Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Fullerene C_{70}/Porphyrin Hybrid Nanoarchitectures: Single-Cocrystal Nanoribbons with Ambipolar Charge Transport Properties

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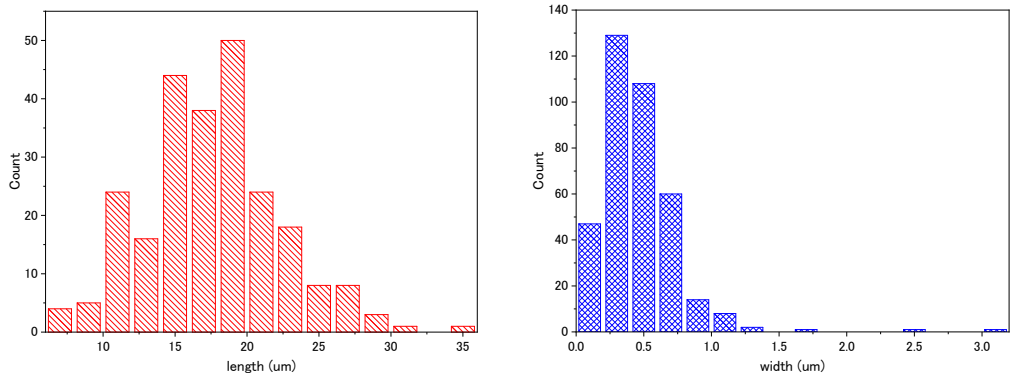

Figure S1. The size distribution histograms of C_{70}/3,5-TPP nanoribbons.

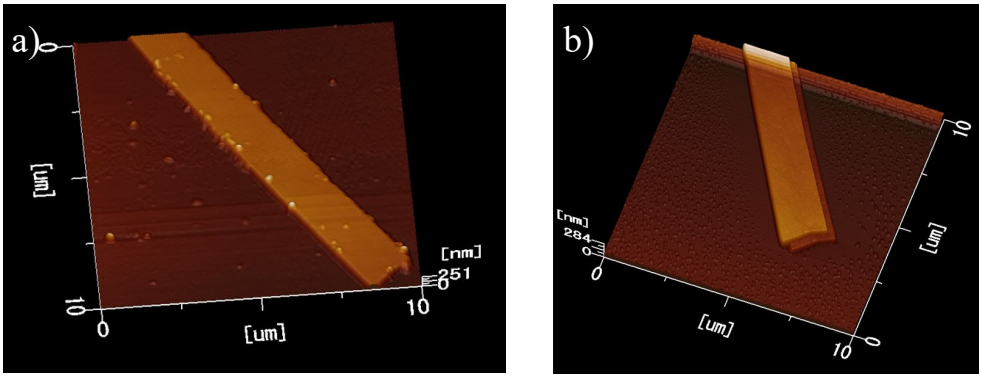

Figure S2. The AFM images of C_{70}/3,5-TPP nanoribbons.

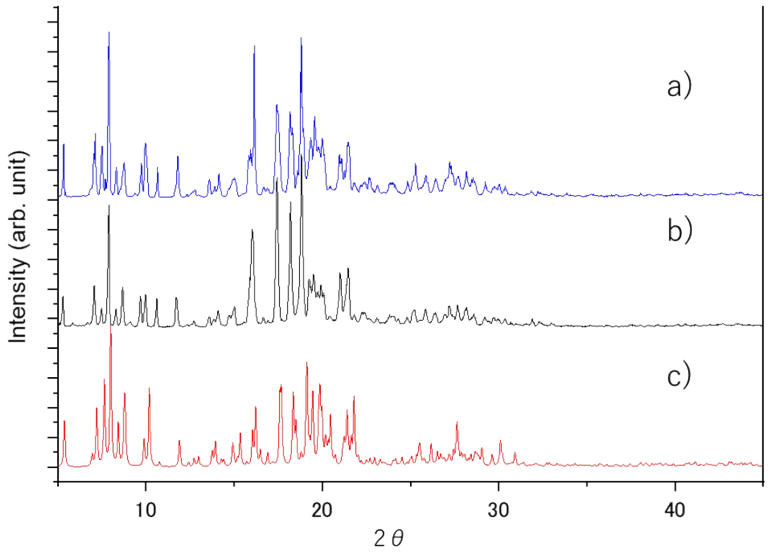

Figure S3. The experimental XRD pattern of C_{70}/3,5-TPP nanoribbons a)without annealing, b) after annealing at 80℃ for 1h, and c) simulated XRD pattern from single crystal data

