419	-4.303474	3.034775
H	3.389860	5.200802	-2.121164	H	-6.114419	-3.034775	4.303474
H	4.279923	4.279923	-4.279923	H	-1.191785	-4.289107	4.289107
H	3.389860	2.121164	-5.200802	H	-2.461377	2.461377	2.461377
H	2.121164	3.389860	-5.200802	H	-2.461377	-2.461377	-2.461377
H	5.200802	3.389860	-2.121164	H	-2.462049	-1.192076	6.119099
H	5.200802	2.121164	-3.389860	H	-1.192076	-2.462049	6.119099
				H	-1.192076	-6.119099	2.462049
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				H	1.191785	4.289107	4.289107
				H	1.191785	-4.289107	-4.289107
				H	0.635291	4.287165	-2.462077
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				H	4.289107	4.289107	1.191785
				H	-0.635016	0.635016	6.117468
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						H	3.034775	-6.114419	-4.303474
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T6	C	-1.824141	1.824141	1.824141	T7	C	2.078781	0.409999	-10.437414
	C	-2.731260	2.731260	0.904544		C	0.844000	-0.352539	-11.014431
	C	-1.824603	3.650516	-0.002423		C	0.810928	-1.813486	-10.463398
	C	-0.913419	2.738674	-0.913419		C	0.690230	-1.774849	-8.887292
	C	0.000000	1.825811	0.000000		C	1.923566	-1.000019	-8.284651
	C	-0.912655	0.912655	0.912655		C	1.968209	0.466396	-8.861100
	C	-3.650516	1.824603	-0.002423		C	-0.629805	-1.015824	-8.479802
	C	-4.558044	2.732372	-0.922045		C	-0.604374	0.450471	-9.057719
	C	-3.651888	3.651888	-1.829726		C	-0.473417	0.394202	-10.632474
	C	-2.732372	4.558044	-0.922045		C	0.638631	1.208683	-8.453805
	C	-4.560273	4.560273	-2.749454		C	-0.758415	-0.970096	-6.905762
	C	-5.479592	3.655150	-3.655150		C	-0.785164	-2.438029	-6.327178
	C	-6.385121	2.741148	-2.741148		C	0.534446	-3.196123	-6.733894

C	-5.476144	1.827371	-1.827371	C	0.655082	-3.242681	-8.308532
C	-3.655150	5.479592	-3.655150	C	1.810914	-0.954192	-6.709392
C	-4.572852	6.382825	-4.572852	C	0.483229	-0.201845	-6.306271
C	-5.467776	5.467776	-5.467776	C	1.767493	-2.422228	-6.132082
C	-6.382825	4.572852	-4.572852	C	-2.080565	-0.211338	-6.497710
C	-4.560273	2.749454	-4.560273	C	-2.054591	1.254225	-7.074726
C	-3.655150	3.655150	-5.479592	C	-1.930618	1.201932	-8.648924
C	-4.572852	4.572852	-6.382825	C	0.517948	1.268313	-6.879603
C	-2.749454	4.560273	-4.560273	C	-0.812484	2.012547	-6.471720
C	-3.651888	1.829726	-3.651888	C	-0.914057	-2.392637	-4.754044
C	-2.740173	2.740173	-2.740173	C	-0.940735	-3.860902	-4.175917
C	-4.558044	0.922045	-2.732372	C	0.378815	-4.618891	-4.582361
C	-1.827371	5.476144	-1.827371	C	0.499375	-4.664911	-6.156058
C	-2.741148	6.385121	-2.741148	C	1.655261	-2.376733	-4.557675
C	-1.829726	3.651888	-3.651888	C	0.327618	-1.623883	-4.155074
C	-0.922045	4.558044	-2.732372	C	1.611844	-3.845101	-3.980827
C	-3.650516	0.002423	-1.824603	C	-2.235960	-1.633694	-4.346788
C	-2.738674	0.913419	-0.913419	C	-2.209546	-0.165794	-4.924588
C	-4.557352	0.905147	0.905147	C	0.362377	-0.151365	-4.729125
C	-5.475210	0.000000	0.000000	C	-0.967418	0.602181	-4.325558
C	-6.383081	0.913527	-0.913527	C	-3.381563	2.006112	-6.666961
C	-4.557352	-0.905147	-0.905147	C	-3.505901	2.058626	-5.093761
C	-1.826505	1.826505	-1.826505	C	-3.531918	0.593136	-4.517032
C	-0.002423	3.650516	-1.824603	C	-0.933189	2.072607	-4.898429
C	-0.913527	6.383081	-0.913527	C	-1.088522	0.652812	-2.749068
C	0.000000	5.475210	0.000000	C	-1.122959	-0.819906	-2.175515
C	-0.905147	4.557352	0.905147	C	-2.365175	-1.588431	-2.774230
C	0.002423	3.650516	1.824603	C	-3.661033	0.638725	-2.944511
C	-0.904544	2.731260	2.731260	C	-3.687353	-0.829217	-2.367116
C	0.913419	2.738674	0.913419	C	-2.418835	1.406655	-2.345678
C	0.905147	4.557352	-0.905147	C	-2.263876	2.816953	-4.491043
C	-1.825811	0.000000	0.000000	C	-2.391482	-3.056717	-2.196522
C	-2.731260	0.904544	2.731260	C	-1.069615	-3.815716	-2.603366
C	-3.650516	-0.002423	1.824603	C	0.206816	-1.573772	-2.578544
C	-2.738674	-0.913419	0.913419	C	0.172069	-3.046902	-2.004600
C	0.912655	0.912655	-0.912655	C	1.499691	-3.799811	-2.406998
C	0.000000	0.000000	-1.825811	C	0.343811	-6.088006	-4.005386
C	-0.913419	0.913419	-2.738674	C	0.223271	-6.042486	-2.431912
C	0.904544	2.731260	-2.731260	C	-1.096269	-5.284406	-2.025606
C	-0.002423	1.824603	-3.650516	C	0.051312	-2.997008	-0.428637
C	1.824141	1.824141	-1.824141	C	-1.278448	-2.243001	-0.025822
C	1.824603	3.650516	0.002423	C	-2.520675	-3.011619	-0.624397
C	-0.912655	-0.912655	-0.912655	C	-1.225133	-5.239725	-0.453302
C	-1.824603	0.002423	-3.650516	C	-2.546991	-4.480368	-0.046670
C	-2.731260	-0.904544	-2.731260	C	0.016567	-4.470747	0.145330
C	-2.732372	0.922045	-4.558044	C	1.456310	-5.268605	-1.830516
C	-0.922045	2.732372	-4.558044	C	-1.244041	-0.769646	-0.599487
C	-3.650516	-1.824603	0.002423	C	-3.842838	-2.252268	-0.217490
C	-1.824141	-1.824141	-1.824141	C	-3.816671	-0.783905	-0.795007
C	1.825811	0.000000	0.000000	C	-2.574360	-0.015431	-0.196421
C	0.912655	-0.912655	0.912655	C	1.450522	-0.803976	-1.978828
C	0.000000	0.000000	1.825811	C	1.330071	-0.753712	-0.402752
C	1.826505	1.826505	1.826505	C	0.000000	0.000000	0.000000
C	0.913419	0.913419	2.738674	C	0.155466	1.422121	-2.149314

C	2.738674	0.913419	0.913419	C	0.034697	1.472931	-0.573280
C	2.731260	2.731260	-0.904544	C	-2.540068	1.457367	-0.769777
C	-0.913419	-0.913419	2.738674	C	1.485521	0.668746	-2.552337
C	-1.826505	-1.826505	1.826505	C	1.295033	-2.227071	0.170866
C	0.000000	-1.825811	0.000000	C	-0.120727	0.050428	1.575519
C	-1.824603	-0.002423	3.650516	C	-0.155409	-1.423129	2.148652
C	0.002423	1.824603	3.650516	C	-1.399447	-2.192890	1.549581
C	-0.913419	-2.738674	0.913419	C	-2.695488	0.034901	1.378965
C	-2.731260	-2.731260	-0.904544	C	-2.729702	-1.438525	1.952182
C	-4.558044	-0.922045	2.732372	C	-1.451322	0.804441	1.978052
C	-3.651888	-1.829726	3.651888	C	-1.295935	2.226596	-0.170220
C	-2.740173	-2.740173	2.740173	C	-3.971962	-2.207019	1.354201
C	-4.558044	-2.732372	0.922045	C	-1.433853	-3.666816	2.123086
C	-3.651888	-3.651888	1.829726	C	-2.676061	-4.435513	1.525147
C	-1.824603	-3.650516	0.002423	C	1.174596	-2.176956	1.746312
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C	-0.002423	-3.650516	1.824603	C	1.139589	-3.650886	2.319771
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C	-1.829726	-3.651888	3.651888	C	2.623158	-2.979778	-0.231261
C	-0.922045	-2.732372	4.558044	C	2.734937	-3.024984	-1.804717
C	-2.732372	-4.558044	0.922045	C	2.778657	-1.556591	-2.381094
C	-0.922045	-4.558044	2.732372	C	2.418835	-1.406655	2.345678
C	1.824141	-1.824141	1.824141	C	2.453994	0.066777	1.772533
C	-0.905147	0.905147	4.557352	C	2.574304	0.016439	0.197084
C	0.905147	-0.905147	4.557352	C	3.858684	-2.204595	0.371127
C	1.824603	0.002423	3.650516	C	3.902512	-0.736122	-0.205041
C	-1.827371	-1.827371	5.476144	C	2.467600	-4.403673	1.918270
C	0.000000	0.000000	5.475210	C	3.746902	-2.159239	1.944143
C	2.731260	-0.904544	2.731260	C	1.123862	0.820382	2.174870
C	2.738674	-0.913419	-0.913419	C	2.609415	1.489242	-0.376209
C	1.826505	-1.826505	-1.826505	C	1.279248	2.242536	0.026598
C	0.913419	-2.738674	-0.913419	C	2.729702	1.438525	-1.952182
C	2.731260	-2.731260	0.904544	C	4.014168	-0.781545	-1.778499
C	1.824603	-3.650516	-0.002423	C	-1.416784	2.277419	1.405172
C	3.650516	0.002423	1.824603	C	1.158656	2.293361	1.602009
C	3.650516	-1.824603	-0.002423	C	-2.850745	-1.388477	3.525147
C	0.913419	-0.913419	-2.738674	C	-1.605724	-0.619067	4.114100
C	0.002423	-3.650516	-1.824603	C	-0.275962	-1.372870	3.721907
C	-0.904544	-2.731260	-2.731260	C	-1.554839	-3.616966	3.696103
C	-0.905147	-4.557352	-0.905147	C	-0.309868	-2.847160	4.284939
C	0.905147	-4.557352	0.905147	C	-2.884436	-2.862641	4.088416
C	0.002423	-1.824603	-3.650516	C	-1.571958	0.854844	3.551297
C	2.731260	0.904544	-2.731260	C	0.969378	-0.603127	4.310911
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C	3.650516	1.824603	0.002423	C	1.019505	-3.601031	3.892857
C	3.650516	-0.002423	-1.824603	C	2.298813	-1.356600	3.918721
C	-0.905147	-0.905147	-4.557352	C	-0.172069	3.046902	2.004601
C	0.905147	0.905147	-4.557352	C	-0.326494	1.624373	4.140318
C	0.922045	2.732372	4.558044	C	-4.026291	0.789377	1.781807
C	1.829726	3.651888	3.651888	C	-3.992380	2.262365	1.208912
C	2.740173	2.740173	2.740173	C	-3.870907	2.211510	-0.366433
C	2.732372	0.922045	4.558044	C	-5.139256	-0.024471	-0.387927

C	3.651888	1.829726	3.651888	C	-5.113264	1.443663	-0.965151
C	1.827371	1.827371	5.476144	C	-5.268703	0.021031	1.183841
C	0.922045	4.558044	2.732372	C	-2.747885	3.031371	1.808008
C	3.651888	3.651888	1.829726	C	-3.836907	3.682063	-0.938993
C	2.732372	4.558044	0.922045	C	-2.592599	4.441706	-0.335733
C	4.558044	2.732372	0.922045	C	-1.261375	3.697424	-0.742637
C	4.558044	0.922045	2.732372	C	-2.384682	2.877115	-2.918353
C	1.827371	5.476144	1.827371	C	-1.140708	3.636940	-2.314923
C	4.557352	0.905147	-0.905147	C	-3.715695	3.621659	-2.511380
C	4.557352	-0.905147	0.905147	C	-4.983737	1.397841	-2.537368
C	-0.913527	-0.913527	6.383081	C	0.190121	2.892897	-2.721859
C	-6.383081	-0.913527	0.913527	C	-0.016962	4.457329	-0.139079
C	-4.560273	-2.749454	4.560273	C	1.313975	3.713365	-0.545806
C	-5.479592	-3.655150	3.655150	C	-2.713492	4.502210	1.236210
C	-6.385121	-2.741148	2.741148	C	-0.137471	4.517687	1.432789
C	-4.560273	-4.560273	2.749454	C	1.434394	3.652880	-2.118111
C	-2.749454	-4.560273	4.560273	C	-2.902133	1.608737	3.943682
C	-3.655150	-3.655150	5.479592	C	-4.147480	0.839578	3.354797
C	-3.655150	-5.479592	3.655150	C	-2.868627	3.082356	3.381007
C	-1.827371	-5.476144	1.827371	C	-0.292605	3.097840	3.577576
C	-2.741148	-2.741148	6.385121	C	-5.294638	-1.447645	1.760955
C	0.000000	-5.475210	0.000000	C	-4.180720	-0.634431	3.917768
C	-2.741148	-6.385121	2.741148	C	1.606025	0.618110	-4.128873
C	-0.913527	-6.383081	0.913527	C	2.890482	-1.601961	-3.954981
C	0.913527	0.913527	6.383081	C	4.057831	0.686505	-2.354569
C	0.913527	6.383081	0.913527	C	2.934115	-0.133954	-4.531465
C	2.749454	4.560273	4.560273	C	0.310697	2.832484	-4.294595
C	3.655150	5.479592	3.655150	C	2.764876	2.908990	-2.524779
C	2.741148	6.385121	2.741148	C	1.641154	2.088542	-4.701676
C	4.560273	4.560273	2.749454	C	3.703318	-3.628181	2.520232
C	4.560273	2.749454	4.560273	C	2.264657	-2.830768	4.481954
C	3.655150	3.655150	5.479592	C	2.403699	3.063259	2.201736
C	5.479592	3.655150	3.655150	C	3.734151	2.310193	1.799440
C	5.476144	1.827371	1.827371	C	3.698736	0.837195	2.372220
C	2.741148	2.741148	6.385121	C	2.249109	1.640623	4.337385
C	5.475210	0.000000	0.000000	C	3.578853	0.887404	3.945310
C	6.385121	2.741148	2.741148	C	2.283364	3.114247	3.774767
C	6.383081	0.913527	0.913527	C	3.854120	2.259328	0.223980
C	-4.572852	-6.382825	4.572852	C	5.026949	0.084762	1.970724
C	-5.467776	-5.467776	5.467776	C	5.138427	0.039148	0.397582
C	-6.382825	-4.572852	4.572852	C	4.982957	-1.384026	2.546457
C	-4.572852	-4.572852	6.382825	C	3.544295	-0.586613	4.508180
C	6.382825	4.572852	4.572852	C	5.182387	1.507393	-0.178269
C	5.467776	5.467776	5.467776	C	2.558642	4.473592	0.057969
C	4.572852	6.382825	4.572852	C	3.889426	3.729889	-0.348480
C	4.572852	4.572852	6.382825	C	2.438498	4.534101	1.629969
C	0.000000	0.000000	-5.475210	C	5.293858	1.461460	-1.751866
C	-1.827371	1.827371	-5.476144	C	4.009321	3.669477	-1.920968
C	0.922045	-2.732372	-4.558044	C	4.169753	0.640809	-3.928404
C	1.829726	-3.651888	-3.651888	C	2.885216	2.848826	-4.097505
C	2.740173	-2.740173	-2.740173	C	-1.468687	5.262083	1.839367
C	2.732372	-0.922045	-4.558044	C	-1.622812	3.851479	3.970192
C	3.651888	-1.829726	-3.651888	C	1.107236	5.278028	2.036242
C	1.827371	-1.827371	-5.476144	C	0.953112	3.867424	4.167066

C	0.922045	-4.558044	-2.732372	C	-4.127550	-3.630938	3.500758
C	3.651888	-3.651888	-1.829726	C	-5.423918	-1.402586	3.330099
C	2.732372	-4.558044	-0.922045	C	-4.957813	2.863383	-3.113971
C	4.558044	-2.732372	-0.922045	C	-0.138882	-5.895644	2.294646
C	4.558044	-0.922045	-2.732372	C	1.188692	-6.649000	1.893050
C	1.827371	-5.476144	-1.827371	C	1.300838	-6.693230	0.319592
C	0.913527	-6.383081	-0.913527	C	-1.251819	-6.709031	0.124496
C	2.741148	-6.385121	-2.741148	C	0.067761	-7.467407	-0.281795
C	3.655150	-5.479592	-3.655150	C	-1.380636	-6.664905	1.696679
C	2.749454	-4.560273	-4.560273	C	2.424177	-5.873139	2.494645
C	4.560273	-4.560273	-2.749454	C	0.188298	-7.512003	-1.855308
C	3.655150	-3.655150	-5.479592	C	0.985471	-5.075701	4.456428
C	4.560273	-2.749454	-4.560273	C	-0.259409	-5.846355	3.867644
C	2.741148	-2.741148	-6.385121	C	2.312907	-5.828342	4.065349
C	5.476144	-1.827371	-1.827371	C	3.591997	-3.583154	4.090752
C	5.479592	-3.655150	-3.655150	C	-2.702647	-5.904874	2.102809
C	6.385121	-2.741148	-2.741148	C	-1.588696	-5.091635	4.259688
C	6.383081	-0.913527	-0.913527	C	4.871718	-1.338855	4.116980
C	0.913527	-0.913527	-6.383081	C	3.553748	-5.055062	4.661012
C	6.382825	-4.572852	-4.572852	C	4.833066	-2.810633	4.686892
C	5.467776	-5.467776	-5.467776	C	-2.831920	-5.860189	3.672137
C	4.572852	-6.382825	-4.572852	C	-5.323823	3.016855	1.612079
C	4.572852	-4.572852	-6.382825	C	-5.290134	4.487584	1.040150
C	-0.913527	0.913527	-6.383081	C	-5.168439	4.426941	-0.532050
C	-2.741148	2.741148	-6.385121	C	-6.436520	2.203056	-0.558040
H	-3.374366	3.374366	1.548102	C	-6.410833	3.668778	-1.134664
H	-5.200291	3.375373	-0.278045	C	-6.566496	2.249174	1.013991
H	-3.375373	5.200291	-0.278045	C	-4.045101	5.247032	1.643003
H	-5.202504	5.202504	-2.105194	C	-6.285285	3.615571	-2.707517
H	-7.032397	2.105445	-3.375421	C	-4.199230	3.836385	3.773892
H	-7.032397	3.375421	-2.105445	C	-5.445269	3.067724	3.184956
H	-5.216910	7.027857	-3.948209	C	-4.165687	5.307843	3.212480
H	-3.948209	7.027857	-5.216910	C	-1.589087	5.322716	3.408693
H	-6.107015	6.107015	-6.107015	C	-6.591947	0.780522	1.590805
H	-7.027857	5.216910	-3.948209	C	-5.477996	1.593761	3.747684
H	-7.027857	3.948209	-5.216910	C	-4.833066	2.810633	-4.686892
H	-5.202504	2.105194	-5.202504	C	0.987001	5.338662	3.605580
H	-5.216910	3.948209	-7.027857	C	-2.919836	6.072511	3.808803
H	-3.948209	5.216910	-7.027857	C	-0.343811	6.088006	4.005386
H	-2.105194	5.202504	-5.202504	C	-6.721477	0.825649	3.160099
H	-5.200291	0.278045	-3.375373	C	2.275057	-7.301050	4.636227
H	-3.375421	7.032397	-2.105445	C	1.034961	-8.075048	4.041401
H	-2.105445	7.032397	-3.375421	C	1.145700	-8.119350	2.469640
H	-0.278045	5.200291	-3.375373	C	-0.087686	-8.894635	1.867686
H	-5.199602	1.548640	1.548640	C	0.032805	-8.938003	0.294685
H	-7.030257	1.548343	-0.278304	C	-1.407671	-8.135155	2.274489
H	-7.030257	0.278304	-1.548343	C	-0.293408	-7.321689	4.431971
H	-5.199602	-1.548640	-1.548640	C	-1.537622	-8.090972	3.844782
H	-1.548343	7.030257	-0.278304	C	-5.496971	6.058445	3.613085
H	-0.278304	7.030257	-1.548343	C	-6.743129	5.294867	3.017461
H	-1.548640	5.199602	1.548640	C	-6.622308	5.233235	1.447027
H	-1.548102	3.374366	3.374366	C	-7.865776	4.475280	0.843746
H	1.548640	5.199602	-1.548640	C	-7.739223	4.421492	-0.728457
H	-3.374366	1.548102	3.374366	C	-7.890743	3.008728	1.421031

H	1.548102	3.374366	-3.374366	C	-6.776480	3.822193	3.578513
H	-3.374366	-1.548102	-3.374366	C	-8.021108	3.053621	2.991269
H	-3.375373	0.278045	-5.200291	C	5.337822	2.927113	-2.327090
H	-0.278045	3.375373	-5.200291	C	4.213645	2.106410	-4.503767
H	3.374366	3.374366	-1.548102	C	6.418960	2.282632	0.424487
H	-3.374366	-3.374366	-1.548102	C	6.307958	2.328868	1.997968
H	-5.200291	-0.278045	3.375373	C	4.979476	3.080633	2.399546
H	-5.200291	-3.375373	0.278045	C	5.134384	4.490716	0.255380
H	-3.375373	-0.278045	5.200291	C	5.014992	4.551373	1.827756
H	1.548102	-3.374366	3.374366	C	6.463160	3.748469	-0.150722
H	-0.278045	-3.375373	5.200291	C	6.263533	0.860098	2.573332
H	-3.375373	-5.200291	0.278045	C	4.859857	3.131513	3.972563
H	-0.278045	-5.200291	3.375373	C	4.824827	1.657536	4.535115
H	-1.548640	1.548640	5.199602	C	3.529426	3.884226	4.364583
H	1.548640	-1.548640	5.199602	C	3.683555	5.294873	2.233693
H	3.374366	-1.548102	3.374366	C	6.152516	0.905339	4.144041
H	3.374366	-3.374366	1.548102	C	6.113101	-0.566620	4.713466
H	-1.548102	-3.374366	-3.374366	C	7.394785	1.677627	4.741154
H	-1.548640	-5.199602	-1.548640	C	7.435189	3.149297	4.172572
H	1.548640	-5.199602	1.548640	C	7.545520	3.104279	2.600803
H	3.374366	1.548102	-3.374366	C	6.106412	3.901939	4.563134
H	-1.548640	-1.548640	-5.199602	C	7.590521	4.570955	2.025049
H	1.548640	1.548640	-5.199602	C	6.260584	5.312981	2.431649
H	0.278045	3.375373	5.200291	C	7.705028	4.517093	0.451926
H	3.375373	0.278045	5.200291	C	3.563479	5.355687	3.803209
H	0.278045	5.200291	3.375373	C	6.140585	5.374617	4.002145
H	3.375373	5.200291	0.278045	C	4.809084	6.122240	4.400762
H	5.200291	3.375373	0.278045	C	2.232163	6.104402	4.202563
H	5.200291	0.278045	3.375373	C	6.578752	3.695199	-1.724337
H	5.199602	1.548640	-1.548640	C	7.392038	6.136363	4.596939
H	5.199602	-1.548640	1.548640	C	8.697073	5.380584	4.191008
H	-0.278304	-1.548343	7.030257	C	8.676384	3.928676	4.766016
H	-1.548343	-0.278304	7.030257	C	8.830485	5.339069	2.635509
H	-7.030257	-1.548343	0.278304	C	5.454210	2.874312	-3.900650
H	-7.030257	-0.278304	1.548343	C	-5.454210	-2.874312	3.900649
H	-5.202504	-2.105194	5.202504	C	-4.158291	-5.102800	4.071592
H	-7.032397	-2.105445	3.375421	C	-6.750937	-0.646249	3.730285
H	-7.032397	-3.375421	2.105445	C	-2.863139	-7.332856	4.243521
H	-5.202504	-5.202504	2.105194	C	-8.049467	1.582026	3.560771
H	-2.105194	-5.202504	5.202504	C	0.990498	-9.550378	4.608495
H	-2.105445	-3.375421	7.032397	C	-0.242569	-10.297236	4.007792
H	-3.375421	-2.105445	7.032397	C	-0.123253	-10.363470	2.452004
H	-3.375421	-7.032397	2.105445	C	-1.561700	-9.566177	4.413434
H	-2.105445	-7.032397	3.375421	C	-8.079714	6.040593	3.414455
H	-1.548343	-7.030257	0.278304	C	-9.298503	5.269190	2.815631
H	-0.278304	-7.030257	1.548343	C	-9.193465	5.227501	1.257964
H	1.548343	0.278304	7.030257	C	-9.347567	3.817107	3.388470
H	0.278304	1.548343	7.030257	C	3.046259	-0.179603	-6.105874
H	0.278304	7.030257	1.548343	C	1.761683	2.028482	-6.274981
H	1.548343	7.030257	0.278304	C	3.090236	1.286071	-6.681514
H	2.105194	5.202504	5.202504	C	4.330476	2.053849	-6.077540
H	2.105445	7.032397	3.375421	C	3.207578	1.233737	-8.256219
H	3.375421	7.032397	2.105445	H	3.005169	-0.113971	-10.734592
H	5.202504	5.202504	2.105194	H	2.104907	1.433509	-10.853106

