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Supporting Information

for

Enhanced host–guest interaction between [10]cycloparaphenylene ([10]CPP) and [5]CPP by cationic charges

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Experimental procedures and computation data

General. ^{1}H NMR (400 MHz) experiments were carried out in anhydrous conditions under nitrogen atmosphere for CD_2Cl_2 or 1,1,2,2-tetrachloroethane-d_2 (TCE-d_2) solution of a sample and are reported in parts per million (δ) from residual solvent peak. UV–vis–NIR spectra were measured in CH_2Cl_2 at room temperature. Cyclic voltammetry was conducted with a Pt electrode for 1,2-dichloroethane of a sample (1 mmol/L) in the presence of supporting electrolyte, $Bu_4NB(C_6F_5)_4$ (0.1 mol/L) at room temperature under nitrogen atmosphere. Scan rates of 100 mV/s were employed. The potentials were calibrated with respect to the ferrocene/ferrocenium couple (Fc/Fc^+).

Materials. [*n*]CPPs (*n* = 5, 8–12),[1] $[5]CPP^{2+}$ $[B(C_6F_5)_4]_2$,[2] $[10]CPP^{2+}$ $(SbF_6)_2$,[2] $[5]CPP^{\bullet+}$ $SbCl_6$,[2] and $[10]CPP^{\bullet+}$ $SbCl_6$ [2] were prepared according to literature procedures. CD_2Cl_2 or 1,1,2,2-tetrachloroethane-d_2 (TCE-d_2) was used after dried over molecular sieves.

1. Experimental procedures of titration experiment

A solution of $[5]CPP^{2+}$ TCE-d_2 (1.63×10^{-2} mol L^{-1}) was added to a solution of $[10]CPP^{2+}$ in TCE-d_2 (1.30×10^{-4} mol L^{-1}) at 50 °C. The changes in the chemical shift ($\Delta\delta_{obs}$) of [10]CPP were monitored as a function of the added ($[5]CPP^{2+}$), and the $\Delta\delta_{obs}$ and $[[5]CPP^{2+}]$ were fitted by non-linear curve fitting with least squares method by using eq. 1 to obtain association constant K_a.

$$\Delta\delta_{obs} = \frac{K_a \Delta\delta_{CP}[G]}{1 + K_a[G]}$$

$\Delta\delta_{obs}$: the change in the chemical shift from free [10]CPP

$\Delta\delta_{cp}$: $\Delta\delta_{obs}$ at 100% complexation

[G]: concentration of $[5]CPP^{2+}$

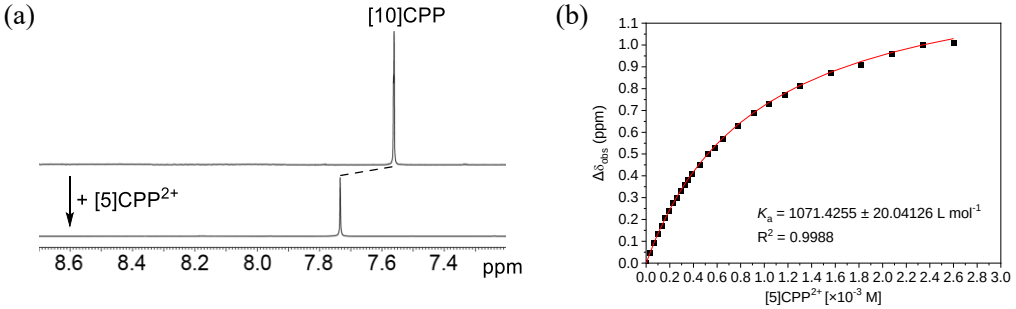


Figure S1. Titration experiments for [5]CPP. (a) ^{1}H NMR spectra of a 1:1 mixture of $[5]CPP^{2+}$ and [10]CPP in TCE-d_2 at 25 °C, and (b) determination of K_a for $[10]CPP \supset [5]CPP^{2+}$ by the least-square method in TCE-d_2 at 50 °C.

2. Theoretical calculations

DFT calculations were carried using Gaussian 16, Revision A.03 [3]. Geometry optimizations were performed with standard gradient techniques at ωB97X-D levels of theory with the 6-31G* basis set. All stationary points were optimized without any symmetry assumptions and characterized by normal coordinate analysis at the same level of theory.

Table S1. Energies (*E*), zero-point correction (*ZPE*), thermal correction to enthalpy (*H*) at 298.15 K, thermal correction to Gibbs free energy at 298.15 K and entropy (*S*) at 298.15 K under 1 atmosphere of pressure of the structures calculated at the (U)B3LYP/6-31G* level of theory.

