

Supporting Information

Charge Delocalization and Aromaticity of Doubly Reduced Double-walled Carbon Nanohoops

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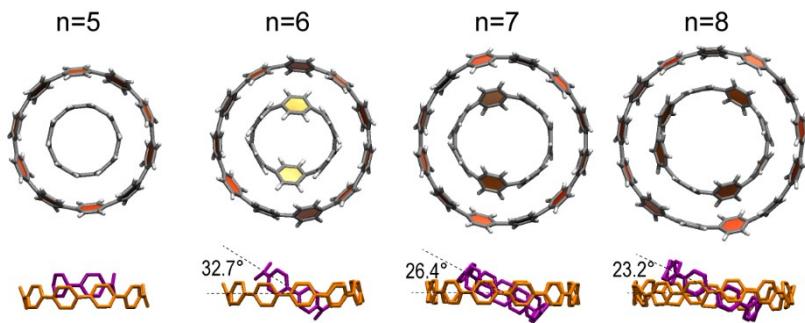


Figure S1. Optimized geometries (B97D3/TZVP) of neutral $[n+5]\text{CPP} \supset [n]\text{CPP}$ ($n = 5-8$) complexes.

Table S1. Averaged C_{ipso} - C_{ipso} , C_{ipso} - C_{ortho} and C_{ortho} - C_{ortho} bond lengths (\AA) of optimized (B97D3/TZVP) $[n]\text{CPPs}$ ($n=5-8, 10-13$) molecules and complexed $[n+5]\text{CPP} \supset [n]\text{CPP}$ ($n=5-8$) at 0, 2- and 2+ charge states.

Charge		0			2-			2+
	Bond	$i - i$	$i - o$	$o - o$	$i - i$	$i - o$	$o - o$	$i - i$
[5]CPP	free	1.485	1.411	1.389	1.441	1.435	1.379	1.438
	guest	1.483	1.411	1.388	1.473	1.415	1.386	1.460
[6]CPP	free	1.481	1.409	1.390	1.445	1.431	1.380	1.443
	guest	1.480	1.409	1.388	1.480	1.410	1.389	1.460
[7]CPP	free	1.480	1.409	1.389	1.448	1.427	1.380	1.448
	guest	1.477	1.408	1.388	1.471 (1.475)	1.411 (1.411)	1.386 (1.387)	1.461
[8]CPP	free	1.479	1.408	1.389	1.452	1.424	1.382	1.452
	guest	1.476	1.407	1.388	1.472 (1.476)	1.409 (1.410)	1.388 (1.388)	1.462
[10]CPP	free	1.478	1.407	1.390	1.457	1.420	1.383	1.458
	host	1.476	1.407	1.389	1.460	1.417	1.384	1.466
[11]CPP	free	1.478	1.407	1.389	1.459	1.419	1.384	1.460
	host	1.477	1.407	1.389	1.457	1.418	1.383	1.468
[12]CPP	free	1.477	1.406	1.390	1.460	1.417	1.384	1.462
	host	1.477	1.407	1.389	1.464 (1.461)	1.416 (1.415)	1.385 (1.384)	1.469
[13]CPP	free	1.477	1.406	1.390	1.461	1.416	1.384	1.463
	host	1.477	1.407	1.389	1.463 (1.464)	1.415 (1.416)	1.384 (1.385)	1.470

Table S2. Averaged dihedral angles of adjacent phenylenes of optimized (B97D3/TZVP) [n]CPPs (n=5-8,9-11) molecules and complexed [n]CPP \subset [n+5]CPP (n=5-8) at 0, 2- and 2+ charge states.

		Dihedral angle (°)		
		0	2-	2+
[5]CPP	free	18.2	0.0	0.0
	guest	0.5	8.3	0.0
[6]CPP	free	27.8	0.0	0.0
	guest	23.6	21.8	11.6
[7]CPP	free	25.7	6.3	7.9
	guest	21.9	20.4 (17.4)	8.7
[8]CPP	free	30.9	12.6	14.7
	guest	26.6	26.5 (25.1)	18.7
[10]CPP	free	32.6	17.7	20.1
	host	28.1	17.9	22.2
[11]CPP	free	31.7	18.2	20.7
	host	28.0	17.9	17.8
[12]CPP	free	33.5	21.0	23.3
	host	29.2	17.6 (21.7)	20.9
[13]CPP	free	32.9	21.2	23.5
	host	29.3	17.3 (22.0)	21.1

Table S3. Averaged Mayer Bond Orders (MBO) of C_{ipso} - C_{ipso} , C_{ipso} - C_{ortho} and C_{ortho} - C_{ortho} bonds of optimized (B97D3/TZVP) $[n]$ CPPs ($n=5-8, 10-13$) molecules and complexed $[n+5]\text{CPP} \supset [n]\text{CPP}$ ($n=5-8$) at 0, 2- and 2+ charge states.

Charge	Bond	0			2-			2+
		$i - i$	$i - o$	$o - o$	$i - i$	$i - o$	$o - o$	$i - i$
[5]CPP	free	1.03	1.325	1.465	1.143	1.178	1.582	1.206
	guest	0.981	1.22	1.469	1.018	1.26	1.454	1.052
[6]CPP	free	0.997	1.33	1.461	1.127	1.197	1.564	1.17
	guest	0.992	1.301	1.447	0.995	1.305	1.446	1.041
[7]CPP	free	0.993	1.331	1.461	1.112	1.218	1.552	1.142
	guest	0.972	1.309	1.453	0.970 (1.000)	1.297 (1.299)	1.433 (1.460)	1.030
[8]CPP	free	0.974	1.339	1.456	1.091	1.241	1.54	1.111
	guest	0.976	1.317	1.447	0.977 (0.983)	1.314 (1.311)	1.426 (1.454)	1.002
[10]CPP	free	0.96	1.343	1.451	1.058	1.27	1.521	1.066
	host	0.988	1.336	1.469	1.073	1.283	1.535	1.066
[11]CPP	free	0.967	1.343	1.451	1.049	1.278	1.515	1.052
	host	0.984	1.338	1.456	1.061	1.275	1.519	1.042
[12]CPP	free	0.951	1.345	1.448	1.035	1.289	1.508	1.036
	host	0.968	1.339	1.459	1.050 (1.041)	1.287 (1.291)	1.507 (1.511)	1.030
[13]CPP	free	0.94967	1.345	1.448	1.029	1.293	1.503	1.027
	host	0.978	1.341	1.457	1.045 (1.032)	1.288 (1.296)	1.502 (1.504)	1.021

Table S4. Averaged Multicenter Delocalization Indices (MCI) of optimized (B97D3/TZVP) $[n]$ CPPs ($n=5-8,10-13$) molecules and complexed $[n+5]\text{CPP} \supset [n]\text{CPP}$ ($n=5-8$) at 0 and 2- charge states, calculated with the pseudo- π approach with the wB97XD functional.

	Charge	0	2-
[5]CPP	free	0.019578	0.011243
	guest	0.019517	0.018226
[6]CPP	free	0.019475	0.012181
	guest	0.019449	0.019436
[7]CPP	free	0.019431	0.012994
	guest	0.019396 (0.018312)	0.018231
[8]CPP	free	0.019421	0.013700
	guest	0.019378 (0.018446)	0.018378
[10]CPP	free	0.019409	0.014780
	host	0.019367	0.015422
[11]CPP	free	0.019407	0.015193
	host	0.019382	0.015180
[12]CPP	free	0.019404	0.015546
	host	0.019383 (0.016158)	0.016185
[13]CPP	free	0.019405	0.015836
	host	0.019396 (0.016388)	0.016402

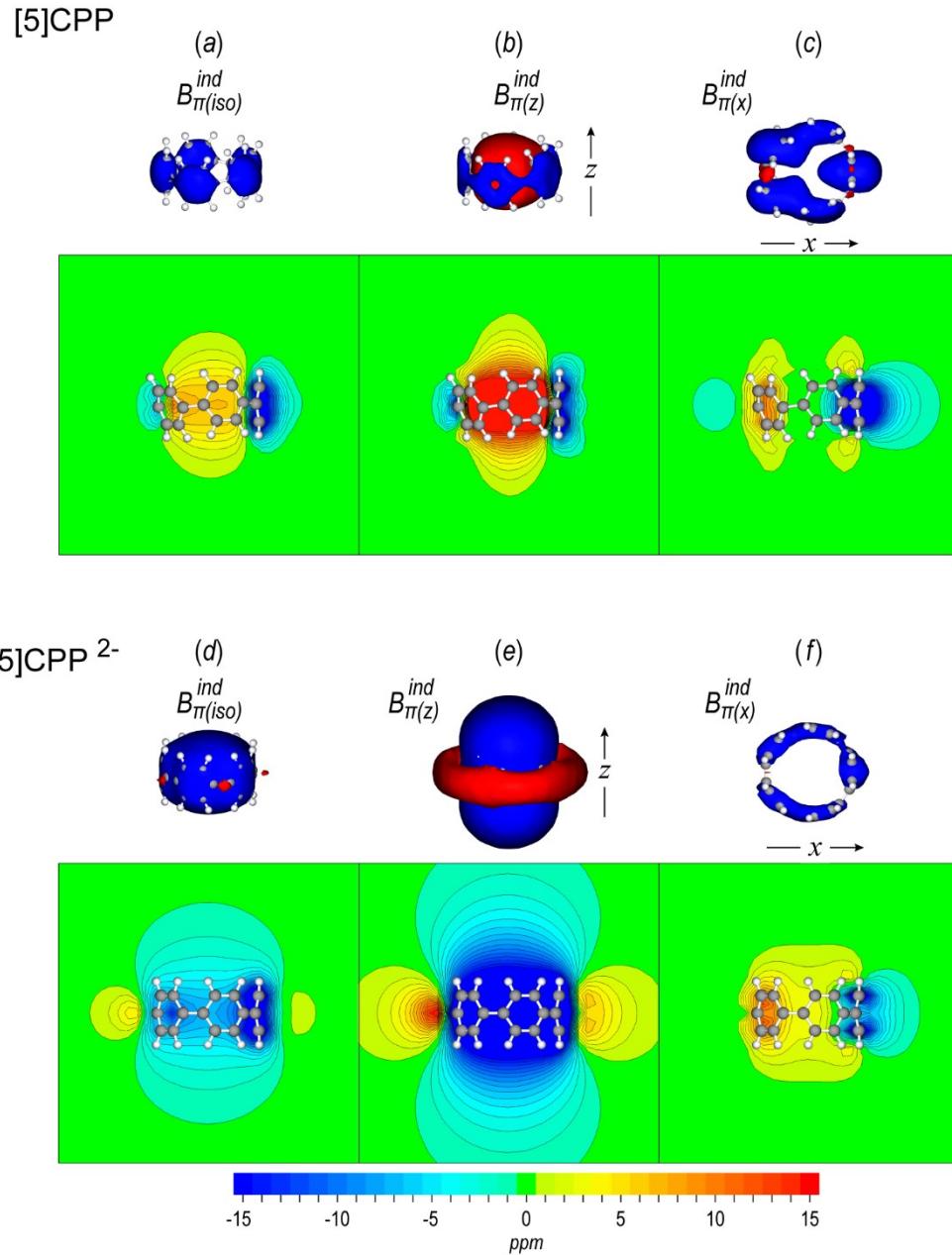


Figure S2. Isosurfaces of pseudo- π and contour maps of π contributions to the isotropic ($B_{\pi(iso)}^{ind}$), out-of-plane ($B_{\pi(z)}^{ind}$) and in-plane ($B_{\pi(x)}^{ind}$) components of the induced magnetic field of neutral and dianion [5]CPP^{0,2-}. Isosurface isovalue ± 5 ppm. Blue: shielding; red: deshielding.

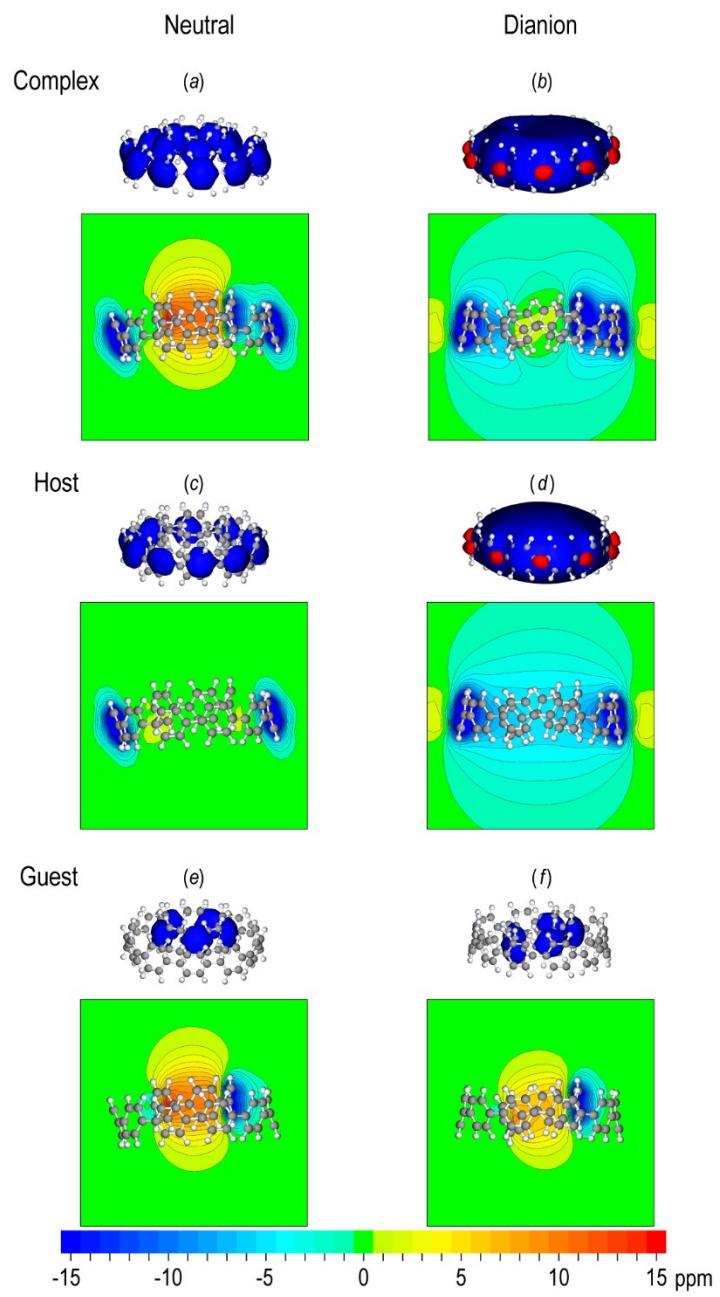


Figure S3. π contributions to the isotropic component of the induced magnetic field, $B_{\pi(iso)}^{ind}$, of $[10]\text{CPP} \supset [5]\text{CPP}^q$ ($q = 0, 2-$) complexes and NBO-dissected contributions of hosts and guests. Isosurface isovalue ± 5 ppm. Blue: shielding; red: deshielding.