H	5.202504	2.105194	5.202504	H	0.928549	-0.387855	-12.117826
H	3.375421	2.105445	7.032397	H	-0.052330	-2.349725	-10.897318
H	2.105445	3.375421	7.032397	H	1.736634	-2.338652	-10.760590
H	7.032397	3.375421	2.105445	H	2.860774	-1.531128	-8.566707
H	7.032397	2.105445	3.375421	H	-1.506657	-1.558162	-8.900504
H	7.030257	1.548343	0.278304	H	-0.448664	1.417703	-11.048272
H	7.030257	0.278304	1.548343	H	-1.337366	-0.140850	-11.066486
H	-5.216910	-7.027857	3.948209	H	0.662948	2.246762	-8.856038
H	-3.948209	-7.027857	5.216910	H	-1.662341	-2.980013	-6.748455
H	-6.107015	-6.107015	6.107015	H	-0.209861	-3.788940	-8.731452
H	-7.027857	-3.948209	5.216910	H	1.580904	-3.777855	-8.594587
H	-7.027857	-5.216910	3.948209	H	2.705104	-2.952979	-6.414657
H	-3.948209	-5.216910	7.027857	H	-2.957234	-0.754194	-6.918920
H	-5.216910	-3.948209	7.027857	H	-1.915208	2.231684	-9.054830
H	7.027857	5.216910	3.948209	H	-2.804804	0.671562	-9.073062
H	7.027857	3.948209	5.216910	H	-0.787623	3.050742	-6.874454
H	6.107015	6.107015	6.107015	H	-1.817866	-4.402570	-4.597677
H	3.948209	7.027857	5.216910	H	-0.365579	-5.210731	-6.579461
H	5.216910	7.027857	3.948209	H	1.425276	-5.199646	-6.442589
H	5.216910	3.948209	7.027857	H	2.549479	-4.375537	-4.263887
H	3.948209	5.216910	7.027857	H	-3.112878	-2.176168	-4.768769
H	0.278045	-3.375373	-5.200291	H	-3.365702	3.035664	-7.073293
H	3.375373	-0.278045	-5.200291	H	-4.255343	1.475464	-7.091526
H	0.278045	-5.200291	-3.375373	H	-4.408259	0.050111	-4.938687
H	3.375373	-5.200291	-0.278045	H	-4.564006	-1.371834	-2.789457
H	5.200291	-3.375373	-0.278045	H	-2.238698	3.854959	-4.894223
H	5.200291	-0.278045	-3.375373	H	-3.268367	-3.598933	-2.618894
H	0.278304	-7.030257	-1.548343	H	-0.521122	-6.633596	-4.429128
H	1.548343	-7.030257	-0.278304	H	1.269740	-6.622511	-4.292255
H	3.375421	-7.032397	-2.105445	H	-1.973372	-5.825829	-2.447737
H	2.105445	-7.032397	-3.375421	H	-3.423853	-5.022325	-0.469433
H	2.105194	-5.202504	-5.202504	H	2.393972	-5.798795	-2.113947
H	5.202504	-5.202504	-2.105194	H	-4.719462	-2.794628	-0.640217
H	5.202504	-2.105194	-5.202504	H	-4.874573	-4.217768	1.508267
H	2.105445	-3.375421	-7.032397	H	3.516976	-4.979360	0.061045
H	3.375421	-2.105445	-7.032397	H	3.672430	-3.555969	-2.088418
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H	7.030257	-0.278304	-1.548343	H	-1.690574	-0.583394	5.224438
H	7.030257	-1.548343	-0.278304	H	-0.394951	-2.811080	5.395250
H	0.278304	-1.548343	-7.030257	H	-2.968712	-2.826397	5.198474
H	1.548343	-0.278304	-7.030257	H	0.884065	-0.567456	5.421215
H	7.027857	-3.948209	-5.216910	H	-0.411573	1.659643	5.250652
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H	6.107015	-6.107015	-6.107015	H	-2.567658	5.479641	-0.739962
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H	3.948209	-7.027857	-5.216910	H	-3.690266	4.659526	-2.914901
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H	5.216910	-3.948209	-7.027857	H	0.007511	5.495259	-0.543339
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H	-3.375421	2.105445	-7.032397	H	-6.170634	-1.989943	1.337648
H	-2.105445	3.375421	-7.032397	H	-4.264773	-0.598572	5.027855
				H	3.827951	-2.133204	-4.238291

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H	-6.328792	-3.414554	3.490065
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H	-4.251572	-5.072151	5.174177
H	-7.625316	-1.186846	3.319733
H	-6.843807	-0.616306	4.832924
H	-3.738308	-7.872217	3.832965
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H	1.915151	-10.090232	4.335310
H	-0.266869	-11.328785	4.409281
H	-0.988164	-10.914835	2.040931
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					H	4.363878	3.083510	-6.482532	
					H	4.142525	0.714565	-8.542087	
					H	3.241357	2.263602	-8.660721	
T8	C	0.912972	-0.912972	0.912972	T9	C	-1.825949	-1.825949	1.825949
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	C	-2.730672	2.730672	-2.730672		C	1.825261	1.825261	-1.825261
	C	4.566646	-4.566646	4.566646		C	2.736640	2.736640	-2.736640
	C	3.652937	-3.652937	3.652937		C	-5.479748	-5.479748	5.479748
	C	0.912466	-2.738372	-0.912466		C	-4.566036	-4.566036	4.566036
	C	-0.000358	-1.825667	-1.825667		C	-1.825493	-0.000657	3.651174
	C	-2.730894	0.904525	-4.556840		C	-0.912590	0.912590	2.738321
	C	4.558847	-6.384346	2.748557		C	1.825493	3.651174	0.000657
	C	3.651102	-5.476664	1.829014		C	2.736890	4.562649	-0.910659
	C	0.912466	0.912466	2.738372		C	-5.471946	-3.661660	7.297417
	C	-0.000358	1.825667	1.825667		C	-4.564206	-2.742132	6.389708
	C	-2.730894	4.556840	-0.904525		C	-1.825493	-3.651174	0.000657
	C	4.558847	-2.748557	6.384346		C	-0.912590	-2.738321	-0.912590
	C	3.651102	-1.829014	5.476664		C	1.825493	-0.000657	-3.651174
	C	0.904525	-4.556840	-2.730894		C	2.736890	0.910659	-4.562649
	C	-0.002486	-3.650197	-3.650197		C	-5.471946	-7.297417	3.661660
	C	-2.731744	-0.921520	-6.383109		C	-4.564206	-6.389708	2.742132
	C	0.904525	2.730894	4.556840		C	-1.817654	1.817654	5.469462
	C	-0.002486	3.650197	3.650197		C	-0.910659	2.736890	4.562649
	C	-2.731744	6.383109	0.921520		C	1.826391	5.476933	1.826391
	C	-2.740043	-2.740043	-8.209137		C	2.737476	6.388706	0.915438
	C	-2.740043	8.209137	2.740043		C	-1.817654	-5.469462	-1.817654
	C	-0.912466	0.912466	-2.738372		C	-0.910659	-4.562649	-2.736890
	C	-1.823846	1.823846	-3.649837		C	1.826391	-1.826391	-5.476933
	C	-0.912466	2.738372	-0.912466		C	2.737476	-0.915438	-6.388706
	C	-1.823846	3.649837	-1.823846		C	1.834644	7.296075	3.644860
	C	-0.913248	-0.913248	-4.564046		C	2.739841	8.213925	2.739841
	C	-1.824330	-0.002268	-5.475823		C	1.834644	-3.644860	-7.296075
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	C	6.386749	-6.386749	4.575946		C	0.000657	-1.825493	-3.651174
	C	5.478351	-5.478351	3.656243		C	0.913153	-0.913153	-4.564032
	C	2.738703	-2.738703	0.913778		C	0.008611	5.469743	3.643950
	C	1.825667	-0.000358	1.825667		C	0.915438	6.388706	2.737476
	C	6.386749	-4.575946	6.386749		C	0.008611	-3.643950	-5.469743
	C	5.478351	-3.656243	5.478351		C	0.915438	-2.737476	-6.388706
	C	2.738703	-0.913778	2.738703		C	-2.738635	-0.913455	2.738635
	C	-0.912972	-0.912972	-0.912972		C	-7.299848	-5.489047	7.299848

C	-1.825667	-0.000358	-1.825667	C	-6.391449	-4.569348	6.391449
C	6.399333	-8.209310	6.399333	C	-3.651730	-1.826888	3.651730
C	5.481640	-7.306067	5.481640	C	-2.738635	-2.738635	0.913455
C	2.739899	-4.564830	2.739899	C	-7.299848	-7.299848	5.489047
C	1.826409	-3.651691	1.826409	C	-6.391449	-6.391449	4.569348
C	-0.912972	0.912972	0.912972	C	-3.651730	-3.651730	1.826888
C	-1.825667	1.825667	0.000358	C	0.000000	0.000000	1.825702
C	6.399333	-6.399333	8.209310	C	0.912879	0.912879	0.912879
C	5.481640	-5.481640	7.306067	C	-7.312431	-7.312431	9.122408
C	2.739899	-2.739899	4.564830	C	3.643546	3.643546	-1.817512
C	1.826409	-1.826409	3.651691	C	-6.394738	-6.394738	8.219165
C	1.823846	-3.649837	-1.823846	C	-3.653007	-3.653007	5.477880
C	2.730894	-4.556840	-0.904525	C	-2.739517	-2.739517	4.564696
C	1.823846	1.823846	3.649837	C	0.000000	-1.825702	0.000000
C	2.730894	0.904525	4.556840	C	0.912879	-0.912879	-0.912879
C	-0.913778	-2.738703	-2.738703	C	-7.312431	-9.122408	7.312431
C	-1.826409	-1.826409	-3.651691	C	3.643546	1.817512	-3.643546
C	2.731744	-6.383109	0.921520	C	-6.394738	-8.219165	6.394738
C	1.824330	-5.475823	0.002268	C	-3.653007	-5.477880	3.653007
C	-0.913778	2.738703	2.738703	C	-2.739517	-4.564696	2.739517
C	-1.826409	3.651691	1.826409	C	-2.736890	0.910659	4.562649
C	2.731744	-0.921520	6.383109	C	-3.643950	-0.008611	5.469743
C	1.824330	-0.002268	5.475823	C	-2.736890	-4.562649	-0.910659
C	-0.921998	-4.557471	-4.557471	C	-3.643950	-5.469743	0.008611
C	-1.829014	-3.651102	-5.476664	C	0.000657	1.825493	3.651174
C	-0.921998	4.557471	4.557471	C	0.913455	2.738635	2.738635
C	-1.829014	5.476664	3.651102	C	3.643950	5.469743	0.008611
C	6.399333	6.399333	-8.209310	C	-3.644860	-1.834644	7.296075
C	6.399333	8.209310	-6.399333	C	-2.737476	-0.915438	6.388706
C	8.209310	6.399333	-6.399333	C	0.000657	-3.651174	-1.825493
C	7.294261	7.294261	-7.294261	C	0.913455	-2.738635	-2.738635
C	0.912972	0.912972	-0.912972	C	3.643950	-0.008611	-5.469743
C	0.000358	1.825667	-1.825667	C	-3.644860	-7.296075	1.834644
C	8.209310	-6.399333	6.399333	C	-2.737476	-6.388706	0.915438
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C	4.564830	-2.739899	2.739899	C	0.915620	4.563221	4.563221
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C	3.656243	-5.478351	5.478351	C	0.915620	-4.563221	-4.563221
C	0.912466	-0.912466	-2.738372	C	3.644860	-1.834644	-7.296075
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C	4.557471	-4.557471	0.921998	C	3.653137	-3.653137	-9.122157
C	3.650197	-3.650197	0.002486	C	-7.299848	7.299848	-5.489047
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C	4.567615	-8.211513	4.567615	C	-8.219165	6.394738	-6.394738
C	3.653890	-7.302439	3.653890	C	-7.312431	9.122408	-7.312431
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C	3.653890	-3.653890	7.302439	C	-9.122408	7.312431	-7.312431
C	0.904525	-2.730894	-4.556840	C	-8.207357	8.207357	-8.207357
C	-0.002268	-1.824330	-5.475823	C	-1.825702	0.000000	0.000000
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C	-0.002268	5.475823	1.824330	C	-9.122408	-7.312431	7.312431
C	0.000358	-1.825667	1.825667	C	1.817512	3.643546	-3.643546
C	-2.738372	0.912466	-0.912466	C	-8.219165	-6.394738	6.394738
C	-3.649837	1.823846	-1.823846	C	-5.477880	-3.653007	3.653007
C	0.913778	-2.738703	2.738703	C	-4.564696	-2.739517	2.739517
C	0.000000	-3.651264	0.000000	C	-5.489047	-7.299848	7.299848
C	-2.738703	-0.913778	-2.738703	C	-4.569348	-6.391449	6.391449
C	-3.650197	-0.002486	-3.650197	C	-1.825261	1.825261	1.825261
C	0.913248	-4.564046	0.913248	C	-0.912590	2.738321	0.912590
C	0.000000	0.000000	3.651264	C	1.817654	5.469462	-1.817654
C	-2.738703	2.738703	0.913778	C	-5.470524	-1.835106	5.470524
C	-3.650197	3.650197	0.002486	C	-4.563221	-0.915620	4.563221
C	0.913248	-0.913248	4.564046	C	-1.825261	-1.825261	-1.825261
C	-0.002268	-5.475823	-1.824330	C	-0.912590	-0.912590	-2.738321
C	-2.739899	-2.739899	-4.564830	C	1.817654	1.817654	-5.469462
C	-3.651102	-1.829014	-5.476664	C	-5.470524	-5.470524	1.835106
C	0.905101	-6.382721	-0.905101	C	-4.563221	-4.563221	0.915620
C	-0.002268	1.824330	5.475823	C	-5.480708	-5.480708	9.124597
C	-2.739899	4.564830	2.739899	C	-4.566991	-4.566991	8.215507
C	-3.651102	5.476664	1.829014	C	-5.480708	-9.124597	5.480708
C	0.905101	0.905101	6.382721	C	-4.566991	-8.215507	4.566991
C	-2.748557	-4.558847	-6.384346	C	-1.817512	3.643546	3.643546
C	-3.653890	-3.653890	-7.302439	C	-0.910659	4.562649	2.736890
C	-2.748557	6.384346	4.558847	C	1.818298	7.295463	0.008114
C	-3.653890	7.302439	3.653890	C	-1.817512	-3.643546	-3.643546
C	2.738372	-0.912466	-0.912466	C	-0.910659	-2.736890	-4.562649
C	1.825667	0.000358	-1.825667	C	1.818298	-0.008114	-7.295463
C	-0.904525	2.730894	-4.556840	C	1.826425	9.121199	1.826425
C	6.384346	-4.558847	2.748557	C	1.826425	-1.826425	-9.121199
C	5.476664	-3.651102	1.829014	C	-0.913455	-2.738635	2.738635
C	2.738372	0.912466	0.912466	C	1.825702	0.000000	0.000000
C	1.825667	1.825667	-0.000358	C	2.738321	0.912590	-0.912590
C	-0.904525	4.556840	-2.730894	C	-1.826888	-3.651730	3.651730
C	6.384346	-2.748557	4.558847	C	-0.913153	-0.913153	4.564032
C	5.476664	-1.829014	3.651102	C	1.825949	1.825949	1.825949
C	-0.912466	-2.738372	0.912466	C	2.738635	2.738635	0.913455
C	-1.825667	-1.825667	-0.000358	C	-1.826391	-1.826391	5.476933
C	-4.556840	0.904525	-2.730894	C	-0.913153	-4.564032	0.913153
C	2.748557	-6.384346	4.558847	C	1.825949	-1.825949	-1.825949
C	1.829014	-5.476664	3.651102	C	2.738635	-0.913455	-2.738635
C	-0.912466	-0.912466	2.738372	C	-1.826391	-5.476933	1.826391
C	-1.825667	0.000358	1.825667	C	-0.911011	0.911011	6.388398
C	-4.556840	2.730894	-0.904525	C	1.826888	3.651730	3.651730
C	2.748557	-4.558847	6.384346	C	2.739517	4.564696	2.739517
C	1.829014	-3.651102	5.476664	C	-1.818298	-0.008114	7.295463
C	2.730672	-2.730672	-2.730672	C	-0.911011	-6.388398	-0.911011
C	1.823846	-1.823846	-3.649837	C	1.826888	-3.651730	-3.651730
C	-0.905101	0.905101	-6.382721	C	2.739517	-2.739517	-4.564696
C	2.730672	2.730672	2.730672	C	-1.818298	-7.295463	0.008114
C	1.823846	3.649837	1.823846	C	1.835106	5.470524	5.470524
C	-0.905101	6.382721	-0.905101	C	2.742132	6.389708	4.564206
C	-0.913248	-4.564046	-0.913248	C	1.835106	-5.470524	-5.470524
C	-1.826409	-3.651691	-1.826409	C	2.742132	-4.564206	-6.389708
C	-4.557471	-0.921998	-4.557471	C	-3.651174	-0.000657	1.825493

C	2.740043	-8.209137	2.740043	C	-2.738321	0.912590	0.912590
C	1.826713	-7.300962	1.826713	C	-0.000657	3.651174	-1.825493
C	-0.913248	0.913248	4.564046	C	0.910659	4.562649	-2.736890
C	-1.826409	1.826409	3.651691	C	-7.297417	-3.661660	5.471946
C	-4.557471	4.557471	0.921998	C	-6.389708	-2.742132	4.564206
C	2.740043	-2.740043	8.209137	C	-3.651174	-1.825493	0.000657
C	1.826713	-1.826713	7.300962	C	-2.738321	-0.912590	-0.912590
C	-0.913287	-0.913287	-8.208333	C	-0.000657	1.825493	-3.651174
C	-0.913287	8.208333	0.913287	C	0.910659	2.736890	-4.562649
C	-0.921520	-6.383109	-2.731744	C	-7.297417	-5.471946	3.661660
C	-1.829014	-5.476664	-3.651102	C	-6.389708	-4.564206	2.742132
C	-4.558847	-2.748557	-6.384346	C	-0.000657	-1.825493	3.651174
C	-0.921520	2.731744	6.383109	C	0.912590	-0.912590	2.738321
C	-1.829014	3.651102	5.476664	C	3.651174	1.825493	0.000657
C	-4.558847	6.384346	2.748557	C	4.562649	2.736890	-0.910659
C	-4.567615	-4.567615	-8.211513	C	-3.661660	-5.471946	7.297417
C	-4.567615	8.211513	4.567615	C	-2.742132	-4.564206	6.389708
C	0.913778	2.738703	-2.738703	C	-0.000657	-3.651174	1.825493
C	0.002486	3.650197	-3.650197	C	0.912590	-2.738321	0.912590
C	0.913248	0.913248	-4.564046	C	3.651174	-0.000657	-1.825493
C	0.002268	1.824330	-5.475823	C	4.562649	0.910659	-2.736890
C	0.913248	4.564046	-0.913248	C	-3.661660	-7.297417	5.471946
C	0.002268	5.475823	-1.824330	C	-2.742132	-6.389708	4.564206
C	0.905101	-0.905101	-6.382721	C	-3.643546	1.817512	3.643546
C	0.000000	0.000000	-7.300575	C	-2.736640	2.736640	2.736640
C	0.905101	6.382721	0.905101	C	0.000000	5.476617	0.000000
C	0.000000	7.300575	0.000000	C	0.911011	6.388398	-0.911011
C	3.651264	0.000000	0.000000	C	-3.643546	-3.643546	-1.817512
C	8.211513	-4.567615	4.567615	C	-2.736640	-2.736640	-2.736640
C	7.302439	-3.653890	3.653890	C	0.000000	0.000000	-5.476617
C	4.564046	-0.913248	0.913248	C	0.911011	0.911011	-6.388398
C	-2.738372	-0.912466	0.912466	C	0.000000	0.000000	5.476617
C	-3.651264	0.000000	0.000000	C	0.913153	0.913153	4.564032
C	0.921998	-4.557471	4.557471	C	3.651730	3.651730	1.826888
C	0.002486	-3.650197	3.650197	C	4.563221	4.563221	0.915620
C	3.649837	-1.823846	-1.823846	C	-3.653137	-3.653137	9.122157
C	4.556840	-2.730894	-0.904525	C	-2.739841	-2.739841	8.213925
C	3.649837	1.823846	1.823846	C	0.000000	-5.476617	0.000000
C	4.556840	0.904525	2.730894	C	0.913153	-4.564032	-0.913153
C	-2.738703	-2.738703	-0.913778	C	3.651730	-1.826888	-3.651730
C	-3.651691	-1.826409	-1.826409	C	4.563221	-0.915620	-4.563221
C	0.921520	-6.383109	2.731744	C	-3.653137	-9.122157	3.653137
C	0.002268	-5.475823	1.824330	C	-2.739841	-8.213925	2.739841
C	-2.738703	0.913778	2.738703	C	0.008114	7.295463	1.818298
C	-3.651691	1.826409	1.826409	C	0.913229	8.213317	0.913229
C	0.921520	-2.731744	6.383109	C	0.008114	-1.818298	-7.295463
C	0.002268	-1.824330	5.475823	C	0.913229	-0.913229	-8.213317
C	-2.739899	-4.564830	-2.739899	C	0.008114	1.818298	7.295463
C	-3.652937	-3.652937	-3.652937	C	0.915438	2.737476	6.388706
C	0.913287	-8.208333	0.913287	C	3.653007	5.477880	3.653007
C	0.000000	-7.300575	0.000000	C	4.564206	6.389708	2.742132
C	-2.739899	2.739899	4.564830	C	0.008114	-7.295463	-1.818298
C	-3.652937	3.652937	3.652937	C	0.915438	-6.388706	-2.737476
C	0.913287	-0.913287	8.208333	C	3.653007	-3.653007	-5.477880