Molecular	*E* (kJ mol^{-1})	*ZEP* (kJ mol^{-1})	*E* + *ZPE* (kJ mol^{-1})	*H* (kJ mol^{-1})	*G* (kJ mol^{-1})	*S* (cal mol^{-1} K^{-1})
[5]CPP^{2+}	-3030185.76	1066.709144	-3029119.05	-3029061.65	-3029245.60	147.461
[10]CPP	-6064134.93	2148.803718	-6061986.12	-6061869.27	-6062188.33	255.773
[10]CPP⊃[5]CPP^{2+} (**1**)	-9094628.84	3223.40249	-9091405.44	-9091231.27	-9091656.36	340.76
[10]CPP⊃[5]CPP^{2+} (**2**)	-9094626.31	3226.2144	-9091400.09	-9091226.76	-9091647.59	337.35
[10]CPP⊃[5]CPP^{2+} (**3**)	-9094624.61	3226.251157	-9091398.36	-9091224.48	-9091651.23	337.35

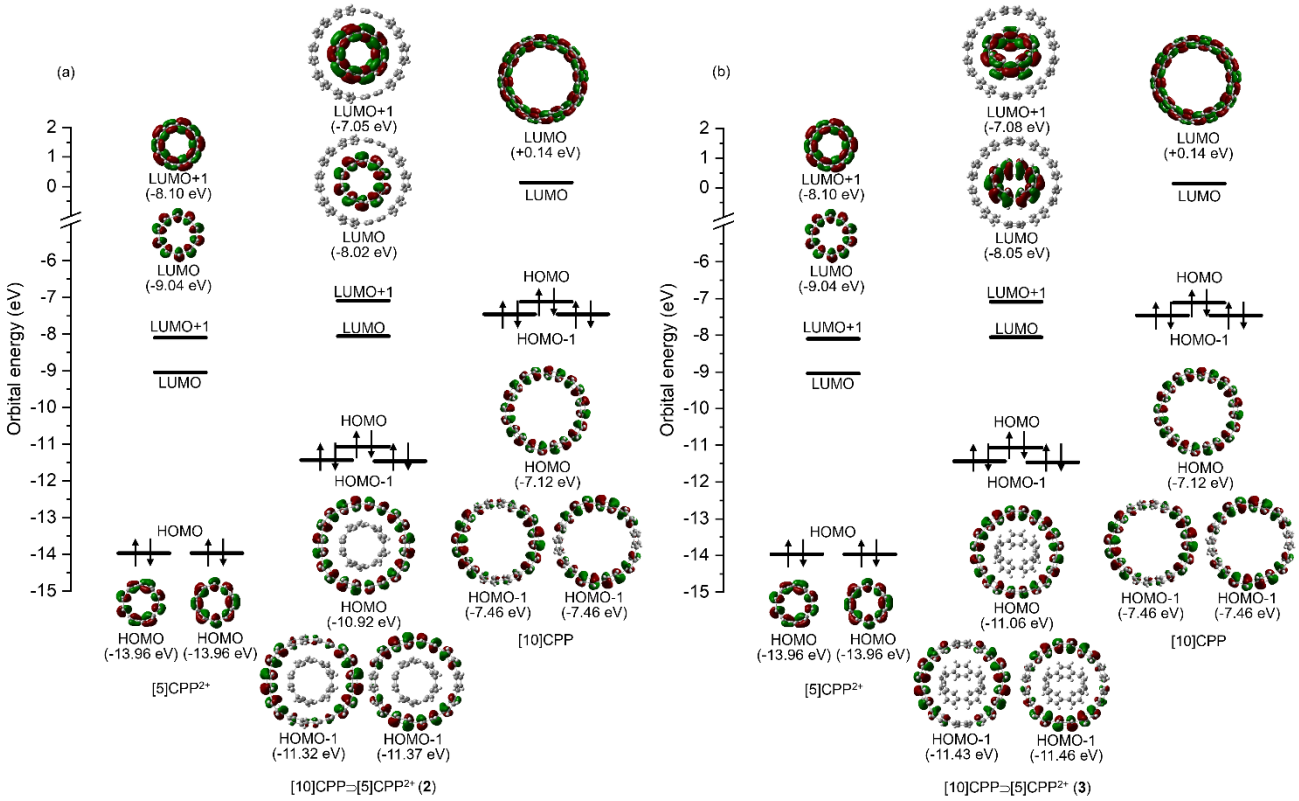
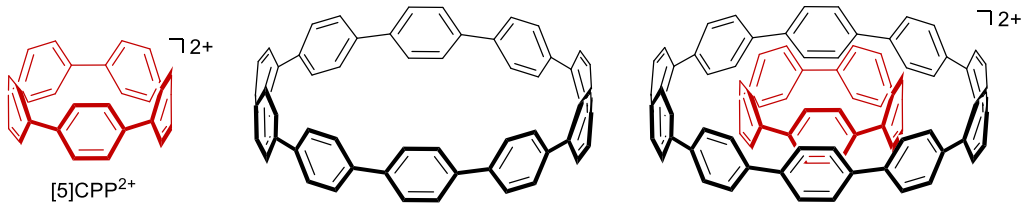


Figure S2. HOMO−1, HOMO, LUMO, and LUMO+1 orbitals of (a) [10]CPP⊃[5]CPP^{2+} (**2**), (b) [10]CPP⊃[5]CPP^{2+} (**3**), [5]CPP^{2+}, and [10]CPP.