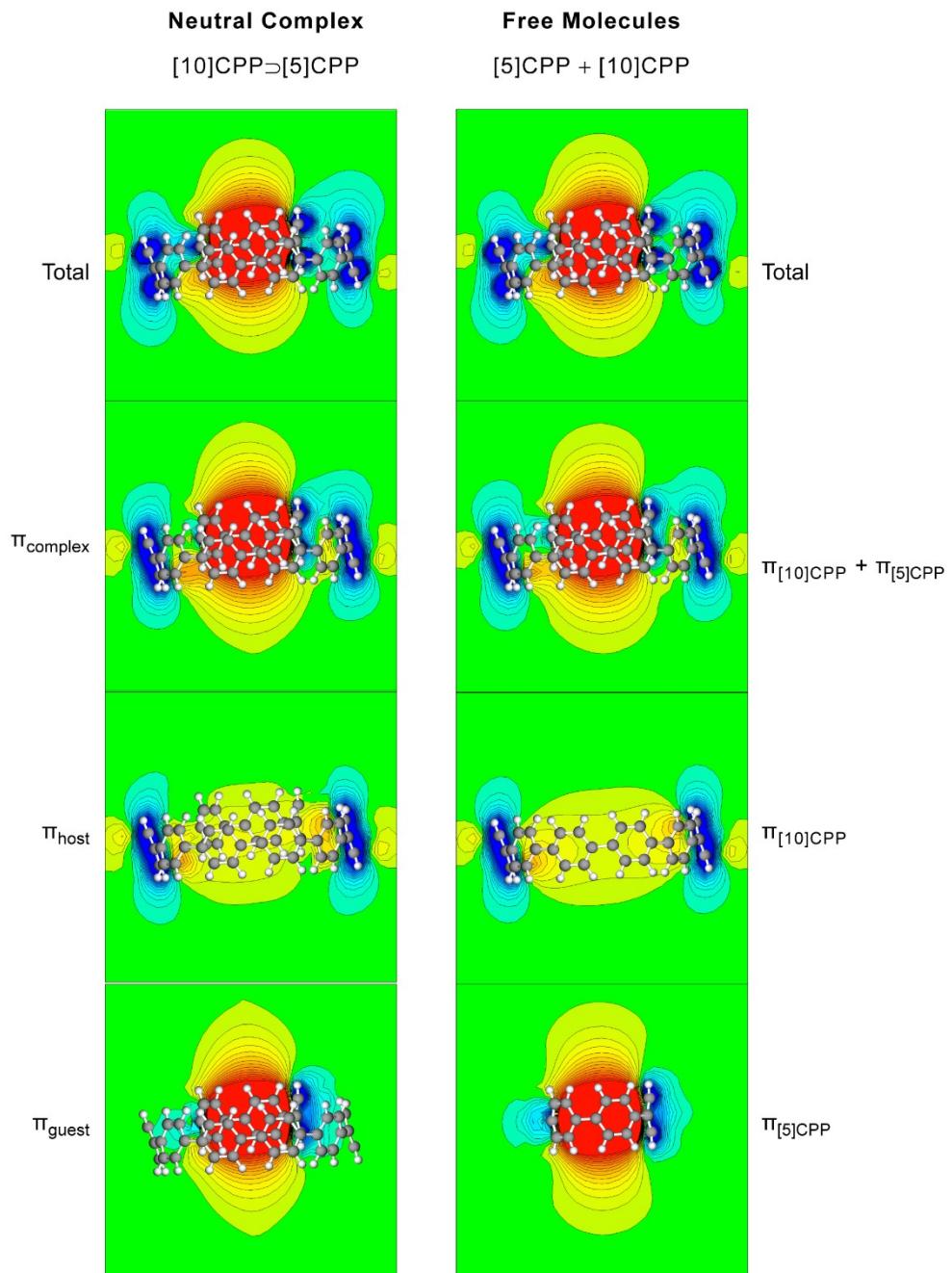


Figure S4. Comparison of out-of-plane magnetic response of the total electrons and π system of neutral complex $[10]\supset[5]\text{CPP}$ and host-guest contributions, with the corresponding free molecules adopting the geometry of the complex and their cumulative effect.

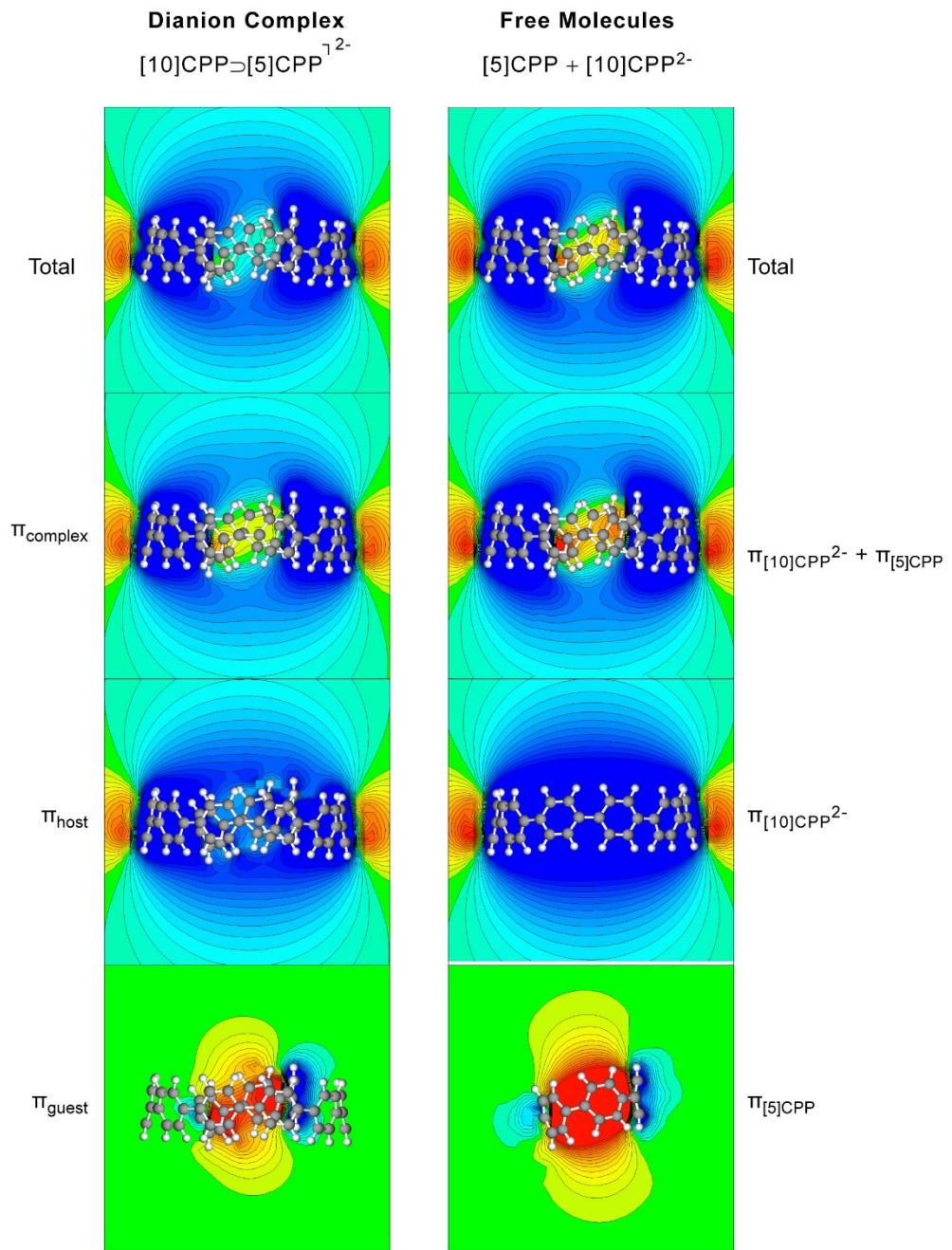


Figure S5. Comparison of out-of-plane magnetic response of the total electrons and π system of dianion complex $[10]\supset[5]\text{CPP}^{2-}$ and host-guest contributions, with the corresponding free molecules adopting the geometry of the complex and their cumulative effect.

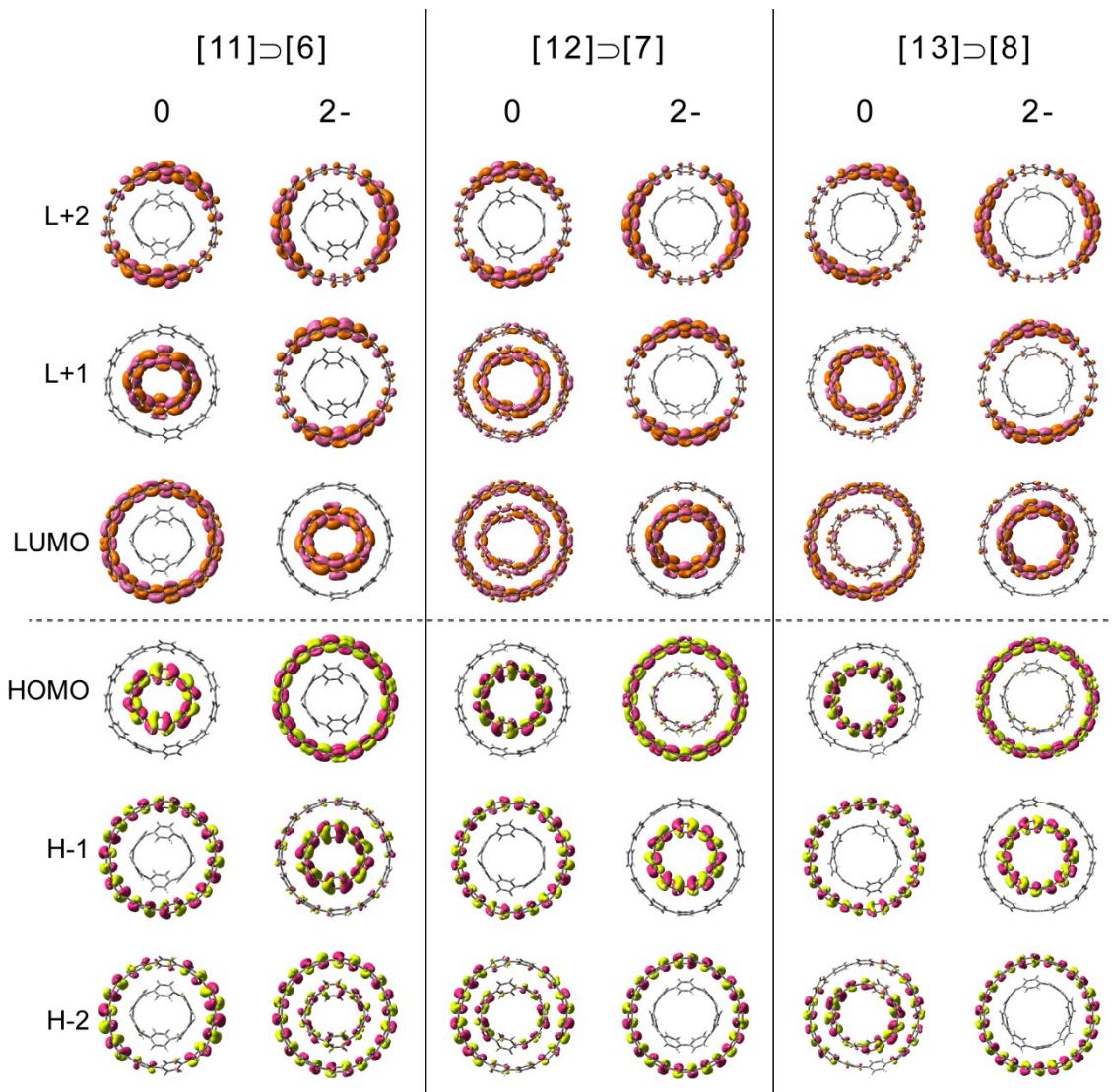


Figure S6. Frontier orbitals of neutral and doubly charged planetary orbit $[n+5]\text{CPP} \supseteq [n]\text{CPP}^q$ ($n = 6-8$; $q = 0, 2-$) complexes.

Table S5. Averaged values of calculated ^1H -NMR chemical shifts (ppm).

		0		2-	
		calc	exp ^a	calc	exp ^c
[5]CPP	free	5.16	7.85	3.35	
	guest	7.20		-1.36	
[6]CPP	free	7.42	7.64	3.12	
	guest	6.07		-3.29	
[7]CPP	free	7.47	7.49	3.08	
	guest	6.23		-1.97	
[8]CPP	free	7.39	7.48	3.21	5.36
	guest	6.23		-1.63	
[10]CPP	free	7.47	7.56	3.71	5.36
	host	7.00		4.22	
[11]CPP	free	7.53	7.58	3.97	
	host	7.47		3.86	
[12]CPP	free	7.54	7.62	4.24	5.36
	host	7.47		4.61	
[13]CPP	free	7.58	7.64	4.45	
	host	7.48		4.81	

Experimental data taken from ^a Ref. 4 and ^c Ref. 51 of main manuscript.

Table S6. HOMO-LUMO gaps calculated at the B97D3/def2TZVP level.