C	0.000000	0.000000	7.300575	C	4.564206	-2.742132	-6.389708
C	-2.748557	-6.384346	-4.558847	C	3.661660	7.297417	5.471946
C	-3.656243	-5.478351	-5.478351	C	4.566991	8.215507	4.566991
C	-2.748557	4.558847	6.384346	C	3.661660	-5.471946	-7.297417
C	-3.656243	5.478351	5.478351	C	4.566991	-4.566991	-8.215507
C	2.738703	0.913778	-2.738703	C	-1.825949	1.825949	-1.825949
C	1.826409	1.826409	-3.651691	C	-0.913455	2.738635	-2.738635
C	6.383109	-2.731744	0.921520	C	-1.825493	3.651174	-0.000657
C	5.475823	-1.824330	0.002268	C	-0.913153	4.564032	-0.913153
C	2.738703	2.738703	-0.913778	C	-1.825493	0.000657	-3.651174
C	1.826409	3.651691	-1.826409	C	-0.913153	0.913153	-4.564032
C	6.383109	-0.921520	2.731744	C	-1.817654	5.469462	1.817654
C	5.475823	-0.002268	1.824330	C	-0.911011	6.388398	0.911011
C	2.730894	-0.904525	-4.556840	C	-1.817654	-1.817654	-5.469462
C	1.824330	0.002268	-5.475823	C	-0.911011	-0.911011	-6.388398
C	2.730894	4.556840	0.904525	C	-4.564032	-0.913153	0.913153
C	1.824330	5.475823	-0.002268	C	-9.124597	-5.480708	5.480708
C	-1.823846	-3.649837	1.823846	C	-8.215507	-4.566991	4.566991
C	-4.564046	-0.913248	-0.913248	C	-5.476933	-1.826391	1.826391
C	-5.475823	-0.002268	-1.824330	C	1.825261	-1.825261	1.825261
C	-0.904525	-4.556840	2.730894	C	2.738321	-0.912590	0.912590
C	-1.823846	-1.823846	3.649837	C	5.469462	1.817654	-1.817654
C	-4.564046	0.913248	0.913248	C	-1.835106	-5.470524	5.470524
C	-5.475823	1.824330	0.002268	C	-0.915620	-4.563221	4.563221
C	-0.904525	-2.730894	4.556840	C	-4.562649	0.910659	2.736890
C	-1.824330	-5.475823	-0.002268	C	-5.469743	-0.008611	3.643950
C	-4.564830	-2.739899	-2.739899	C	-4.562649	-2.736890	-0.910659
C	-5.476664	-1.829014	-3.651102	C	-5.469743	-3.643950	0.008611
C	-0.905101	-6.382721	0.905101	C	1.825493	0.000657	3.651174
C	-1.824330	0.002268	5.475823	C	2.738635	0.913455	2.738635
C	-4.564830	2.739899	2.739899	C	5.469743	3.643950	0.008611
C	-5.476664	3.651102	1.829014	C	-1.834644	-3.644860	7.296075
C	-0.905101	-0.905101	6.382721	C	-0.915438	-2.737476	6.388706
C	-1.826713	-7.300962	-1.826713	C	1.825493	-3.651174	-0.000657
C	-4.566646	-4.566646	-4.566646	C	2.738635	-2.738635	-0.913455
C	-5.478351	-3.656243	-5.478351	C	5.469743	-0.008611	-3.643950
C	-0.913287	-8.208333	-0.913287	C	-1.834644	-7.296075	3.644860
C	-1.826713	1.826713	7.300962	C	-0.915438	-6.388706	2.737476
C	-4.566646	4.566646	4.566646	C	1.826391	1.826391	5.476933
C	-5.478351	5.478351	3.656243	C	2.739517	2.739517	4.564696
C	-0.913287	0.913287	8.208333	C	5.470524	5.470524	1.835106
C	-4.575946	-6.386749	-6.386749	C	-1.826425	-1.826425	9.121199
C	-5.481640	-5.481640	-7.306067	C	-0.913229	-0.913229	8.213317
C	-4.575946	6.386749	6.386749	C	1.826391	-5.476933	-1.826391
C	-5.481640	7.306067	5.481640	C	2.739517	-4.564696	-2.739517
C	4.564046	0.913248	-0.913248	C	5.470524	-1.835106	-5.470524
C	3.651691	1.826409	-1.826409	C	-1.826425	-9.121199	1.826425
C	0.921998	4.557471	-4.557471	C	-0.913229	-8.213317	0.913229
C	8.209137	-2.740043	2.740043	C	1.834644	3.644860	7.296075
C	7.300962	-1.826713	1.826713	C	2.742132	4.564206	6.389708
C	-2.730672	-2.730672	2.730672	C	5.471946	7.297417	3.661660
C	-3.649837	-1.823846	1.823846	C	1.834644	-7.296075	-3.644860
C	-6.382721	0.905101	-0.905101	C	2.742132	-6.389708	-4.564206
C	4.556840	-0.904525	-2.730894	C	5.471946	-3.661660	-7.297417

C	3.650197	0.002486	-3.650197	C	5.480708	9.124597	5.480708
C	0.921520	2.731744	-6.383109	C	5.480708	-5.480708	-9.124597
C	4.556840	2.730894	0.904525	C	-3.651174	1.825493	-0.000657
C	3.650197	3.650197	-0.002486	C	-2.738635	2.738635	-0.913455
C	0.921520	6.383109	-2.731744	C	-0.008611	5.469743	-3.643950
C	-2.730894	-4.556840	0.904525	C	-7.296075	-1.834644	3.644860
C	-3.650197	-3.650197	-0.002486	C	-6.388706	-0.915438	2.737476
C	-6.383109	-0.921520	-2.731744	C	-3.651174	0.000657	-1.825493
C	-2.730894	-0.904525	4.556840	C	-2.738635	0.913455	-2.738635
C	-3.650197	0.002486	3.650197	C	-0.008611	3.643950	-5.469743
C	-6.383109	2.731744	0.921520	C	-7.296075	-3.644860	1.834644
C	0.913287	0.913287	-8.208333	C	-6.388706	-2.737476	0.915438
C	0.913287	8.208333	-0.913287	C	-3.643546	3.643546	1.817512
C	-2.731744	-6.383109	-0.921520	C	-2.736890	4.562649	0.910659
C	-3.651102	-5.476664	-1.829014	C	-0.008114	7.295463	-1.818298
C	-6.384346	-2.748557	-4.558847	C	-3.643546	-1.817512	-3.643546
C	-2.731744	0.921520	6.383109	C	-2.736890	-0.910659	-4.562649
C	-3.651102	1.829014	5.476664	C	-0.008114	1.818298	-7.295463
C	-6.384346	4.558847	2.748557	C	0.000000	9.120920	0.000000
C	-2.740043	-8.209137	-2.740043	C	0.000000	0.000000	-9.120920
C	-3.653890	-7.302439	-3.653890	C	0.910659	-2.736890	4.562649
C	-6.386749	-4.575946	-6.386749	C	3.651174	0.000657	1.825493
C	-2.740043	2.740043	8.209137	C	4.564032	0.913153	0.913153
C	-3.653890	3.653890	7.302439	C	-0.008611	-3.643950	5.469743
C	-6.386749	6.386749	4.575946	C	0.910659	-4.562649	2.736890
C	-6.399333	-6.399333	-8.209310	C	3.651174	-1.825493	-0.000657
C	-6.399333	8.209310	6.399333	C	4.564032	-0.913153	-0.913153
C	2.739899	2.739899	-4.564830	C	-0.008611	-5.469743	3.643950
C	1.829014	3.651102	-5.476664	C	0.911011	-0.911011	6.388398
C	2.739899	4.564830	-2.739899	C	3.651730	1.826888	3.651730
C	1.829014	5.476664	-3.651102	C	4.564696	2.739517	2.739517
C	2.731744	0.921520	-6.383109	C	-0.008114	-1.818298	7.295463
C	1.826713	1.826713	-7.300962	C	0.911011	-6.388398	0.911011
C	2.731744	6.383109	-0.921520	C	3.651730	-3.651730	-1.826888
C	1.826713	7.300962	-1.826713	C	4.564696	-2.739517	-2.739517
C	5.475823	0.002268	-1.824330	C	-0.008114	-7.295463	1.818298
C	6.382721	-0.905101	-0.905101	C	0.913229	0.913229	8.213317
C	5.475823	1.824330	-0.002268	C	3.653007	3.653007	5.477880
C	6.382721	0.905101	0.905101	C	4.566036	4.566036	4.566036
C	-4.556840	-2.730894	0.904525	C	0.000000	0.000000	9.120920
C	-5.475823	-1.824330	-0.002268	C	0.913229	-8.213317	-0.913229
C	-4.556840	-0.904525	2.730894	C	3.653007	-5.477880	-3.653007
C	-5.475823	0.002268	1.824330	C	4.566036	-4.566036	-4.566036
C	-4.557471	-4.557471	-0.921998	C	0.000000	-9.120920	0.000000
C	-5.476664	-3.651102	-1.829014	C	3.661660	5.471946	7.297417
C	-4.557471	0.921998	4.557471	C	4.569348	6.391449	6.391449
C	-5.476664	1.829014	3.651102	C	3.661660	-7.297417	-5.471946
C	-4.558847	-6.384346	-2.748557	C	4.569348	-6.391449	-6.391449
C	-5.478351	-5.478351	-3.656243	C	-5.476617	0.000000	0.000000
C	-4.558847	2.748557	6.384346	C	-4.564032	0.913153	-0.913153
C	-5.478351	3.656243	5.478351	C	-1.826888	3.651730	-3.651730
C	-4.567615	-8.211513	-4.567615	C	-0.915620	4.563221	-4.563221
C	-5.481640	-7.306067	-5.481640	C	-9.122157	-3.653137	3.653137
C	-4.567615	4.567615	8.211513	C	-8.213925	-2.739841	2.739841

C	-5.481640	5.481640	7.306067	C	1.817512	-3.643546	3.643546
C	4.564830	2.739899	-2.739899	C	2.736640	-2.736640	2.736640
C	3.652937	3.652937	-3.652937	C	5.476617	0.000000	0.000000
C	8.208333	-0.913287	0.913287	C	6.388398	0.911011	-0.911011
C	7.300575	0.000000	0.000000	C	-5.469462	1.817654	1.817654
C	4.557471	0.921998	-4.557471	C	-4.562649	2.736890	0.910659
C	3.651102	1.829014	-5.476664	C	-1.826391	5.476933	-1.826391
C	4.557471	4.557471	-0.921998	C	-0.915438	6.388706	-2.737476
C	3.651102	5.476664	-1.829014	C	-5.469462	-1.817654	-1.817654
C	-6.382721	-0.905101	0.905101	C	-4.562649	-0.910659	-2.736890
C	-7.300575	0.000000	0.000000	C	-1.826391	1.826391	-5.476933
C	-6.383109	-2.731744	-0.921520	C	-0.915438	2.737476	-6.388706
C	-7.300962	-1.826713	-1.826713	C	1.817654	-1.817654	5.469462
C	-6.383109	0.921520	2.731744	C	2.736890	-0.910659	4.562649
C	-7.300962	1.826713	1.826713	C	5.476933	1.826391	1.826391
C	-6.384346	-4.558847	-2.748557	C	6.388706	2.737476	0.915438
C	-7.302439	-3.653890	-3.653890	C	1.817654	-5.469462	1.817654
C	-6.384346	2.748557	4.558847	C	2.736890	-4.562649	0.910659
C	-7.302439	3.653890	3.653890	C	5.476933	-1.826391	-1.826391
C	-6.386749	-6.386749	-4.575946	C	6.388706	-0.915438	-2.737476
C	-7.306067	-5.481640	-5.481640	C	-1.818298	7.295463	-0.008114
C	-6.386749	4.575946	6.386749	C	-0.913229	8.213317	-0.913229
C	-7.306067	5.481640	5.481640	C	-1.818298	0.008114	-7.295463
C	-6.399333	-8.209310	-6.399333	C	-0.913229	0.913229	-8.213317
C	-7.294261	-7.294261	-7.294261	C	1.818298	0.008114	7.295463
C	-6.399333	6.399333	8.209310	C	2.737476	0.915438	6.388706
C	-7.294261	7.294261	7.294261	C	5.477880	3.653007	3.653007
C	6.383109	0.921520	-2.731744	C	6.389708	4.564206	2.742132
C	5.476664	1.829014	-3.651102	C	1.818298	-7.295463	-0.008114
C	2.748557	4.558847	-6.384346	C	2.737476	-6.388706	-0.915438
C	6.383109	2.731744	-0.921520	C	5.477880	-3.653007	-3.653007
C	5.476664	3.651102	-1.829014	C	6.389708	-2.742132	-4.564206
C	2.748557	6.384346	-4.558847	C	1.826425	1.826425	9.121199
C	-8.208333	-0.913287	-0.913287	C	2.739841	2.739841	8.213925
C	-8.208333	0.913287	0.913287	C	5.479748	5.479748	5.479748
C	2.740043	2.740043	-8.209137	C	6.391449	6.391449	4.569348
C	2.740043	8.209137	-2.740043	C	1.826425	-9.121199	-1.826425
C	-8.209137	-2.740043	-2.740043	C	2.739841	-8.213925	-2.739841
C	-8.209137	2.740043	2.740043	C	5.479748	-5.479748	-5.479748
C	-8.211513	-4.567615	-4.567615	C	6.391449	-4.569348	-6.391449
C	-8.211513	4.567615	4.567615	C	5.489047	7.299848	7.299848
C	-8.209310	-6.399333	-6.399333	C	6.394738	8.219165	6.394738
C	-8.209310	6.399333	6.399333	C	5.489047	-7.299848	-7.299848
C	7.300962	1.826713	-1.826713	C	6.394738	-6.394738	-8.219165
C	4.566646	4.566646	-4.566646	C	-3.651730	3.651730	-1.826888
C	3.656243	5.478351	-5.478351	C	-2.739517	4.564696	-2.739517
C	8.208333	0.913287	-0.913287	C	-3.651730	1.826888	-3.651730
C	4.558847	2.748557	-6.384346	C	-2.739517	2.739517	-4.564696
C	3.653890	3.653890	-7.302439	C	-3.643950	5.469743	-0.008611
C	4.558847	6.384346	-2.748557	C	-2.737476	6.388706	-0.915438
C	3.653890	7.302439	-3.653890	C	-3.643950	0.008611	-5.469743
C	6.384346	2.748557	-4.558847	C	-2.737476	0.915438	-6.388706
C	5.478351	3.656243	-5.478351	C	7.312431	9.122408	7.312431
C	6.384346	4.558847	-2.748557	C	7.312431	-7.312431	-9.122408

C	5.478351	5.478351	-3.656243	C	-6.388398	0.911011	0.911011
C	8.209137	2.740043	-2.740043	C	-7.295463	-0.008114	1.818298
C	7.302439	3.653890	-3.653890	C	-6.388398	-0.911011	-0.911011
C	4.575946	6.386749	-6.386749	C	-7.295463	-1.818298	0.008114
C	4.567615	4.567615	-8.211513	C	3.643546	-1.817512	3.643546
C	4.567615	8.211513	-4.567615	C	4.562649	-0.910659	2.736890
C	6.386749	4.575946	-6.386749	C	7.295463	1.818298	0.008114
C	5.481640	5.481640	-7.306067	C	3.643546	-3.643546	1.817512
C	6.386749	6.386749	-4.575946	C	4.562649	-2.736890	0.910659
C	5.481640	7.306067	-5.481640	C	7.295463	-0.008114	-1.818298
C	8.211513	4.567615	-4.567615	C	3.643950	0.008611	5.469743
C	7.306067	5.481640	-5.481640	C	4.563221	0.915620	4.563221
H	7.933498	-7.933498	7.933498	C	7.296075	3.644860	1.834644
H	-3.373922	3.373922	-3.373922	C	3.643950	-5.469743	-0.008611
H	-3.374160	1.548016	-5.199838	C	4.563221	-4.563221	-0.915620
H	5.201759	-7.026565	2.104448	C	7.296075	-1.834644	-3.644860
H	-3.374160	5.199838	-1.548016	C	3.644860	1.834644	7.296075
H	5.201759	-2.104448	7.026565	C	4.564206	2.742132	6.389708
H	1.548016	-5.199838	-3.374160	C	7.297417	5.471946	3.661660
H	-3.375006	-0.277776	-7.025328	C	3.644860	-7.296075	-1.834644
H	1.548016	3.374160	5.199838	C	4.564206	-6.389708	-2.742132
H	-3.375006	7.025328	0.277776	C	7.297417	-3.661660	-5.471946
H	-3.374731	-2.104689	-8.856306	C	3.653137	3.653137	9.122157
H	-2.104689	-3.374731	-8.856306	C	4.566991	4.566991	8.215507
H	-2.104689	8.856306	3.374731	C	7.299848	7.299848	5.489047
H	-3.374731	8.856306	2.104689	C	3.653137	-9.122157	-3.653137
H	-0.277776	-3.375006	-7.025328	C	4.566991	-8.215507	-4.566991
H	-0.277776	7.025328	3.375006	C	7.299848	-5.489047	-7.299848
H	7.028966	-7.028966	3.931662	C	-5.476933	1.826391	-1.826391
H	7.028966	-3.931662	7.028966	C	-4.564696	2.739517	-2.739517
H	7.043388	-8.854339	5.774686	C	-1.835106	5.470524	-5.470524
H	5.774686	-8.854339	7.043388	C	-9.121199	-1.826425	1.826425
H	5.774686	-7.043388	8.854339	C	-8.213317	-0.913229	0.913229
H	7.043388	-5.774686	8.854339	C	-5.469743	3.643950	-0.008611
H	3.374160	-5.199838	-1.548016	C	-4.563221	4.563221	-0.915620
H	3.374160	1.548016	5.199838	C	-1.834644	7.296075	-3.644860
H	3.375006	-7.025328	0.277776	C	-5.469743	0.008611	-3.643950
H	3.375006	-0.277776	7.025328	C	-4.563221	0.915620	-4.563221
H	-0.278219	-5.200462	-5.200462	C	-1.834644	3.644860	-7.296075
H	-0.278219	5.200462	5.200462	C	-1.826425	9.121199	-1.826425
H	7.043388	5.774686	-8.854339	C	-1.826425	1.826425	-9.121199
H	5.774686	7.043388	-8.854339	C	5.469462	-1.817654	1.817654
H	5.774686	8.854339	-7.043388	C	6.388398	-0.911011	0.911011
H	7.043388	8.854339	-5.774686	C	5.469743	0.008611	3.643950
H	8.854339	7.043388	-5.774686	C	6.388706	0.915438	2.737476
H	8.854339	5.774686	-7.043388	C	5.469743	-3.643950	-0.008611
H	7.933498	7.933498	-7.933498	C	6.388706	-2.737476	-0.915438
H	8.854339	-5.774686	7.043388	C	5.470524	1.835106	5.470524
H	8.854339	-7.043388	5.774686	C	6.389708	2.742132	4.564206
H	3.931662	-7.028966	7.028966	C	5.470524	-5.470524	-1.835106
H	5.200462	-5.200462	0.278219	C	6.389708	-4.564206	-2.742132
H	5.200462	-0.278219	5.200462	C	5.471946	3.661660	7.297417
H	5.201846	-8.858784	3.931868	C	6.391449	4.569348	6.391449
H	3.931868	-8.858784	5.201846	C	5.471946	-7.297417	-3.661660

H	3.931868	-5.201846	8.858784	C	6.391449	-6.391449	-4.569348
H	5.201846	-3.931868	8.858784	C	5.480708	5.480708	9.124597
H	1.548016	-3.374160	-5.199838	C	6.394738	6.394738	8.219165
H	1.548016	5.199838	3.374160	C	5.480708	-9.124597	-5.480708
H	1.548603	-7.024942	-1.548603	C	6.394738	-8.219165	-6.394738
H	1.548603	1.548603	7.024942	C	7.312431	7.312431	9.122408
H	-2.104448	-5.201759	-7.026565	C	8.207357	8.207357	8.207357
H	-2.104448	7.026565	5.201759	C	7.312431	-9.122408	-7.312431
H	-1.548016	3.374160	-5.199838	C	8.207357	-8.207357	-8.207357
H	7.026565	-5.201759	2.104448	C	-7.295463	1.818298	-0.008114
H	-1.548016	5.199838	-3.374160	C	-6.388706	2.737476	-0.915438
H	7.026565	-2.104448	5.201759	C	-3.653007	5.477880	-3.653007
H	-5.199838	1.548016	-3.374160	C	-2.742132	6.389708	-4.564206
H	2.104448	-7.026565	5.201759	C	-7.295463	0.008114	-1.818298
H	-5.199838	3.374160	-1.548016	C	-6.388706	0.915438	-2.737476
H	2.104448	-5.201759	7.026565	C	-3.653007	3.653007	-5.477880
H	3.373922	-3.373922	-3.373922	C	-2.742132	4.564206	-6.389708
H	-1.548603	1.548603	-7.024942	C	7.295463	0.008114	1.818298
H	3.373922	3.373922	3.373922	C	8.213317	0.913229	0.913229
H	-1.548603	7.024942	-1.548603	C	7.295463	-1.818298	-0.008114
H	-5.200462	-0.278219	-5.200462	C	8.213317	-0.913229	-0.913229
H	3.374731	-8.856306	2.104689	C	-3.644860	7.296075	-1.834644
H	2.104689	-8.856306	3.374731	C	-2.739841	8.213925	-2.739841
H	-5.200462	5.200462	0.278219	C	-3.644860	1.834644	-7.296075
H	2.104689	-3.374731	8.856306	C	-2.739841	2.739841	-8.213925
H	3.374731	-2.104689	8.856306	C	7.296075	1.834644	3.644860
H	-1.548219	-0.278169	-8.855496	C	8.213925	2.739841	2.739841
H	-0.278169	-1.548219	-8.855496	C	7.296075	-3.644860	-1.834644
H	-0.278169	8.855496	1.548219	C	8.213925	-2.739841	-2.739841
H	-1.548219	8.855496	0.278169	C	7.297417	3.661660	5.471946
H	-0.277776	-7.025328	-3.375006	C	8.215507	4.566991	4.566991
H	-5.201759	-2.104448	-7.026565	C	7.297417	-5.471946	-3.661660
H	-0.277776	3.375006	7.025328	C	8.215507	-4.566991	-4.566991
H	-5.201759	7.026565	2.104448	C	7.299848	5.489047	7.299848
H	-3.931868	-5.201846	-8.858784	C	8.219165	6.394738	6.394738
H	-5.201846	-3.931868	-8.858784	C	7.299848	-7.299848	-5.489047
H	-5.201846	8.858784	3.931868	C	8.219165	-6.394738	-6.394738
H	-3.931868	8.858784	5.201846	C	-8.213317	0.913229	-0.913229
H	1.548603	-1.548603	-7.024942	C	-5.477880	3.653007	-3.653007
H	1.548603	7.024942	1.548603	C	-4.566036	4.566036	-4.566036
H	8.858784	-3.931868	5.201846	C	-9.120920	0.000000	0.000000
H	8.858784	-5.201846	3.931868	C	-5.470524	5.470524	-1.835106
H	0.278219	-5.200462	5.200462	C	-4.564206	6.389708	-2.742132
H	5.199838	-3.374160	-1.548016	C	-5.470524	1.835106	-5.470524
H	5.199838	1.548016	3.374160	C	-4.564206	2.742132	-6.389708
H	0.277776	-7.025328	3.375006	C	9.120920	0.000000	0.000000
H	0.277776	-3.375006	7.025328	C	9.121199	1.826425	1.826425
H	1.548219	-8.855496	0.278169	C	9.121199	-1.826425	-1.826425
H	0.278169	-8.855496	1.548219	C	9.122157	3.653137	3.653137
H	0.278169	-1.548219	8.855496	C	9.122157	-3.653137	-3.653137
H	1.548219	-0.278169	8.855496	C	9.124597	5.480708	5.480708
H	-2.104448	-7.026565	-5.201759	C	9.124597	-5.480708	-5.480708
H	-2.104448	5.201759	7.026565	C	9.122408	7.312431	7.312431
H	7.025328	-3.375006	0.277776	C	9.122408	-7.312431	-7.312431