Table S2. TD-DFT vertical one-electron excitations calculated at the ωB97X-D/6-31G* level.

Molecule	Energy (eV)	Wavelength (nm)	Oscillator Strength (*f*)	Description
[10]CPP⊃[5]CPP^{2+} (**1**)	0.6437	1926.10	0.0001	HOMO→LUMO (0.70157)
	1.0255	1208.99	0.0043	d-HOMO-1→LUMO (0.69947)
	1.0265	1207.88	0.0043	d-HOMO-1→LUMO (0.69104)
	1.7968	690.04	0.0547	d-HOMO-3→LUMO (0.42875)
	1.7971	689.90	0.0545	d-HOMO-3→LUMO (0.42982)
	3.0933	400.81	0.4447	d-HOMO-3→LUMO+1 (0.51169)
	3.0942	400.70	0.4443	d-HOMO-3→LUMO+1 (0.51120)
[10]CPP⊃[5]CPP^{2+} (**2**)	0.6809	1820.83	0.0001	HOMO→LUMO (0.69949)
	1.0449	1186.61	0.0010	d-HOMO-1→LUMO (0.69828)
	1.1541	1074.27	0.0043	d-HOMO-1→LUMO (0.0159)
	1.7941	691.07	0.0820	d-HOMO-3→LUMO (0.47820)
	1.8130	683.87	0.0612	d-HOMO-3→LUMO (0.53596)
	3.1295	398.74	0.2627	d-HOMO-3→LUMO+1 (0.46832)
	3.2170	396.18	0.2627	d-HOMO-3→LUMO+1 (0.46832)
[10]CPP⊃[5]CPP^{2+} (**3**)	0.8676	1428.98	0.0027	HOMO→LUMO (0.70057)
	1.1812	1049.60	0.0007	d-HOMO-1→LUMO (0.69678)
	1.7951	690.69	0.0125	HOMO→LUMO+1 (0.66245)
	1.8204	681.09	0.0869	d-HOMO-3→LUMO (0.47820)
	3.1764	390.33	0.2492	d-HOMO-3→LUMO+1 (0.43617)
	3.2853	377.39	0.2944	d-HOMO-3→LUMO+1 (0.43429)

Table S3. Averaged C–C bond lengths (Å), dihedral angles (deg), and Mullikene charge for the optimized structures of [5]CPP^{2+}, [10]CPP, and [5] and [10]CPP unit in the complex [10]CPP⊃[5]CPP^{2+}.



Molecule	C_{ipso}-C_{ipso} (Å)	C_{ipso}-C_{ortho} (Å)	C_{ortho}-C_{ortho} (Å)	C_{ortho}-C_{ipso}-C_{ipso}-C_{ortho} (°)	*Mulliken Charge*
[10]CPP⊃[5]CPP^{2+} (**1**)					2.00
[10]CPP	1.485	1.400	1.387	30.66	1.86
[5]CPP	1.431	1.430	1.365	0.04	0.14
[10]CPP⊃[5]CPP^{2+} (**2**)					2.00
[10]CPP	1.486	1.401	1.388	25.50	1.75
[5]CPP	1.431	1.429	1.366	0.01	0.25
[10]CPP⊃[5]CPP^{2+} (**3**)					2.00
[10]CPP	1.485	1.400	1.389	32.44	1.71
[5]CPP	1.431	1.430	1.366	1.42	0.25
Free [10]CPP	1.486	1.400	1.388	36.86	
Free [5]CPP^{2+}	1.432	1.431	1.366	0.11	
[10]CPP⊃[5]CPP^{2+} $B(C_6F_5)_4]_2$ (**X-ray**)					
[10]CPP	1.486(4)	1.399(4)	1.381(4)	17.6(4)	
[5]CPP	1.425(6)	1.429(4)	1.355(4)	1.08(4)	

3. X-ray crystallographic structures

A suitable single crystal was obtained by vapor diffusion of hexane into a sample solution in dichloroethane or dichloromethane. The intensity data were collected at 103 K on Rigaku Saturn70 CCD diffractometer with the VariMax Optix using Mo Kα radiation (λ = 0.71073 Å). The intensity data were corrected for Lorentz and polarization effects and for absorption (multiscan). The structures were solved by direct methods (SHELXT 2014/5) and refined by least-squares calculations on F^2 for all reflections (SHELXL-2019/3) [4]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. All calculations were performed by using Yadokari-XG [5] and Olex-2 1.5 [6]. The crystallographic data and the summary of solution and refinement are given in Table S4.