	HOMO-LUMO Gap (ev)	
	0	2-
[10]CPP \supset [5]CPP	1.2626	0.2275
[11]CPP \supset [6]CPP	1.7165	0.0318
[12]CPP \supset [7]CPP	1.7916	0.2817 (0.1287)
[13]CPP \supset [8]CPP	1.8991	0.2942 (0.2044)

Cartesian coordinates of optimized structures B97D3/defTZVP

[5]CPP

C 3.4497960 1.6676530 0.9497430
 C 2.6308310 2.7923040 0.9212480
 C 1.7619480 3.0257350 -0.1673860
 C 2.0542860 2.3142560 -1.3480560
 C 2.8728480 1.1928810 -1.3205730
 C 3.4333210 0.7368540 -0.1111440
 H 3.9900180 1.4366880 1.8647140
 H 2.5586790 3.4072670 1.8148450
 H 1.4684700 2.4935910 -2.2442660
 H 2.8863080 0.5490150 -2.1948350
 C 0.3640470 3.4919990 0.0146810
 C -0.5194790 3.6747310 -1.0712250
 C -0.2478250 3.2417670 1.2593450
 C -1.8379920 3.2390820 -0.9967250
 H -0.1386160 4.0163710 -2.0303700
 C -1.5662140 2.8148780 1.3342280
 H 0.3614500 3.1708650 2.1552520
 C -2.3303420 2.6063260 0.1670590
 H -2.4363610 3.2562600 -1.9033910
 H -1.9202600 2.4465940 2.2913430
 C -3.2147190 1.4153420 0.0955780
 C -3.4411980 0.6114160 1.2340480
 C -3.4231400 0.7694260 -1.1422480
 C -3.4238700 -0.7741060 1.1413090
 H -3.4537190 1.0552390 2.2249530
 C -3.4384110 -0.6161070 -1.2350040
 H -3.3922300 1.3389680 -2.0661960
 C -3.2126060 -1.4197410 -0.0962040
 H -3.3939700 -1.3436180 2.0653090
 H -3.4485530 -1.0598790 -2.2259500
 C -2.3266750 -2.6096170 -0.1668200
 C -1.5625190 -2.8185060 -1.3339160
 C -1.8332210 -3.2404980 0.9975170
 C -0.2435200 -3.2434640 -1.2588260
 H -1.9173320 -2.4519770 -2.2914230
 C -0.5141510 -3.6743990 1.0721940
 H -2.4312800 -3.2574350 1.9043820
 C 0.3689760 -3.4915640 -0.0140270
 H 0.3654150 -3.1727430 -2.1549760
 H -0.1327100 -4.0145520 2.0316320
 C 3.4343850 -0.7319760 0.1107080
 C 2.8749990 -1.1887820 1.3203420
 C 3.4517840 -1.6627690 -0.9501670
 C 2.0580340 -2.3113150 1.3481360
 H 2.8878820 -0.5448930 2.1945930
 C 2.6343780 -2.7885450 -0.9213790
 H 3.9913530 -1.4310640 -1.8653350
 C 1.7662140 -3.0231970 0.1675760
 H 1.4728810 -2.4914790 2.2446100
 H 2.5628000 -3.4036020 -1.8149540

[5]CPP²⁻

C 3.1694860 1.5535690 1.1958110
 C 2.3318820 2.6489340 1.1958050
 C 1.6760820 3.0961070 -0.0003300
 C 2.3312750 2.6486390 -1.1962490
 C 3.1690050 1.5530320 -1.1962940
 C 3.4289310 0.8033240 -0.0003470

H 3.5024590 1.1658780 2.1575450
 H 2.0451190 3.0719140 2.1575520
 H 2.0440080 3.0706550 -2.1582860
 H 3.5007380 1.1650810 -2.1583640
 C 0.2952230 3.5077170 0.0002150
 C -0.4981660 3.4928060 -1.1958960
 C -0.4979830 3.4924270 1.1962270
 C -1.7990270 3.0351220 -1.1959340
 H -0.0261340 3.6887520 -2.1576090
 C -1.7990080 3.0347430 1.1961610
 H -0.0260820 3.6876960 2.1581430
 C -2.4273330 2.5504390 0.0001740
 H -2.2897090 2.8925530 -2.1577020
 H -2.2894010 2.8918300 2.1580560
 C -3.2463530 1.3648760 -0.0003700
 C -3.4774890 0.6058320 1.1959680
 C -3.4773400 0.6057820 -1.1960960
 C -3.4442740 -0.7728720 1.1960490
 H -3.5179280 1.1152690 2.1577290
 C -3.4442070 -0.7729250 -1.1960200
 H -3.5179820 1.1151390 -2.1578680
 C -3.1768460 -1.5199590 0.0000070
 H -3.4603770 -1.2836040 2.1578170
 H -3.4598380 -1.2837090 -2.1577900
 C -2.3014030 -2.6644840 -0.0001520
 C -1.6504660 -3.1179480 -1.1961220
 C -1.6504230 -3.1181500 1.1959760
 C -0.3288800 -3.5123310 -1.1961890
 H -2.1472200 -2.9988900 -2.1580050
 C -0.3290000 -3.5125500 1.1959450
 H -2.1473770 -2.9992340 2.1577420
 C 0.4641470 -3.4893360 -0.0001860
 H 0.1518690 -3.6847120 -2.1580980
 H 0.1519620 -3.6853900 2.1576630
 C 3.4636100 -0.6370270 0.0003320
 C 3.2402710 -1.3984260 1.1962710
 C 3.2407120 -1.3989000 -1.1958270
 C 2.4564870 -2.5332420 1.1962360
 H 3.5530240 -0.9950010 2.1583290
 C 2.4570300 -2.5334610 -1.1958240
 H 3.5546460 -0.9956320 -2.1575550
 C 1.8235910 -3.0117580 0.0003240
 H 2.1900060 -2.9686970 2.1582700
 H 2.1910040 -2.9697860 -2.1575730

[5]CPP²⁺

C -0.7806890 -3.3877620 1.2127860
 C 0.5897450 -3.4260080 1.2127610
 C 1.3148660 -3.1925180 0.0000810
 C 0.5896470 -3.4267390 -1.2124330
 C -0.7807940 -3.3885260 -1.2123940
 C -1.4917160 -3.1141240 0.0001550
 H -1.3074790 -3.4347750 2.1595970
 H 1.1131340 -3.5024920 2.1595300
 H 1.1129880 -3.5039290 -2.1591700
 H -1.3077040 -3.4363000 -2.1591070
 C 2.5015970 -2.3808320 -0.0001220
 C 2.9820530 -1.7895300 -1.2127380
 C 2.9828100 -1.7898320 1.2123620

C 3.4423720 -0.4981240 -1.2127430
 H 2.8635650 -2.3049820 -2.1595520
 C 3.4430480 -0.4983950 1.2123880
 H 2.8650870 -2.3055990 2.1590980
 C 3.4441380 0.2638000 -0.0001100
 H 3.6769570 -0.0241820 -2.1595950
 H 3.6782230 -0.0246580 2.1591920
 C 3.0379400 1.6429080 0.0000310
 C 2.6237930 2.2824630 1.2126390
 C 2.6239610 2.2827010 -1.2124970
 C 1.5374650 3.1188570 1.2126740
 H 3.0777700 2.0110780 2.1594440
 C 1.5375750 3.1190110 -1.2124970
 H 3.0780520 2.0115410 -2.1593190
 C 0.8131780 3.3555580 0.0000500
 H 1.1591500 3.4883470 2.1595310
 H 1.1593260 3.4886930 -2.1593010
 C -0.6239470 3.3955920 0.0000820
 C -1.3604380 3.1999530 -1.2124930
 C -1.3603360 3.1996900 1.2126430
 C -2.4920400 2.4259570 -1.2125460
 H -0.9620880 3.5479780 -2.1592590
 C -2.4918740 2.4256160 1.2126010
 H -0.9619660 3.5475450 2.1594680
 C -2.9413790 1.8104100 -0.0000230
 H -2.9608490 2.1810260 -2.1593310
 H -2.9605320 2.1803860 2.1593800
 C -2.6309630 -2.2370320 -0.0000140
 C -3.0781920 -1.6199390 1.2124860
 C -3.0775290 -1.6198540 -1.2126840
 C -3.4654160 -0.3047910 1.2124520
 H -2.9896460 -2.1414620 2.1592320
 C -3.4647690 -0.3047130 -1.2127770
 H -2.9883200 -2.1412320 -2.1594490
 C -3.4240920 0.4561360 -0.0001430
 H -3.6734540 0.1816460 2.1591830
 H -3.6722780 0.1817650 -2.1596050

[6]CPP

C -1.83676500 -3.34721200 -1.26563900
 C -2.91236900 -2.46914200 -1.26558400
 C -3.58863800 -2.14924700 -0.07273400
 C -3.34045100 -2.99192100 1.03099300
 C -2.26314000 -3.87116400 1.03100500
 C -1.38783400 -3.94554700 -0.07274500
 H -1.22425000 -3.40998300 -2.16010200
 H -3.09632100 -1.88141100 -2.15996500
 H -3.92324400 -2.87458700 1.94125100
 H -2.03153200 -4.41858100 1.94131900
 C -4.11189500 -0.77109500 0.07270600
 C -3.81866900 -0.08300500 1.26567800
 C -4.48473900 0.02407700 -1.03120300
 C -3.59595400 1.28749900 1.26557100
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 C -4.26170800 1.39662800 -1.03130900
 H -4.84272100 -0.45032200 -1.94158100
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 H -3.17953900 1.74085700 2.16013400
 H -4.45098100 1.95998400 -1.94170000
 C 0.06726700 -4.18178400 0.07275500
 C 0.68248600 -3.75612800 1.26561500
 C 0.92107700 -4.38817400 -1.03102200
 C 1.98077100 -3.26383800 1.26565300

H 0.08149900 -3.62139300 2.15993900
 C 2.22126700 -3.89507500 -1.03100900
 H 0.52794100 -4.83395400 -1.94136900
 C 2.72352700 -3.17449200 0.07280900
 H 2.34128900 -2.76457100 2.16004500
 H 2.81118100 -3.96816700 -1.94131200
 C -2.72353000 3.17447500 -0.07283900
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 C -1.98073900 3.26376000 -1.26566300
 C -0.92109600 4.38817200 1.03099700
 H -2.81120500 3.96817500 1.94126500
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 H -2.34120800 2.76443000 -2.16003700
 C -0.06726400 4.18176400 -0.07276800
 H -0.52797000 4.83400000 1.94132200
 H -0.08146300 3.62128600 -2.15993300
 C 1.38784700 3.94554100 0.07276800
 C 2.26315800 3.87116400 -1.03097400
 C 1.83678900 3.34723000 1.26566700
 C 3.34047900 2.99194900 -1.03095600
 H 2.03154000 4.41854400 -1.94130800
 C 2.91240900 2.46917100 1.26561900
 H 1.22427600 3.40998000 2.16013200
 C 3.58867100 2.14927600 0.07277300
 H 3.92326800 2.87462900 -1.94121800
 H 3.09634900 1.88144000 2.16000200
 C 4.11191800 0.77111000 -0.07270600
 C 3.81861500 0.08304300 -1.26566900
 C 4.48475900 -0.02409500 1.03119000
 C 3.59585900 -1.28745600 -1.26557300
 H 3.56737100 0.64472100 -2.16041900
 C 4.26168900 -1.39663400 1.03127300
 H 4.84279600 0.45028900 1.94155400
 C 3.65616300 -2.03287100 -0.07257300
 H 3.17936200 -1.74076100 -2.16012200
 H 4.45091800 -1.95999100 1.94167600

[6]CPP²⁻

C -3.39067300 2.50664500 -1.19538500
 C -2.39960800 3.46640700 -1.19530200
 C -1.71109800 3.84515100 0.00038900
 C -2.39903700 3.46558800 1.19610700
 C -3.39006600 2.50574700 1.19600100
 C -3.79134000 1.83043400 0.00018000
 H -3.76963900 2.16766700 -2.15745500
 H -2.04829700 3.83423800 -2.15727800
 H -2.04709000 3.83245700 2.15821400
 H -3.76810700 2.16575900 2.15806100
 C -0.31009000 4.19704200 0.00029200
 C 0.47584900 4.18777200 1.19590400
 C 0.47551800 4.18809900 -1.19550400
 C 1.80272900 3.80993200 1.19565300
 H -0.00722700 4.34589200 2.15804800
 C 1.80243200 3.81026500 -1.19574000
 H -0.00785500 4.34621700 -2.15749600
 C 2.47528500 3.40397900 -0.00019400
 H 2.29696000 3.68960900 2.15760300
 H 2.29633200 3.69024100 -2.15789300
 C -4.18758600 0.44125600 -0.00018700
 C -4.20404400 -0.34480400 1.19527400
 C -4.20269300 -0.34417300 -1.19600700
 C -3.86745300 -1.68274300 1.19511400
 H -4.34813600 0.14275900 2.15736100

C -3.86606200 -1.68214200 -1.19614800
 H -4.34512800 0.14395300 -2.15805500
 C -3.48107000 -2.36715500 -0.00049300
 H -3.76357700 -2.18067500 2.15707900
 H -3.76059000 -2.17934600 -2.15830300
 C 3.48106000 2.36715000 -0.00038500
 C 3.86705700 1.68260200 1.19521500
 C 3.86640700 1.68226900 -1.19604900
 C 4.20367200 0.34463100 1.19531200
 H 3.76257400 2.18027000 2.15724800
 C 4.20302600 0.34433200 -1.19597100
 H 3.76147200 2.17971800 -2.15814000
 C 4.18758200 -0.44125800 -0.00020400
 H 4.34720700 -0.14309200 2.15740600
 H 4.34596800 -0.14364500 -2.15801400
 C 3.79134400 -1.83043900 0.00012200
 C 3.39054900 -2.50659300 -1.19539400
 C 3.39019100 -2.50579800 1.19598900
 C 2.39952700 -3.46644400 -1.19522900
 H 3.76919100 -2.16744600 -2.15752000
 C 2.39913000 -3.46557200 1.19617600
 H 3.76851400 -2.16594200 2.15799600
 C 1.71111300 -3.84517300 0.00048000
 H 2.04805000 -3.83411800 -2.15720900
 H 2.04733300 -3.83256800 2.15828500
 C 0.31010100 -4.19705700 0.00028900
 C -0.47544500 -4.18803600 -1.19557500
 C -0.47589300 -4.18782800 1.19583200
 C -1.80231700 -3.81016300 -1.19583400
 H 0.00796400 -4.34630300 -2.15753200
 C -1.80280500 -3.80998700 1.19555800
 H 0.00714900 -4.34577000 2.15801500
 C -2.47526500 -3.40395700 -0.00028200
 H -2.29627600 -3.69017300 -2.15796300
 H -2.29694800 -3.68956300 2.15753700

[6]CPP²⁺

C 4.07725800 -0.84278200 -1.20962100
 C 3.58143100 -2.12304900 -1.20961500
 C 3.12061200 -2.72586500 0.00008700
 C 3.58125100 -2.12296900 1.20982400
 C 4.07701500 -0.84267600 1.20982200
 C 4.14252700 -0.08679000 0.00006900
 H 4.31291900 -0.37744300 -2.16007700
 H 3.44201500 -2.62575000 -2.16004400
 H 3.44168000 -2.62560300 2.16026700
 H 4.31240000 -0.37722100 2.16029000
 C 1.99611400 -3.63048300 0.00005100
 C 1.30855800 -3.95136000 1.20976800
 C 1.30868000 -3.95136100 -1.20975300
 C -0.04814100 -4.16188400 1.20967300
 H 1.82930500 -3.92262800 2.16026100
 C -0.04803000 -4.16176300 -1.20983300
 H 1.82955300 -3.92265800 -2.16017500
 C -0.80046900 -4.06447700 -0.00010800
 H -0.55334800 -4.29228700 2.16006300
 H -0.55314600 -4.29201800 -2.16028700
 C 3.92101300 1.33932400 -0.00003500
 C 3.62957200 2.03999200 1.20960900
 C 3.62921600 2.03958900 -1.20982800
 C 2.76857400 3.10941500 1.20955200
 H 3.99549200 1.66830300 2.16007700
 C 2.76815500 3.10895400 -1.20989300