H	7.025328	-0.277776	3.375006	C	-7.296075	3.644860	-1.834644
H	3.374160	-1.548016	-5.199838	C	-6.389708	4.564206	-2.742132
H	3.374160	5.199838	1.548016	C	-3.661660	7.297417	-5.471946
H	-1.548016	-5.199838	3.374160	C	-7.296075	1.834644	-3.644860
H	-1.548016	-3.374160	5.199838	C	-6.389708	2.742132	-4.564206
H	-1.548603	-7.024942	1.548603	C	-3.661660	5.471946	-7.297417
H	-1.548603	-1.548603	7.024942	C	-3.653137	9.122157	-3.653137
H	-0.278169	-8.855496	-1.548219	C	-3.653137	3.653137	-9.122157
H	-1.548219	-8.855496	-0.278169	C	-9.121199	1.826425	-1.826425
H	-1.548219	0.278169	8.855496	C	-8.213925	2.739841	-2.739841
H	-0.278169	1.548219	8.855496	C	-5.479748	5.479748	-5.479748
H	-3.931662	-7.028966	-7.028966	C	-4.569348	6.391449	-6.391449
H	-3.931662	7.028966	7.028966	C	-5.471946	7.297417	-3.661660
H	0.278219	5.200462	-5.200462	C	-4.566991	8.215507	-4.566991
H	8.856306	-2.104689	3.374731	C	-5.471946	3.661660	-7.297417
H	8.856306	-3.374731	2.104689	C	-4.566991	4.566991	-8.215507
H	-3.373922	-3.373922	3.373922	C	-7.297417	5.471946	-3.661660
H	-7.024942	1.548603	-1.548603	C	-6.391449	6.391449	-4.569348
H	5.199838	-1.548016	-3.374160	C	-7.297417	3.661660	-5.471946
H	0.277776	3.375006	-7.025328	C	-6.391449	4.569348	-6.391449
H	5.199838	3.374160	1.548016	C	-9.122157	3.653137	-3.653137
H	0.277776	7.025328	-3.375006	C	-8.215507	4.566991	-4.566991
H	-3.374160	-5.199838	1.548016	C	-5.489047	7.299848	-7.299848
H	-7.025328	-0.277776	-3.375006	C	-5.480708	9.124597	-5.480708
H	-3.374160	-1.548016	5.199838	C	-5.480708	5.480708	-9.124597
H	-7.025328	3.375006	0.277776	H	-8.846595	-8.846595	8.846595
H	1.548219	0.278169	-8.855496	H	-6.114843	-3.017534	7.939632
H	0.278169	1.548219	-8.855496	H	-6.114843	-7.939632	3.017534
H	0.278169	8.855496	-1.548219	H	-2.461039	2.461039	6.112444
H	1.548219	8.855496	-0.278169	H	-2.461039	-6.112444	-2.461039
H	-3.375006	-7.025328	-0.277776	H	1.190853	7.938289	4.288079
H	-7.026565	-2.104448	-5.201759	H	1.190853	-4.288079	-7.938289
H	-3.375006	0.277776	7.025328	H	-0.634962	6.112715	4.287157
H	-7.026565	5.201759	2.104448	H	-0.634962	-4.287157	-6.112715
H	-2.104689	-8.856306	-3.374731	H	-7.942064	-4.844759	7.942064
H	-3.374731	-8.856306	-2.104689	H	-7.942064	-7.942064	4.844759
H	-7.028966	-3.931662	-7.028966	H	-7.956487	-6.687783	9.767436
H	-3.374731	2.104689	8.856306	H	-6.687783	-7.956487	9.767436
H	-2.104689	3.374731	8.856306	H	4.286740	4.286740	-2.460871
H	-7.028966	7.028966	3.931662	H	-6.687783	-9.767436	7.956487
H	-5.774686	-7.043388	-8.854339	H	-7.956487	-9.767436	6.687783
H	-7.043388	-5.774686	-8.854339	H	4.286740	2.460871	-4.286740
H	-7.043388	8.854339	5.774686	H	-4.287157	0.634962	6.112715
H	-5.774686	8.854339	7.043388	H	-4.287157	-6.112715	-0.634962
H	3.375006	0.277776	-7.025328	H	4.287157	6.112715	-0.634962
H	3.375006	7.025328	-0.277776	H	-4.288079	-1.190853	7.938289
H	7.024942	-1.548603	-1.548603	H	4.287157	0.634962	-6.112715
H	7.024942	1.548603	1.548603	H	-4.288079	-7.938289	1.190853
H	-5.199838	-3.374160	1.548016	H	-0.634962	4.287157	6.112715
H	-5.199838	-1.548016	3.374160	H	4.288079	7.938289	1.190853
H	-5.200462	-5.200462	-0.278219	H	-0.634962	-6.112715	-4.287157
H	-5.200462	0.278219	5.200462	H	4.288079	-1.190853	-7.938289
H	-5.201759	-7.026565	-2.104448	H	3.017757	9.769323	4.287803
H	-5.201759	2.104448	7.026565	H	4.287803	9.769323	3.017757

H	-3.931868	-8.858784	-5.201846	H	3.017757	-4.287803	-9.769323
H	-5.201846	-8.858784	-3.931868	H	4.287803	-3.017757	-9.769323
H	-5.201846	3.931868	8.858784	H	-7.942064	7.942064	-4.844759
H	-3.931868	5.201846	8.858784	H	-7.942064	4.844759	-7.942064
H	8.855496	-0.278169	1.548219	H	-9.771867	4.844954	-6.114933
H	8.855496	-1.548219	0.278169	H	-9.771867	6.114933	-4.844954
H	5.200462	0.278219	-5.200462	H	-7.956487	9.767436	-6.687783
H	5.200462	5.200462	-0.278219	H	-6.687783	9.767436	-7.956487
H	-7.024942	-1.548603	1.548603	H	-6.687783	7.956487	-9.767436
H	-7.025328	-3.375006	-0.277776	H	-7.956487	6.687783	-9.767436
H	-7.025328	0.277776	3.375006	H	-9.767436	6.687783	-7.956487
H	-7.026565	-5.201759	-2.104448	H	-9.767436	7.956487	-6.687783
H	-7.026565	2.104448	5.201759	H	-8.846595	8.846595	-8.846595
H	-7.028966	-7.028966	-3.931662	H	-9.767436	-7.956487	6.687783
H	-7.028966	3.931662	7.028966	H	-9.767436	-6.687783	7.956487
H	-5.774686	-8.854339	-7.043388	H	2.460871	4.286740	-4.286740
H	-7.043388	-8.854339	-5.774686	H	-4.844759	-7.942064	7.942064
H	-7.933498	-7.933498	-7.933498	H	2.461039	6.112444	-2.461039
H	-7.043388	5.774686	8.854339	H	-6.113492	-1.191284	6.113492
H	-5.774686	7.043388	8.854339	H	2.461039	2.461039	-6.112444
H	-7.933498	7.933498	7.933498	H	-6.113492	-6.113492	1.191284
H	7.025328	0.277776	-3.375006	H	-6.114933	-4.844954	9.771867
H	2.104448	5.201759	-7.026565	H	-4.844954	-6.114933	9.771867
H	7.025328	3.375006	-0.277776	H	-4.844954	-9.771867	6.114933
H	2.104448	7.026565	-5.201759	H	-6.114933	-9.771867	4.844954
H	-8.855496	-0.278169	-1.548219	H	-2.460871	4.286740	4.286740
H	-8.855496	-1.548219	-0.278169	H	2.461712	7.937677	-0.635480
H	-8.855496	0.278169	1.548219	H	-2.460871	-4.286740	-4.286740
H	-8.855496	1.548219	0.278169	H	2.461712	0.635480	-7.937677
H	2.104689	3.374731	-8.856306	H	2.461308	9.768360	1.191255
H	3.374731	2.104689	-8.856306	H	1.191255	9.768360	2.461308
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H	2.104689	8.856306	-3.374731	H	2.461308	-1.191255	-9.768360
H	-8.856306	-2.104689	-3.374731	H	-2.461712	0.635480	7.937677
H	-8.856306	-3.374731	-2.104689	H	-2.461712	-7.937677	-0.635480
H	-8.856306	2.104689	3.374731	H	1.191284	6.113492	6.113492
H	-8.856306	3.374731	2.104689	H	1.191284	-6.113492	-6.113492
H	-8.858784	-5.201846	-3.931868	H	-7.939632	-3.017534	6.114843
H	-8.858784	-3.931868	-5.201846	H	-7.939632	-6.114843	3.017534
H	-8.858784	5.201846	3.931868	H	-3.017534	-6.114843	7.939632
H	-8.858784	3.931868	5.201846	H	-3.017534	-7.939632	6.114843
H	-8.854339	-7.043388	-5.774686	H	-4.286740	2.460871	4.286740
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H	-8.854339	7.043388	5.774686	H	-4.287803	-3.017757	9.769323
H	-8.854339	5.774686	7.043388	H	-3.017757	-4.287803	9.769323
H	8.855496	1.548219	-0.278169	H	-3.017757	-9.769323	4.287803
H	8.855496	0.278169	-1.548219	H	-4.287803	-9.769323	3.017757
H	5.201759	2.104448	-7.026565	H	-0.635480	7.937677	2.461712
H	5.201759	7.026565	-2.104448	H	-0.635480	-2.461712	-7.937677
H	7.026565	2.104448	-5.201759	H	-0.635480	2.461712	7.937677
H	7.026565	5.201759	-2.104448	H	-0.635480	-7.937677	-2.461712
H	8.856306	3.374731	-2.104689	H	3.017534	7.939632	6.114843
H	8.856306	2.104689	-3.374731	H	3.017534	-6.114843	-7.939632
H	3.931662	7.028966	-7.028966	H	-2.461039	6.112444	2.461039

H	3.931868	5.201846	-8.858784	H	-2.461039	-2.461039	-6.112444
H	5.201846	3.931868	-8.858784	H	-9.771867	-6.114933	4.844954
H	5.201846	8.858784	-3.931868	H	-9.771867	-4.844954	6.114933
H	3.931868	8.858784	-5.201846	H	6.112444	2.461039	-2.461039
H	7.028966	3.931662	-7.028966	H	-1.191284	-6.113492	6.113492
H	7.028966	7.028966	-3.931662	H	-6.112715	0.634962	4.287157
H	8.858784	5.201846	-3.931868	H	-6.112715	-4.287157	-0.634962
H	8.858784	3.931868	-5.201846	H	6.112715	4.287157	-0.634962
				H	-1.190853	-4.288079	7.938289
				H	6.112715	0.634962	-4.287157
				H	-1.190853	-7.938289	4.288079
				H	6.113492	6.113492	1.191284
				H	-2.461308	-1.191255	9.768360
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				H	6.113492	-1.191284	-6.113492
				H	-1.191255	-9.768360	2.461308
				H	-2.461308	-9.768360	1.191255
				H	1.190853	4.288079	7.938289
				H	6.114843	7.939632	3.017534
				H	1.190853	-7.938289	-4.288079
				H	6.114843	-3.017534	-7.939632
				H	6.114933	9.771867	4.844954
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				H	6.114933	-4.844954	-9.771867
				H	4.844954	-6.114933	-9.771867
				H	0.634962	6.112715	-4.287157
				H	-7.938289	-1.190853	4.288079
				H	0.634962	4.287157	-6.112715
				H	-7.938289	-4.288079	1.190853
				H	-4.286740	4.286740	2.460871
				H	0.635480	7.937677	-2.461712
				H	-4.286740	-2.460871	-4.286740
				H	0.635480	2.461712	-7.937677
				H	-0.635027	9.768080	0.635027
				H	0.635027	9.768080	-0.635027
				H	0.635027	0.635027	-9.768080
				H	-0.635027	-0.635027	-9.768080
				H	0.634962	-4.287157	6.112715
				H	0.634962	-6.112715	4.287157
				H	0.635480	-2.461712	7.937677
				H	0.635480	-7.937677	2.461712
				H	-0.635027	0.635027	9.768080
				H	0.635027	-0.635027	9.768080
				H	0.635027	-9.768080	0.635027
				H	-0.635027	-9.768080	-0.635027
				H	3.017534	6.114843	7.939632
				H	3.017534	-7.939632	-6.114843
				H	-9.769323	-4.287803	3.017757
				H	-9.769323	-3.017757	4.287803
				H	2.460871	-4.286740	4.286740
				H	-6.112444	2.461039	2.461039
				H	-6.112444	-2.461039	-2.461039
				H	2.461039	-2.461039	6.112444
				H	2.461039	-6.112444	2.461039

H	-2.461712	7.937677	0.635480
H	-2.461712	-0.635480	-7.937677
H	2.461712	-0.635480	7.937677
H	2.461712	-7.937677	0.635480
H	1.191255	2.461308	9.768360
H	2.461308	1.191255	9.768360
H	2.461308	-9.768360	-1.191255
H	1.191255	-9.768360	-2.461308
H	4.844759	7.942064	7.942064
H	4.844759	-7.942064	-7.942064
H	-4.287157	6.112715	0.634962
H	-4.287157	-0.634962	-6.112715
H	6.687783	9.767436	7.956487
H	7.956487	9.767436	6.687783
H	7.956487	-6.687783	-9.767436
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H	-7.937677	0.635480	2.461712
H	-7.937677	-2.461712	-0.635480
H	4.286740	-2.460871	4.286740
H	7.937677	2.461712	-0.635480
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H	4.287157	-0.634962	6.112715
H	7.938289	4.288079	1.190853
H	4.287157	-6.112715	0.634962
H	7.938289	-1.190853	-4.288079
H	4.288079	1.190853	7.938289
H	7.939632	6.114843	3.017534
H	4.288079	-7.938289	-1.190853
H	7.939632	-3.017534	-6.114843
H	3.017757	4.287803	9.769323
H	4.287803	3.017757	9.769323
H	7.942064	7.942064	4.844759
H	4.287803	-9.769323	-3.017757
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H	-9.768360	-2.461308	1.191255
H	-9.768360	-1.191255	2.461308
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H	-1.190853	7.938289	-4.288079
H	-6.112715	-0.634962	-4.287157
H	-1.190853	4.288079	-7.938289
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H	6.113492	1.191284	6.113492
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H	6.114843	3.017534	7.939632
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H	4.844954	6.114933	9.771867
H	6.114933	4.844954	9.771867
H	6.114933	-9.771867	-4.844954
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H	-6.113492	1.191284	-6.113492
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T10	C	-2.738922	-2.738922	-2.738922
	C	-1.825806	-1.825806	-1.825806
	C	-9.120387	-9.120387	-9.120387
	C	0.912770	0.912770	0.912770
	C	1.825315	1.825315	1.825315
	C	-6.392782	-6.392782	-6.392782
	C	-5.479070	-5.479070	-5.479070
	C	-2.738493	-4.564036	-0.913717
	C	-1.825557	-3.651099	-0.000466
	C	0.912956	-0.912956	2.738492
	C	1.825557	-0.000466	3.651099
	C	-6.384977	-8.210434	-4.574691
	C	-5.477241	-7.302711	-3.655172
	C	-2.738493	-0.913717	-4.564036
	C	-1.825557	-0.000466	-3.651099
	C	0.912956	2.738492	-0.912956
	C	1.825557	3.651099	-0.000466
	C	-6.384977	-4.574691	-8.210434
	C	-5.477241	-3.655172	-7.302711
	C	-2.730700	-6.382199	0.904548
	C	-1.823721	-5.475276	1.823721
	C	0.913717	-2.738493	4.564036
	C	1.826225	-1.826225	5.476875
	C	-2.730700	0.904548	-6.382199
	C	-1.823721	1.823721	-5.475276
	C	0.913717	4.564036	-2.738493
	C	1.826225	5.476875	-1.826225
	C	0.921658	-4.556958	6.382661
	C	1.828505	-3.650534	7.301613
	C	0.921658	6.382661	-4.556958
	C	1.828505	7.301613	-3.650534
	C	-0.912770	-0.912770	0.912770
	C	0.000000	0.000000	1.825557
	C	2.730422	2.730422	4.556233
	C	-0.912770	0.912770	-0.912770
	C	0.000000	1.825557	0.000000
	C	2.730422	4.556233	2.730422
	C	-0.912209	-2.738089	2.738089
	C	0.000466	-1.825557	3.651099
	C	2.730700	0.904548	6.382199
	C	-0.912209	2.738089	-2.738089
	C	0.000466	3.651099	-1.825557

C	2.730700	6.382199	0.904548
C	-0.904449	-4.556438	4.556438
C	0.002422	-3.649891	5.475509
C	2.731378	-0.921200	8.208282
C	-0.904449	4.556438	-4.556438
C	0.002422	5.475509	-3.649891
C	2.731378	8.208282	-0.921200
C	2.739466	-2.739466	10.034091
C	2.739466	10.034091	-2.739466
C	-3.651601	-3.651601	-1.826497
C	-8.212880	-8.212880	-6.402077
C	-7.304480	-7.304480	-5.482382
C	-4.564726	-4.564726	-2.739931
C	-3.651601	-1.826497	-3.651601
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C	-7.304480	-5.482382	-7.304480
C	-4.564726	-2.739931	-4.564726
C	-0.912956	-2.738492	-0.912956
C	0.000000	-1.825557	0.000000
C	-8.225460	-10.035439	-8.225460
C	2.738089	0.912209	2.738089
C	3.649482	1.823531	3.649482
C	-7.307768	-9.132196	-7.307768
C	-4.566046	-6.390888	-4.566046
C	-3.652558	-5.477680	-3.652558
C	-0.912956	-0.912956	-2.738492
C	0.000000	0.000000	-1.825557
C	-8.225460	-8.225460	-10.035439
C	2.738089	2.738089	0.912209
C	3.649482	3.649482	1.823531
C	-7.307768	-7.307768	-9.132196
C	-4.566046	-4.566046	-6.390888
C	-3.652558	-3.652558	-5.477680
C	-3.649891	-5.475509	-0.002422
C	-4.556958	-6.382661	-0.921658
C	-3.649891	-0.002422	-5.475509
C	-4.556958	-0.921658	-6.382661
C	-0.912384	-4.563791	0.912384
C	0.000466	-3.651099	1.825557
C	2.738493	-0.913717	4.564036
C	3.649891	-0.002422	5.475509
C	-4.557899	-8.209031	-2.747685
C	-3.650534	-7.301613	-1.828505
C	-0.912384	0.912384	-4.563791
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C	2.738493	4.564036	-0.913717
C	3.649891	5.475509	-0.002422
C	-4.557899	-2.747685	-8.209031
C	-3.650534	-1.828505	-7.301613
C	-0.904548	-6.382199	2.730700
C	0.002422	-5.475509	3.649891
C	2.739451	-2.739451	6.389845
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C	-0.904548	2.730700	-6.382199

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C	-2.730422	-4.556233	2.730422
C	-1.823531	-3.649482	3.649482

C	0.913125	-0.913125	6.389336
C	1.824142	-0.002138	7.301115
C	-2.730422	2.730422	-4.556233
C	-1.823531	3.649482	-3.649482
C	0.913125	6.389336	-0.913125
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C	0.921200	-2.731378	8.208282
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C	4.556438	4.556438	0.904449
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C	0.913717	-4.564036	2.738493
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C	-2.731378	-8.208282	-0.921200
C	-1.824142	-0.002138	-7.301115
C	0.913717	2.738493	-4.564036
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C	4.556958	6.382661	-0.921658
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C	0.921658	-6.382661	4.556958
C	1.828670	-5.476212	5.476212
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C	4.557899	8.209031	-2.747685
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C	-4.564036	-2.738493	-0.913717
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C	-0.912956	0.912956	2.738492
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C	-7.302711	-5.477241	-3.655172
C	-4.564036	-0.913717	-2.738493
C	-3.651099	-0.000466	-1.825557
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C	3.651099	-0.000466	1.825557
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C	-0.913717	-2.738493	-4.564036
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C	0.002138	-7.301115	1.824142
C	2.739931	-4.564726	4.564726
C	3.652558	-3.652558	5.477680
C	-0.905083	0.905083	-8.208045
C	0.002138	1.824142	-7.301115
C	2.739931	4.564726	-4.564726
C	3.652558	5.477680	-3.652558
C	2.748139	-6.383531	6.383531
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C	3.655172	7.302711	-5.477241
C	-2.738492	0.912956	0.912956
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C	-2.738089	-0.912209	2.738089
C	-1.825557	0.000466	3.651099

C	0.904548	2.730700	6.382199
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C	0.904548	6.382199	2.730700
C	-2.730422	-2.730422	4.556233
C	-1.823721	-1.823721	5.475276
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C	-9.128523	-5.480021	-5.480021
C	-6.389845	-2.739451	-2.739451
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C	4.563791	0.912384	0.912384
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C	-1.828670	-5.476212	-5.476212
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C	0.912384	-4.563791	-0.912384
C	1.825557	-3.651099	0.000466
C	4.564036	-0.913717	2.738493
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C	1.825557	0.000466	-3.651099
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C	1.826225	-5.476875	1.826225
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C	-2.739466	-10.034091	-2.739466
C	-1.826321	-9.126133	-1.826321
C	0.913125	0.913125	-6.389336
C	1.826225	1.826225	-5.476875
C	4.564726	4.564726	-2.739931
C	5.476212	5.476212	-1.828670
C	-2.739466	-2.739466	-10.034091
C	-1.826321	-1.826321	-9.126133
C	0.921200	-8.208282	2.731378
C	1.828505	-7.301613	3.650534
C	4.566046	-4.566046	6.390888
C	5.477241	-3.655172	7.302711

C	0.921200	2.731378	-8.208282
C	1.828505	3.650534	-7.301613
C	4.566046	6.390888	-4.566046
C	5.477241	7.302711	-3.655172
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C	-3.651099	1.825557	0.000466
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C	-7.301613	-1.828505	-3.650534
C	-4.556233	-2.730422	2.730422
C	-3.649482	-1.823531	3.649482
C	-0.913125	0.913125	6.389336
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C	-0.921658	-4.556958	-6.382661
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C	2.738493	-4.564036	0.913717
C	3.651601	-3.651601	1.826497
C	6.382661	-0.921658	4.556958
C	-0.921200	-8.208282	-2.731378
C	-0.002138	-1.824142	-7.301115
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C	3.651601	1.826497	-3.651601
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C	-0.921200	-2.731378	-8.208282

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C	3.655172	-7.302711	5.477241
C	6.384977	-4.574691	8.210434
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C	-5.475276	-1.823721	1.823721
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C	-5.475276	1.823721	-1.823721
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C	1.823721	-5.475276	-1.823721
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C	0.904548	-2.730700	-6.382199
C	1.823721	-1.823721	-5.475276
C	4.564036	0.913717	-2.738493
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C	-2.730700	-0.904548	6.382199
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C	1.824142	-7.301115	0.002138
C	4.564726	-4.564726	2.739931
C	5.477680	-3.652558	3.652558
C	0.905083	-0.905083	-8.208045
C	1.824142	0.002138	-7.301115
C	4.564726	2.739931	-4.564726
C	5.477680	3.652558	-3.652558

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C	1.826321	-9.126133	1.826321
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C	5.479070	-5.479070	5.479070
C	0.913118	0.913118	-10.033638
C	1.826321	1.826321	-9.126133
C	4.566046	4.566046	-6.390888
C	5.479070	5.479070	-5.479070
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C	-4.564036	2.738493	0.913717
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C	-0.921658	6.382661	4.556958
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C	-3.649891	5.475509	0.002422
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C	3.649891	-5.475509	0.002422
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C	7.302711	-3.655172	5.477241

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H	-1.548091	-10.680800	-0.278037
H	-0.278037	-10.680800	-1.548091
H	7.026488	7.026488	-2.104295
H	-0.278037	-1.548091	-10.680800
H	-1.548091	-0.278037	-10.680800
H	2.103868	-8.851243	5.201092
H	7.027866	-3.930557	8.852648
H	2.103868	5.201092	-8.851243
H	7.027866	8.852648	-3.930557
H	-10.682308	-3.930766	-5.200813