Table S4. Crystal data and structure refinement parameters of ([10]CPP⊃[5]CPP^{2+} $[B(C_6F_5)_4]_2$).

Identification code		Identification code	
Data deposition	CCDC 2314282	Density (calculated)	1.612 g/m^3
Empirical formula	$C_{60}H_{40}$, $(C_{24}BF_{20})_2$, $C_{30}H_{20}$, $(CH_2Cl_2)_{4.33}$	Absorption coefficient μ	0.326 mm^{-1}
		F(000)	11519
Formula weight	2867.21	Crystal size	0.04, 0.10, 0.15 Å
Temperature	103(2) K	θ range for data collection	1.6440 to 28.8400°
Wavelength	0.71073 Å	Index ranges	-36<=h<=36,
Crystal system	monoclinic		-27<=k<=27,
Space group	C2/c		-55<=l<=55
Unit cell dimensions	a = 28.4017(4) Å	Reflection collected	1777842
	b = 20.3156(3) Å	Data/restraints/parameters	28748/0/1913
	c = 41.3026(8) Å	Goodness-of-fit on F^2	1.027
	α = 90°	Final R indices [I>2σ(I)]	R_1 = 0.0575, wR_2 = 0.1120
	β = 97.433(2)°	R indices (all data)	R_1 = 0.1053, wR_2 = 0.1288
	γ = 90°		
Volume	23631.2(7) Å^3		
Z	8		

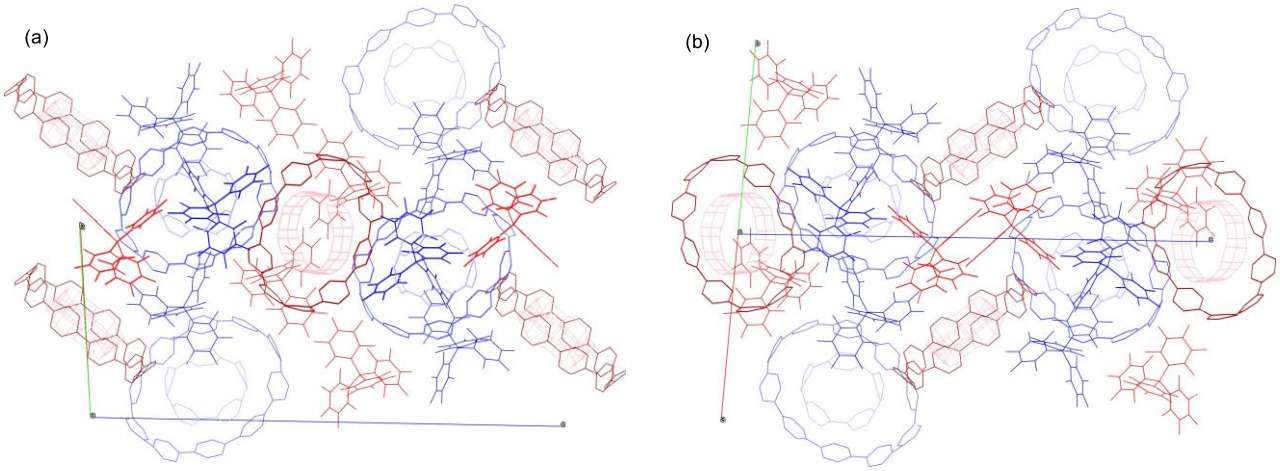


Figure S3. Wire-flame view of packing structure of crystalline unit lattices viewed from a) 45° and b)135° directions of the a, b-axes.