H 3.99475400 1.66751700 -2.16029000
 C 2.14634000 3.54363900 -0.00014900
 H 2.48328900 3.54627500 2.15993700
 H 2.48241000 3.54536000 -2.16034900
 C -2.14634900 -3.54364200 -0.00010900
 C -2.76831100 -3.10920400 1.20965200
 C -2.76842400 -3.10915700 -1.20979600
 C -3.62936900 -2.03983700 1.20970400
 H -2.48270700 -3.54584200 2.16004600
 C -3.62942500 -2.03973400 -1.20973500
 H -2.48298400 -3.54577700 -2.16024400
 C -3.92101900 -1.33932400 0.00001600
 H -3.99508500 -1.66799800 2.16019000
 H -3.99516100 -1.66779800 -2.16017800
 C -4.14253000 0.08678500 0.00010900
 C -4.07740100 0.84284500 -1.20956100
 C -4.07685000 0.84259400 1.20988500
 C -3.58163800 2.12313700 -1.20953700
 H -4.31318700 0.37755200 -2.16001000
 C -3.58101800 2.12286200 1.20990400
 H -4.31210300 0.37708900 2.16036100
 C -3.12060700 2.72586000 0.00014300
 H -3.44245200 2.62595000 -2.15994300
 H -3.44120500 2.62538200 2.16037000
 C -1.99611900 3.63048400 0.00001800
 C -1.30867000 3.95124800 -1.20978700
 C -1.30857900 3.95147500 1.20973300
 C 0.04802800 4.16177700 -1.20983000
 H -1.82948700 3.92239400 -2.16023700
 C 0.04812900 4.16188600 1.20967500
 H -1.82938500 3.92288700 2.16019600
 C 0.80046600 4.06449000 -0.00010700
 H 0.55314500 4.29209600 -2.16027700
 H 0.55333100 4.29222600 2.16007200

[7]CPP

C -3.81638100 2.32777500 1.35016200
 C -4.36781700 1.05612900 1.29541400
 C -4.83610200 0.51608500 0.08341000
 C -4.97390200 1.41677700 -0.99144100
 C -4.42704000 2.69373000 -0.93311900
 C -3.70469300 3.13067800 0.19793600
 H -3.32110900 2.62495300 2.26840400
 H -4.27472900 0.41413300 2.16638200
 H -5.43212400 1.08226600 -1.91889700
 H -4.48070900 3.32087300 -1.81857500
 C -4.77306100 -0.95093400 -0.09300000
 C -4.21299300 -1.45410800 -1.28190500
 C -4.88039000 -1.85224200 0.98558700
 C -3.55565400 -2.67741700 -1.30311400
 H -4.13336900 -0.80726800 -2.15077800
 C -4.22263800 -3.07670100 0.96412300
 H -5.40409600 -1.54990000 1.88902800
 C -3.42809100 -3.45476600 -0.13694200
 H -2.98539600 -2.94404700 -2.18816700
 H -4.24663600 -3.70480000 1.85116100
 C 1.58625000 4.58324000 -0.19796100
 C 2.09241300 3.95003500 -1.35019300
 C 2.43042200 4.57647500 0.93310500
 C 3.21592400 3.13834000 -1.29537500
 H 1.51496600 3.95265400 -2.26850600
 C 3.55277900 3.75795500 0.99146300
 H 2.15621600 5.14306800 1.81855000

C 3.89429400 2.91315400 -0.08335200
 H 3.46386900 2.53890800 -2.16636100
 H 4.11758600 3.70447300 1.91891400
 C -2.23739500 -4.32315200 -0.00358900
 C -1.58442300 -4.90236500 -1.11002100
 C -1.50871700 -4.26620800 1.19897300
 C -0.21678800 -5.15209700 -1.08495100
 H -2.13507400 -5.07062400 -2.03222800
 C -0.14259200 -4.51318800 1.22305900
 H -1.97622100 -3.85359400 2.08815600
 C 0.56065600 -4.83066100 0.04622900
 H 0.26971500 -5.51154200 -1.98820400
 H 0.40802600 -4.28456100 2.13070000
 C 1.98507300 -4.43962000 -0.04616000
 C 2.81764400 -4.31899600 1.08502300
 C 2.42772300 -3.80777100 -1.22305500
 C 3.86603900 -3.40595300 1.11005300
 H 2.58286800 -4.87641600 1.98829800
 C 3.47627900 -2.89790300 -1.19903300
 H 1.83759400 -3.89246100 -2.13071800
 C 4.13175200 -2.57461500 0.00355900
 H 4.42535800 -3.26935400 2.03227600
 H 3.66764400 -2.30455700 -2.08828900
 C 4.71191900 -1.21988000 0.13689700
 C 4.42457900 -0.48645200 1.30309400
 C 5.20188800 -0.48901000 -0.96416200
 C 4.36490400 0.90099300 1.28192800
 H 4.07054800 -1.00699600 2.18814200
 C 5.14194300 0.89963600 -0.98560300
 H 5.54327000 -1.01674200 -1.85122200
 C 4.58934400 1.61967100 0.09301500
 H 3.96610500 1.41638500 2.15082800
 H 5.43768900 1.42707800 -1.88905400
 C -2.60708900 4.12023900 0.10917800
 C -1.85958900 4.49933100 1.24282600
 C -2.02937800 4.43527300 -1.13750600
 C -0.52041400 4.84954100 1.13749600
 H -2.28802200 4.40114200 2.23569600
 C -0.69911400 4.81793800 -1.24282600
 H -2.58120500 4.24851400 -2.05368600
 C 0.13718700 4.87360400 -0.10918800
 H 0.04944200 4.97068700 2.05366500
 H -0.28071100 4.95236900 -2.23571800

[7]CPP²⁻

C -3.59575300 -3.23316000 1.23128700
 C -2.53690000 -4.11878100 1.21843400
 C -1.89391400 -4.51580100 0.00835400
 C -2.63876500 -4.20458700 -1.16936700
 C -3.69670000 -3.31817000 -1.15662100
 C -4.11657600 -2.65364100 0.03534300
 H -3.94122500 -2.87279100 2.19712400
 H -2.10210100 -4.40133700 2.17416500
 H -2.30942000 -4.59244100 -2.13101100
 H -4.14477500 -3.04621500 -2.10985900
 C -0.49025000 -4.87025100 -0.02844100
 C 0.27141100 -4.79419400 -1.23245700
 C 0.30516600 -4.98431400 1.15181300
 C 1.62467700 -4.51996300 -1.22971300
 H -0.24046400 -4.80138600 -2.19155500
 C 1.65807200 -4.71063300 1.15446100
 H -0.17537400 -5.19740400 2.10446600
 C 2.35112000 -4.29591200 -0.02284800

H 2.10263800 -4.32403800 -2.18641000
 H 2.18088600 -4.72252700 2.10869600
 C -3.98173400 2.85152500 -0.03539000
 C -3.43312800 3.40482200 -1.23132800
 C -3.53000000 3.49483700 1.15656800
 C -2.33226500 4.23764900 -1.21843800
 H -3.79572800 3.06170100 -2.19717200
 C -2.43001200 4.32850200 1.16934800
 H -3.99092500 3.24521300 2.10978700
 C -1.67074300 4.60284500 -0.00832800
 H -1.88410100 4.49855300 -2.17414900
 H -2.08223700 4.69990300 2.13099400
 C 3.50501000 -3.42129000 0.01764500
 C 4.09471900 -2.86997600 -1.15992200
 C 3.91465200 -2.77949800 1.22386300
 C 4.72442800 -1.64161500 -1.15914500
 H 3.96765600 -3.37991000 -2.11275500
 C 4.54446600 -1.55059700 1.22462200
 H 3.59247400 -3.18284200 2.18067900
 C 4.82723200 -0.84225100 0.01933100
 H 5.06513800 -1.23995500 -2.11133700
 H 4.68291000 -1.05428800 2.18197500
 C 4.86268500 0.60537800 -0.01942300
 C 4.79909800 1.40875700 1.15909000
 C 4.61491300 1.32676800 -1.22468300
 C 4.23021600 2.66644500 1.15992600
 H 5.11970500 0.99083100 2.11126800
 C 4.04598200 2.58501600 -1.22386500
 H 4.72888900 0.82433300 -2.18206300
 C 3.66820700 3.24601300 -0.01761800
 H 4.12821200 3.18192400 2.11278900
 H 3.74391900 3.00368200 -2.18066100
 C 2.55847400 4.17600300 0.02291200
 C 1.84384600 4.43521800 1.22978700
 C 1.88651200 4.62412500 -1.15438200
 C 0.50559000 4.77521200 1.23254300
 H 2.31166500 4.21613800 2.18647500
 C 0.54858000 4.96352900 -1.15172400
 H 2.40928300 4.61050300 -2.10861800
 C -0.25145500 4.88836800 0.02852400
 H -0.00529900 4.80737600 2.19165300
 H 0.07900400 5.19985800 -2.10436500
 C -4.71480000 -1.33514400 0.01962100
 C -4.87240700 -0.55451100 1.20469700
 C -4.87242000 -0.58785100 -1.18618300
 C -4.83780600 0.82519800 1.18613000
 H -4.90526200 -1.04835900 2.17312700
 C -4.83932100 0.79189400 -1.20475100
 H -4.89301200 -1.10738500 -2.14139800
 C -4.64370600 1.56386500 -0.01966900
 H -4.83295900 1.34512200 2.14134300
 H -4.84791500 1.28676500 -2.17317700

[7]CPP²⁺

C -3.49579900 -3.22395100 1.25538600
 C -2.42993500 -4.09263000 1.23743700
 C -1.81595400 -4.47435400 0.01093700
 C -2.56520200 -4.20836500 -1.17198800
 C -3.63214200 -3.34215600 -1.15376900
 C -4.02064600 -2.68079100 0.04815700
 H -3.85549100 -2.87247900 2.21545500
 H -1.98841100 -4.38504700 2.18327000
 H -2.25433600 -4.62994600 -2.12155000

H -4.12308700 -3.10607900 -2.09123300
 C -0.40811500 -4.80994200 -0.03333100
 C 0.32073900 -4.70554500 -1.25126800
 C 0.37099300 -4.94961700 1.15254300
 C 1.66548200 -4.41517100 -1.24944000
 H -0.19888100 -4.72732800 -2.20227600
 C 1.71411500 -4.65833900 1.15451200
 H -0.10432400 -5.21961400 2.08923200
 C 2.36849100 -4.20891200 -0.02945900
 H 2.15047300 -4.21805200 -2.19863900
 H 2.25689800 -4.70849200 2.09219900
 C -3.96158700 2.76700100 -0.04806100
 C -3.42524100 3.29865100 -1.25535800
 C -3.55874500 3.41982700 1.15381100
 C -2.34082300 4.14406100 -1.23753900
 H -3.79255200 2.95502100 -2.21538000
 C -2.47334400 4.26279000 1.17189700
 H -4.05459100 3.19444900 2.09133000
 C -1.71862800 4.51246900 -0.01110400
 H -1.89317900 4.42684300 -2.18342700
 H -2.15335300 4.67759100 2.12141600
 C 3.51097400 -3.31985000 0.01495100
 C 4.10603600 -2.79457900 -1.16923800
 C 3.88406400 -2.69008800 1.23509400
 C 4.71691500 -1.56343700 -1.16681300
 H 4.02191300 -3.33294000 -2.10706000
 C 4.49574400 -1.45754800 1.23752700
 H 3.57330700 -3.11184300 2.18408900
 C 4.77329500 -0.77561100 0.01996900
 H 5.09623900 -1.16774400 -2.10274400
 H 4.64210400 -0.95789400 2.18830200
 C 4.78898700 0.67225800 -0.01964100
 C 4.74954000 1.46122700 1.16707000
 C 4.52646800 1.35994500 -1.23729000
 C 4.16551500 2.70533200 1.16928800
 H 5.12009500 1.05751800 2.10308700
 C 3.94161000 2.60543800 -1.23505700
 H 4.66208500 0.85713200 -2.18799600
 C 3.58211100 3.24326400 -0.01501500
 H 4.09294400 3.24548400 2.10704800
 H 3.64018800 3.03371200 -2.18414100
 C 2.45911200 4.15682400 0.02926800
 C 1.76071300 4.37828600 1.24923000
 C 1.81460300 4.62023100 -1.15472800
 C 0.42255500 4.69762000 1.25103200
 H 2.24132500 4.17080400 2.19844900
 C 0.47807600 4.94041000 -1.15278700
 H 2.35834100 4.65867900 -2.09241000
 C -0.30387300 4.81760200 0.03308500
 H -0.09648100 4.73067700 2.20203900
 H 0.00873500 5.22061800 -2.08948600
 C -4.63750800 -1.37112600 0.02848800
 C -4.81048800 -0.61117900 1.22132100
 C -4.81228300 -0.65923800 -1.19353200
 C -4.79662900 0.76308400 1.19376900
 H -4.86389800 -1.10759200 2.18356000
 C -4.79631300 0.71500000 -1.22108200
 H -4.85588300 -1.19297500 -2.13607200
 C -4.60665200 1.47100600 -0.02828300
 H -4.82846000 1.29766500 2.13630500
 H -4.83910800 1.21246500 -2.18330900
 C -5.24442700 -1.80636100 0.05644700
 C -5.76005400 -1.11426500 -1.05696900
 C -5.86051600 0.27237000 -1.05696300
 C -5.45005600 1.03158300 0.05644800
 C -5.16510200 0.32195200 1.23720300
 C -5.06472300 -1.06305500 1.23719000
 C -4.98569000 2.43106700 -0.05642900
 C -4.86095200 3.28513300 1.05693700
 C -3.95147200 4.33665800 1.05692600
 C -3.12429800 4.58314300 -0.05644200
 C -3.42452900 3.87978900 -1.23716800
 C -4.33295300 2.82951600 -1.23716900
 C -1.80635700 5.24436800 0.05640800
 C -1.11425200 5.75999300 -1.05700200
 C 0.27238200 5.86046200 -1.05698400
 C 1.03158400 5.45000200 0.05643300
 C 0.32194600 5.16502700 1.23717800
 C -1.06306000 5.06464900 1.23715500
 C 2.43107500 4.98565900 -0.05642000
 C 3.28512300 4.86092600 1.05696000
 C 4.33666000 3.95146000 1.05696300
 C 4.58317600 3.12429400 -0.05640400
 C 3.87983000 3.42451500 -1.23713900
 C 2.82954500 4.33292300 -1.23715400
 C 5.76006300 1.11426800 -1.05695800
 C 5.86053300 -0.27236800 -1.05695100
 C 5.45005100 -1.03157900 0.05645000
 C 5.16507200 -0.32195300 1.23720400
 C 5.06468900 1.06305400 1.23718900
 C 4.98569400 -2.43106700 -0.05643000
 C 4.86094900 -3.28513200 1.05693800
 C 3.95147300 -4.33665800 1.05692600
 C 3.12430000 -4.58314800 -0.05644500
 C 3.42452600 -3.87978400 -1.23716500
 C 4.33295100 -2.82951200 -1.23716700
 C 1.80636400 -5.24437800 0.05639900
 C 1.11425500 -5.75998200 -1.05701700
 C -0.27238000 -5.86044300 -1.05699700
 C -1.03157800 -5.45000000 0.05642800
 C -0.32193400 -5.16506600 1.23718100
 C 1.06307300 -5.06469100 1.23715500
 C -2.43106800 -4.98564700 -0.05642100
 C -3.28511000 -4.86090800 1.05696400
 C -4.33664900 -3.95144800 1.05697000
 C -4.58317400 -3.12428700 -0.05640000
 C -3.87983900 -3.42451200 -1.23713800
 C -2.82955300 -4.33292000 -1.23715500
 C 5.24441400 1.80635900 0.05644700
 H -6.01029200 -1.66259700 -1.96168100
 H -6.18715500 0.77889400 -1.96169400
 H -4.86121700 0.86546300 2.12707500
 H -4.68563500 -1.55707700 2.12705300
 H -5.42568900 3.07446200 1.96163700
 H -3.82439400 4.92588500 1.96160900
 H -2.82523900 4.04914200 -2.12700000
 H -4.41419400 2.21207800 -2.12699800
 H -1.66257500 6.01022500 -1.96172300
 H 0.77891500 6.18710500 -1.96171000
 H 0.86545900 4.86112700 2.12704500
 H -1.55708800 4.68555100 2.12701000
 H 3.07441700 5.42566000 1.96165500
 H 4.92587600 3.82437800 1.96165400
 H 4.04920500 2.82523400 -2.12697200