H	-10.682308	-5.200813	-3.930766
H	1.547886	-5.199591	-5.199591
H	-7.025166	-3.374016	1.548015
H	-7.025166	1.548015	-3.374016
H	1.548015	-7.025166	-3.374016
H	1.548015	-3.374016	-7.025166
H	-3.374016	-1.548015	7.025166
H	-3.374016	7.025166	-1.548015
H	1.548588	-8.850255	-1.548588
H	1.548588	-1.548588	-8.850255
H	0.278037	-10.680800	1.548091
H	1.548091	-10.680800	0.278037
H	1.548091	0.278037	-10.680800
H	0.278037	1.548091	-10.680800
H	3.930557	-8.852648	7.027866
H	3.930557	7.027866	-8.852648
H	-0.278037	5.200129	7.025618
H	-0.278037	7.025618	5.200129
H	-5.199591	-1.547886	5.199591
H	-0.277555	3.374741	8.850494
H	-5.199591	5.199591	-1.547886
H	-0.277555	8.850494	3.374741
H	-1.548091	0.278037	10.680800
H	-0.278037	1.548091	10.680800
H	-0.278037	10.680800	1.548091
H	-1.548091	10.680800	0.278037
H	5.757789	-8.855095	8.855095
H	5.757789	8.855095	-8.855095
H	-8.850494	-3.374741	-0.277555
H	-8.850494	-0.277555	-3.374741
H	3.373714	-5.199394	-3.373714
H	3.373714	-3.373714	-5.199394
H	3.374016	-7.025166	-1.548015
H	3.374016	-1.548015	-7.025166
H	3.374741	-8.850494	0.277555
H	3.374741	0.277555	-8.850494
H	2.104263	-10.681250	3.374319
H	3.374319	-10.681250	2.104263
H	3.374319	2.104263	-10.681250
H	2.104263	3.374319	-10.681250
H	-10.681250	-2.104263	-3.374319
H	-10.681250	-3.374319	-2.104263
H	-7.025166	-1.548015	3.374016
H	-7.025166	3.374016	-1.548015
H	-3.374741	0.277555	8.850494
H	-3.374741	8.850494	0.277555
H	5.199394	-3.373714	-3.373714
H	8.850255	1.548588	1.548588
H	7.600812	-8.869516	10.680466
H	8.869516	-7.600812	10.680466
H	8.869516	10.680466	-7.600812
H	7.600812	10.680466	-8.869516
H	5.199591	-5.199591	-1.547886
H	8.850494	-0.277555	3.374741

H	5.199591	-1.547886	-5.199591
H	8.850494	3.374741	-0.277555
H	5.200129	-7.025618	0.278037
H	8.851243	-2.103868	5.201092
H	5.200129	0.278037	-7.025618
H	8.851243	5.201092	-2.103868
H	5.201092	-8.851243	2.103868
H	8.852648	-3.930557	7.027866
H	5.201092	2.103868	-8.851243
H	8.852648	7.027866	-3.930557
H	3.930766	-10.682308	5.200813
H	5.200813	-10.682308	3.930766
H	8.855095	-5.757789	8.855095
H	5.200813	3.930766	-10.682308
H	3.930766	5.200813	-10.682308
H	8.855095	8.855095	-5.757789
H	5.757975	-10.684889	7.027957
H	7.027957	-10.684889	5.757975
H	7.027957	5.757975	-10.684889
H	5.757975	7.027957	-10.684889
H	-8.850255	-1.548588	1.548588
H	-8.850255	1.548588	-1.548588
H	7.025166	-3.374016	-1.548015
H	7.025166	-1.548015	-3.374016
H	-5.200129	0.278037	7.025618
H	-5.200129	7.025618	0.278037
H	7.025618	-5.200129	0.278037
H	7.025618	0.278037	-5.200129
H	7.026488	-7.026488	2.104295
H	7.026488	2.104295	-7.026488
H	7.027866	-8.852648	3.930557
H	7.027866	3.930557	-8.852648
H	-2.104295	7.026488	7.026488
H	-10.680800	-0.278037	-1.548091
H	-10.680800	-1.548091	-0.278037
H	-7.025618	0.278037	5.200129
H	-2.103868	5.201092	8.851243
H	-7.025618	5.200129	0.278037
H	-2.103868	8.851243	5.201092
H	-2.104263	3.374319	10.681250
H	-3.374319	2.104263	10.681250
H	-3.374319	10.681250	2.104263
H	-2.104263	10.681250	3.374319
H	8.850255	-1.548588	-1.548588
H	7.600812	-10.680466	8.869516
H	8.869516	-10.680466	7.600812
H	9.759624	-9.759624	9.759624
H	8.869516	7.600812	-10.680466
H	7.600812	8.869516	-10.680466
H	9.759624	9.759624	-9.759624
H	8.850494	-3.374741	0.277555
H	8.850494	0.277555	-3.374741
H	8.851243	-5.201092	2.103868
H	8.851243	2.103868	-5.201092

H	8.852648	-7.027866	3.930557
H	8.852648	3.930557	-7.027866
H	8.855095	-8.855095	5.757789
H	8.855095	5.757789	-8.855095
H	-8.850494	0.277555	3.374741
H	-8.850494	3.374741	0.277555
H	-5.201092	2.103868	8.851243
H	-5.201092	8.851243	2.103868
H	10.680466	-7.600812	8.869516
H	10.680466	-8.869516	7.600812
H	10.680466	8.869516	-7.600812
H	10.680466	7.600812	-8.869516
H	10.680800	-1.548091	0.278037
H	10.680800	-0.278037	1.548091
H	10.680800	1.548091	-0.278037
H	10.680800	0.278037	-1.548091
H	10.681250	-3.374319	2.104263
H	10.681250	-2.104263	3.374319
H	10.681250	2.104263	-3.374319
H	10.681250	3.374319	-2.104263
H	10.682308	-3.930766	5.200813
H	10.682308	-5.200813	3.930766
H	10.682308	5.200813	-3.930766
H	10.682308	3.930766	-5.200813
H	10.684889	-5.757975	7.027957
H	10.684889	-7.027957	5.757975
H	10.684889	5.757975	-7.027957
H	10.684889	7.027957	-5.757975
H	-10.680800	1.548091	0.278037
H	-10.680800	0.278037	1.548091
H	-7.026488	2.104295	7.026488
H	-7.026488	7.026488	2.104295
H	-8.851243	2.103868	5.201092
H	-3.930557	7.027866	8.852648
H	-8.851243	5.201092	2.103868
H	-3.930557	8.852648	7.027866
H	-5.200813	3.930766	10.682308
H	-3.930766	5.200813	10.682308
H	-5.200813	10.682308	3.930766
H	-3.930766	10.682308	5.200813
H	-10.681250	3.374319	2.104263
H	-10.681250	2.104263	3.374319
H	-7.027866	3.930557	8.852648
H	-7.027866	8.852648	3.930557

Table S2. Cartesian coordinates of BLYP/3-21G optimized compounds in [Å]. Names of model structures are given in the main text.

A	C	0.000000	0.000000	0.000000	T2	C	-1.674316	1.674316	-1.674316
	C	0.000000	0.000000	1.450000		C	-0.837153	2.511478	-0.837153
	C	1.367073	0.000000	-0.483333		C	0.000000	1.674317	0.000000
	C	0.683537	1.183920	1.933333		C	-0.837158	0.837158	0.837158
	H	-1.026719	0.000000	1.813000		C	-1.674317	0.000000	0.000000
	H	0.513360	-0.889165	1.813000		C	-2.511478	0.837153	-0.837153
	C	0.000000	2.367840	1.450000		C	0.000000	0.000000	1.674317
	H	0.683537	1.183920	3.022333		C	-0.837153	-0.837153	2.511478
	C	2.050610	1.183920	1.450000		C	-1.674316	-1.674316	1.674316
	C	0.000000	2.367840	0.000000		C	-2.511478	-0.837153	0.837153
	H	-1.026719	2.367840	1.813000		C	0.837158	-0.837158	0.837158
	H	0.513360	3.257005	1.813000		C	0.000000	-1.674317	0.000000
	C	-0.683537	1.183920	-0.483333		C	-0.837158	-0.837158	-0.837158
	H	-0.513360	3.257005	-0.363000		C	0.000000	0.000000	-1.674317
	C	1.367073	2.367840	-0.483333		C	0.837158	0.837158	-0.837158
	H	-1.710256	1.183920	-0.120333		C	-0.837153	-2.511478	0.837153
	H	-0.683537	1.183920	-1.572333		C	-0.837153	0.837153	-2.511478
	C	2.050610	1.183920	0.000000		C	1.674317	0.000000	0.000000
	H	3.077329	1.183920	-0.363000		C	0.837153	2.511478	0.837153
	H	-0.513360	-0.889165	-0.363000		C	1.674316	1.674316	1.674316
	H	1.367073	0.000000	-1.572333		C	0.837153	0.837153	2.511478
	H	1.880433	-0.889165	-0.120333		C	2.511478	0.837153	0.837153
	H	1.367073	2.367840	-1.572333		C	2.511478	-0.837153	-0.837153
	H	1.880433	3.257005	-0.120333		C	1.674316	-1.674316	-1.674316
	H	2.563969	0.294755	1.813000		C	0.837153	-2.511478	-0.837153
	H	2.563969	2.073085	1.813000		C	0.837153	-0.837153	-2.511478
						H	-0.208423	-1.465899	3.140205
						H	-1.465899	-0.208423	3.140205
						H	-2.303050	-2.303050	2.303050
						H	-0.208423	-3.140205	1.465899
						H	-1.465899	-3.140205	0.208423
						H	1.465892	-1.465892	1.465892
						H	-1.465892	1.465892	1.465892
						H	-1.465892	-1.465892	-1.465892
						H	-3.140205	-0.208423	1.465899
						H	-3.140205	-1.465899	0.208423
						H	0.208423	1.465899	3.140205
						H	1.465899	0.208423	3.140205
						H	1.465899	-3.140205	-0.208423
						H	0.208423	-3.140205	-1.465899
						H	2.303050	-2.303050	-2.303050
						H	2.303050	2.303050	2.303050
						H	-3.140205	0.208423	-1.465899
						H	-3.140205	1.465899	-0.208423
						H	-2.303050	2.303050	-2.303050
						H	1.465899	-0.208423	-3.140205
						H	0.208423	-1.465899	-3.140205
						H	-0.208423	1.465899	-3.140205
						H	-1.465899	0.208423	-3.140205
						H	3.140205	1.465899	0.208423

					H	3.140205	0.208423	1.465899	
					H	3.140205	-0.208423	-1.465899	
					H	3.140205	-1.465899	-0.208423	
					H	-0.208423	3.140205	-1.465899	
					H	-1.465899	3.140205	-0.208423	
					H	1.465899	3.140205	0.208423	
					H	0.208423	3.140205	1.465899	
					H	1.465892	1.465892	-1.465892	
T3	C	-2.743949	-2.743949	2.743949	T4	C	-4.185771	2.511442	2.511442
	C	-1.830199	-1.830199	3.646647		C	-3.348652	3.348652	3.348652
	C	-0.914727	-0.914727	2.736997		C	-2.511442	2.511442	4.185771
	C	-1.819469	-0.008659	1.819469		C	-1.674327	1.674327	3.348703
	C	-2.736997	-0.914727	0.914727		C	-2.511484	0.837171	2.511484
	C	-3.646647	-1.830199	1.830199		C	-3.348703	1.674327	1.674327
	C	-0.008659	-1.819469	1.819469		C	-0.837171	2.511484	2.511484
	C	0.911262	-0.911262	0.911262		C	-1.674327	3.348703	1.674327
	C	0.000000	0.000000	0.000000		C	-2.511442	4.185771	2.511442
	C	-0.911262	0.911262	0.911262		C	-2.511484	2.511484	0.837171
	C	1.819469	0.008659	1.819469		C	0.000068	1.674363	1.674363
	C	0.914727	0.914727	2.736997		C	0.837324	0.837324	2.511509
	C	0.008659	1.819469	1.819469		C	0.000000	0.000000	3.348731
	C	0.914727	2.736997	0.914727		C	-0.837150	0.837150	4.185882
	C	1.819469	1.819469	0.008659		C	-1.674363	-0.000068	1.674363
	C	0.911262	0.911262	-0.911262		C	-0.837164	0.837164	0.837164
	C	-1.819469	1.819469	-0.008659		C	-0.837324	-0.837324	2.511509
	C	-2.736997	0.914727	-0.914727		C	0.837324	2.511509	0.837324
	C	-1.819469	0.008659	-1.819469		C	0.000000	3.348731	0.000000
	C	-0.911262	-0.911262	-0.911262		C	-0.837150	4.185882	0.837150
	C	-0.008659	1.819469	-1.819469		C	-1.674363	1.674363	-0.000068
	C	-0.914727	2.736997	-0.914727		C	-0.837324	2.511509	-0.837324
	C	-1.819469	-1.819469	0.008659		C	-0.000068	-1.674363	1.674363
	C	2.736997	0.914727	0.914727		C	0.837164	-0.837164	0.837164
	C	1.819469	-0.008659	-1.819469		C	1.674363	0.000068	1.674363
	C	2.736997	-0.914727	-0.914727		C	2.511484	-0.837171	2.511484
	C	1.819469	-1.819469	-0.008659		C	1.674327	-1.674327	3.348703
	C	0.008659	-1.819469	-1.819469		C	0.837150	-0.837150	4.185882
	C	0.914727	-2.736997	-0.914727		C	0.837171	-2.511484	2.511484
	C	-0.914727	-2.736997	0.914727		C	0.000000	0.000000	0.000000
	C	-0.914727	0.914727	-2.736997		C	2.511509	0.837324	0.837324
	C	0.914727	-0.914727	-2.736997		C	1.674363	1.674363	0.000068
	C	0.000000	0.000000	3.644203		C	0.837164	0.837164	-0.837164
	C	0.000000	3.644203	0.000000		C	-2.511509	-0.837324	0.837324
	C	-3.644203	0.000000	0.000000		C	-1.674363	-1.674363	0.000068
	C	3.646647	1.830199	1.830199		C	-0.837164	-0.837164	-0.837164
	C	2.743949	2.743949	2.743949		C	-2.511509	0.837324	-0.837324
	C	1.830199	1.830199	3.646647		C	-1.674363	0.000068	-1.674363
	C	3.644203	0.000000	0.000000		C	-0.000068	1.674363	-1.674363
	C	1.830199	3.646647	1.830199		C	-3.348731	0.000000	0.000000
	C	-1.830199	1.830199	-3.646647		C	-0.837324	-2.511509	0.837324
	C	-2.743949	2.743949	-2.743949		C	0.000068	-1.674363	-1.674363
	C	-3.646647	1.830199	-1.830199		C	0.837324	-2.511509	-0.837324
	C	0.000000	0.000000	-3.644203		C	1.674363	-1.674363	-0.000068
	C	-1.830199	3.646647	-1.830199		C	1.674363	-0.000068	-1.674363

C	0.000000	-3.644203	0.000000	C	2.511509	-0.837324	-0.837324
C	1.830199	-3.646647	-1.830199	C	0.837324	-0.837324	-2.511509
C	2.743949	-2.743949	-2.743949	C	-0.837324	0.837324	-2.511509
C	3.646647	-1.830199	-1.830199	C	3.348731	0.000000	0.000000
C	1.830199	-1.830199	-3.646647	C	2.511484	-2.511484	0.837171
C	-1.830199	-3.646647	1.830199	C	3.348703	-1.674327	1.674327
H	-3.361714	-3.361714	3.361714	C	0.000000	-3.348731	0.000000
H	-2.484915	-1.174722	4.181691	C	1.674327	-3.348703	1.674327
H	-1.174722	-2.484915	4.181691	C	4.185882	-0.837150	0.837150
H	-2.436769	0.610034	2.436769	C	0.837150	-4.185882	0.837150
H	-4.181691	-1.174722	2.484915	C	-0.837150	-4.185882	-0.837150
H	-4.181691	-2.484915	1.174722	C	-1.674327	-3.348703	-1.674327
H	0.610034	-2.436769	2.436769	C	-2.511484	-2.511484	-0.837171
H	2.436769	-0.610034	2.436769	C	-0.837171	-2.511484	-2.511484
H	-0.610034	2.436769	2.436769	C	-3.348703	-1.674327	-1.674327
H	2.436769	2.436769	-0.610034	C	-2.511484	-0.837171	-2.511484
H	-2.436769	2.436769	0.610034	C	-4.185882	-0.837150	-0.837150
H	-2.436769	-0.610034	-2.436769	C	0.000000	0.000000	-3.348731
H	0.610034	2.436769	-2.436769	C	-1.674327	-1.674327	-3.348703
H	-2.436769	-2.436769	-0.610034	C	-0.837150	-0.837150	-4.185882
H	2.436769	0.610034	-2.436769	C	2.511484	0.837171	-2.511484
H	2.436769	-2.436769	0.610034	C	1.674327	1.674327	-3.348703
H	-0.610034	-2.436769	-2.436769	C	0.837171	2.511484	-2.511484
H	-0.654742	0.654742	4.179865	C	2.511484	2.511484	-0.837171
H	0.654742	-0.654742	4.179865	C	1.674327	3.348703	-1.674327
H	-0.654742	4.179865	0.654742	C	3.348703	1.674327	-1.674327
H	0.654742	4.179865	-0.654742	C	0.837150	0.837150	-4.185882
H	-4.179865	0.654742	0.654742	C	0.837150	4.185882	-0.837150
H	-4.179865	-0.654742	-0.654742	C	4.185882	0.837150	-0.837150
H	4.181691	2.484915	1.174722	C	-4.185882	0.837150	0.837150
H	4.181691	1.174722	2.484915	C	-2.511442	-2.511442	-4.185771
H	3.361714	3.361714	3.361714	C	-3.348652	-3.348652	-3.348652
H	1.174722	2.484915	4.181691	C	-2.511442	-4.185771	-2.511442
H	2.484915	1.174722	4.181691	C	-4.185771	-2.511442	-2.511442
H	4.179865	0.654742	-0.654742	C	2.511442	-2.511442	4.185771
H	4.179865	-0.654742	0.654742	C	3.348652	-3.348652	3.348652
H	1.174722	4.181691	2.484915	C	2.511442	-4.185771	2.511442
H	2.484915	4.181691	1.174722	C	4.185771	-2.511442	2.511442
H	-1.174722	2.484915	-4.181691	C	2.511442	4.185771	-2.511442
H	-2.484915	1.174722	-4.181691	C	3.348652	3.348652	-3.348652
H	-3.361714	3.361714	-3.361714	C	2.511442	2.511442	-4.185771
H	-4.181691	2.484915	-1.174722	C	4.185771	2.511442	-2.511442
H	-4.181691	1.174722	-2.484915	H	-4.843987	3.169465	1.853309
H	0.654742	0.654742	-4.179865	H	-4.843987	1.853309	3.169465
H	-0.654742	-0.654742	-4.179865	H	-4.006831	4.006831	4.006831
H	-2.484915	4.181691	-1.174722	H	-3.169465	1.853309	4.843987
H	-1.174722	4.181691	-2.484915	H	-1.853309	3.169465	4.843987
H	-0.654742	-4.179865	-0.654742	H	-3.169668	0.179000	3.169668
H	0.654742	-4.179865	0.654742	H	-0.179000	3.169668	3.169668
H	1.174722	-4.181691	-2.484915	H	-3.169465	4.843987	1.853309
H	2.484915	-4.181691	-1.174722	H	-1.853309	4.843987	3.169465
H	3.361714	-3.361714	-3.361714	H	-3.169668	3.169668	0.179000
H	4.181691	-1.174722	-2.484915	H	1.495522	1.495522	3.169644
H	4.181691	-2.484915	-1.174722	H	-1.495093	0.179144	4.844112

H	2.484915	-1.174722	-4.181691	H	-0.179144	1.495093	4.844112
H	1.174722	-2.484915	-4.181691	H	-1.495522	-1.495522	3.169644
H	-2.484915	-4.181691	1.174722	H	1.495522	3.169644	1.495522
H	-1.174722	-4.181691	2.484915	H	-1.495093	4.844112	0.179144
				H	-0.179144	4.844112	1.495093
				H	-1.495522	3.169644	-1.495522
				H	3.169668	-0.179000	3.169668
				H	0.179144	-1.495093	4.844112
				H	1.495093	-0.179144	4.844112
				H	0.179000	-3.169668	3.169668
				H	3.169644	1.495522	1.495522
				H	-3.169644	-1.495522	1.495522
				H	-3.169644	1.495522	-1.495522
				H	-1.495522	-3.169644	1.495522
				H	1.495522	-3.169644	-1.495522
				H	3.169644	-1.495522	-1.495522
				H	1.495522	-1.495522	-3.169644
				H	-1.495522	1.495522	-3.169644
				H	3.169668	-3.169668	0.179000
				H	4.844112	-0.179144	1.495093
				H	4.844112	-1.495093	0.179144
				H	0.179144	-4.844112	1.495093
				H	1.495093	-4.844112	0.179144
				H	-1.495093	-4.844112	-0.179144
				H	-0.179144	-4.844112	-1.495093
				H	-3.169668	-3.169668	-0.179000
				H	-0.179000	-3.169668	-3.169668
				H	-3.169668	-0.179000	-3.169668
				H	-4.844112	-1.495093	-0.179144
				H	-4.844112	-0.179144	-1.495093
				H	-0.179144	-1.495093	-4.844112
				H	-1.495093	-0.179144	-4.844112
				H	3.169668	0.179000	-3.169668
				H	0.179000	3.169668	-3.169668
				H	3.169668	3.169668	-0.179000
				H	1.495093	0.179144	-4.844112
				H	0.179144	1.495093	-4.844112
				H	0.179144	4.844112	-1.495093
				H	1.495093	4.844112	-0.179144
				H	4.844112	1.495093	-0.179144
				H	4.844112	0.179144	-1.495093
				H	-4.844112	1.495093	0.179144
				H	-4.844112	0.179144	1.495093
				H	-1.853309	-3.169465	-4.843987
				H	-3.169465	-1.853309	-4.843987
				H	-4.006831	-4.006831	-4.006831
				H	-1.853309	-4.843987	-3.169465
				H	-3.169465	-4.843987	-1.853309
				H	-4.843987	-3.169465	-1.853309
				H	-4.843987	-1.853309	-3.169465
				H	1.853309	-3.169465	4.843987
				H	3.169465	-1.853309	4.843987
				H	4.006831	-4.006831	4.006831
				H	3.169465	-4.843987	1.853309

					H	1.853309	-4.843987	3.169465
					H	4.843987	-1.853309	3.169465
					H	4.843987	-3.169465	1.853309
					H	1.853309	4.843987	-3.169465
					H	3.169465	4.843987	-1.853309
					H	4.006831	4.006831	-4.006831
					H	3.169465	1.853309	-4.843987
					H	1.853309	3.169465	-4.843987
					H	4.843987	3.169465	-1.853309
					H	4.843987	1.853309	-3.169465
O2	C	0.000000	1.674300	-1.674300	O3	C	0.000000	5.022900
	C	0.000000	-1.674300	-1.674300		C	0.000000	3.348600
	C	1.674300	0.000000	-1.674300		C	1.674302	3.348600
	C	-1.674300	0.000000	-1.674300		C	-1.674302	3.348600
	C	0.837150	-0.837150	-2.511450		C	0.000000	-1.674302
	C	-0.837150	0.837150	-2.511450		C	0.000000	3.348600
	C	-0.837150	-0.837150	2.511450		C	1.674301	1.674301
	C	0.837150	0.837150	2.511450		C	3.348600	0.000000
	C	0.000000	1.674300	1.674300		C	-1.674301	1.674301
	C	0.000000	-1.674300	1.674300		C	0.000000	1.674300
	C	1.674300	0.000000	1.674300		C	1.674301	-1.674301
	C	-1.674300	0.000000	1.674300		C	-3.348600	0.000000
	C	0.837150	2.511450	0.837150		C	-1.674301	-1.674301
	C	-0.837150	-2.511450	0.837150		C	0.000000	-3.348600
	C	-2.511450	-0.837150	0.837150		C	0.000000	5.022900
	C	0.837150	-0.837150	0.837150		C	1.674302	3.348600
	C	2.511450	0.837150	0.837150		C	3.348600	1.674302
	C	-0.837150	0.837150	0.837150		C	5.022900	0.000000
	C	1.674300	1.674300	0.000000		C	-1.674302	3.348600
	C	-1.674300	1.674300	0.000000		C	0.000000	1.674300
	C	1.674300	-1.674300	0.000000		C	1.674300	0.000000
	C	-1.674300	-1.674300	0.000000		C	3.348600	-1.674302
	C	0.000000	0.000000	0.000000		C	-3.348600	1.674302
	C	-0.837150	2.511450	-0.837150		C	-1.674300	0.000000
	C	0.837150	-2.511450	-0.837150		C	0.000000	-1.674300
	C	2.511450	-0.837150	-0.837150		C	1.674302	-3.348600
	C	-0.837150	-0.837150	-0.837150		C	-5.022900	0.000000
	C	-2.511450	0.837150	-0.837150		C	-3.348600	-1.674302
	C	0.837150	0.837150	-0.837150		C	-1.674302	-3.348600
	C	0.000000	0.000000	-3.357820		C	0.000000	-5.022900
	C	0.000000	0.000000	3.357820		C	0.000000	0.000000
	C	0.000000	3.357820	0.000000		C	0.000000	1.674302
	C	0.000000	-3.357820	0.000000		C	1.674302	0.000000
	C	-3.357820	0.000000	0.000000		C	-1.674302	0.000000
	C	3.357820	0.000000	0.000000		C	0.000000	-1.674302
	H	0.628730	2.303030	-2.303030		C	0.000000	3.348600
	H	-0.628730	-2.303030	-2.303030		C	1.674301	1.674301
	H	2.303030	0.628730	-2.303030		C	3.348600	0.000000
	H	-2.303030	-0.628730	-2.303030		C	-1.674301	1.674301
	H	1.462390	-1.462390	-3.147110		C	0.000000	0.000000
	H	-1.462390	1.462390	-3.147110		C	1.674301	-1.674301
	H	-1.462390	-1.462390	3.147110		C	-3.348600	0.000000
	H	1.462390	1.462390	3.147110		C	-1.674301	-1.674301