Cartesian Coordination

[5]CPP^{2+}

C	3.099	1.563	1.210
C	2.256	2.637	1.210
C	1.611	3.043	-0.001
C	2.252	2.634	-1.213
C	3.095	1.559	-1.213
C	3.339	0.839	-0.001
C	0.234	3.435	0.000
C	-0.527	3.426	1.212
C	-0.529	3.429	-1.211
C	-1.809	2.957	1.212
C	-1.811	2.959	-1.210
C	-2.396	2.472	0.001
C	-3.195	1.284	0.001
C	-3.423	0.557	1.212
C	-3.423	0.558	-1.211
C	-3.373	-0.808	1.211
C	-3.373	-0.807	-1.212
C	-3.092	-1.515	-0.001
C	-2.208	-2.642	-0.001
C	-1.587	-3.082	-1.212
C	-1.589	-3.084	1.210
C	-0.273	-3.456	-1.212
C	-0.275	-3.458	1.211
C	0.486	-3.408	0.000
C	3.392	-0.591	0.001
C	3.205	-1.331	-1.210
C	3.202	-1.328	1.213
C	2.444	-2.464	-1.210
C	2.440	-2.461	1.213
C	1.830	-2.916	0.001
H	-3.511	1.078	-2.158
H	-3.422	-1.334	2.158
H	-3.423	-1.331	-2.159
H	-2.108	-3.004	-2.160
H	-2.111	-3.009	2.157
H	3.478	1.195	2.157
H	1.989	3.093	2.157
H	1.982	3.086	-2.160
H	3.470	1.189	-2.160
H	-0.059	3.669	2.159
H	-0.062	3.674	-2.158
H	-2.323	2.841	2.160
H	-2.327	2.845	-2.157
H	-3.511	1.076	2.159
H	0.211	-3.664	-2.159
H	0.208	-3.669	2.158
H	3.556	-0.936	-2.157
H	3.548	-0.931	2.160
H	2.211	-2.938	-2.157
H	2.204	-2.932	2.160

1

C	1.960	2.836	0.674
C	1.296	3.198	1.888
C	-0.045	3.449	1.889
C	-0.797	3.353	0.676
C	-0.040	3.491	-0.529
C	1.303	3.239	-0.530
C	-2.090	2.740	0.676
C	-2.677	2.240	-0.528
C	-3.331	1.040	-0.528
C	-3.435	0.277	0.676
C	-3.293	1.021	1.889
C	-2.640	2.218	1.890
C	-3.251	-1.142	0.676
C	-2.925	-1.826	1.889
C	-1.988	-2.818	1.888
C	-1.324	-3.182	0.674
C	-2.019	-2.848	-0.530
C	-2.957	-1.854	-0.529
C	0.082	-3.446	0.673
C	0.849	-3.385	-0.532
C	2.084	-2.799	-0.533
C	2.617	-2.244	0.671
C	2.067	-2.765	1.884
C	0.835	-3.349	1.885
C	3.444	-0.243	1.884
C	3.268	1.110	1.885
C	2.943	1.796	0.673
C	3.307	1.118	-0.532
C	3.482	-0.238	-0.533
C	3.303	-0.987	0.671
H	1.819	3.154	2.836
H	-0.547	3.597	2.838
H	-0.547	3.678	-1.468
H	1.841	3.230	-1.470
H	-2.502	2.750	-1.468
H	-3.666	0.618	-1.468
H	-3.589	0.588	2.838
H	-2.436	2.701	2.838
H	-3.320	-1.483	2.838
H	-1.668	-3.234	2.836
H	-1.720	-3.295	-1.470
H	-3.386	-1.528	-1.469
H	0.406	-3.692	-1.472
H	2.601	-2.652	-1.474
H	2.562	-2.590	2.832
H	0.387	-3.621	2.834
H	3.563	-0.754	2.833
H	3.254	1.633	2.834
H	3.328	1.657	-1.472
H	3.638	-0.752	-1.474
C	-6.619	2.822	-1.437
C	-5.954	4.039	-1.437
C	-5.269	4.485	-0.297
C	-5.459	3.768	0.888
C	-6.125	2.551	0.888
C	-6.625	2.005	-0.298
C	-4.168	5.477	-0.379
C	-3.713	6.206	0.728
C	-3.380	5.509	-1.537
C	-2.457	6.801	0.728
C	-2.128	6.102	-1.537
C	-1.606	6.692	-0.379
C	-6.864	0.542	-0.380
C	-6.466	-0.138	-1.538
C	-7.230	-0.234	0.727
C	-6.288	-1.512	-1.538
C	-7.052	-1.613	0.727
C	-6.501	-2.271	-0.380
C	-5.898	-3.625	-0.297
C	-5.684	-4.414	-1.436
C	-5.275	-4.026	0.889
C	-4.731	-5.422	-1.436
C	-4.321	-5.033	0.889
C	-3.955	-5.678	-0.296
C	-0.141	6.917	-0.297
C	0.639	7.165	-1.436
C	0.535	6.610	0.888
C	2.001	6.908	-1.437