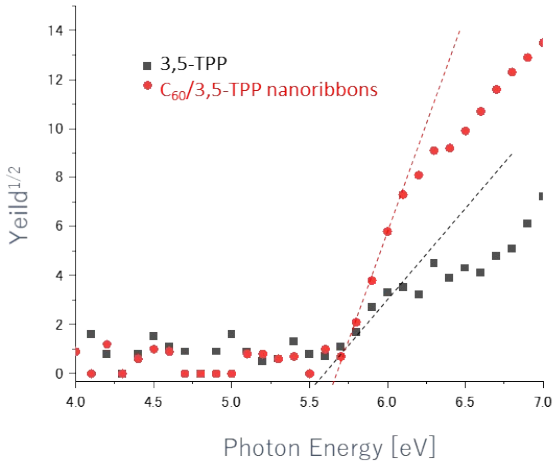

Figure S4. PYSA spectra of 3,5-TPP and C_{60}/3,5-TPP cocrystals.

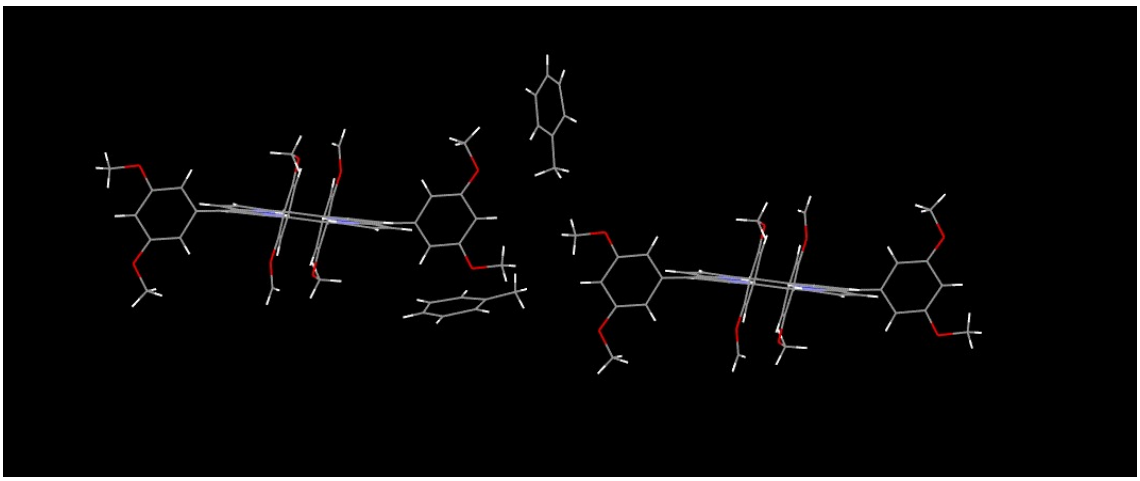

Figure S5. The [(3,5-TPP) toluene$_2$ (3,5-TPP)] unit structure in C_{60}/3,5-TPP cocrystals