H 2.21211900 4.41415700 -2.12699100
 H 6.01031300 1.66258900 -1.96167300
 H 6.18719200 -0.77888200 -1.96167900
 H 4.86116800 -0.86547500 2.12706200
 H 4.68558000 1.55707900 2.12704200
 H 5.42568800 -3.07444400 1.96163400
 H 3.82438800 -4.92589100 1.96160600
 H 2.82523800 -4.04913000 -2.12699900
 H 4.41418800 -2.21208100 -2.12700000
 H 1.66257100 -6.01020600 -1.96174300
 H -0.77890600 -6.18707300 -1.96173000
 H -0.86543900 -4.86118900 2.12705900
 H 1.55711100 -4.68561700 2.12701700
 H -3.07440600 -5.42563900 1.96166100
 H -4.92586400 -3.82436900 1.96166100
 H -4.04921900 -2.82523000 -2.12696900
 H -2.21213500 -4.41415400 -2.12699800

[8]CPP²⁻

C 3.02913600 4.69144100 0.02456700
 C 3.75193200 4.32294700 -1.14696200
 C 4.67820200 3.29834300 -1.14691000
 C 4.97205300 2.54220900 0.02466300
 C 4.46692700 3.10707900 1.22963900
 C 3.54028500 4.13210400 1.22959200
 C 5.45889500 1.17551500 -0.02438000
 C 5.71036300 0.40377300 1.14689900
 C 5.64101000 -0.97574900 1.14680600
 C 5.31335100 -1.71824200 -0.02454500
 C 5.35408300 -0.96143200 -1.22942700
 C 5.42351900 0.41857400 -1.22934300
 C 4.69166500 -3.02909900 0.02447000
 C 4.32307000 -3.75179200 -1.14710600
 C 3.29840600 -4.67798800 -1.14708600
 C 2.54228500 -4.97184800 0.02450400
 C 3.10725900 -4.46687500 1.22949500
 C 4.13237500 -3.54034000 1.22948500
 C 1.17553100 -5.45852000 -0.02450200
 C 0.40384700 -5.71010500 1.14678200
 C -0.97567400 -5.64072900 1.14675800
 C -1.71821600 -5.31296100 -0.02452100
 C -0.96146600 -5.35344100 -1.22944300
 C 0.41854600 -5.42286600 -1.22943100
 C -3.75193600 -4.32293600 -1.14698700
 C -4.67823100 -3.29835400 -1.14694700
 C -4.97212700 -2.54223300 0.02464000
 C -4.46705200 -3.10715800 1.22961300
 C -3.54039000 -4.13215300 1.22957500
 C -5.45894900 -1.17554200 -0.02437900
 C -5.71029700 -0.40380700 1.14693300
 C -5.64091000 0.97570200 1.14686100
 C -5.31334200 1.71821100 -0.02450300
 C -5.35420500 0.96143200 -1.22939900
 C -5.42367900 -0.41858200 -1.22934300
 C -4.69158900 3.02904700 0.02450500
 C -4.32307900 3.75180100 -1.14705100
 C -3.29841000 4.67801300 -1.14704100
 C -2.54224200 4.97183600 0.02451200
 C -3.10709600 4.46674500 1.22950800
 C -4.13218900 3.54019500 1.22950600
 C -1.17551600 5.45859400 -0.02451800
 C -0.40383800 5.71026600 1.14674500
 C 0.97569300 5.64090900 1.14672500

C 1.71821900 5.31304800 -0.02453400
 C 0.96147200 5.35349600 -1.22945800
 C -0.41853600 5.42292200 -1.22945100
 C -3.02915100 -4.69142800 0.02456200
 H 3.52146200 4.80832600 -2.09301100
 H 5.13798600 3.02016300 -2.09292000
 H 4.69329600 2.62904900 2.17914600
 H 3.08738600 4.40540600 2.17906900
 H 5.89169900 0.90982500 2.09280700
 H 5.77059000 -1.49755000 2.09266800
 H 5.17521700 -1.45941100 -2.17880100
 H 5.29563700 0.93211200 -2.17867200
 H 4.80842600 -3.52128700 -2.09315700
 H 3.02017600 -5.13773600 -2.09310100
 H 2.62925300 -4.69330800 2.17900100
 H 4.40581200 -3.08759200 2.17899500
 H 0.90995200 -5.89155000 2.09263700
 H -1.49743900 -5.77041900 2.09261800
 H -1.45949000 -5.17432000 -2.17874700
 H 0.93205600 -5.29469200 -2.17873600
 H -3.52141500 -4.80829000 -2.09304400
 H -5.13801300 -3.02018300 -2.09296700
 H -4.69352200 -2.62920400 2.17913300
 H -3.08756200 -4.40550400 2.17907000
 H -5.89156000 -0.90987700 2.09283900
 H -5.77042000 1.49749400 2.09273100
 H -5.17541600 1.45942200 -2.17878500
 H -5.29591000 -0.93209900 -2.17870000
 H -4.80846000 3.52132900 -2.09309900
 H -3.02022200 5.13776500 -2.09306900
 H -2.62899300 4.69309100 2.17898400
 H -4.40551500 3.08733500 2.17899200
 H -0.90993800 5.89177300 2.09259300
 H 1.49746100 5.77069100 2.09257400
 H 1.45950500 5.17435200 -2.17875200
 H -0.93205200 5.29474700 -2.17875300

[8]CPP²⁺

C 2.76269000 4.77624500 0.02584200
 C 3.50805300 4.48282300 -1.15032700
 C 4.48119200 3.50988900 -1.15027800
 C 4.77486800 2.76456700 0.02588800
 C 4.24273900 3.27015200 1.24135300
 C 3.26833600 4.24423100 1.24130500
 C 5.33069000 1.42378500 -0.02570500
 C 5.64973700 0.68910800 1.15053800
 C 5.65022300 -0.68697600 1.15039600
 C 5.33170200 -1.42162400 -0.02600800
 C 5.31336600 -0.68767800 -1.24138000
 C 5.31286800 0.69009400 -1.24124500
 C 4.77652200 -2.76264900 0.02542900
 C 4.48267600 -3.50785300 -1.15078400
 C 3.50969100 -4.48091600 -1.15063500
 C 2.76463900 -4.77469900 0.02568100
 C 3.27065200 -4.24285600 1.24109800
 C 4.24484700 -3.26858800 1.24095200
 C 1.42379800 -5.33031700 -0.02565900
 C 0.68925500 -5.64927100 1.15069600
 C -0.68682500 -5.64966400 1.15072800
 C -1.42159000 -5.33117600 -0.02560700
 C -0.68782000 -5.31276800 -1.24106600
 C 0.68995200 -5.31232200 -1.24110600
 C -3.50789200 -4.48253900 -1.15041600

C -4.48111600	-3.50969100	-1.15038400	C 2.82612600	6.31133000	-0.04615600
C -4.77502900	-2.76453000	0.02583900	C 3.25976800	5.66808700	-1.21891300
C -4.24304400	-3.27028300	1.24130600	C 4.38334800	4.85175900	-1.21891300
C -3.26858900	-4.24428900	1.24126500	C 5.12911000	4.63811300	-0.04615600
C -5.33088200	-1.42377000	-0.02572700	C 4.80295600	5.42809200	1.07238900
C -5.64981700	-0.68908900	1.15056300	C 3.67822800	6.24525500	1.07238900
C -5.65023500	0.68697300	1.15047100	C 5.99609000	3.44481800	0.04615600
C -5.33174000	1.42162900	-0.02592900	C 5.96882600	2.66953500	1.21891300
C -5.31353600	0.68774600	-1.24133000	C 6.39799500	1.34868800	1.21891300
C -5.31313400	-0.69003500	-1.24125300	C 6.87575200	0.73749700	0.04615600
C -4.77645600	2.76260200	0.02548900	C 7.07622600	1.56831200	-1.07238900
C -4.48272000	3.50783500	-1.15071100	C 6.64661800	2.89051000	-1.07238900
C -3.50969900	4.48090200	-1.15058800	C 6.87575200	-0.73749700	-0.04615600
C -2.76453100	4.77456600	0.02565500	C 6.39799500	-1.34868800	-1.21891300
C -3.27034000	4.24259200	1.24109200	C 5.96882600	-2.66953500	-1.21891300
C -4.24453800	3.26833000	1.24098200	C 5.99609000	-3.44481800	-0.04615600
C -1.42370000	5.33027000	-0.02570900	C 6.64661800	-2.89051000	1.07238900
C -0.68921400	5.64952800	1.15059000	C 7.07622600	-1.56831200	1.07238900
C 0.68688500	5.64997700	1.15064700	C 4.38334800	-4.85175900	1.21891300
C 1.42164000	5.33132200	-0.02563100	C 3.25976800	-5.66808700	1.21891300
C 0.68791900	5.31254100	-1.24109500	C 2.82612600	-6.31133000	0.04615600
C -0.68985800	5.31204100	-1.24114800	C 3.67822800	-6.24525500	-1.07238900
C -2.76263400	-4.77606800	0.02581500	C 4.80295600	-5.42809200	-1.07238900
H 3.27817300	4.99163800	-2.08049600	C 1.42332300	-6.76712800	-0.04615600
H 4.99009700	3.28016000	-2.08042500	C 0.69441000	-6.50162200	-1.21891300
H 4.50244100	2.80292800	2.18454600	C -0.69441000	-6.50162200	-1.21891300
H 2.80075400	4.50381100	2.18437400	C -1.42332300	-6.76712800	-0.04615600
H 5.84636000	1.21127800	2.08092700	C -0.69512000	-7.21452600	1.07238900
H 5.84706900	-1.20924700	2.08068700	C 0.69512000	-7.21452600	1.07238900
H 5.16725800	-1.20169800	-2.18466500	C -2.82612600	-6.31133000	0.04615600
H 5.16644300	1.20414200	-2.18446100	C -3.25976800	-5.66808700	1.21891300
H 4.99123600	-3.27794600	-2.08106900	C -4.38334800	-4.85175900	1.21891300
H 3.27969800	-4.98972000	-2.08077500	C -5.12911000	-4.63811300	0.04615600
H 2.80370400	-4.50276100	2.18437900	C -4.80295600	-5.42809200	-1.07238900
H 4.50484500	-2.80137900	2.18407900	C -3.67822800	-6.24525500	-1.07238900
H 1.21157300	-5.84590600	2.08099900	C 5.12911000	-4.63811300	0.04615600
H -1.20903700	-5.84644100	2.08106100	C -5.99609000	-3.44481800	-0.04615600
H -1.20197500	-5.16649700	-2.18426200	C -5.96882600	-2.66953500	-1.21891300
H 1.20388300	-5.16576800	-2.18436900	C -6.39799500	-1.34868800	-1.21891300
H -3.27789500	-4.99116500	-2.08065600	C -6.87575200	-0.73749700	-0.04615600
H -4.98989400	-3.27992000	-2.08059000	C -7.07622600	-1.56831200	1.07238900
H -4.50300700	-2.80328800	2.18453600	C -6.64661800	-2.89051000	1.07238900
H -2.80124500	-4.50404300	2.18439500	C -6.87575200	0.73749700	0.04615600
H -5.84640100	-1.21131100	2.08092500	C -6.39799500	1.34868800	1.21891300
H -5.84698700	1.20927800	2.08076000	C -5.96882600	2.66953500	1.21891300
H -5.16743900	1.20179700	-2.18461000	C -5.99609000	3.44481800	0.04615600
H -5.16685800	-1.20401700	-2.18452900	C -6.64661800	2.89051000	-1.07238900
H -4.99137400	3.27799200	-2.08096600	C -7.07622600	1.56831200	-1.07238900
H -3.27981500	4.98975100	-2.08073700	C -5.12911000	4.63811300	-0.04615600
H -2.80316800	4.50235500	2.18430000	C -4.80295600	5.42809200	1.07238900
H -4.50434500	2.80092200	2.18406400	C -3.67822800	6.24525500	1.07238900
H -1.21155400	5.84638000	2.08084100	C -2.82612600	6.31133000	-0.04615600
H 1.20913300	5.84697600	2.08092500	C -3.25976800	5.66808700	-1.21891300
H 1.20214000	5.16594600	-2.18420900	C -4.38334800	4.85175900	-1.21891300
H -1.20380600	5.16518700	-2.18435800	H -1.22550600	7.51237200	-1.97330600
[10]CPP			H 1.22550600	7.51237200	-1.97330600
C -1.42332300	6.76712800	0.04615600	H 1.21799600	6.15773100	2.10634900
C -0.69512000	7.21452600	-1.07238900	H -1.21799600	6.15773100	2.10634900
C 0.69512000	7.21452600	-1.07238900	H 2.63404500	5.69762900	-2.10634900
C 1.42332300	6.76712800	0.04615600	H 4.60480300	4.26579000	-2.10634900
C 0.69441000	6.50162200	1.21891300	H 5.40711600	5.35730200	1.97330600
C -0.69441000	6.50162200	1.21891300	H 3.42420600	6.79797100	1.97330600

H 6.23273200 0.74446100 2.10634900
 H 7.52339200 1.15592500 -1.97330600
 H 6.76598800 3.48697600 -1.97330600
 H 6.23273200 -0.74446100 -2.10634900
 H 5.47996900 -3.06122600 -2.10634900
 H 6.76598800 -3.48697600 1.97330600
 H 7.52339200 -1.15592500 1.97330600
 H 4.60480300 -4.26579000 2.10634900
 H 2.63404500 -5.69762900 2.10634900
 H 3.42420600 -6.79797100 -1.97330600
 H 5.40711600 -5.35730200 -1.97330600
 H 1.21799600 -6.15773100 -2.10634900
 H -1.21799600 -6.15773100 -2.10634900
 H -1.22550600 -7.51237200 1.97330600
 H 1.22550600 -7.51237200 1.97330600
 H -2.63404500 -5.69762900 2.10634900
 H -4.60480300 -4.26579000 2.10634900
 H -5.40711600 -5.35730200 -1.97330600
 H -3.42420600 -6.79797100 -1.97330600
 H -5.47996900 -3.06122600 -2.10634900
 H -6.23273200 -0.74446100 -2.10634900
 H -7.52339200 -1.15592500 1.97330600
 H -6.76598800 -3.48697600 1.97330600
 H -6.23273200 0.74446100 2.10634900
 H -5.47996900 3.06122600 2.10634900
 H -6.76598800 3.48697600 -1.97330600
 H -7.52339200 1.15592500 -1.97330600
 H -5.40711600 5.35730200 1.97330600
 H -3.42420600 6.79797100 1.97330600
 H -2.63404500 5.69762900 -2.10634900
 H -4.60480300 4.26579000 -2.10634900