C	1.898	6.354	0.888
C	2.638	6.395	-0.297
C	3.922	5.654	-0.380
C	4.755	5.447	0.727
C	4.195	4.914	-1.537
C	5.710	4.437	0.728
C	5.148	3.907	-1.537
C	5.870	3.594	-0.379
C	-2.637	-6.356	-0.378
C	-2.011	-6.943	0.729
C	-1.868	-6.188	-1.536
C	-0.645	-7.198	0.729
C	-0.505	-6.442	-1.536
C	0.151	-6.877	-0.378
C	1.625	-6.722	-0.296
C	2.441	-6.765	-1.435
C	2.199	-6.253	0.889
C	3.695	-6.172	-1.436
C	3.453	-5.660	0.889
C	4.180	-5.513	-0.297
C	6.538	2.270	-0.296
C	7.015	1.606	-1.435
C	6.455	1.534	0.889
C	7.194	0.231	-1.435
C	6.634	0.158	0.889
C	6.902	-0.533	-0.296
C	6.594	-1.983	-0.379
C	6.653	-2.839	0.728
C	5.976	-2.471	-1.537
C	5.987	-4.059	0.728
C	5.312	-3.687	-1.537
C	5.234	-4.471	-0.379
H	-7.099	2.483	-2.350
H	-5.927	4.627	-2.350
H	-4.979	4.102	1.803
H	-6.147	1.967	1.803
H	-4.335	6.284	1.615
H	-3.709	4.980	-2.427
H	-2.124	7.332	1.616
H	-1.511	6.022	-2.427
H	-6.200	0.424	-2.429
H	-7.631	0.246	1.615
H	-5.889	-1.988	-2.429
H	-7.317	-2.180	1.615
H	-6.235	-4.209	-2.349
H	-5.445	-3.466	1.804
H	-4.555	-5.984	-2.349
H	-3.771	-5.232	1.804
H	0.167	7.516	-2.349
H	-0.028	6.448	1.804
H	2.568	7.065	-2.350
H	2.364	5.999	1.803
H	4.636	6.062	1.615
H	3.591	5.063	-2.428
H	6.317	4.285	1.616
H	5.263	3.296	-2.427
H	-2.592	-7.175	1.618
H	-2.321	-5.762	-2.428
H	-0.187	-7.625	1.618
H	0.071	-6.209	-2.427
H	2.074	-7.225	-2.348
H	1.614	-6.239	1.804
H	4.283	-6.180	-2.349
H	3.814	-5.199	1.803
H	7.204	2.163	-2.348
H	6.128	2.019	1.805
C	-6.814	-1.422	-0.222
C	-2.896	-6.622	-1.175
H	7.518	-0.260	-2.348
H	6.441	-0.394	1.804
H	7.201	-2.537	1.616
H	5.932	-1.851	-2.427
H	6.028	-4.684	1.616
H	4.766	-3.985	-2.428

2

C	-1.904	-3.121	-0.552
C	-3.160	0.678	2.086
C	-3.064	1.395	0.851
C	-1.295	-2.863	1.775
C	-3.483	-0.688	-0.311
C	-2.200	-2.542	0.719
C	0.401	-3.415	0.134
C	-0.026	-3.284	1.489
C	-0.642	-3.558	-0.834
C	-3.485	0.682	-0.310
C	-1.911	3.118	-0.550
C	-2.206	2.537	0.721
C	-1.301	2.860	1.777
C	-3.158	-0.686	2.085
C	-3.061	-1.402	0.850
C	3.430	-1.445	0.504
C	1.957	2.557	-1.578
C	1.705	2.985	-0.237
C	2.723	-1.443	-1.812
C	3.426	1.451	0.505
C	3.281	-0.710	-0.716
C	1.712	-2.982	-0.238
C	1.963	-2.553	-1.579
C	2.666	-2.551	0.737
C	2.660	2.556	0.738
C	-0.033	3.284	1.491
C	0.394	3.415	0.136
C	-0.650	3.557	-0.832
C	2.720	1.449	-1.811
C	3.279	0.717	-0.715
C	-5.729	3.281	-1.449
C	-6.376	2.824	-0.294
C	-2.807	-5.935	1.111
C	-3.521	-5.991	-0.090
C	-4.934	4.418	-1.421
C	-7.213	0.687	-1.358
C	-1.560	-6.996	-1.111
C	-6.596	0.687	0.956
C	-1.474	-6.309	1.174
C	-5.535	-4.801	0.863
C	-5.723	-3.292	-1.448
C	-6.817	1.409	-0.223
C	-0.789	-6.754	0.037
C	-6.594	-0.699	0.956
C	-5.546	4.791	0.861
C	-4.733	-5.146	-0.233
C	-6.339	-3.669	0.833
C	1.388	-6.562	-1.203
C	-4.925	-4.428	-1.419
C	-7.211	-0.701	-1.358
C	-6.348	3.658	0.831
C	1.457	-6.572	1.179
C	-6.370	-2.836	-0.293
C	0.699	-6.710	0.008
C	-3.533	5.985	-0.091
C	-4.744	5.137	-0.234
C	-2.909	6.616	-1.176
C	-2.819	5.930	1.110
H	-7.487	-1.230	-2.265
H	-6.923	3.394	1.714