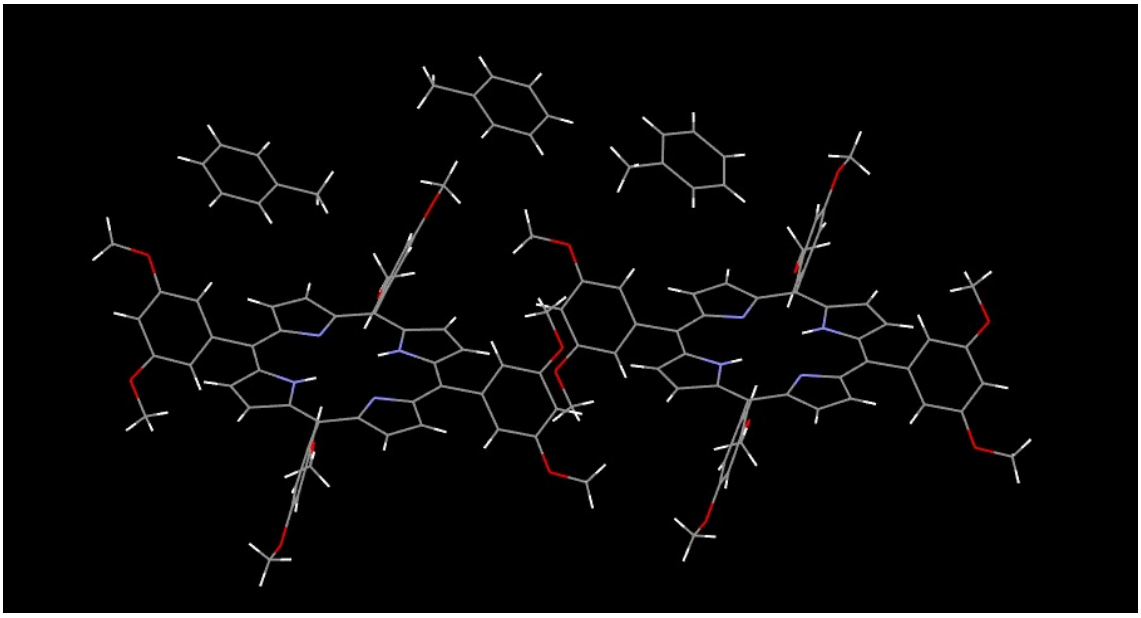

Figure S6. The [(3,5-TPP)$_2$ toluene$_3$] unit structure in C_{70}/3,5-TPP nanoribbons