[10]CPP²

C -1.44610400 6.80593400 0.02642800
 C -0.69143900 7.11204600 -1.13787300
 C 0.69143900 7.11204600 -1.13787300
 C 1.44610400 6.80593400 0.02642800
 C 0.69157400 6.72218700 1.22571300
 C -0.69157400 6.72218700 1.22571300
 C 2.83050500 6.35611500 -0.02642800
 C 3.39170700 5.84486000 -1.22571300
 C 4.51069700 5.03186700 -1.22571300
 C 5.17035000 4.65611800 -0.02642800
 C 4.73974200 5.34734800 1.13787300
 C 3.62097000 6.16018400 1.13787300
 C 6.02595700 3.47847600 0.02642800
 C 6.17947100 2.73499500 1.22571300
 C 6.60688700 1.41954400 1.22571300
 C 6.91969900 0.72782300 0.02642800
 C 6.97762400 1.54014500 -1.13787300
 C 6.55029100 2.85534100 -1.13787300
 C 6.91969900 -0.72782300 -0.02642800
 C 6.60688700 -1.41954400 -1.22571300
 C 6.17947100 -2.73499500 -1.22571300
 C 6.02595700 -3.47847600 -0.02642800
 C 6.55029100 -2.85534100 1.13787300
 C 6.97762400 -1.54014500 1.13787300
 C 4.51069700 -5.03186700 1.22571300
 C 3.39170700 -5.84486000 1.22571300
 C 2.83050500 -6.35611500 0.02642800
 C 3.62097000 -6.16018400 -1.13787300
 C 4.73974200 -5.34734800 -1.13787300
 C 1.44610400 -6.80593400 -0.02642800

C 0.69157400 -6.72218700 -1.22571300
 C -0.69157400 -6.72218700 -1.22571300
 C -1.44610400 -6.80593400 -0.02642800
 C -0.69143900 -7.11204600 1.13787300
 C 0.69143900 -7.11204600 1.13787300
 C -2.83050500 -6.35611500 0.02642800
 C -3.39170700 -5.84486000 1.22571300
 C -4.51069700 -5.03186700 1.22571300
 C -5.17035000 -4.65611800 0.02642800
 C -6.02595700 -3.47847600 -0.02642800
 C -4.73974200 -5.34734800 -1.13787300
 C -3.62097000 -6.16018400 -1.13787300
 C -6.91969900 -0.72782300 -0.02642800
 C -6.0688700 1.41954400 1.22571300
 C -6.97762400 1.54014500 -1.13787300
 C -6.55029100 2.85534100 1.13787300
 C -6.91969900 0.72782300 0.02642800
 C -6.60688700 1.54014500 -1.13787300
 C -6.17947100 2.73499500 1.22571300
 C -6.02595700 3.47847600 0.02642800
 C -6.55029100 2.85534100 -1.13787300
 C -6.97762400 1.54014500 -1.13787300
 C -4.51069700 5.03186700 -1.22571300
 C -1.20961000 7.30629000 -2.07432800
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H 1.20179500 6.51347700 2.16218700
 H -1.20179500 6.51347700 2.16218700
 H 2.85625300 5.97591100 -2.16218700
 H 4.80079800 4.56311600 -2.16218700
 H 5.27312400 5.19992200 2.07432800
 H 3.31593500 6.62190400 2.07432800
 H 5.82330900 3.15575000 2.16218700
 H 6.56606000 0.86980000 2.16218700
 H 7.32248500 1.10736100 -2.07432800
 H 6.57490500 3.40817500 -2.07432800
 H 6.56606000 -0.86980000 -2.16218700
 H 5.82330900 -3.15575000 -2.16218700
 H 6.57490500 -3.40817500 2.07432800
 H 7.32248500 -1.10736100 2.07432800
 H 4.80079800 -4.56311600 2.16218700
 H 2.85625300 -5.97591100 2.16218700
 H 3.31593500 -6.62190400 -2.07432800
 H 5.27312400 -5.19992200 -2.07432800
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 H -1.20179500 -6.51347700 -2.16218700
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 H 1.20961000 -7.30629000 2.07432800
 H -2.85625300 -5.97591100 2.16218700
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 H -5.27312400 -5.19992200 -2.07432800
 H -3.31593500 -6.62190400 -2.07432800
 H -5.82330900 -3.15575000 -2.16218700
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 H -6.57490500 -3.40817500 2.07432800
 H -6.56606000 0.86980000 2.16218700

H -5.82330900 3.15575000 2.16218700
H -6.57490500 3.40817500 -2.07432800
H -7.32248500 1.10736100 -2.07432800
H -5.27312400 5.19992200 2.07432800
H -3.31593500 6.62190400 2.07432800
H -2.85625300 5.97591100 -2.16218700
H -4.80079800 4.56311600 -2.16218700

[10]CPP²⁺

C -1.42469500 6.74196100 0.02753800
C -0.68945200 7.07900200 -1.13845000
C 0.68945200 7.07900200 -1.13845000
C 1.42469500 6.74196100 0.02753800
C 0.69005800 6.63420900 1.23355300
C -0.69005800 6.63420900 1.23355300
C 2.81022300 6.29177600 -0.02753800
C 3.34122100 5.77279300 -1.23355300
C 4.45775900 4.96158100 -1.23355300
C 5.11542800 4.61694600 -0.02753800
C 4.71871100 5.32178300 1.13845000
C 3.60315500 6.13228200 1.13845000
C 5.97173100 3.43834600 0.02753800
C 6.09626800 2.70636700 1.23355300
C 6.52274700 1.39379900 1.23355300
C 6.85224100 0.72841500 0.02753800
C 6.94558300 1.53182400 -1.13845000
C 6.51947900 2.84323900 -1.13845000
C 6.85224100 -0.72841500 -0.02753800
C 6.52274700 -1.39379900 -1.23355300
C 6.09626800 -2.70636700 -1.23355300
C 5.97173100 -3.43834600 -0.02753800
C 6.51947900 -2.84323900 1.13845000
C 6.94558300 -1.53182400 1.13845000
C 4.45775900 -4.96158100 1.23355300
C 3.34122100 -5.77279300 1.23355300
C 2.81022300 -6.29177600 0.02753800
C 3.60315500 -6.13228200 -1.13845000
C 4.71871100 -5.32178300 -1.13845000
C 1.42469500 -6.74196100 -0.02753800
C 0.69005800 -6.63420900 -1.23355300
C -0.69005800 -6.63420900 -1.23355300
C -1.42469500 -6.74196100 -0.02753800
C -0.68945200 -7.07900200 1.13845000
C 0.68945200 -7.07900200 1.13845000
C -2.81022300 -6.29177600 0.02753800
C -3.34122100 -5.77279300 1.23355300
C -4.45775900 -4.96158100 1.23355300
C -5.11542800 -4.61694600 0.02753800
C -4.71871100 -5.32178300 -1.13845000
C -3.60315500 -6.13228200 -1.13845000
C 5.11542800 -4.61694600 0.02753800
C -5.97173100 -3.43834600 -0.02753800
C -6.09626800 -2.70636700 -1.23355300
C -6.52274700 -1.39379900 -1.23355300
C -6.85224100 -0.72841500 -0.02753800
C -6.94558300 -1.53182400 1.13845000
C -6.51947900 -2.84323900 1.13845000
C -6.85224100 0.72841500 0.02753800
C -6.52274700 1.39379900 1.23355300
C -6.09626800 2.70636700 1.23355300
C -5.97173100 3.43834600 0.02753800
C -6.51947900 2.84323900 -1.13845000
C -6.94558300 1.53182400 -1.13845000

C -5.11542800 4.61694600 -0.02753800
C -4.71871100 5.32178300 1.13845000
C -3.60315500 6.13228200 1.13845000
C -2.81022300 6.29177600 -0.02753800
C -3.34122100 5.77279300 -1.23355300
C -4.45775900 4.96158100 -1.23355300
H -1.21354500 7.31005300 -2.06024800
H 1.21354500 7.31005300 -2.06024800
H 1.20655400 6.42616200 2.16423300
H -1.20655400 6.42616200 2.16423300
H 2.80108100 5.90806900 -2.16423300
H 4.75332600 4.48968000 -2.16423300
H 5.27852000 5.20065300 2.06024800
H 3.31496300 6.62726100 2.06024800
H 5.73879800 3.13329400 2.16423300
H 6.48448900 0.83829300 2.16423300
H 7.32728000 1.10478100 -2.06024800
H 6.57726800 3.41308000 -2.06024800
H 6.48448900 -0.83829300 -2.16423300
H 5.73879800 -3.13329400 -2.16423300
H 6.57726800 -3.41308000 2.06024800
H 7.32728000 -1.10478100 2.06024800
H 4.75332600 -4.48968000 2.16423300
H 2.80108100 -5.90806900 2.16423300
H 3.31496300 -6.62726100 -2.06024800
H 5.27852000 -5.20065300 -2.06024800
H 1.20655400 -6.42616200 -2.16423300
H -1.20655400 -6.42616200 -2.16423300
H -1.21354500 -7.31005300 2.06024800
H 1.21354500 -7.31005300 2.06024800
H -2.80108100 -5.90806900 2.16423300
H -4.75332600 -4.48968000 2.16423300
H -5.27852000 -5.20065300 -2.06024800
H -3.31496300 -6.62726100 -2.06024800
H -5.73879800 -3.13329400 -2.16423300
H -6.48448900 -0.83829300 -2.16423300
H -7.32728000 -1.10478100 2.06024800
H -6.57726800 -3.41308000 2.06024800
H -6.48448900 0.83829300 2.16423300
H -5.73879800 3.13329400 2.16423300
H -6.57726800 3.41308000 -2.06024800
H -7.32728000 1.10478100 -2.06024800
H -5.27852000 5.20065300 2.06024800
H -3.31496300 6.62726100 2.06024800
H -2.80108100 5.90806900 -2.16423300
H -4.75332600 4.48968000 -2.16423300

[11]CPP

C 0.79594200 -7.54085500 -1.13245800
C -0.58745600 -7.55472900 -1.25215500
C -1.42203500 -7.44765100 -0.12369300
C -0.79390400 -7.54088100 1.13250400
C 0.58949600 -7.55438300 1.25219900
C 1.42405400 -7.44726200 0.12372300
H 1.39413400 -7.50348100 -2.03807600
H -1.02318900 -7.57304300 -2.24683900
H -1.39212000 -7.50350300 2.03810800
H 1.02521700 -7.57242200 2.24689300
C -6.22820000 -4.39698500 -0.07057900
C -6.29920700 -3.67396200 1.13259500
C -6.92147600 -3.87436100 -1.17772400
C -6.87643500 -2.41060800 1.17797400
H -5.77948000 -4.04873900 2.01019400

C -7.50571500 -2.61439400 -1.12953400
 H -6.95761800 -4.44367600 -2.10316200
 C -7.41606800 -1.81364900 0.02478500
 H -6.79177900 -1.82848000 2.09118900
 H -7.99357100 -2.22194700 -2.01794600
 C 3.47098500 6.74548800 -0.03553000
 C 2.72248900 6.69414000 1.15349900
 C 2.86696100 7.36030300 -1.14785900
 C 1.38894900 7.08097600 1.18244800
 H 3.15271700 6.22668500 2.03466600
 C 1.53258300 7.74945400 -1.11813600
 H 3.43838300 7.49164500 -2.06323800
 C 0.73743400 7.54009100 0.02422300
 H 0.81171000 6.90532800 2.08569800
 H 1.08550900 8.17912600 -2.01090000
 C -7.61772600 -0.35004900 -0.01347100
 C -7.92394500 0.40702200 1.13286900
 C -7.25943800 0.36113000 -1.17248100
 C -7.71969800 1.78219800 1.16355400
 H -8.28183600 -0.09551200 2.02779900
 C -7.05801300 1.73447700 -1.14275600
 H -7.01252900 -0.18408300 -2.07877800
 C -7.20225800 2.46710500 0.04840900
 H -7.92041100 2.32819800 2.08186900
 H -6.65997500 2.22552800 -2.02613900
 C -6.58614100 3.80645600 0.14765400
 C -6.47043600 4.66801600 -0.95920500
 C -5.86847400 4.15129500 1.30631700
 C -5.55637900 5.71524700 -0.96330000
 H -7.07039300 4.48339700 -1.84664200
 C -4.95537900 5.19825400 1.30245000
 H -5.93131900 3.51243600 2.18271900
 C -4.71510800 5.95138100 0.13980800
 H -5.45754700 6.33077000 -1.85381100
 H -4.32797000 5.35113300 2.17603500
 C -3.47282400 6.74453600 0.03552900
 C -2.72429700 6.69333800 -1.15348800
 C -2.86898300 7.35954500 1.14784700
 C -1.39086100 7.08053900 -1.18243300
 H -3.15438200 6.22572300 -2.03463900
 C -1.53471200 7.74905900 1.11812800
 H -3.44045200 7.49075000 2.06321600
 C -0.73949200 7.53987800 -0.02421500
 H -0.81356200 6.90501400 -2.08566800
 H -1.08776300 8.17887700 2.01088400
 C 7.61783000 -0.34798100 0.01347000
 C 7.92383000 0.40917300 -1.13287400
 C 7.25937100 0.36310500 1.17248600
 C 7.71920000 1.78429200 -1.16356000
 H 8.28185600 -0.09326100 -2.02780700
 C 7.05756400 1.73639400 1.14275800
 H 7.01263700 -0.18217500 2.07879200
 C 7.20157800 2.46905400 -0.04841400
 H 7.91975100 2.33034300 -2.08187900
 H 6.65940900 2.22734200 2.02614700
 C 6.58508300 3.80822700 -0.14766000
 C 5.86728500 4.15283900 -1.30631000
 C 6.46916500 4.66977100 0.95918600
 C 4.95391300 5.19955500 -1.30244500
 H 5.93026700 3.51396900 -2.18269300
 C 5.55482900 5.71675900 0.96327900
 H 7.06917700 4.48532100 1.84662000
 C 4.71347200 5.95265100 -0.13981500
 H 4.32643800 5.35223800 -2.17601700
 H 5.45584700 6.33226500 1.85378400
 C 2.83192600 -7.00893200 0.23290600
 C 3.23976400 -6.25328900 1.34783400
 C 3.74754700 -7.11023500 -0.83304800
 C 4.41701300 -5.51917100 1.33488000
 H 2.57123700 -6.13955000 2.19515200
 C 4.92010200 -6.36231800 -0.85373300
 H 3.51763700 -7.74690500 -1.68294900
 C 5.24540300 -5.48935300 0.19989400
 H 4.63401600 -4.85803900 2.16917500
 H 5.57452400 -6.42301900 -1.71986400
 C 6.22940400 -4.39529900 0.07056600
 C 6.30024100 -3.67226200 -1.13260400
 C 6.92252400 -3.87247700 1.17772700
 C 6.87712100 -2.40874500 -1.17797500
 H 5.78063600 -4.04717400 -2.01021600
 C 7.50641000 -2.61235200 1.12954500
 H 6.95881500 -4.44179100 2.10316000
 C 7.41657100 -1.81163400 -0.02478600
 H 6.79231500 -1.82665100 -2.09119700
 H 7.99415200 -2.21976700 2.01796100
 C -5.24388800 -5.49075900 -0.19991800
 C -4.91843500 -6.36372900 0.85365300
 C -4.41540500 -5.52022800 -1.33484700
 C -3.74568100 -7.11134200 0.83298200
 H -5.57290700 -6.42468200 1.71972900
 C -3.23795900 -6.25402900 -1.34778500
 H -4.63252700 -4.85906300 -2.16908500
 C -2.83001800 -7.00968500 -0.23289900
 H -3.51565000 -7.74804300 1.68282800
 H -2.56936800 -6.14003300 -2.19502100