C	2.758	6.129	1.142
C	3.399	5.833	-0.068
C	5.800	-3.141	-1.162
C	6.434	-2.789	0.036
C	1.443	6.574	1.179
C	5.408	4.758	1.050
C	5.417	-4.747	1.050
C	4.919	4.224	-1.225
C	4.928	-4.214	-1.226
C	7.432	-0.686	-0.934
C	6.707	0.701	1.346
C	4.631	4.997	-0.095
C	4.641	-4.988	-0.096
C	5.793	3.152	-1.161
C	1.375	6.565	-1.203
C	6.959	-1.407	0.170
C	7.431	0.701	-0.934
C	2.770	-6.124	1.142
C	6.709	-0.688	1.346
C	6.284	3.682	1.117
C	2.701	6.156	-1.240
C	2.713	-6.150	-1.240
C	6.956	1.421	0.170
C	3.411	-5.826	-0.068
C	-0.803	6.752	0.037
C	0.685	6.711	0.008
C	-1.488	6.306	1.173
C	-1.574	6.993	-1.111
C	6.428	2.802	0.036
C	6.291	-3.669	1.116
H	-2.663	-3.137	-1.326
H	-3.122	1.207	3.032
H	-1.543	-2.628	2.803
H	-3.655	-1.216	-1.241
H	0.691	-3.373	2.297
H	-0.416	-3.919	-1.830
H	-3.658	1.210	-1.240
H	-2.671	3.133	-1.323
H	-1.548	2.623	2.805
H	-3.120	-1.215	3.031
H	4.070	-1.063	1.291
H	1.428	3.015	-2.405
H	2.784	-1.054	-2.822
H	4.067	1.071	1.291
H	1.435	-3.012	-2.407
H	2.716	-3.038	1.703
H	2.710	3.042	1.705
H	0.684	3.374	2.299
H	-0.425	3.919	-1.828
H	2.781	1.061	-2.821
H	-5.764	2.688	-2.359
H	-3.261	-5.483	1.988
H	-4.368	4.684	-2.310
H	-7.490	1.214	-2.266
H	-1.108	-7.449	-1.988
H	-6.308	1.210	1.863
H	-0.944	-6.141	2.104
H	-5.497	-5.397	1.771
H	-5.759	-2.700	-2.358
H	-6.305	-1.221	1.863
H	-5.509	5.387	1.768
H	-6.914	-3.406	1.716
H	0.873	-6.710	-2.147
H	-4.360	-4.693	-2.308
H	-1.024	-4.086	0.957
H	-3.001	-3.087	0.041
H	-3.026	-0.186	3.244
H	-1.050	-1.205	4.177
H	1.010	-6.771	2.147
H	-3.458	6.776	-2.100
H	-3.273	5.477	1.987
H	-3.445	-6.783	-2.099
H	3.265	5.956	2.086
H	5.901	-2.500	-2.033
H	0.996	6.771	2.148
H	5.306	5.395	1.923
H	5.317	-5.385	1.922
H	4.376	4.381	-2.151
H	4.386	-4.373	-2.151
H	7.750	-1.215	-1.829
H	6.399	1.227	2.246
H	5.895	2.512	-2.032
H	0.860	6.712	-2.146
H	7.747	1.230	-1.828
H	3.278	-5.951	2.086
H	6.401	-1.215	2.246
H	6.832	3.504	2.038
H	3.177	6.046	-2.209
H	3.188	-6.038	-2.209
H	-0.957	6.139	2.104
H	-1.123	7.446	-1.988
H	6.839	-3.490	2.037

3

C	2.579	1.550	-1.312
C	3.099	0.300	-1.790
C	3.556	-0.631	-0.906
C	3.496	-0.359	0.499
C	3.497	1.022	0.865
C	3.040	1.956	-0.020
C	3.025	-1.359	1.411
C	2.574	-0.997	2.716
C	1.455	-1.581	3.244
C	0.729	-2.549	2.488
C	1.450	-3.197	1.444
C	2.573	-2.618	0.920
C	-0.712	-2.553	2.487
C	-1.429	-3.206	1.445
C	-2.556	-2.634	0.920
C	-3.015	-1.378	1.410
C	-2.565	-1.011	2.714
C	-1.443	-1.589	3.242
C	-3.493	-0.381	0.498
C	-3.504	1.000	0.863
C	-3.054	1.937	-0.022
C	-2.589	1.533	-1.313
C	-3.100	0.280	-1.791
C	-3.551	-0.654	-0.907
C	-0.685	1.439	-2.902
C	0.677	1.444	-2.901
C	1.398	2.122	-1.863
C	0.672	3.150	-1.173
C	-0.693	3.146	-1.174
C	-1.411	2.113	-1.864
H	3.026	0.038	-2.840
H	3.851	-1.614	-1.256
H	3.716	1.327	1.881
H	2.909	2.979	0.318
H	3.030	-0.169	3.246
H	1.061	-1.200	4.179
H	1.050	-4.079	0.956
H	3.021	-3.067	0.040
C	-2.847	6.302	0.251
C	-0.720	6.568	-1.004
C	-1.440	6.771	0.179
C	-3.705	6.313	-0.857