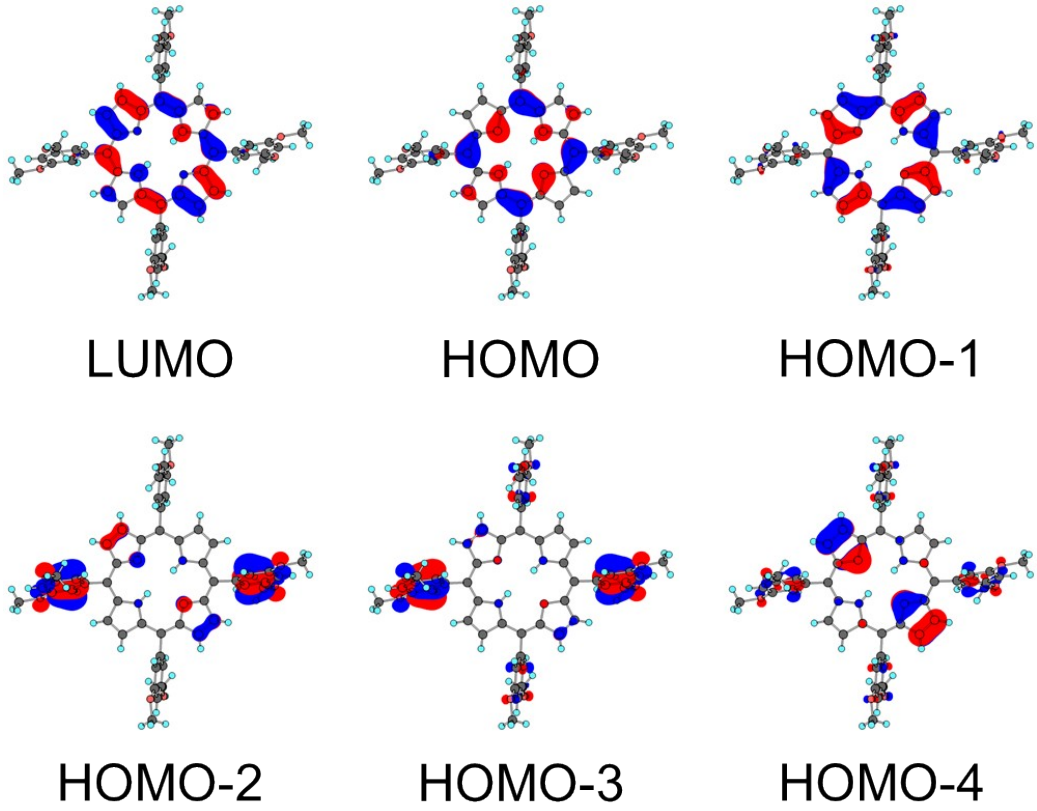

Figure S7. Molecular orbitals of 3,5-TPP.

Table S1. Coupling constant between 3,5-TPPs of C_{60}- and C_{70}-based cocrystals.

		Coupling constant (eV)	
A	**B**	**TPPs of C_{60} cocrystal**	**TPPs of C_{70} cocrystal**
HOMO	HOMO	1.47×10^{-6}	8.8×10^{-4}
HOMO-1	HOMO-1	9.2×10^{-5}	3.3×10^{-3}
HOMO-2	HOMO-2	2.3×10^{-5}	1.5×10^{-2}
HOMO-3	HOMO-3	4.1×10^{-4}	5.3×10^{-2}
HOMO-4	HOMO-4	7.7×10^{-5}	1.7×10^{-2}

Here, we explain the calculation technique for coupling constants. The coupling constants were evaluated based on $\langle \phi_A | H_{AB} | \phi_B \rangle$. Here, $\phi_{A(B)}$ is the molecular orbital for each TPP molecule $A(B)$, and H_{AB} is the Fock operator with both TPPs, which is obtained from the DFT calculation. This method assumes that a hole is localized on each TPP site, and hole-hopping occurs between those. To numerically estimate the coupling constants, we need to execute matrix operations between the Fock matrix and the coefficient vectors of molecular orbitals. For such matrix calculations based on quantum chemistry, we employed a Python-based quantum chemistry program tool.[1, 2] In the tool, the core part is developed by C++, but the Python interfaces are prepared. Thus, we can easily handle with matrix operations based on quantum chemistry without compromising calculation speeds. The tool has been employed to investigate the ground and excited electronic structures of various materials and molecules.[3-5]

1. T. Shimazaki, M. Hashimoto and T. Maeda, *Proceedings of the 3rd International Workshop on Software Engineering for High Performance Computing in Computational Science and Engineering*, 2015, 9 [DOI: 10.1145/2830168.2830170].
2. T. Shimazaki, in *Recent Advances of the Fragment Molecular Orbital Method*, eds. Y. Mochizuki, S. Tanaka and K. Fukuzawa, Springer, Singapore2021, pp. 589-600.
3. T. Shimazaki and T. Nakajima, *Physical Chemistry Chemical Physics*, 2016, **18**, 27554-27563.
4. T. Shimazaki, K. Kitaura, D. G. Fedorov and T. Nakajima, *J Chem Phys*, 2017, **146**, 084109.
5. T. Shimazaki and M. Tachikawa, *Physical Chemistry Chemical Physics*, 2021, **23**, 21078-21086.

We employed molecular geometries from the corresponding experimental ones. We show those

below in the XYZ-format.