[11]CPP²

C 7.54807500 -1.32396900 -1.16455500
 C 7.18071300 -2.65581200 -1.22580000
 C 6.85625300 -3.40661500 -0.06501500
 C 7.14880600 -2.75932800 1.16363300
 C 7.52279900 -1.42934300 1.22489000
 C 7.63271100 -0.61880300 0.06415600
 H 7.67932800 -0.78880900 -2.10106300
 H 7.07620700 -3.11133600 -2.20685000
 H 6.98499000 -3.28539900 2.10014800
 H 7.66916600 -0.98546200 2.20592100
 C 2.60008900 -7.18692000 -0.02217100
 C 1.85885700 -7.19422700 1.18636600
 C 1.88699800 -7.61161200 -1.17344000
 C 0.49181500 -7.40912500 1.20756000
 H 2.34548100 -6.89210900 2.10993200
 C 0.52106100 -7.82881900 -1.15155900
 H 2.41843700 -7.73397100 -2.11451600
 C -0.25277600 -7.63828900 0.02289100
 H -0.03424000 -7.26635600 2.14760400
 H 0.02588000 -8.11538000 -2.07648600
 C -5.61225700 5.19219400 -0.00793000
 C -5.91409300 4.50656000 1.19568200
 C -6.27405700 4.70548700 -1.16504900
 C -6.64582300 3.33215000 1.20824100
 H -5.45166800 4.83210200 2.12358000
 C -7.00642600 3.53168000 -1.15231400
 H -6.17407900 5.24575600 -2.10371100
 C -7.14043600 2.74065900 0.01843500
 H -6.72514200 2.78852000 2.14573600

H -7.45687100	3.19046100	-2.08155300	C 5.54863500	5.54743000	1.17395500
C -1.69893900	-7.44997500	-0.00940600	C 4.24871500	6.09364200	-1.20690400
C -2.49727200	-7.42169000	1.16368600	H 5.57031100	4.69502100	-2.10955600
C -2.35909300	-7.05320100	-1.19983100	C 4.49018300	6.43775400	1.15228400
C -3.76401900	-6.86502900	1.17624700	H 6.06710800	5.37818600	2.11499600
H -2.09216900	-7.81140000	2.09473600	C 3.72881200	6.67360900	-0.02210100
C -3.62604200	-6.49720100	-1.18738900	H 3.72444200	6.24273000	-2.14696100
H -1.81287800	-7.06060000	-2.13909000	H 4.21365400	6.93840000	2.07732400
C -4.34464400	-6.28852900	0.01671800	C 3.91517700	-6.56206600	-0.09636400
H -4.30964600	-6.83674600	2.11668800	C 4.71921100	-6.31652900	1.04683400
H -4.01708200	-6.09330300	-2.11728800	C 4.36575300	-5.95099100	-1.29322700
C -5.46043300	-5.35071300	0.07458900	C 5.75425400	-5.39849000	1.03377900
C -6.15218300	-4.90907400	-1.08327200	H 4.49479400	-6.83300200	1.97751400
C -5.76645600	-4.64810800	1.26734800	C 5.39780700	-5.03050900	-1.30528300
C -6.91769200	-3.75661000	-1.08573700	H 3.80796600	-6.10734900	-2.21270000
H -6.04978800	-5.46682200	-2.01133200	C 6.07514400	-4.63709200	-0.12165400
C -6.53255700	-3.49563900	1.26500900	H 6.30235500	-5.22926900	1.95725500
H -5.28252700	-4.93956700	2.19559800	H 5.60299700	-4.51261500	-2.23747600
C -7.05931300	-2.94478600	0.06959800			
H -7.39019100	-3.44832500	-2.01561400			
H -6.61567300	-2.93383200	2.19145400			
C -7.49075900	-1.55277600	0.00754000			
C -7.39427300	-0.80980900	-1.19604400			
C -7.80632500	-0.79391800	1.16444300			
C -7.41361700	0.57375500	-1.20872100			
H -7.16634300	-1.32749400	-2.12387500			
C -7.82641600	0.58948500	1.15159400			
H -8.00050500	-1.30786200	2.10312900			
C -7.53169600	1.33585300	-0.01903500			
H -7.20021400	1.08000300	-2.14621800			
H -8.03605400	1.11440900	2.08075700			
C 2.39252700	7.25769100	0.01012000			
C 1.69383300	7.64440500	-1.16316700			
C 1.62222300	7.25844300	1.20050700			
C 0.32139600	7.82006400	-1.17590800			
H 2.24193500	7.76910600	-2.09422200			
C 0.24993500	7.43487100	1.18788000			
H 2.09393200	6.98374900	2.13999600			
C -0.47332300	7.62574500	-0.01635700			
H -0.16083900	8.07645500	-2.11647200			
H -0.29340800	7.29066100	2.11778500			
C -1.91287100	7.39726500	-0.07437100			
C -2.53687400	6.95238900	-1.26711600			
C -2.73362500	7.37625200	1.08325000			
C -3.78771600	6.36040300	-1.26494800			
H -1.97141300	6.95177200	-2.19504200			
C -3.98400100	6.78399700	1.08553300			
H -2.35830100	7.80150600	2.01123900			
C -4.52379400	6.16130400	-0.06976500			
H -4.14845400	5.92131600	-2.19118800			
H -4.54818400	6.76409500	2.01519300			
C 7.60008800	0.83827000	0.12108700			
C 7.22399800	1.52489000	1.30501700			
C 7.71833200	1.65618900	-1.03422400			
C 6.81566000	2.84614000	1.29337400			
H 7.13273600	0.97525500	2.23715300			
C 7.30618900	2.97688300	-1.04688000			
H 8.10012700	1.22849800	-1.95787500			
C 6.74468700	3.60217100	0.09657600			
H 6.41929100	3.26795800	2.21313400			
H 7.38046300	3.53523200	-1.97747300			
C 5.94056200	4.81596200	0.02256000			
C 5.30918400	5.20464000	-1.18589800			

C -3.31310700	-7.10555500	-1.06638400	H 6.55920200	-2.62577800	-2.22853900
H -1.61042900	-8.00377500	-1.97497200	C 7.57351000	-0.12260600	-0.15052400
C -3.13548200	-6.59987100	1.28605900	H 8.22630300	-0.46370800	1.89627500
H -1.26673400	-7.01181100	2.20989200	H 7.04370900	-0.26570400	-2.25273200
C -3.87998100	-6.50726800	0.08661600			
H -3.89473400	-7.17436700	-1.98021200			
H -3.53945800	-6.18828700	2.20483700			
C -5.05582400	-5.64432000	0.01940400			
C -5.39050400	-4.99543000	-1.19238700			
C -5.77293000	-5.24898900	1.17614300			
C -6.22750300	-3.89692600	-1.20970700			
H -4.89548800	-5.28400000	-2.11346400			
C -6.61072100	-4.15230000	1.15839000			
H -5.64607200	-5.79804200	2.10383000			
C -6.78400000	-3.37861300	-0.01665000			
H -6.35989900	-3.36218400	-2.14408800			
H -7.12144900	-3.86767700	2.07277800			
C -2.37984000	7.19224000	0.00626300			
C -3.16391300	7.11988300	-1.17234500			
C -2.97852700	6.72520100	1.20016400			
C -4.36921900	6.44739900	-1.19009700			
H -2.80466000	7.57606500	-2.08930500			
C -4.18488300	6.05330300	1.18266400			
H -2.43570000	6.78818700	2.13706700			
C -4.86931400	5.80441500	-0.03019100			
H -4.92563800	6.39224100	-2.12038900			
H -4.54551100	5.61302000	2.10607200			
C -5.89227300	4.76441900	-0.09267800			
C -6.09322000	4.03643400	-1.28899400			
C -6.56352200	4.29327400	1.06341300			
C -6.74555100	2.81888400	-1.28605100			
H -5.63011500	4.37362200	-2.21015600			
C -7.21459500	3.07640300	1.06658600			
H -6.54697200	4.88201900	1.97507900			
C -7.23724000	2.25255400	-0.08644600			
H -6.77169300	2.24282300	-2.20486500			
H -7.69310900	2.73907600	1.98056300			
C 5.55351000	5.14733400	0.15103800			
C 4.82304800	5.42080900	1.33320100			
C 5.21091300	5.90984100	-0.99549900			
C 3.71420700	6.24226200	1.32127700			
H 5.06339600	4.90094400	2.25342400			
C 4.09428400	6.72107600	-1.01154900			
H 5.81132400	5.83667500	-1.89600100			
C 3.25346600	6.83649400	0.12290700			
H 3.12618300	6.33284800	2.22839300			
H 3.84865000	7.25919200	-1.92177900			
C 1.88598100	7.33847800	0.04002900			
C 1.17216900	7.25477100	-1.17844700			
C 1.14980600	7.71875500	1.18978700			
C -0.20642100	7.33902300	-1.20715000			
H 1.69659000	7.00117500	-2.09377300			
C -0.22675200	7.80822900	1.15960200			
H 1.67006000	7.92065100	2.12085300			
C -0.95637600	7.51685600	-0.02043300			
H -0.71696100	7.14867700	-2.14505600			
H -0.75469100	8.07965700	2.06812800			
C 6.99081200	-2.91601900	-0.12323000			
C 7.53955300	-2.26876600	1.01136800			
C 6.93646000	-2.16573900	-1.32140600			
C 7.82829600	-0.91910700	0.99574000			
H 7.71644200	-2.83359600	1.92137300			
C 7.21259700	-0.81366700	-1.33290000			

[12]CPP

C 4.85827300	-6.24164000	-1.20637200
C 3.69149100	-6.99520600	-1.20645700
C 3.23311900	-7.62952000	-0.03862100
C 4.08074500	-7.59934000	1.08409000
C 5.24853700	-6.84508400	1.08418800
C 5.62481000	-6.08480500	-0.03842000
H 5.11424000	-5.66899300	-2.09332200
H 3.06435800	-6.99289500	-2.09348500
H 3.79859300	-8.14173400	1.98284100
H 5.85886800	-6.81102400	1.98301600
C -6.08482500	-5.62481500	0.03841900
C -6.24167100	-4.85828300	1.20637200
C -6.84510300	-5.24854100	-1.08419100
C -6.99524300	-3.69150400	1.20645900
H -5.66902300	-5.11424500	2.09332100
C -7.59936300	-4.08075300	-1.08409200
H -6.81103800	-5.85887000	-1.98302100
C -7.62955200	-3.23312900	0.03862300
H -6.99292500	-3.06437400	2.09348800
H -8.14175600	-3.79860200	-1.98284400
C 1.01479000	8.22383000	0.03841200
C 0.30092300	7.90342000	1.20632100
C 0.26542900	8.62171800	-1.08408500
C -1.08631100	7.83417300	1.20647500
H 0.84308600	7.58766000	2.09315600
C -1.12304700	8.55245700	-1.08391000
H 0.78083000	8.95046300	-1.98289100
C -1.82882500	8.08194300	0.03875400
H -1.59407700	7.46602600	2.09347500
H -1.66883000	8.82831400	-1.98256900
C -8.08194400	-1.82882800	-0.03875600
C -8.55244600	-1.12304800	1.08391400
C -7.83419500	-1.08631300	-1.20648000
C -8.62171000	0.26542600	1.08408900
H -8.82829100	-1.66883200	1.98257500
C -7.90345000	0.30092200	-1.20632800
H -7.46606100	-1.59407400	-2.09348700
C -8.22384200	1.01479100	-0.03841600
H -8.95044900	0.78082400	1.98289900
H -7.58770600	0.84307800	-2.09317300
C -7.91347000	2.45713400	0.03925300
C -7.96846600	3.30392800	-1.08314500
C -7.32721300	2.97593300	1.20691300
C -7.33430100	4.54106400	-1.08318200
H -8.48050000	2.96938500	-1.98174000
C -6.69358300	4.21194000	1.20686100
H -7.26189000	2.35180500	2.09365700
C -6.61466500	4.99079600	0.03919600
H -7.36168300	5.15207700	-1.98178000
H -6.14872100	4.52328500	2.09360200
C -5.62480700	6.08481500	-0.03841900
C -4.85827700	6.24166300	-1.20637200
C -5.24853600	6.84509500	1.08419100
C -3.69150100	6.99523900	-1.20646100
H -5.11423500	5.66901200	-2.09332100
C -4.08075000	7.59935900	1.08409000
H -5.85886400	6.81102900	1.98302100