H	-0.628730	2.303030	2.303030	C	0.000000	-3.348600	-1.674302
H	0.628730	-2.303030	2.303030	C	-0.837151	0.837151	4.185750
H	2.303030	-0.628730	2.303030	C	0.837151	-0.837151	4.185750
H	-2.303030	0.628730	2.303030	C	-0.837151	2.511451	2.511451
H	1.462390	3.147110	1.462390	C	0.837151	0.837151	2.511450
H	-1.462390	-3.147110	1.462390	C	2.511451	-0.837151	2.511451
H	-3.147110	-1.462390	1.462390	C	-2.511451	0.837151	2.511451
H	3.147110	1.462390	1.462390	C	-0.837151	-0.837151	2.511450
H	2.303030	2.303030	-0.628730	C	0.837151	-2.511451	2.511451
H	-2.303030	2.303030	0.628730	C	-0.837151	4.185750	0.837151
H	2.303030	-2.303030	0.628730	C	0.837151	2.511450	0.837151
H	-2.303030	-2.303030	-0.628730	C	2.511450	0.837151	0.837151
H	-1.462390	3.147110	-1.462390	C	4.185750	-0.837151	0.837151
H	1.462390	-3.147110	-1.462390	C	-2.511451	2.511451	0.837151
H	3.147110	-1.462390	-1.462390	C	-0.837151	0.837151	0.837151
H	-3.147110	1.462390	-1.462390	C	0.837151	-0.837151	0.837151
H	0.625240	0.625240	-3.993480	C	2.511451	-2.511451	0.837151
H	-0.625240	-0.625240	-3.993480	C	-4.185750	0.837151	0.837151
H	-0.625240	0.625240	3.993480	C	-2.511450	-0.837151	0.837151
H	0.625240	-0.625240	3.993480	C	-0.837151	-2.511450	0.837151
H	-0.625240	3.993480	0.625240	C	0.837151	-4.185750	0.837151
H	0.625240	3.993480	-0.625240	C	-0.837151	-0.837151	-4.185750
H	0.625240	-3.993480	0.625240	C	0.837151	0.837151	-4.185750
H	-0.625240	-3.993480	-0.625240	C	-2.511451	-0.837151	-2.511451
H	-3.993480	-0.625240	-0.625240	C	-0.837151	0.837151	-2.511450
H	-3.993480	0.625240	0.625240	C	0.837151	2.511451	-2.511451
H	3.993480	0.625240	-0.625240	C	-0.837151	-2.511451	-2.511451
H	3.993480	-0.625240	0.625240	C	0.837151	-0.837151	-2.511450
				C	2.511451	0.837151	-2.511451
				C	-4.185750	-0.837151	-0.837151
				C	-2.511450	0.837151	-0.837151
				C	-0.837151	2.511450	-0.837151
				C	0.837151	4.185750	-0.837151
				C	-2.511451	-2.511451	-0.837151
				C	-0.837151	-0.837151	-0.837151
				C	0.837151	0.837151	-0.837151
				C	2.511451	2.511451	-0.837151
				C	-0.837151	-4.185750	-0.837151
				C	0.837151	-2.511450	-0.837151
				C	2.511450	-0.837151	-0.837151
				C	4.185750	0.837151	-0.837151
H	0.658182	0.658182	5.681080				
H	-0.658182	-0.658182	5.681080				
H	0.658182	2.332484	4.006780				
H	2.332484	0.658182	4.006780				
H	-2.332484	-0.658182	4.006780				
H	-0.658182	-2.332484	4.006780				
H	0.658182	4.006780	2.332484				
H	2.332482	2.332482	2.332482				
H	4.006780	0.658182	2.332484				
H	-4.006780	-0.658182	2.332484				
H	-2.332482	-2.332482	2.332482				
H	-0.658182	-4.006780	2.332484				
H	0.658182	5.681080	0.658182				

H	-0.658182	5.681080	-0.658182
H	2.332484	4.006780	0.658182
H	4.006780	2.332484	0.658182
H	5.681080	-0.658182	-0.658182
H	5.681080	0.658182	0.658182
H	-2.332484	4.006780	-0.658182
H	4.006780	-2.332484	-0.658182
H	-4.006780	2.332484	-0.658182
H	2.332484	-4.006780	-0.658182
H	-5.681080	0.658182	-0.658182
H	-5.681080	-0.658182	0.658182
H	-4.006780	-2.332484	0.658182
H	-2.332484	-4.006780	0.658182
H	-0.658182	-5.681080	0.658182
H	0.658182	-5.681080	-0.658182
H	0.658182	-0.658182	-5.681080
H	-0.658182	0.658182	-5.681080
H	-0.658182	2.332484	-4.006780
H	2.332484	-0.658182	-4.006780
H	-2.332484	0.658182	-4.006780
H	0.658182	-2.332484	-4.006780
H	-0.658182	4.006780	-2.332484
H	4.006780	-0.658182	-2.332484
H	-2.332482	2.332482	-2.332482
H	2.332482	-2.332482	-2.332482
H	-4.006780	0.658182	-2.332484
H	0.658182	-4.006780	-2.332484
H	-1.495333	1.495333	4.843930
H	1.495333	-1.495333	4.843930
H	-1.495333	3.169632	3.169632
H	3.169632	-1.495333	3.169632
H	-3.169632	1.495333	3.169632
H	1.495333	-3.169632	3.169632
H	-1.495333	4.843930	1.495333
H	4.843930	-1.495333	1.495333
H	-3.169632	3.169632	1.495333
H	3.169632	-3.169632	1.495333
H	-4.843930	1.495333	1.495333
H	1.495333	-4.843930	1.495333
H	-1.495333	-1.495333	-4.843930
H	1.495333	1.495333	-4.843930
H	-3.169632	-1.495333	-3.169632
H	1.495333	3.169632	-3.169632
H	-1.495333	-3.169632	-3.169632
H	3.169632	1.495333	-3.169632
H	-4.843930	-1.495333	-1.495333
H	1.495333	4.843930	-1.495333
H	-3.169632	-3.169632	-1.495333
H	3.169632	3.169632	-1.495333
H	-1.495333	-4.843930	-1.495333
H	4.843930	1.495333	-1.495333

Table S3. A_1 -mode frequencies of tetrahedral and octahedral compounds at the SCC-DFTB level of theory.

A	719.7	A	719.7
O2	486.1	T2	485.5
O3	373.9	T3	376.3
O4	302.7	T4	308.6
O5	254.1	T5	262.5
O6	218.8	T6	229.1
O7	192.1	T7	203.5
O8	171.1	T8	183.3
		T9	166.9
		T10	153.3

Table S4. T_2 -mode vibrational frequencies and Raman intensities of tetrahedral compounds computed at the SCC-DFTB level of theory.

A		T2		T3		T4		T5		T6		T7		T8		T9		T10	
1102.7	0.020	1153.3	0.054	1112.4	0.082	1102.0	0.000	1109.6	0.000	1104.4	0.047	1105.7	0.043	1100.2	0.130	1102.6	0.079	1101.2	0.006
		1197.5	0.000	1124.5	0.000	1115.6	0.056	1114.4	0.012	1107.6	0.093	1107.7	0.007	1100.4	0.000	1104.0	0.028	1102.5	0.000
		1243.6	0.000	1141.4	0.002	1119.6	0.000	1115.1	0.000	1112.2	0.001	1107.7	0.000	1104.7	0.000	1105.5	0.000	1102.6	0.003
		1281.8	0.013	1171.9	0.073	1124.5	0.000	1117.5	0.130	1112.2	0.000	1110.7	0.000	1105.6	0.000	1106.7	0.000	1103.9	0.014
		1297.3	0.000	1203.2	0.000	1132.0	0.105	1125.9	0.008	1114.5	0.064	1115.1	0.004	1107.6	0.000	1107.5	0.011	1104.8	0.000
				1238.2	0.000	1142.8	0.030	1126.4	0.000	1118.5	0.000	1116.6	0.142	1111.4	0.000	1108.9	0.031	1105.1	0.000
				1263.4	0.004	1151.3	0.000	1141.6	0.000	1120.8	0.004	1117.0	0.000	1112.4	0.001	1110.9	0.000	1106.4	0.000
				1267.0	0.000	1173.7	0.016	1142.9	0.011	1123.4	0.000	1118.4	0.000	1113.2	0.000	1111.9	0.000	1107.3	0.020
				1291.2	0.000	1182.2	0.093	1149.8	0.133	1124.9	0.000	1120.4	0.087	1114.2	0.028	1112.9	0.016	1108.1	0.000
						1204.4	0.000	1155.4	0.066	1131.3	0.000	1120.6	0.000	1115.4	0.108	1114.1	0.000	1109.2	0.000
						1235.6	0.000	1166.8	0.000	1132.2	0.008	1125.6	0.000	1116.6	0.063	1114.2	0.005	1109.5	0.042
						1250.8	0.000	1167.7	0.007	1135.2	0.165	1125.6	0.068	1118.6	0.002	1116.1	0.000	1110.6	0.000
						1253.3	0.000	1185.9	0.162	1138.2	0.000	1129.4	0.000	1119.5	0.000	1116.3	0.121	1112.0	0.033
						1268.9	0.000	1194.9	0.010	1141.9	0.000	1130.1	0.029	1120.5	0.000	1116.9	0.004	1113.4	0.026
						1273.1	0.001	1204.9	0.000	1145.0	0.000	1132.5	0.000	1120.6	0.000	1117.4	0.000	1114.2	0.038
						1287.5	0.000	1233.8	0.000	1151.5	0.022	1134.9	0.011	1122.7	0.000	1117.5	0.035	1114.4	0.109
						1290.2	0.000	1246.8	0.001	1160.9	0.000	1136.1	0.000	1124.6	0.000	1119.7	0.056	1114.6	0.000
						1297.3	0.045	1248.3	0.000	1162.6	0.123	1137.5	0.026	1125.0	0.000	1119.8	0.000	1115.6	0.000
								1261.4	0.000	1163.3	0.151	1142.6	0.000	1127.5	0.000	1122.6	0.000	1116.2	0.028
								1269.6	0.000	1173.7	0.021	1146.0	0.178	1128.3	0.046	1123.4	0.008	1117.5	0.000
								1273.5	0.003	1176.4	0.000	1148.8	0.000	1131.3	0.068	1125.2	0.026	1117.8	0.025
								1284.7	0.000	1186.1	0.028	1149.9	0.053	1132.2	0.000	1125.7	0.026	1118.9	0.010
								1287.3	0.000	1191.0	0.237	1153.9	0.000	1133.4	0.000	1126.0	0.000	1120.0	0.000
								1288.7	0.000	1205.0	0.001	1156.4	0.018	1133.8	0.070	1126.6	0.000	1120.4	0.091
								1290.4	0.000	1205.1	0.000	1159.3	0.000	1136.1	0.000	1127.4	0.000	1121.7	0.025
								1294.4	0.084	1232.3	0.000	1159.4	0.013	1137.4	0.157	1128.3	0.008	1121.9	0.000
								1298.0	0.000	1242.4	0.007	1167.0	0.095	1140.0	0.000	1130.2	0.032	1122.8	0.002
										1245.9	0.000	1173.7	0.349	1140.4	0.003	1131.9	0.000	1123.6	0.000
										1256.4	0.000	1178.1	0.000	1144.5	0.000	1132.0	0.144	1123.8	0.000
										1261.7	0.000	1180.3	0.000	1145.0	0.043	1134.0	0.006	1124.2	0.000
										1265.1	0.000	1183.4	0.000	1147.7	0.000	1134.8	0.009	1125.9	0.000
										1270.4	0.000	1189.2	0.010	1147.8	0.013	1136.3	0.000	1126.1	0.004
										1273.2	0.005	1193.6	0.342	1149.2	0.043	1136.8	0.000	1126.2	0.000
										1283.1	0.000	1199.0	0.030	1152.0	0.014	1138.0	0.000	1127.6	0.029
										1285.9	0.000	1205.2	0.000	1154.5	0.149	1138.4	0.000	1128.7	0.000
										1286.4	0.000	1210.9	0.000	1158.1	0.000	1139.8	0.009	1129.4	0.003
										1286.5	0.000	1231.1	0.000	1158.7	0.142	1143.2	0.000	1130.8	0.003
										1287.2	0.000	1239.1	0.016	1159.4	0.000	1143.5	0.006	1131.0	0.000
										1292.5	0.133	1244.1	0.000	1164.8	0.111	1145.4	0.170	1131.8	0.082
										1292.5	0.000	1254.8	0.000	1167.2	0.000	1147.6	0.000	1132.6	0.000
										1293.5	0.003	1259.7	0.000	1170.3	0.013	1147.9	0.000	1132.6	0.093
										1294.5	0.000	1262.8	0.000	1173.1	0.000	1148.0	0.151	1133.6	0.001

1298.1	0.000	1265.8	0.000	1173.2	0.083	1149.4	0.000	1134.4	0.000
		1271.2	0.000	1180.3	0.426	1151.8	0.000	1135.1	0.011
		1272.4	0.007	1184.0	0.048	1152.4	0.151	1135.2	0.000
		1282.2	0.000	1186.3	0.000	1155.0	0.006	1136.4	0.000
		1283.9	0.000	1192.8	0.000	1157.7	0.000	1137.0	0.008
		1284.6	0.000	1192.8	0.031	1159.5	0.004	1137.4	0.000
		1284.7	0.000	1195.9	0.470	1162.7	0.154	1140.0	0.010
		1285.1	0.000	1200.8	0.028	1163.1	0.205	1140.0	0.000
		1286.2	0.000	1205.3	0.000	1164.0	0.000	1141.4	0.260
		1286.6	0.000	1206.3	0.009	1164.9	0.004	1142.1	0.025
		1288.9	0.000	1214.0	0.002	1166.5	0.013	1142.4	0.000
		1290.4	0.009	1230.1	0.000	1167.5	0.000	1143.9	0.000
		1291.0	0.160	1236.7	0.028	1170.3	0.263	1144.3	0.003
		1292.4	0.000	1242.6	0.000	1171.0	0.000	1146.4	0.000
		1294.2	0.027	1252.4	0.000	1178.0	0.133	1146.9	0.002
		1294.6	0.000	1257.5	0.000	1178.1	0.000	1150.1	0.000
		1295.5	0.001	1260.7	0.000	1183.4	0.263	1150.3	0.000
				1262.6	0.000	1185.3	0.184	1151.9	0.000
				1264.1	0.000	1186.1	0.000	1152.8	0.109
				1264.7	0.002	1188.2	0.150	1152.9	0.000
				1271.6	0.000	1190.2	0.000	1154.6	0.168
				1271.8	0.007	1194.6	0.050	1156.6	0.001
				1281.6	0.000	1198.0	0.654	1157.6	0.000
				1282.8	0.000	1201.3	0.000	1159.0	0.250
				1283.5	0.000	1201.8	0.027	1160.1	0.043
				1283.5	0.000	1205.4	0.000	1160.7	0.122
				1284.5	0.000	1207.8	0.002	1160.8	0.000
				1284.6	0.000	1210.8	0.003	1161.6	0.000
				1284.7	0.000	1215.7	0.007	1163.5	0.000
				1286.1	0.000	1229.2	0.000	1165.7	0.035
				1286.9	0.000	1234.7	0.043	1170.1	0.003
				1287.6	0.002	1241.3	0.000	1170.4	0.000
				1289.2	0.000	1249.9	0.000	1172.2	0.591
				1289.3	0.097	1256.3	0.000	1173.2	0.176
				1290.8	0.004	1260.3	0.000	1174.7	0.000
				1291.2	0.101	1262.0	0.000	1175.9	0.000
				1291.3	0.000	1262.2	0.003	1178.9	0.001
				1292.6	0.078	1264.0	0.000	1179.4	0.026
				1292.8	0.000	1264.6	0.000	1180.0	0.000
				1296.7	0.000	1271.7	0.000	1181.7	0.207
				1296.8	0.000	1271.8	0.006	1188.4	0.580
				1299.1	0.000	1281.2	0.000	1189.1	0.000
				1299.9	0.034	1282.3	0.000	1190.6	0.151
						1282.6	0.000	1193.0	0.000
						1282.6	0.000	1195.0	0.000
						1282.8	0.000	1196.1	0.000
						1283.3	0.000	1197.0	0.035
						1284.0	0.000	1199.1	0.846
						1284.4	0.000	1203.2	0.081
						1284.8	0.000	1205.4	0.000
						1285.5	0.000	1207.0	0.000
						1286.1	0.002	1207.5	0.006
						1286.3	0.000	1212.3	0.000
						1286.7	0.000	1213.6	0.000
						1287.8	0.028	1216.4	0.018
						1288.8	0.001	1228.5	0.000
						1289.1	0.000	1233.2	0.061
						1289.4	0.088	1240.1	0.000
						1290.7	0.000	1247.7	0.000
						1291.3	0.269	1255.0	0.000
						1291.9	0.000	1259.2	0.000
						1292.0	0.001	1259.3	0.003
						1293.3	0.000	1261.2	0.000
						1293.8	0.000	1261.6	0.000
						1296.1	0.000	1262.9	0.000
						1297.9	0.014	1264.6	0.000
						1298.0	0.028	1264.8	0.000
						1298.3	0.000	1271.7	0.000
								1271.8	0.007
								1280.9	0.000
								1281.7	0.000
								1281.9	0.000

1281.9	0.000
1282.6	0.000
1282.9	0.000
1283.0	0.000
1283.4	0.000
1283.9	0.000
1284.4	0.000
1285.0	0.001
1285.2	0.000
1285.3	0.000
1286.4	0.000
1286.4	0.001
1286.6	0.000
1286.9	0.007
1287.7	0.004
1288.2	0.000
1288.3	0.059
1289.1	0.000
1290.2	0.000
1290.6	0.000
1290.6	0.445
1291.3	0.000
1291.5	0.000
1293.4	0.000
1293.7	0.000
1294.0	0.000
1295.3	0.000
1295.3	0.000
1296.5	0.048
1299.1	0.000
1299.2	0.000
1299.4	0.000

Table S5. T_2 -mode vibrational frequencies and Raman intensities of octahedral compounds computed at the SCC-DFTB level of theory.

A		O2		O3		O4		O5		O6		O7		O8	
1102.7	0.020	1107.0	0.133	1103.9	0.000	1103.5	0.000	1100.3	0.000	1101.0	0.000	1100.7	0.000	1100.5	0.000
		1152.6	0.075	1112.3	0.088	1105.1	0.000	1101.9	0.000	1103.1	0.059	1101.6	0.379	1100.5	0.093
		1197.9	0.000	1120.8	0.000	1106.9	0.049	1102.0	0.053	1104.0	0.000	1102.0	0.000	1100.6	0.000
		1206.8	0.000	1123.1	0.077	1111.7	0.004	1103.7	0.222	1105.0	0.061	1103.3	0.001	1100.9	0.000
		1240.9	0.000	1141.6	0.013	1113.9	0.000	1107.4	0.000	1105.8	0.077	1103.8	0.000	1101.1	0.018
		1251.0	0.000	1156.3	0.004	1123.4	0.001	1107.4	0.055	1106.9	0.000	1104.0	0.012	1102.1	0.040
		1272.2	0.000	1178.6	0.225	1126.8	0.000	1110.0	0.036	1107.0	0.003	1104.4	0.000	1102.6	0.073
				1200.0	0.000	1132.0	0.001	1112.1	0.017	1107.3	0.000	1105.0	0.006	1102.8	0.000
				1215.9	0.000	1133.5	0.000	1114.4	0.000	1109.9	0.127	1107.0	0.001	1103.1	0.000
				1233.1	0.000	1139.5	0.001	1117.1	0.000	1110.2	0.000	1107.3	0.051	1103.2	0.315
				1236.7	0.000	1146.9	0.000	1118.9	0.021	1112.1	0.019	1107.5	0.000	1104.0	0.011
				1242.7	0.000	1148.2	0.154	1121.3	0.039	1112.5	0.001	1108.5	0.000	1104.2	0.000
				1250.6	0.008	1156.0	0.000	1121.3	0.000	1113.1	0.000	1110.0	0.000	1104.9	0.293
				1266.0	0.000	1163.6	0.498	1124.5	0.071	1113.9	0.000	1110.2	0.112	1105.6	0.000
				1276.8	0.000	1175.9	0.012	1124.9	0.000	1115.9	0.000	1110.7	0.005	1105.8	0.000
				1278.6	0.000	1184.0	0.000	1125.2	0.074	1116.1	0.002	1111.3	0.000	1106.6	0.000
				1287.1	0.008	1200.1	0.000	1127.9	0.000	1119.5	0.000	1111.4	0.001	1106.8	0.046
				1292.2	0.000	1202.4	0.167	1128.5	0.003	1119.6	0.001	1111.7	0.000	1107.3	0.000
				1297.2	0.002	1220.1	0.000	1134.4	0.000	1120.9	0.005	1111.9	0.000	1107.3	0.035
						1229.2	0.000	1135.5	0.000	1121.3	0.000	1112.6	0.000	1107.8	0.189
						1235.4	0.000	1136.0	0.010	1122.5	0.040	1113.7	0.000	1108.2	0.018
						1242.9	0.000	1136.4	0.002	1124.2	0.000	1113.9	0.000	1109.1	0.000
						1247.5	0.004	1140.8	0.014	1124.7	0.000	1114.6	0.017	1109.5	0.024
						1250.9	0.000	1146.7	0.001	1126.0	0.000	1115.0	0.022	1109.8	0.000
						1252.6	0.000	1153.0	0.000	1127.2	0.000	1115.2	0.084	1109.8	0.068
						1255.5	0.002	1153.0	0.004	1128.1	0.000	1115.5	0.000	1110.6	0.000
						1268.0	0.000	1156.0	0.000	1128.3	0.001	1116.0	0.094	1111.3	0.000
						1269.0	0.000	1158.7	0.019	1128.9	0.000	1116.7	0.000	1111.8	0.115
						1276.2	0.000	1165.5	0.001	1130.2	0.005	1117.8	0.002	1111.9	0.000
						1279.1	0.001	1169.1	0.000	1132.9	0.010	1118.8	0.000	1112.7	0.017
						1282.2	0.001	1174.7	0.000	1133.0	0.000	1119.1	0.002	1112.9	0.000
						1284.6	0.000	1177.8	0.000	1136.5	0.000	1121.1	0.000	1113.7	0.003