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TPPs from C60/3,5-TPP

C	8.909562000	9.029039000	20.865231000
C	9.222536000	8.570314000	22.163545000
H	8.805132000	7.844836000	22.611445000
C	10.238668000	9.353502000	22.669700000
H	10.654499000	9.264957000	23.520246000
C	10.542577000	10.320180000	21.670562000
C	11.507135000	11.340562000	21.749590000
C	12.415303000	11.353988000	22.923718000
C	13.431073000	10.382835000	22.998982000
H	13.468638000	9.687476000	22.352986000
C	14.373594000	10.434302000	24.007528000
C	14.315775000	11.436782000	25.006666000
H	14.915483000	11.441705000	25.742509000
C	13.349247000	12.401223000	24.858018000
C	12.391580000	12.340805000	23.896513000
H	11.694118000	12.986712000	23.889833000
C	15.702335000	8.720239000	23.128814000
H	15.810540000	9.230027000	22.299624000
H	14.987316000	8.059363000	23.015804000
H	16.541439000	8.259299000	23.341022000
C	14.258107000	13.515587000	26.797963000
H	14.175880000	12.784895000	27.444994000
H	14.183016000	14.374812000	27.262685000
H	15.128934000	13.460630000	26.351305000
C	11.702587000	12.316191000	20.759860000
C	12.662663000	13.392515000	20.882165000
H	13.240849000	13.562623000	21.617124000
C	12.568500000	14.092909000	19.755078000
H	13.066101000	14.871778000	19.534835000
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C	11.214771000	13.900468000	17.611918000
C	11.949104000	15.137905000	17.160330000

C	11.347525000	16.388768000	17.293925000
H	10.464822000	16.469146000	17.638562000
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C	13.333957000	17.420339000	16.418974000
H	13.801200000	18.205406000	16.158502000
C	13.913500000	16.198566000	16.307959000
C	13.244060000	15.028259000	16.672992000
H	13.665091000	14.181096000	16.589825000
C	10.424228000	18.984477000	17.794435000
H	10.647493000	18.815107000	18.733398000
H	9.698533000	18.386144000	17.518270000
H	10.139325000	19.915173000	17.688067000
C	15.865890000	17.051122000	15.212859000
H	16.069324000	17.736433000	15.883843000
H	15.292078000	17.435264000	14.517734000
H	16.699930000	16.732319000	14.809083000
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H	8.549328000	13.111843000	14.112057000
C	8.661250000	12.056620000	15.961742000
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C	6.788524000	11.022812000	14.708586000
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H	4.288344000	10.935095000	11.889795000

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H	7.509708000	9.390088000	13.742470000
C	3.501491000	13.656561000	14.503490000
H	3.393287000	13.146773000	15.332680000
H	4.216510000	14.317437000	14.616500000
H	2.662388000	14.117501000	14.291281000
C	4.945720000	8.861213000	10.834340000
H	5.027947000	9.591905000	10.187309000
H	5.020810000	8.001988000	10.369619000
H	4.074893000	8.916170000	11.280998000
C	7.501239000	10.060609000	16.872443000
C	6.541163000	8.984285000	16.750138000
H	5.962978000	8.814177000	16.015179000
C	6.635327000	8.283891000	17.877226000
H	6.137725000	7.505022000	18.097469000
C	7.640519000	8.928343000	18.712663000
C	7.989055000	8.476332000	20.020385000
C	7.254723000	7.238895000	20.471973000
C	7.856301000	5.988032000	20.338378000
H	8.739005000	5.907654000	19.993742000
C	7.149716000	4.878142000	20.712820000
C	5.869870000	4.956461000	21.213329000
H	5.402627000	4.171394000	21.473801000
C	5.290327000	6.178234000	21.324345000
C	5.959766000	7.348541000	20.959311000
H	5.538735000	8.195704000	21.042479000
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H	8.556334000	3.561693000	18.898905000
H	9.505293000	3.990656000	20.114033000
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C	20.144490360	10.320180000	40.486713720
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C	17.590968360	8.476332000	38.836536720
C	16.856636360	7.238895000	39.288124720
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H	18.340918360	5.907654000	38.809893720
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C	15.471783360	4.956461000	40.029480720
H	15.004540360	4.171394000	40.289952720
C	14.892240360	6.178234000	40.140496720
C	15.561679360	7.348541000	39.775462720
H	15.140648360	8.195704000	39.858630720
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C	12.939850360	5.325678000	41.235596720
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H	12.105810360	5.644481000	41.639372720
O	15.608313360	8.970859000	30.643984720
O	17.330398360	3.613853000	39.397258720
O	13.427865360	12.801767000	32.292279720
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N	17.763042360	9.975577000	36.872130720
H	18.408125360	10.504520000	37.153356720
N	19.096503360	12.264724000	35.841005720