H	-3.726	1.304	1.879
H	-2.930	2.960	0.316
H	-3.025	0.017	-2.841
H	-3.839	-1.640	-1.257
H	-1.206	0.816	-3.620
H	1.202	0.824	-3.619
H	1.192	3.879	-0.560
H	-1.218	3.872	-0.561
C	3.722	-6.204	0.610
C	4.856	-5.399	0.640
C	5.153	-4.529	-0.418
C	4.356	-4.617	-1.567
C	3.221	-5.415	-1.593
C	2.839	-6.170	-0.477
C	6.046	-3.351	-0.270
C	6.644	-2.723	-1.373
C	6.073	-2.668	0.950
C	7.066	-1.402	-1.301
C	6.494	-1.346	1.021
C	6.904	-0.655	-0.125
C	1.441	-6.671	-0.410
C	0.720	-6.573	0.787
C	0.720	-6.998	-1.567
C	-0.671	-6.578	0.786
C	-0.667	-7.003	-1.567
C	-1.391	-6.681	-0.411
C	-2.792	-6.190	-0.478
C	-3.676	-6.231	0.609
C	-3.179	-5.438	-1.594
C	-4.815	-5.434	0.639
C	-4.320	-4.648	-1.568
C	-5.118	-4.566	-0.419
C	6.877	0.830	-0.128
C	7.079	1.592	1.032
C	6.389	1.494	-1.258
C	6.653	2.913	1.105
C	5.959	2.811	-1.184
C	6.003	3.520	0.022
C	5.124	4.706	0.179
C	4.796	5.545	-0.894
C	4.366	4.830	1.350
C	3.656	6.338	-0.859
C	3.222	5.616	1.383
C	2.799	6.321	0.249
C	-6.020	-3.394	-0.271
C	-6.623	-2.770	-1.374
C	-6.052	-2.711	0.949
C	-7.054	-1.453	-1.302
C	-6.482	-1.393	1.020
C	-6.898	-0.705	-0.125
C	-6.883	0.780	-0.128
C	-7.091	1.541	1.032
C	-6.399	1.448	-1.257
C	-6.675	2.864	1.106
C	-5.980	2.769	-1.183
C	-6.030	3.476	0.023
C	1.388	6.780	0.178
C	0.667	7.170	1.315
C	0.669	6.573	-1.004
C	-0.721	7.165	1.316
C	-3.265	5.593	1.384
C	-4.839	5.511	-0.892
C	-4.403	4.798	1.351
C	-5.160	4.669	0.180
H	3.505	-6.839	1.464
H	5.495	-5.419	1.518
H	4.566	-3.979	-2.421
H	2.573	-5.372	-2.464
H	6.740	-3.258	-2.314
H	5.648	-3.130	1.837
H	7.484	-0.932	-2.186
H	6.387	-0.814	1.962
H	1.244	-6.388	1.721
H	1.248	-7.200	-2.494
H	-1.197	-6.396	1.720
H	-1.194	-7.209	-2.494
H	-3.454	-6.865	1.463
H	-2.532	-5.390	-2.464
H	-5.455	-5.459	1.516
H	-4.535	-4.011	-2.421
H	7.547	1.140	1.902
H	6.236	0.947	-2.183
H	6.789	3.463	2.031
H	5.480	3.255	-2.052
H	5.413	5.544	-1.788
H	4.607	4.217	2.215
H	3.407	6.946	-1.724
H	2.599	5.601	2.272
H	-6.714	-3.306	-2.315
H	-5.623	-3.170	1.836
H	-7.476	-0.986	-2.187
H	-6.380	-0.861	1.962
H	-7.556	1.084	1.902
H	-6.243	0.903	-2.183
H	-6.816	3.413	2.032
H	-5.505	3.217	-2.051
H	1.197	7.435	2.226
H	1.193	6.300	-1.916
H	-1.252	7.426	2.227
H	-1.243	6.292	-1.915
H	-3.461	6.924	-1.722
H	-2.641	5.582	2.274
H	-5.456	5.506	-1.786
H	-4.640	4.184	2.216

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