1288.9	0.001	1181.4	1.147	1137.5	0.000	1121.6	0.099	1113.7	0.000
1289.0	0.000	1187.0	0.000	1137.6	0.019	1122.3	0.000	1114.1	0.000
1295.2	0.002	1198.7	0.014	1140.1	0.000	1123.6	0.004	1115.0	0.000
1296.7	0.000	1200.1	0.000	1141.2	0.253	1124.3	0.011	1115.3	0.026
1298.1	0.000	1202.7	0.002	1142.9	0.000	1124.4	0.000	1116.1	0.000
		1212.1	0.100	1143.9	0.051	1126.0	0.019	1116.7	0.000
		1222.2	0.000	1144.6	0.076	1126.0	0.021	1116.9	0.015
		1227.1	0.000	1145.6	0.000	1126.5	0.000	1117.0	0.016
		1234.3	0.000	1149.1	0.000	1127.4	0.017	1117.9	0.002
		1244.3	0.000	1150.5	0.009	1127.7	0.000	1118.3	0.000
		1246.0	0.000	1153.0	0.000	1127.8	0.000	1118.6	0.000
		1246.6	0.003	1153.2	0.014	1129.8	0.001	1119.2	0.000
		1251.4	0.002	1156.6	0.096	1129.9	0.007	1119.6	0.000
		1251.5	0.000	1160.8	0.000	1130.9	0.000	1119.9	0.004
		1251.7	0.000	1161.2	0.000	1131.2	0.000	1120.1	0.000
		1256.0	0.001	1161.7	0.023	1132.6	0.010	1122.1	0.000
		1261.0	0.000	1165.7	0.006	1133.1	0.013	1122.3	0.000
		1264.0	0.000	1166.3	0.000	1133.5	0.000	1122.6	0.000
		1270.4	0.000	1170.8	0.071	1134.4	0.000	1123.4	0.020
		1271.9	0.000	1173.1	0.014	1135.2	0.005	1123.6	0.000
		1275.0	0.000	1176.8	0.005	1135.7	0.003	1123.6	0.000
		1279.0	0.000	1181.3	0.034	1136.1	0.000	1123.6	0.000
		1279.1	0.000	1182.6	0.000	1137.4	0.002	1124.4	0.001
		1281.0	0.001	1185.2	0.915	1137.8	0.009	1125.1	0.001
		1282.4	0.000	1188.8	0.168	1138.3	0.000	1125.6	0.000
		1283.7	0.001	1194.8	0.387	1139.2	0.001	1126.3	0.007
		1286.3	0.000	1197.0	0.335	1139.7	0.001	1126.4	0.000
		1288.9	0.000	1197.3	0.000	1139.8	0.000	1126.6	0.000
		1289.9	0.004	1200.1	0.000	1143.8	0.001	1126.7	0.006
		1293.9	0.001	1203.0	0.000	1144.8	0.000	1127.2	0.002
		1294.6	0.000	1209.6	0.009	1145.4	0.000	1127.7	0.000
		1294.7	0.001	1211.5	0.007	1146.6	0.000	1127.9	0.000
		1296.1	0.000	1215.6	0.046	1147.0	0.112	1129.0	0.000
		1298.3	0.000	1223.3	0.000	1147.6	0.001	1129.0	0.222
		1299.2	0.000	1226.1	0.000	1149.8	0.000	1129.8	0.001
		1299.3	0.000	1233.7	0.000	1150.8	0.007	1129.9	0.000
				1243.7	0.000	1150.8	0.000	1130.0	0.018
				1245.8	0.000	1151.9	0.086	1130.6	0.000
				1246.2	0.003	1152.9	0.010	1130.8	0.000
				1248.5	0.001	1154.3	0.063	1131.0	0.000
				1249.1	0.000	1155.7	0.275	1131.6	0.008
				1250.9	0.000	1156.5	0.000	1132.5	0.021
				1253.6	0.002	1157.2	0.000	1133.2	0.000
				1255.2	0.000	1158.0	0.000	1133.3	0.004
				1256.0	0.000	1158.1	0.014	1134.0	0.000
				1256.4	0.000	1163.1	0.002	1134.4	0.001
				1259.4	0.000	1163.6	0.000	1134.4	0.000
				1266.4	0.000	1166.8	0.000	1135.8	0.001
				1266.5	0.000	1167.2	0.005	1136.0	0.005
				1270.4	0.000	1169.8	0.164	1136.2	0.000
				1274.2	0.001	1171.5	0.001	1137.2	0.000
				1275.5	0.000	1173.3	0.000	1137.2	0.047
				1276.0	0.000	1173.4	0.086	1138.5	0.047
				1277.0	0.000	1174.2	0.000	1138.5	0.000
				1279.1	0.002	1176.7	0.000	1138.8	0.003
				1280.1	0.000	1176.8	0.009	1140.0	0.015
				1282.5	0.004	1181.3	0.016	1140.3	0.000
				1283.1	0.000	1183.9	0.000	1140.4	0.004
				1284.5	0.000	1184.6	0.000	1141.1	0.000
				1286.1	0.000	1185.3	0.025	1141.4	0.000
				1286.4	0.000	1189.6	0.111	1142.4	0.000
				1287.9	0.001	1191.0	0.961	1143.1	0.001
				1289.2	0.000	1192.6	1.502	1143.5	0.001
				1289.9	0.008	1195.3	0.080	1144.8	0.000
				1290.8	0.002	1196.9	0.001	1145.9	0.008
				1292.0	0.000	1198.7	0.000	1146.3	0.000
				1292.6	0.001	1200.1	0.000	1147.5	0.067
				1292.8	0.000	1202.4	0.006	1147.7	0.000
				1294.4	0.000	1206.5	0.111	1147.8	0.011
				1295.1	0.000	1207.7	0.000	1148.3	0.001
				1296.0	0.000	1208.4	0.134	1148.9	0.000
				1296.7	0.000	1210.7	0.000	1149.5	0.000

1299.9	0.001	1214.4	0.005	1150.9	0.001
1300.0	0.000	1215.4	0.015	1151.3	0.000
		1216.4	0.008	1152.2	0.019
		1223.8	0.000	1155.0	0.000
		1225.5	0.000	1155.1	0.018
		1233.4	0.000	1156.3	0.000
		1243.1	0.000	1156.7	0.004
		1245.7	0.000	1159.0	0.000
		1245.8	0.004	1159.2	0.000
		1246.6	0.000	1159.9	0.011
		1247.2	0.000	1160.9	0.000
		1249.8	0.000	1161.3	0.064
		1252.5	0.002	1162.5	0.034
		1252.9	0.000	1162.7	0.000
		1254.3	0.001	1163.1	0.000
		1254.6	0.000	1164.1	0.176
		1255.9	0.000	1165.4	0.000
		1256.3	0.000	1165.5	0.589
		1257.5	0.000	1166.8	0.000
		1261.7	0.000	1167.5	0.068
		1262.2	0.000	1168.3	0.023
		1268.5	0.000	1168.4	0.007
		1268.8	0.000	1172.0	0.000
		1270.0	0.000	1174.1	0.024
		1273.8	0.000	1175.2	0.000
		1274.3	0.000	1175.4	0.002
		1276.3	0.000	1176.2	0.091
		1276.8	0.000	1177.0	0.001
		1278.6	0.006	1178.2	0.009
		1279.1	0.001	1179.0	0.000
		1280.1	0.000	1179.7	0.000
		1281.5	0.000	1181.6	0.000
		1282.8	0.006	1183.3	0.006
		1283.4	0.000	1186.1	0.000
		1283.9	0.001	1187.9	0.102
		1285.4	0.000	1188.6	0.055
		1285.8	0.000	1189.9	0.046
		1285.9	0.002	1191.0	0.171
		1287.3	0.000	1191.2	0.000
		1287.3	0.001	1192.6	0.000
		1287.6	0.000	1193.6	0.031
		1288.9	0.004	1195.7	3.699
		1288.9	0.000	1198.7	0.000
		1289.3	0.009	1199.1	0.000
		1290.3	0.000	1199.3	0.068
		1290.9	0.005	1200.1	0.012
		1291.1	0.000	1200.1	0.009
		1291.7	0.001	1202.2	0.003
		1292.1	0.000	1203.7	0.058
		1292.9	0.000	1205.7	0.004
		1294.4	0.001	1206.9	0.006
		1295.9	0.000	1207.6	0.000
		1296.1	0.001	1210.2	0.000
		1296.8	0.012	1213.0	0.000
		1297.9	0.000	1213.1	0.018
		1298.5	0.008	1214.2	0.067
		1299.1	0.000	1214.3	0.000
		1299.9	0.000	1215.7	0.012
				1216.3	0.000
				1217.1	0.007
				1224.2	0.000
				1225.2	0.000
				1233.2	0.000
				1242.5	0.000
				1244.7	0.002
				1245.2	0.000
				1246.1	0.002
				1246.2	0.000
				1248.5	0.000
				1251.4	0.002
				1252.0	0.000
				1252.9	0.001

1253.5	0.000
1254.4	0.000
1254.7	0.000
1255.3	0.001
1256.7	0.000
1257.2	0.000
1258.6	0.000
1260.5	0.000
1264.2	0.000
1264.9	0.000
1269.1	0.000
1269.4	0.000
1271.0	0.000
1273.1	0.000
1274.3	0.000
1276.3	0.000
1276.8	0.000
1277.9	0.000
1278.0	0.006
1279.6	0.004
1280.3	0.000
1280.9	0.006
1281.9	0.005
1282.5	0.000
1284.0	0.000
1284.2	0.000
1284.9	0.001
1285.1	0.000
1285.2	0.000
1285.3	0.000
1285.5	0.000
1286.1	0.000
1286.5	0.000
1286.6	0.001
1287.4	0.000
1287.4	0.000
1287.5	0.000
1287.8	0.009
1288.1	0.000
1288.7	0.000
1289.7	0.000
1290.0	0.028
1290.3	0.001
1291.8	0.000
1291.9	0.000
1292.6	0.005
1293.8	0.000
1294.3	0.000
1294.3	0.002
1295.3	0.000
1295.8	0.000
1296.4	0.001
1296.9	0.000
1296.9	0.020
1297.8	0.000
1298.2	0.000
1298.8	0.004
1299.0	0.000
1299.6	0.009

Table S6. T_2 -mode vibrational frequencies and Raman intensities of tetrahedral compounds computed at the SCC-DFTB level of theory with masses of hydrogen set to 10,000 amu.

A		T2		T3		T4		T5		T6		T7		T8		T9		T10	
1120.1	0.000	1133.3	0.000	1101.5	0.000	1103.6	0.016	1100.2	0.005	1102.8	0.008	1100.5	0.000	1101.5	0.000	1100.4	0.042	1100.4	0.000
1161.6	0.000	1136.0	0.005	1118.2	0.000	1108.8	0.011	1106.8	0.000	1105.7	0.000	1102.7	0.002	1101.6	0.006	1101.8	0.000	1101.2	0.000

1200.2	0.010	1145.5	0.000	1122.5	0.004	1111.5	0.000	1110.0	0.002	1107.4	0.000	1103.3	0.000	1103.1	0.000	1102.4	0.001	1101.7	0.000
1249.7	0.068	1153.9	0.059	1138.7	0.052	1125.1	0.000	1115.7	0.000	1109.7	0.000	1104.2	0.000	1103.1	0.001	1102.8	0.000	1102.9	0.000
		1184.2	0.000	1139.3	0.000	1125.9	0.002	1120.6	0.000	1112.2	0.013	1104.8	0.017	1104.6	0.000	1103.9	0.000	1103.4	0.000
		1205.7	0.074	1149.6	0.002	1130.4	0.000	1121.7	0.020	1114.4	0.026	1108.7	0.000	1106.7	0.010	1105.5	0.000	1104.6	0.005
		1211.8	0.000	1161.8	0.049	1138.9	0.017	1126.1	0.000	1119.6	0.000	1108.8	0.001	1108.0	0.000	1105.6	0.000	1104.9	0.000
		1258.9	0.101	1164.5	0.000	1142.6	0.000	1129.1	0.014	1121.4	0.001	1111.8	0.004	1108.1	0.006	1106.4	0.000	1105.2	0.001
				1178.5	0.197	1147.8	0.050	1131.5	0.025	1121.9	0.000	1112.6	0.000	1109.6	0.000	1107.0	0.000	1106.5	0.000
				1186.9	0.006	1154.5	0.000	1134.5	0.004	1123.5	0.000	1114.6	0.000	1112.2	0.017	1107.6	0.000	1107.2	0.000
				1191.4	0.000	1157.4	0.030	1136.1	0.000	1128.3	0.012	1116.1	0.002	1112.8	0.000	1108.9	0.008	1107.8	0.006
				1207.4	0.002	1160.9	0.000	1143.6	0.037	1128.4	0.000	1121.1	0.004	1114.2	0.001	1110.3	0.000	1108.6	0.000
				1221.9	0.050	1165.5	0.013	1145.5	0.000	1129.2	0.000	1121.5	0.000	1115.8	0.026	1111.5	0.000	1110.1	0.010
				1238.6	0.000	1166.3	0.173	1151.4	0.000	1134.8	0.000	1123.6	0.000	1116.2	0.000	1111.5	0.004	1111.2	0.001
				1265.2	0.162	1178.2	0.038	1153.5	0.000	1136.8	0.000	1125.3	0.015	1117.3	0.000	1112.5	0.011	1111.4	0.000
						1184.1	0.083	1154.8	0.000	1139.3	0.032	1126.4	0.001	1118.6	0.000	1113.4	0.000	1111.5	0.000
						1191.4	0.000	1158.3	0.008	1141.1	0.004	1127.1	0.000	1119.4	0.002	1113.6	0.002	1112.4	0.000
						1191.6	0.250	1158.4	0.000	1143.2	0.078	1129.2	0.040	1121.3	0.001	1113.8	0.013	1113.0	0.004
						1208.8	0.025	1159.1	0.008	1143.6	0.000	1129.2	0.000	1121.6	0.000	1115.3	0.000	1113.0	0.000
						1218.0	0.000	1163.3	0.095	1147.0	0.014	1130.6	0.007	1123.4	0.010	1118.2	0.000	1114.0	0.005
						1226.4	0.012	1169.1	0.146	1147.4	0.000	1131.5	0.000	1125.4	0.014	1118.6	0.002	1115.3	0.000
						1237.8	0.018	1169.3	0.000	1149.8	0.000	1133.0	0.000	1126.4	0.000	1120.8	0.000	1115.4	0.023
						1251.0	0.000	1170.6	0.000	1154.5	0.003	1133.6	0.008	1127.5	0.003	1121.6	0.000	1116.2	0.000
						1269.0	0.235	1177.7	0.359	1156.2	0.001	1136.3	0.000	1127.5	0.000	1121.9	0.000	1117.4	0.000
								1181.9	0.001	1156.8	0.000	1138.8	0.014	1129.5	0.000	1123.0	0.000	1117.4	0.001
								1185.3	0.117	1160.6	0.000	1139.6	0.000	1129.9	0.007	1124.2	0.000	1118.0	0.000
								1185.3	0.000	1161.7	0.065	1141.2	0.018	1130.9	0.000	1124.5	0.002	1118.2	0.000
								1195.6	0.226	1163.1	0.000	1141.3	0.000	1131.3	0.000	1124.8	0.000	1118.8	0.002
								1198.0	0.093	1163.3	0.001	1144.3	0.030	1134.4	0.005	1125.9	0.004	1119.7	0.016
								1208.5	0.078	1165.2	0.123	1146.0	0.000	1134.7	0.001	1126.4	0.000	1119.9	0.000
								1211.5	0.000	1170.9	0.000	1147.2	0.016	1135.0	0.000	1127.0	0.015	1120.3	0.025
								1222.1	0.017	1173.3	0.055	1149.8	0.007	1137.6	0.000	1127.4	0.000	1120.9	0.000
								1234.0	0.000	1175.9	0.154	1151.0	0.000	1137.9	0.004	1128.5	0.026	1122.3	0.001
								1237.5	0.019	1178.7	0.311	1152.3	0.000	1139.4	0.013	1129.0	0.000	1123.2	0.001
								1250.9	0.005	1179.9	0.000	1152.7	0.058	1140.4	0.000	1129.4	0.000	1123.6	0.000
								1257.9	0.000	1182.3	0.101	1155.7	0.000	1141.8	0.000	1130.2	0.000	1123.8	0.004
								1271.6	0.319	1185.6	0.063	1157.1	0.026	1141.8	0.002	1130.8	0.026	1124.6	0.009
										1186.5	0.000	1158.3	0.001	1142.9	0.126	1132.1	0.000	1124.7	0.000
										1188.7	0.329	1159.1	0.000	1143.7	0.000	1133.5	0.002	1126.1	0.000
										1196.8	0.000	1160.1	0.000	1144.4	0.000	1134.0	0.000	1127.8	0.000
										1196.9	0.486	1160.3	0.000	1145.1	0.003	1134.8	0.000	1128.1	0.000
										1201.9	0.030	1162.9	0.113	1146.2	0.001	1134.9	0.001	1128.3	0.006
										1204.9	0.000	1164.4	0.040	1147.2	0.000	1136.8	0.032	1129.1	0.003
										1206.7	0.057	1165.8	0.000	1151.0	0.000	1137.4	0.000	1129.8	0.000
										1210.9	0.002	1168.1	0.070	1151.7	0.000	1138.0	0.000	1130.8	0.000
										1221.5	0.054	1168.2	0.000	1153.5	0.000	1139.5	0.009	1130.8	0.003
										1225.3	0.000	1170.9	0.000	1154.2	0.005	1139.9	0.000	1131.8	0.000
										1235.3	0.005	1173.2	0.223	1156.7	0.000	1140.9	0.043	1131.9	0.001
										1244.1	0.000	1174.3	0.000	1157.3	0.029	1141.2	0.000	1133.0	0.000
										1245.4	0.029	1176.1	0.122	1158.4	0.020	1141.5	0.000	1133.7	0.000
										1258.9	0.002	1178.4	0.005	1159.3	0.000	1142.9	0.023	1134.0	0.005
										1262.3	0.000	1180.8	0.098	1160.2	0.000	1143.3	0.000	1134.4	0.003
										1273.6	0.411	1182.6	0.000	1160.2	0.010	1144.4	0.000	1135.2	0.000
												1185.5	0.879	1161.3	0.000	1145.5	0.000	1136.0	0.000
												1187.8	0.000	1161.8	0.203	1145.9	0.002	1136.8	0.000
												1188.1	0.023	1164.1	0.020	1146.7	0.000	1137.1	0.000
												1192.8	0.279	1164.5	0.003	1148.3	0.040	1137.8	0.059
												1193.0	0.000	1165.6	0.013	1148.9	0.008	1138.2	0.010
												1194.1	0.033	1166.3	0.000	1149.8	0.000	1139.3	0.000
												1195.1	0.322	1169.9	0.004	1150.9	0.031	1139.4	0.000

1199.6	0.003	1170.2	0.000	1151.7	0.000	1139.9	0.000
1200.3	0.000	1172.1	0.000	1153.0	0.009	1140.2	0.004
1203.8	0.496	1172.6	0.293	1153.3	0.000	1141.7	0.038
1213.1	0.016	1173.6	0.057	1154.3	0.005	1142.7	0.000
1213.2	0.000	1174.4	0.000	1154.9	0.000	1142.8	0.037
1220.8	0.007	1175.7	0.003	1155.1	0.005	1143.0	0.001
1222.0	0.000	1177.4	0.048	1157.0	0.000	1143.8	0.000
1222.5	0.001	1179.9	0.369	1157.8	0.001	1145.2	0.000
1231.5	0.026	1180.1	0.000	1158.4	0.000	1145.5	0.012
1235.0	0.000	1182.6	0.004	1159.5	0.041	1146.5	0.031
1244.8	0.001	1183.2	0.000	1160.5	0.000	1147.3	0.000
1250.9	0.000	1184.0	0.011	1161.4	0.003	1147.4	0.023
1251.8	0.045	1185.7	0.485	1162.9	0.016	1147.6	0.000
1263.8	0.001	1187.6	0.000	1163.2	0.118	1148.3	0.009
1265.5	0.000	1189.6	0.000	1163.6	0.000	1149.3	0.000
1275.1	0.512	1190.3	0.753	1164.5	0.000	1150.0	0.000
		1193.0	0.739	1165.7	0.097	1150.4	0.000
		1196.0	0.000	1166.1	0.070	1151.3	0.000
		1196.2	0.028	1166.5	0.000	1152.2	0.005
		1196.9	0.007	1166.8	0.002	1153.6	0.000
		1198.0	0.000	1168.2	0.000	1155.0	0.000
		1198.1	0.456	1170.5	0.153	1155.1	0.007
		1203.9	0.066	1170.6	0.000	1155.9	0.000
		1205.6	0.182	1171.3	0.000	1155.9	0.000
		1208.3	0.140	1171.4	0.144	1156.3	0.058
		1208.6	0.000	1173.6	0.004	1156.6	0.000
		1212.5	0.000	1176.8	0.080	1156.6	0.010
		1212.9	0.087	1177.0	0.158	1157.7	0.000
		1222.7	0.018	1178.7	0.000	1158.4	0.002
		1224.5	0.000	1180.0	0.232	1159.6	0.000
		1228.9	0.008	1180.2	0.000	1159.9	0.006
		1233.7	0.000	1181.8	0.000	1161.0	0.054
		1234.5	0.000	1181.8	0.051	1161.1	0.000
		1239.4	0.012	1183.6	0.437	1161.7	0.009
		1242.5	0.000	1183.6	0.000	1162.3	0.000
		1251.3	0.000	1184.0	0.000	1162.9	0.131
		1255.8	0.000	1184.9	0.058	1163.0	0.000
		1256.8	0.065	1188.6	0.383	1163.4	0.014
		1267.2	0.002	1190.3	0.360	1165.1	0.001
		1267.9	0.000	1190.8	0.680	1165.4	0.000
		1276.3	0.620	1192.7	0.000	1166.2	0.016
				1193.3	0.000	1167.4	0.003
				1194.4	0.922	1167.6	0.000
				1194.5	0.000	1170.3	0.000
				1194.7	0.100	1170.7	0.175
				1197.5	0.003	1171.3	0.127
				1198.0	0.000	1171.5	0.000
				1199.3	0.862	1171.8	0.151
				1200.7	0.117	1173.3	0.191
				1201.7	0.000	1173.8	0.000
				1203.4	0.000	1174.6	0.005
				1205.7	0.139	1175.7	0.055
				1208.2	0.000	1176.4	0.009
				1209.0	0.265	1177.6	0.000
				1211.4	0.000	1179.5	0.173
				1213.3	0.002	1180.0	0.000
				1218.4	0.010	1180.2	0.006
				1220.5	0.000	1181.1	0.228

1222.2	0.047	1181.8	0.000
1223.3	0.000	1182.5	0.055
1231.1	0.009	1182.5	0.000
1232.9	0.000	1184.0	0.052
1235.2	0.013	1185.0	0.000
1241.6	0.000	1186.0	0.758
1243.0	0.000	1186.9	0.000
1245.7	0.006	1187.9	0.142
1248.5	0.000	1189.9	0.000
1256.2	0.001	1190.3	0.998
1259.4	0.000	1191.3	0.134
1260.6	0.089	1192.5	0.001
1269.7	0.003	1192.7	0.000
1269.9	0.000	1193.1	0.457
1277.3	0.736	1193.5	0.000
		1195.1	1.704
		1196.5	0.000
		1197.7	0.082
		1198.7	0.246
		1198.9	0.000
		1199.4	0.306
		1201.2	0.004
		1201.8	0.501
		1204.3	0.000
		1205.1	0.004
		1205.6	0.000
		1206.8	0.002
		1208.4	0.423
		1210.8	0.135
		1212.0	0.000
		1213.6	0.000
		1215.6	0.015
		1217.8	0.008
		1221.3	0.000
		1222.4	0.000
		1226.7	0.004
		1227.9	0.000
		1229.5	0.027
		1232.9	0.000
		1237.7	0.003
		1239.5	0.000
		1240.8	0.020
		1247.4	0.000
		1249.0	0.000
		1250.8	0.004
		1253.3	0.000
		1260.0	0.002
		1262.3	0.000
		1263.5	0.118
		1271.5	0.000
		1271.6	0.004
		1278.1	0.859

Table S7. T_2 -mode vibrational frequencies and Raman intensities of octahedral compounds computed at the SCC-DFTB level of theory with masses of hydrogen set to 10,000 amu.