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TPPs from C70/3,5-TPP

O	7.036909000	5.578862000	27.054926000
O	8.730964000	9.940323000	26.223271000
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O	15.420140000	-0.079525000	24.440080000
O	13.366989000	0.628907000	13.838282000
O	14.892249000	5.065670000	13.065816000
O	4.694636000	5.930698000	15.281360000
O	5.970166000	10.383322000	16.319126000
N	11.423852000	5.056033000	22.051776000
N	12.756550000	4.089217000	19.668881000
H	11.967534000	4.476511000	19.832928000
N	9.316905000	6.337768000	20.506545000
H	10.075813000	5.942146000	20.337690000
N	10.636535000	5.354012000	18.120344000
C	8.599522000	8.660258000	25.777098000
C	13.029807000	2.315469000	15.563185000
H	12.599953000	1.703747000	16.149370000
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C	13.496289000	1.894704000	14.321411000
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C	12.503477000	4.442696000	22.633755000
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C	8.901859000	6.846362000	24.227359000
C	8.856073000	6.642648000	21.758534000
C	11.397435000	4.853730000	17.096098000
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C	14.294858000	4.107044000	13.839484000
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C	16.412807000	3.377829000	24.398618000
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H	7.568348000	8.137079000	27.473458000
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C	15.534363000	3.942762000	23.463907000
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C	10.765401000	5.143120000	15.827284000
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C	0.557756150	16.625307030	35.589304730
C	1.042847150	16.155638030	34.373970730
H	1.480925150	16.742737030	33.767955730
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C	1.725933150	13.370826030	26.016859730
H	1.103202150	13.641218030	25.352256730
C	-1.333473850	14.091838030	26.451615730
H	-1.335998850	13.156556030	26.623174730
C	1.495979150	18.799260030	35.257002730
H	2.396877150	18.423448030	35.165064730
H	1.548422150	19.667678030	35.708884730
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C	-1.325044850	13.975007030	38.227585730
H	-1.973653850	14.699401030	38.103498730
H	-0.563964850	14.303952030	38.749473730
H	-1.752098850	13.232202030	38.704405730
C	-4.066555850	14.318356030	24.049490730
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H	-4.605888850	14.969638030	24.544036730
H	-4.646292850	13.600643030	23.714785730
C	-0.658603850	19.068624030	26.392426730
H	0.289970150	18.891509030	26.220566730
H	-0.842612850	18.964892030	27.350271730
H	-0.874019850	19.983484030	26.115408730
C	0.872697150	14.800361030	34.058494730
C	-0.444538850	14.923099030	27.119823730
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H	-2.804938850	16.369758030	24.607132730
C	-0.457668850	16.307943030	26.899891730
H	0.130138150	16.879731030	27.380316730
C	2.868520150	12.666731030	25.814654730
H	3.197794150	12.353616030	24.979694730
O	7.062825150	12.523541030	23.132506730
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H	4.047945150	12.258853030	29.868071730
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C	5.634944150	9.421970030	24.501372730
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H	4.711774150	9.304540030	26.322721730
C	6.291836150	10.272586030	23.606021730
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C	4.466767150	12.676451030	34.073817730
H	5.089497150	12.406059030	34.738420730
C	7.526174150	11.955439030	33.639061730
H	7.528699150	12.890721030	33.467502730
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H	5.093014150	7.131139030	25.721814730
C	7.517745150	12.072270030	21.863091730
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C	6.851304150	6.978653030	33.698250730
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H	7.066720150	6.063793030	33.975268730
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H	8.997639150	9.677519030	35.483544730
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C	3.324180150	13.380546030	34.276022730
H	2.994906150	13.693661030	35.110982730