C -3.23312700 7.62955100 -0.03862600
 H -3.06437100 6.99292600 -2.09349000
 H -3.79859900 8.14175300 1.98284300
 C 7.62955200 3.23311900 0.03862500
 C 7.59936100 4.08074500 -1.08408700
 C 6.99523300 3.69148400 1.20646000
 C 6.84509200 5.24852800 -1.08418700
 H 8.14175900 3.79859900 -1.98283900
 C 6.24165100 4.85825500 1.20637200
 H 6.99292700 3.06435300 2.09349000
 C 6.08480800 5.62479100 0.03841900
 H 6.81102400 5.85885900 -1.98301500
 H 5.66900200 5.11422000 2.09332000
 C 4.99078600 6.61464900 -0.03918900
 C 4.21193300 6.69356200 -1.20685500
 C 4.54105900 7.33428800 1.08318800
 C 2.97592900 7.32719500 -1.20691100
 H 4.52327900 6.14869000 -2.09358800
 C 3.30392400 7.96845600 1.08314800
 H 5.15207600 7.36167300 1.98178400
 C 2.45713400 7.91345600 -0.03925200
 H 2.35179500 7.26186900 -2.09365000
 H 2.96937700 8.48049500 1.98173900
 C 6.61467800 -4.99079300 0.03919400
 C 6.69358300 -4.21193200 1.20685600
 C 7.33432700 -4.54107100 -1.08318000
 C 7.32721500 -2.97592600 1.20690900
 H 6.14870500 -4.52327200 2.09358800
 C 7.96849400 -3.30393500 -1.08314100
 H 7.36171700 -5.15208900 -1.98177400
 C 7.91348600 -2.45713700 0.03925200
 H 7.26188000 -2.35178800 2.09364500
 H 8.48053600 -2.96939400 -1.98173300
 C 8.22385900 -1.01479400 -0.03842000
 C 7.90344800 -0.30092800 -1.20632700
 C 8.62174200 -0.26543200 1.08408000
 C 7.83419100 1.08630700 -1.20647800
 H 7.58768400 -0.84308600 -2.09316400
 C 8.55247600 1.12304300 1.08390800
 H 8.95049000 -0.78083300 1.98288600
 C 8.08195700 1.82882100 -0.03875500
 H 7.46603700 1.59407100 -2.09347400
 H 8.82833200 1.66882800 1.98256600
 C -4.99080400 -6.61467200 -0.03919600
 C -4.54107800 -7.33431700 1.08317800
 C -4.21194000 -6.69357100 -1.20685700
 C -3.30393800 -7.96847700 1.08314200
 H -5.15209500 -7.36171100 1.98177300
 C -2.97593000 -7.32719100 -1.20690700
 H -4.52328600 -6.14869800 -2.09359200
 C -2.45713900 -7.91346100 -0.03924800
 H -2.96939400 -8.48051600 1.98173400
 H -2.35178900 -7.26185800 -2.09364100
 C -1.01479300 -8.22382700 0.03841700
 C -0.30092900 -7.90342400 1.20632700
 C -0.26543100 -8.62169800 -1.08408700
 C 1.08630600 -7.83416100 1.20647700
 H -0.84308900 -7.58767100 2.09316600
 C 1.12304300 -8.55242700 -1.08391500
 H -0.78083400 -8.95044400 -1.98289300
 C 1.82881800 -8.08191500 0.03875200
 H 1.59407000 -7.46601200 2.09347500
 H 1.66883100 -8.82827600 -1.98257300

[12]CPP²

C -6.16578300 5.24489500 -1.22268400
 C -5.18193600 6.21856200 -1.22289700
 C -4.74634600 6.84659800 -0.03008100
 C -5.50378000 6.54417800 1.12992700
 C -6.48751000 5.57058100 1.13015100
 C -6.79803000 4.81607600 -0.02963100
 H -6.36221900 4.71281900 -2.14955100
 H -4.64798600 6.40923900 -2.14989500
 H -5.28783200 7.06634300 2.05915200
 H -7.01168100 5.36027900 2.05953800
 C 4.81615700 6.79789400 0.02964800
 C 5.24508900 6.16574800 1.22271200
 C 5.57063800 6.48735400 -1.13015100
 C 6.21881400 5.18195700 1.22293500
 H 4.71308300 6.36222800 2.14961300
 C 6.54428800 5.50368600 -1.12992100
 H 5.36027800 7.01147400 -2.05955500
 C 6.84680700 4.74630800 0.03011200
 H 6.40959100 4.64811200 2.14997200
 H 7.06642900 5.28773800 -2.05915700
 C 0.68713300 -8.30329800 0.02399300
 C 1.38017800 -7.98041500 1.21668500
 C 1.49269900 -8.41664900 -1.13750300
 C 2.71894000 -7.62881300 1.21549700
 H 0.82396500 -7.88138700 2.14489200
 C 2.83131700 -8.06485200 -1.13873300
 H 1.04343300 -8.75849000 -2.06703100
 C 3.47909700 -7.56986100 0.02149500
 H 3.15632600 -7.26889700 2.14280100
 H 3.38910200 -8.14194200 -2.06915200
 C 7.57009100 3.47910800 -0.02144700
 C 8.06494000 2.83127800 1.13882500
 C 7.62929500 2.71900000 -1.21546900
 C 8.41677400 1.49267800 1.13759200
 H 8.14188700 3.38901300 2.06928600
 C 7.98093100 1.38025000 -1.21666100
 H 7.26955500 3.15640800 -2.14283400
 C 8.30361100 0.68713000 -0.02395000
 H 8.75849200 1.04340100 2.06715900
 H 7.88211400 0.82411100 -2.14493400
 C 8.29619800 -0.77204500 0.02542500
 C 8.40200300 -1.57869100 -1.13605000
 C 7.96565900 -1.46185300 1.21791000
 C 8.03649900 -2.91362500 -1.13756300
 H 8.74899600 -1.13295000 -2.06536400
 C 7.60036400 -2.79694300 1.21643500
 H 7.87189800 -0.90473600 2.14612500
 C 7.53422200 -3.55636800 0.02234200
 H 8.10851700 -3.47207600 -2.06798300
 H 7.23549000 -3.23074600 2.14349200
 C 6.79803700 -4.81610800 -0.02968300
 C 6.16584100 -5.24502400 -1.22273200
 C 6.48748300 -5.57057600 1.13012700
 C 5.18199900 -6.21869600 -1.22292200
 H 6.36231700 -4.71303600 -2.14964200
 C 5.50376300 -6.54417300 1.12992600
 H 7.01163100 -5.36024500 2.05952000
 C 4.74635400 -6.84665800 -0.03008800
 H 4.64812000 -6.40946300 -2.14994300
 H 5.28780200 -7.06630300 2.05916700
 C -6.84679800 -4.74627900 0.03006500

C -5.18976700 -6.09717500 1.22566300
 H -6.35385500 -4.57556300 2.14752600
 C -4.78950800 -6.73362300 0.02823900
 H -5.35994200 -7.00285900 -2.04880800
 H -4.65357900 -6.29680700 2.14740200
 C -3.52924700 -7.47180200 -0.02508600
 C -2.77913100 -7.51053300 -1.22295600
 C -2.91166900 -7.99875300 1.13540600
 C -1.44671500 -7.87664700 -1.22362900
 H -3.21611500 -7.14120300 -2.14468300
 C -1.58007400 -8.36478800 1.13471400
 H -3.48378900 -8.09980300 2.05231800
 C -0.78101600 -8.22704900 -0.02647200
 H -0.88316300 -7.78220400 -2.14583600
 H -1.13907800 -8.74429600 2.05109600
 C -7.47216200 3.52917100 0.02516200
 C -7.51080600 2.77903400 1.22302300
 C -7.99927700 2.91168500 -1.13529800
 C -7.87700900 1.44664500 1.22369200
 H -7.14132900 3.21599400 2.14470100
 C -8.36540200 1.58011700 -1.13461000
 H -8.10039600 3.48388200 -2.05215500
 C -8.22757800 0.78102100 0.02653800
 H -7.78250900 0.88302100 2.14584700
 H -8.74506700 1.13915600 -2.05094600
 C -8.23658700 -0.67953300 -0.02566600
 C -7.89470000 -1.34941200 -1.22295600
 C -8.38376500 -1.47688100 1.13553900
 C -7.54496500 -2.68621300 -1.22244900
 H -7.79361300 -0.78699100 -2.14514500
 C -8.03410900 -2.81287300 1.13606500
 H -8.75756900 -1.03127000 2.05203600
 C -7.51514300 -3.43679500 -0.02461800
 H -7.18127500 -3.12768300 -2.14428000
 H -8.14183200 -3.38380900 2.05296200
 C 3.52923500 7.47178000 -0.02511600
 C 2.91169300 7.99889000 1.13529800
 C 2.77909100 7.51024100 -1.22299100
 C 1.58008900 8.36492500 1.13456200
 H 3.48383900 8.10007000 2.05218000
 C 1.44668200 7.87635800 -1.22370400
 H 3.21608500 7.14068200 -2.14461800
 C 0.78102800 8.22700900 -0.02658900
 H 1.13910600 8.74457500 2.05089200
 H 0.88307800 7.78171000 -2.14585700
 C -0.67952700 8.23605700 0.02559000
 C -1.34947300 7.89433900 1.22288800
 C -1.47684300 8.38313600 -1.13565000
 C -2.68629900 7.54469000 1.22238500
 H -0.78711800 7.79331300 2.14512500
 C -2.81286100 8.03356600 -1.13617200
 H -1.03120500 8.75677600 -2.05220000
 C -3.43686900 7.51477600 0.02455000
 H -3.12778200 7.18114700 2.14426800
 H -3.38372400 8.14120300 -2.05312400
 C -4.50653200 7.07480400 -1.34553000
 C -3.26667300 7.69803500 -1.34199500
 C -8.03371100 4.66585600 -1.21873800
 C -7.23196600 5.79995000 -1.26245900
 C -8.62360900 0.32954700 -1.17167500
 C -8.45295700 1.70681900 -1.21378400
 C -8.49834500 -3.94471000 -0.95792000
 C -8.99303000 -2.64594800 -0.97639000
 C -5.21370900 -6.85785100 -1.09989200
 C -6.25591000 -5.93996400 -1.08809100
 C 6.52620700 6.18475100 0.13711900
 C 7.25925700 5.76666500 1.26218900
 C 8.05569600 4.62885900 1.21839600
 C 8.14840400 3.84857900 0.05083600
 C 2.86777300 8.44252800 0.24080900
 C 3.30294300 7.68336500 1.34249200
 C 4.53994200 7.05447300 1.34583400
 C 5.40380600 7.13899600 0.24081000
 C -1.40198500 8.82547600 -0.12623700
 C -0.77678700 8.90173900 1.13202500
 C 0.60653600 8.91019000 1.25459100
 C 1.44299000 8.81885500 0.12675600
 C -5.37037000 7.16372600 -0.24082400
 C -4.98947700 8.02046600 0.80682600
 C -3.75305300 8.65769000 0.80227900
 C -2.82845700 8.45564300 -0.24044500
 C -8.13024700 3.88606900 -0.05116700
 C -7.51271800 4.38680400 1.10849500
 C -6.71836800 5.52658500 1.06772900
 C -6.49721300 6.21469700 -0.13728100
 C -8.99648800 -0.32297800 0.01604200
 C -9.32579800 0.48603600 1.11868000
 C -9.15912300 1.86592300 1.07485300
 C -8.65028200 2.50311600 -0.07192000
 C -7.80773000 -4.44513000 0.16099700
 C -7.76791900 -3.63386800 1.30832200
 C -8.26339900 -2.33592500 1.29030500
 C -8.82186900 -1.78583800 0.12364700
 C -4.82877600 -7.53934600 0.06774300
 C -5.62902300 -7.35958900 1.21089800
 C -6.67182500 -6.44010200 1.22300700
 C -6.96539200 -5.65677100 0.09198700
 C -1.59417800 -9.15800800 -1.04957600
 C -2.94352000 -8.82504700 -1.01913300
 C 2.67679700 -8.11930500 -1.26024000
 C 1.32741000 -8.44770000 -1.23047700
 C 6.64162000 -6.47082100 -1.22303500
 C 5.59448600 -7.38535700 -1.21080700
 C 8.25252000 -2.37412900 -1.29060000
 C 7.75105800 -3.66977800 -1.30858700
 C -0.75745700 -8.90820900 0.05329900
 C -1.36688600 -8.44150100 1.23085200
 C -2.71478900 -8.10703700 1.26055000
 C -3.52058200 -8.22411100 0.11467600
 C 3.48208800 -8.23990600 -0.11437400
 C 2.90236500 -8.83805700 1.01953700
 C 1.55152700 -9.16490000 1.05005700
 C 0.71591900 -8.91147500 -0.05284000
 C 6.93895600 -5.68878200 -0.09209500
 C 6.22817000 -5.96848700 1.08802900
 C 5.18160400 -6.88138800 1.09993600
 C 4.79343400 -7.56118900 -0.06762200
 C 8.81340100 -1.82653500 -0.12392800

[13]CPP

C 6.74389800 5.49552900 -1.06787500
 C 7.53296400 4.35207600 -1.10872800
 C 3.79300200 8.64000700 -0.80225200
 C 5.02649900 7.99715400 -0.80698600
 C -0.56516000 8.91371000 -1.25399400
 C 0.81813700 8.89883300 -1.13142400

C 8.98057200 -2.68741700 0.97613400	C 7.11841100 5.19572000 -1.13727500
C 8.47991700 -3.98388600 0.95769100	C 7.84142500 4.01475800 -1.16142100
C 7.78705000 -4.48118300 -0.16124100	C 4.16617500 8.33441400 -0.98882500
C 9.16769800 1.82360300 -1.07523100	C 5.35479200 7.62411000 -0.99366600
C 9.32785700 0.44293100 -1.11903800	C -0.13829500 9.01997700 -1.23011500
C 8.66196000 2.46320400 0.07155700	C 1.24138600 8.94099400 -1.15684200
C 8.46094200 1.666787500 1.21345700	C -4.23979100 7.57768800 -1.31636200
C 8.62507200 0.28981700 1.17135600	C -2.97965600 8.14927200 -1.31871200
C 8.99482000 -0.36450500 -0.01637100	C -7.71811000 5.06282300 -1.20006700
H 6.19289300 5.79092000 -1.95673500	C -6.86881300 6.15551700 -1.22458500
H 7.57854500 3.77829400 -2.03001900	C -8.74955300 0.82100000 -1.19728000
H 3.53052400 9.27891900 -1.64102400	C -8.50824500 2.18392900 -1.22036800
H 5.69799100 8.13854700 -1.65030800	C -8.60200800 -3.47315200 -1.06346300
H -1.00101700 8.93227100 -2.24873300	C -9.02311600 -2.15435200 -1.07285200
H 1.42049300 8.86122100 -2.03440400	C -5.67268600 -6.71690900 -1.15734700
H -4.76375900 6.41510700 -2.16958500	C -6.65901300 -5.74535200 -1.15091200
H -2.58662800 7.50357600 -2.16541500	C 6.84456700 5.88100600 0.07060700
H -8.56230600 4.35516200 -2.11605600	C 7.49616300 5.37755200 1.22358400
H -7.14161000 6.35442400 -2.19315200	C 8.22244100 4.19952700 1.19838500
H -8.35356200 -0.26143200 -2.04229500	C 8.35367700 3.42443100 0.01924200
H -8.05227200 2.15787600 -2.11691300	C 3.31713600 8.37462700 0.14643400
H -8.61582400 -4.57100700 -1.83850500	C 3.84550200 7.78138000 1.32001400
H -9.48838300 -2.27787900 -1.87121100	C 5.03643200 7.07694500 1.31718100
H -4.61679300 -6.96439200 -2.00123600	C 5.80109200 6.90068900 0.13949900
H -6.44869100 -5.35118700 -1.98044200	C -0.95970400 8.96836900 -0.07587000
H 7.17163900 6.32163400 2.19284700	C -0.26732200 9.01789600 1.15931200
H 8.58301200 4.31571200 2.11561500	C 1.11282600 8.94759600 1.23260400
H 2.62239000 7.49226300 2.16626600	C 1.92425200 8.81234100 0.07799600
H 4.79439100 6.39391200 2.17005900	C -5.02002600 7.48653300 -0.13926700
H -1.37939600 8.86626500 2.03492600	C -4.49927100 8.15859900 0.99374500
H 1.04245900 8.92605400 2.24934100	C -3.24082900 8.73635100 0.98936800
H -5.66060100 8.16515900 1.64988200	C -2.39162400 8.68344600 -0.14517100
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