A		O2		O3		O4		O5		O6		O7		O8	
1120.1	0.000	1100.2	0.000	1101.8	0.000	1101.9	0.000	1103.4	0.000	1101.8	0.000	1100.2	0.000	1101.2	0.000
1161.6	0.000	1125.1	0.003	1115.9	0.000	1105.8	0.000	1107.3	0.000	1103.0	0.000	1101.5	0.000	1101.8	0.000
1200.2	0.010	1143.1	0.000	1119.1	0.000	1107.5	0.001	1109.0	0.000	1103.6	0.000	1101.8	0.000	1102.4	0.000
1249.7	0.068	1149.2	0.000	1129.0	0.000	1110.7	0.000	1109.4	0.000	1103.8	0.000	1102.4	0.001	1102.6	0.000
		1151.3	0.000	1129.8	0.000	1113.0	0.000	1109.5	0.000	1104.6	0.000	1104.0	0.000	1102.9	0.000
		1180.9	0.000	1134.3	0.002	1114.2	0.003	1110.0	0.000	1105.7	0.000	1104.1	0.000	1103.4	0.001
		1181.7	0.015	1134.9	0.000	1117.0	0.000	1111.8	0.000	1106.5	0.000	1104.3	0.000	1104.1	0.000
		1183.7	0.021	1143.9	0.000	1117.4	0.000	1113.5	0.000	1107.3	0.001	1106.0	0.000	1104.6	0.000
		1214.5	0.000	1145.4	0.000	1120.5	0.000	1115.3	0.000	1108.4	0.002	1107.0	0.000	1105.3	0.000
		1222.9	0.010	1156.6	0.000	1122.4	0.000	1115.7	0.000	1111.0	0.000	1107.3	0.000	1105.9	0.000
		1237.8	0.091	1160.4	0.010	1125.0	0.000	1116.8	0.000	1111.6	0.000	1107.6	0.000	1106.2	0.000
		1258.5	0.150	1164.9	0.000	1129.2	0.000	1120.3	0.001	1111.7	0.000	1108.3	0.000	1106.5	0.000
				1171.3	0.000	1129.8	0.001	1121.1	0.000	1111.7	0.000	1108.3	0.000	1107.0	0.000
				1172.8	0.000	1131.2	0.000	1122.2	0.000	1111.7	0.000	1109.1	0.000	1107.8	0.000
				1173.7	0.004	1133.7	0.000	1123.9	0.000	1112.8	0.000	1109.9	0.000	1108.0	0.000
				1182.7	0.000	1136.1	0.000	1126.0	0.000	1113.3	0.000	1110.5	0.000	1108.2	0.000
				1190.8	0.000	1143.5	0.000	1126.4	0.005	1114.2	0.000	1111.9	0.000	1109.0	0.000
				1194.8	0.043	1146.2	0.000	1127.1	0.000	1115.1	0.000	1112.4	0.000	1109.1	0.000
				1199.4	0.022	1148.6	0.000	1128.4	0.001	1116.1	0.000	1112.6	0.000	1109.4	0.000
				1203.6	0.189	1149.1	0.000	1130.4	0.001	1117.1	0.000	1113.6	0.000	1109.7	0.000
				1213.4	0.000	1154.6	0.000	1131.2	0.001	1117.7	0.001	1114.2	0.001	1109.9	0.000
				1218.4	0.004	1156.5	0.001	1132.7	0.000	1118.5	0.000	1114.5	0.000	1110.4	0.000
				1238.6	0.000	1159.2	0.000	1135.5	0.000	1120.8	0.000	1115.6	0.000	1110.7	0.000
				1241.1	0.179	1161.5	0.004	1136.2	0.000	1121.7	0.001	1115.7	0.000	1110.7	0.000
				1254.9	0.017	1164.7	0.000	1140.1	0.006	1122.7	0.000	1115.9	0.000	1111.4	0.000
				1264.3	0.242	1167.3	0.001	1140.4	0.000	1123.1	0.000	1116.2	0.001	1111.8	0.000
						1167.6	0.000	1141.7	0.000	1123.4	0.000	1116.4	0.000	1112.5	0.000
						1173.1	0.000	1143.0	0.000	1123.6	0.000	1117.4	0.000	1112.7	0.000
						1175.6	0.000	1144.5	0.000	1123.8	0.000	1117.9	0.000	1113.8	0.000
						1176.7	0.018	1145.4	0.000	1124.5	0.000	1118.3	0.000	1114.0	0.000
						1177.4	0.000	1147.3	0.000	1125.2	0.000	1118.8	0.001	1114.6	0.000
						1179.6	0.024	1148.5	0.000	1127.9	0.000	1119.0	0.000	1115.4	0.000
						1182.2	0.000	1148.6	0.000	1128.2	0.000	1119.9	0.000	1115.4	0.000
						1185.5	0.002	1152.0	0.000	1128.3	0.000	1120.5	0.000	1115.5	0.000
						1189.9	0.072	1155.0	0.000	1129.5	0.000	1120.6	0.000	1116.1	0.000
						1193.0	0.008	1155.9	0.000	1130.0	0.000	1121.0	0.000	1116.5	0.000
						1199.1	0.000	1156.5	0.000	1131.2	0.000	1121.4	0.003	1116.8	0.000
						1200.7	0.010	1158.6	0.000	1131.5	0.000	1122.1	0.000	1117.2	0.000
						1202.5	0.446	1159.0	0.001	1133.2	0.000	1122.2	0.000	1117.3	0.001
						1204.6	0.105	1160.8	0.000	1133.9	0.000	1123.5	0.001	1117.8	0.000
						1205.1	0.000	1161.9	0.000	1134.4	0.000	1124.0	0.000	1117.8	0.000
						1216.0	0.000	1163.1	0.000	1136.6	0.000	1124.6	0.001	1118.1	0.000
						1222.0	0.080	1168.6	0.000	1137.1	0.000	1124.8	0.000	1118.5	0.000
						1230.1	0.001	1169.6	0.000	1137.5	0.000	1125.5	0.000	1118.9	0.000
						1230.2	0.000	1170.5	0.002	1138.7	0.001	1125.9	0.000	1119.1	0.000
						1239.2	0.018	1171.4	0.000	1139.2	0.000	1126.3	0.000	1119.8	0.000
						1248.1	0.000	1172.3	0.000	1140.0	0.000	1126.7	0.000	1120.1	0.000
						1248.7	0.332	1174.2	0.002	1142.1	0.001	1128.2	0.001	1120.2	0.000
						1259.9	0.036	1175.5	0.000	1143.0	0.000	1128.6	0.000	1120.5	0.000
						1271.2	0.260	1176.2	0.000	1144.0	0.001	1129.4	0.000	1121.2	0.000
								1178.8	0.000	1144.4	0.007	1129.6	0.000	1121.7	0.000
								1180.5	0.000	1145.8	0.000	1130.0	0.000	1122.1	0.000
								1182.2	0.000	1146.3	0.000	1130.4	0.000	1122.6	0.000
								1185.1	0.000	1146.9	0.008	1131.1	0.000	1122.9	0.000
								1185.6	0.001	1148.0	0.001	1131.9	0.001	1123.3	0.000
								1188.2	0.000	1148.5	0.000	1132.8	0.000	1123.4	0.000
								1188.3	0.014	1150.7	0.001	1133.2	0.000	1123.9	0.000

1193.4	0.059	1151.1	0.000	1133.7	0.000	1124.8	0.001
1194.9	0.000	1152.5	0.000	1134.2	0.000	1125.0	0.000
1196.2	0.027	1153.4	0.001	1135.3	0.000	1125.5	0.000
1197.9	0.000	1154.1	0.000	1135.4	0.000	1126.0	0.000
1198.2	0.254	1155.6	0.001	1135.8	0.000	1126.2	0.000
1199.1	0.279	1157.0	0.000	1136.8	0.000	1127.7	0.000
1202.0	0.579	1157.2	0.002	1137.1	0.000	1127.7	0.000
1202.5	0.179	1157.7	0.000	1138.9	0.000	1128.1	0.000
1204.0	0.000	1159.0	0.001	1139.1	0.000	1128.1	0.000
1207.1	0.082	1160.8	0.000	1140.0	0.000	1128.5	0.000
1213.0	0.007	1161.3	0.000	1140.3	0.000	1128.5	0.000
1214.9	0.000	1162.2	0.002	1140.6	0.001	1129.0	0.000
1215.4	0.001	1165.0	0.000	1141.6	0.000	1129.0	0.000
1224.2	0.002	1166.4	0.005	1141.7	0.002	1129.1	0.001
1224.2	0.000	1166.6	0.000	1142.5	0.000	1129.8	0.000
1232.5	0.000	1166.9	0.000	1142.6	0.001	1130.4	0.000
1234.2	0.141	1167.1	0.001	1142.9	0.000	1131.0	0.001
1243.3	0.006	1169.5	0.000	1143.7	0.000	1131.1	0.000
1244.2	0.000	1169.5	0.000	1143.9	0.000	1131.8	0.000
1245.7	0.137	1169.5	0.000	1144.7	0.000	1132.0	0.000
1253.3	0.000	1169.5	0.000	1145.6	0.000	1132.6	0.000
1256.5	0.354	1171.0	0.001	1146.7	0.000	1132.8	0.001
1265.8	0.009	1172.8	0.000	1147.3	0.000	1133.3	0.000
1274.2	0.338	1174.1	0.003	1147.8	0.001	1133.5	0.000
		1175.2	0.000	1148.5	0.000	1133.9	0.006
		1175.8	0.003	1148.8	0.001	1134.7	0.001
		1176.8	0.001	1150.3	0.000	1134.9	0.000
		1178.0	0.012	1152.0	0.000	1135.6	0.000
		1178.1	0.000	1152.0	0.001	1135.7	0.000
		1179.2	0.005	1152.9	0.000	1135.9	0.004
		1180.2	0.019	1153.9	0.000	1136.5	0.002
		1183.0	0.000	1154.0	0.002	1137.1	0.001
		1183.4	0.002	1155.0	0.000	1137.3	0.000
		1184.1	0.000	1155.4	0.002	1138.0	0.000
		1184.8	0.000	1155.5	0.001	1138.2	0.000
		1186.7	0.000	1156.6	0.000	1138.2	0.003
		1187.5	0.007	1157.0	0.000	1138.4	0.001
		1188.3	0.000	1157.3	0.002	1139.0	0.000
		1189.4	0.000	1158.0	0.031	1139.3	0.000
		1191.9	0.000	1159.1	0.000	1139.9	0.000
		1192.3	0.007	1159.2	0.000	1140.3	0.000
		1192.7	0.000	1160.1	0.001	1140.4	0.000
		1194.8	0.000	1161.3	0.000	1141.4	0.000
		1195.5	0.010	1162.2	0.000	1141.5	0.000
		1197.8	0.018	1162.8	0.000	1141.8	0.000
		1198.2	0.000	1163.7	0.001	1142.0	0.000
		1198.2	0.000	1164.1	0.000	1142.4	0.000
		1200.8	1.841	1165.5	0.000	1142.5	0.000
		1202.0	0.048	1165.6	0.000	1143.3	0.000
		1202.4	0.556	1166.3	0.000	1143.6	0.000
		1204.6	0.000	1166.7	0.000	1143.8	0.000
		1204.7	0.061	1167.3	0.000	1144.5	0.000
		1205.4	0.000	1167.7	0.001	1145.3	0.000
		1209.0	0.000	1168.7	0.000	1145.7	0.001
		1209.3	0.029	1169.3	0.001	1146.0	0.000
		1211.8	0.031	1170.8	0.000	1146.5	0.000
		1214.6	0.003	1171.5	0.000	1146.9	0.000
		1216.2	0.003	1173.1	0.001	1148.0	0.000

1219.4	0.007	1173.3	0.000	1148.3	0.000
1224.4	0.000	1174.0	0.000	1149.2	0.000
1225.8	0.000	1174.9	0.000	1149.4	0.000
1227.9	0.006	1175.0	0.000	1149.8	0.001
1228.1	0.000	1176.1	0.003	1150.0	0.000
1236.7	0.000	1176.5	0.001	1150.9	0.000
1237.2	0.069	1177.6	0.000	1151.6	0.000
1241.2	0.000	1178.4	0.001	1151.7	0.000
1241.7	0.184	1178.7	0.000	1152.2	0.000
1249.2	0.086	1178.9	0.004	1152.6	0.000
1250.6	0.171	1180.3	0.031	1153.2	0.000
1253.2	0.000	1181.6	0.000	1153.6	0.000
1258.6	0.000	1182.4	0.000	1153.9	0.000
1262.6	0.317	1182.6	0.000	1155.2	0.000
1270.1	0.002	1183.1	0.000	1155.3	0.002
1276.1	0.443	1184.1	0.000	1155.7	0.000
		1184.8	0.004	1155.7	0.000
		1185.6	0.003	1156.1	0.001
		1186.8	0.000	1156.6	0.000
		1187.6	0.004	1157.5	0.000
		1187.8	0.000	1157.6	0.000
		1190.0	0.001	1157.7	0.000
		1190.3	0.015	1159.0	0.000
		1190.4	0.000	1159.0	0.000
		1191.5	0.000	1159.2	0.000
		1193.0	0.031	1160.2	0.000
		1193.4	0.000	1160.8	0.000
		1194.6	0.130	1161.3	0.000
		1196.4	0.082	1162.2	0.001
		1197.1	0.021	1163.1	0.000
		1197.1	0.000	1163.2	0.002
		1197.7	0.210	1163.8	0.000
		1199.5	0.000	1165.0	0.002
		1200.2	0.020	1165.1	0.000
		1200.8	2.152	1165.7	0.055
		1200.8	0.000	1167.0	0.004
		1202.4	0.003	1167.3	0.000
		1203.0	1.166	1167.5	0.000
		1203.1	0.000	1168.3	0.000
		1204.2	0.045	1168.9	0.000
		1204.5	0.251	1169.7	0.003
		1204.9	0.000	1169.9	0.000
		1205.7	0.001	1169.9	0.000
		1207.8	0.020	1170.4	0.000
		1209.2	0.000	1171.2	0.000
		1210.1	0.012	1171.3	0.000
		1210.8	0.000	1171.5	0.000
		1212.3	0.016	1171.7	0.000
		1213.3	0.000	1172.3	0.000
		1213.4	0.012	1172.5	0.000
		1218.5	0.021	1173.6	0.003
		1219.2	0.000	1173.7	0.002
		1220.9	0.039	1174.2	0.000
		1221.3	0.000	1176.1	0.000
		1226.8	0.004	1176.4	0.000
		1228.0	0.010	1176.8	0.008
		1230.7	0.000	1177.5	0.000
		1232.1	0.000	1177.8	0.000

1238.0	0.020	1178.1	0.000
1238.3	0.000	1178.4	0.005
1238.9	0.050	1179.2	0.000
1241.7	0.000	1179.5	0.000
1243.1	0.279	1179.6	0.009
1248.1	0.030	1180.4	0.010
1248.4	0.000	1181.4	0.000
1253.5	0.312	1181.5	0.001
1256.0	0.045	1181.7	0.007
1258.8	0.000	1183.2	0.012
1263.5	0.000	1183.7	0.000
1266.9	0.297	1184.0	0.000
1272.9	0.000	1184.9	0.050
1277.4	0.572	1185.4	0.006
		1186.3	0.000
		1186.6	0.001
		1186.8	0.000
		1188.4	0.000
		1188.5	0.003
		1189.4	0.000
		1189.7	0.001
		1191.5	0.000
		1191.7	0.003
		1192.1	0.000
		1192.2	0.000
		1192.4	0.000
		1192.4	0.000
		1193.3	0.001
		1194.1	0.007
		1195.2	0.004
		1195.7	0.000
		1196.3	0.000
		1197.3	0.043
		1197.7	0.000
		1198.3	0.026
		1199.3	0.000
		1199.6	0.241
		1199.8	0.001
		1200.6	0.000
		1200.8	4.752
		1201.7	0.000
		1202.2	0.036
		1202.6	0.000
		1203.2	0.068
		1203.9	0.004
		1204.2	0.000
		1204.3	0.567
		1204.9	0.341
		1205.5	0.006
		1205.7	0.006
		1206.9	0.000
		1207.3	0.000
		1208.4	0.084
		1208.8	0.003
		1210.3	0.000
		1211.6	0.031
		1211.8	0.000
		1212.3	0.006

1214.5	0.036
1215.0	0.000
1215.9	0.009
1216.7	0.008
1219.2	0.000
1221.6	0.004
1222.6	0.000
1222.9	0.001
1225.4	0.000
1227.3	0.021
1228.8	0.035
1229.5	0.000
1232.1	0.000
1234.9	0.044
1236.9	0.004
1238.1	0.000
1238.2	0.053
1244.7	0.086
1245.1	0.000
1245.7	0.297
1246.1	0.000
1248.9	0.115
1252.7	0.001
1253.7	0.000
1257.7	0.352
1260.9	0.016
1263.1	0.000
1267.2	0.000
1269.8	0.294
1274.9	0.000
1278.4	0.722

Figure S1. Carbon bulk/surface ratio for tetrahedral and octahedral complexes as a function of the number of atoms.

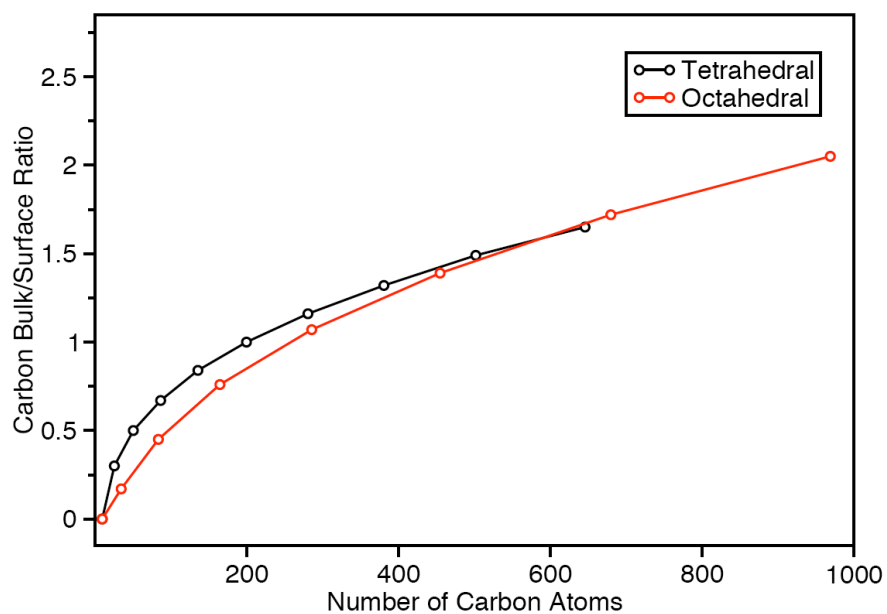


Figure S2. Carbon bulk/surface ratio for tetrahedral and octahedral complexes as a function of the number of carbon network layers surrounding the center of mass.

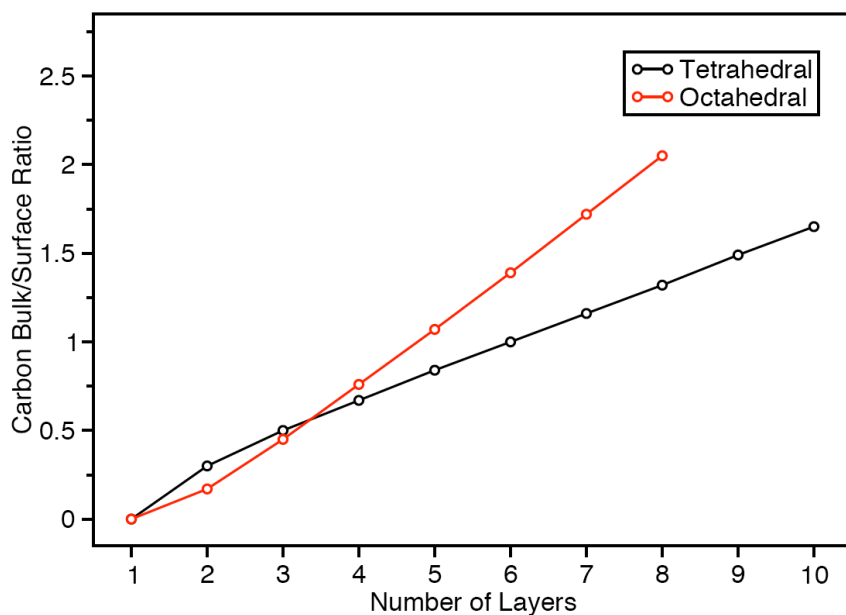


Figure F1. Low-frequency modes of the five largest octahedral models fitted to a simple analytic formula. The red filled circles denote the computed frequencies and the solid black line, the analytical fit.

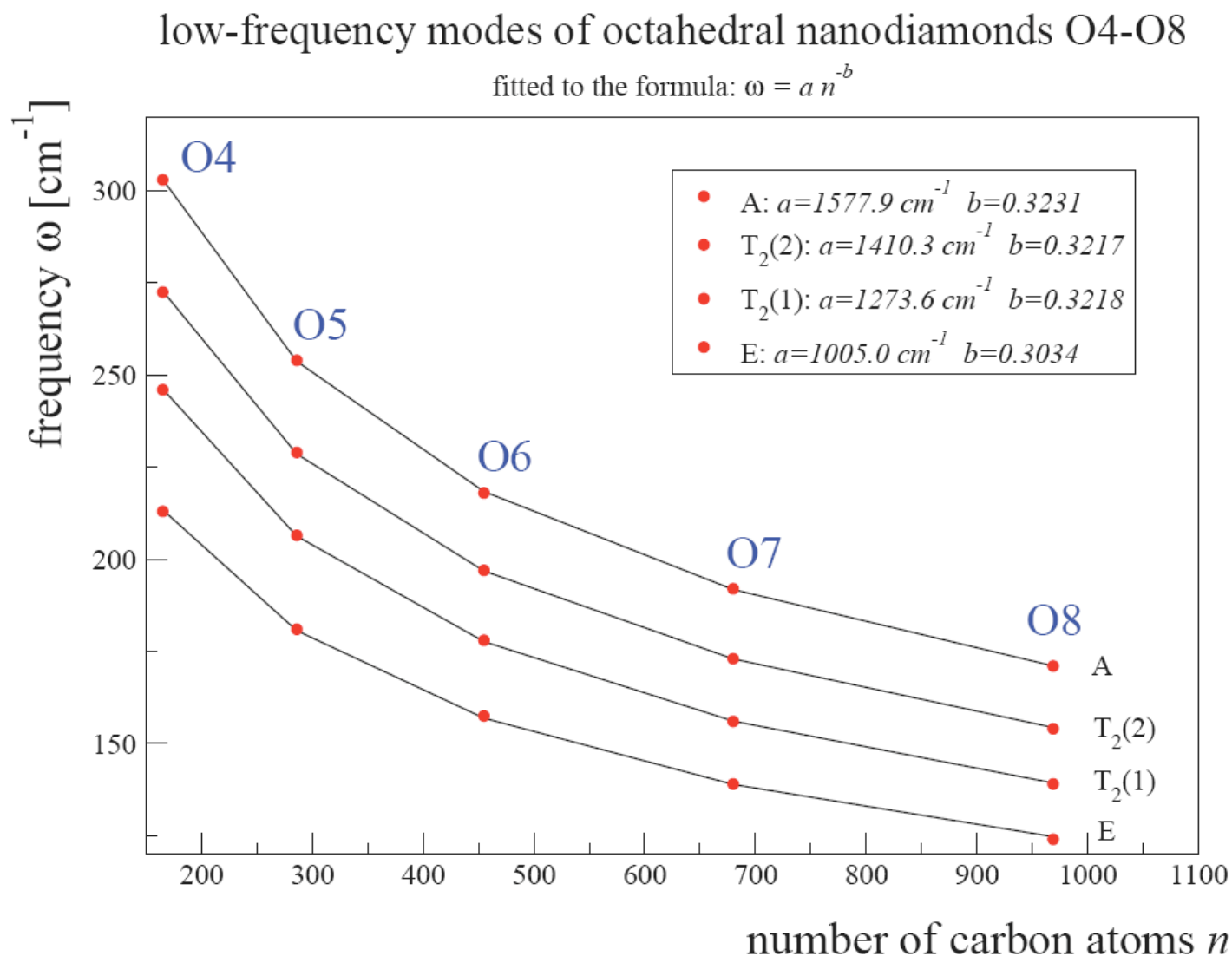


Figure F2. Low-frequency modes of the five largest tetrahedral models fitted to a simple analytic formula. The red filled circles denote the computed frequencies and the solid black line, the analytical fit.

