

Supplementary Information

Molecular magnetoresistance enhanced by destructive quantum interference of a $[\pi\cdots\pi]$ supramolecule

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S1. Details for geometries of the supramolecule and related junction

Geometries of the $[\pi \cdots \pi]$ supramolecule are mainly optimized at the PBE-D2/def2SVP level of theory. To be more reliable, other methods are also considered for the geometry optimization, such as the PBE-D2/def2SVP level with the counterpoise correction (CP) correction, the PBE-D3BJ/def2SVP level without the CP correction and the PBE-D3BJ/def2SVP level with the CP correction. ‘D3BJ’ means the more accurate D3 version of Grimme’s dispersion with Becke-Johnson damping [S. Grimme, S. Ehrlich and L. Goerigk, *J. Comp. Chem.* **32**, 1456-1465 (2011)]. After comparison, the coordinates and frontier molecular orbitals (FMOs) of the supramolecule (including the OPpe and HOMO-LUMO gap) are little influenced by different optimization methods. Here, the FMOs of the supramolecule are calculated using the def2TZVP basis set, and the functional and corrections (e.g. dispersion, CP) are consistent with those for the optimization.

The junction is optimized based on a slab-like model shown in Fig. S1. The initial geometry of the supramolecule takes the one optimized by Gaussian in this slab-like model. Rigid constraints are applied for the electrode surface atoms (marked by blue-dashed lines), while other atoms are fully relaxed without any constraints for geometric optimizations. ‘‘Rigid constraints’’ mean that the marked cobalt atoms are regarded as a rigid body with only translational motions, which is determined by the force on the center-of-mass of the rigid body atoms. This optimization scheme could yield a reasonable (though perhaps not optimal) for each configuration of the supramolecule. The calculation confirms that if d_{mj} is optimized for configuration C1, configuration C2 will be disfavored in the C1-related junction. Although the left and right semi-infinite electrodes are removed in this slab-like model, the optimized geometries of the supramolecule and the interfaces are quite close to those in the full supramolecular junction. This is implied by the fact that the increase of the electrode layers in the slab-like model has negligible impacts on the present optimized geometries of the supramolecule and the interfaces. Moreover, in the optimization calculations, the FHI pseudopotential together with the double- ζ plus polarization (DZP) basis set is used for electrode atoms, while the PseudoDojo pseudopotential together with the medium basis set is used for atoms of tips and the supramolecule.

Considering the periodic boundary condition, the thickness of the vacuum layer d_{vm} is set to be 12 Å, which is large enough to avoid possible interactions between these two surfaces in the z direction. The two other lattice parameters in the x and y directions (L_x, L_y) are 17.4 and 15.0 Å. Other larger supercells, with $L_x > 17.4$ Å and $L_y > 15.0$ Å, are tried as well, but the present optimized geometries are little affected. The force criterion for geometry optimization is less than 0.04 eV/Å.

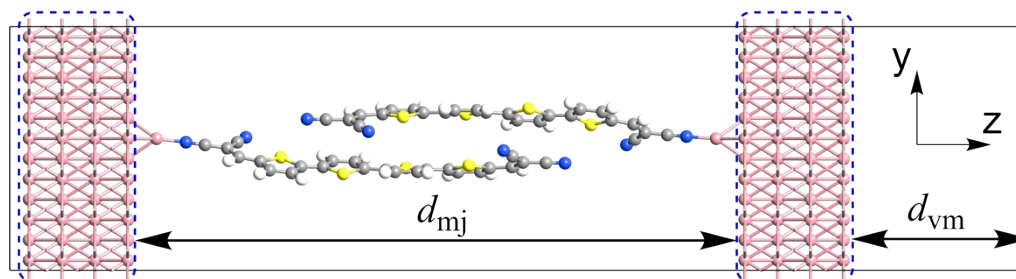


Fig. S1. The slab-like model for optimizing the geometry of the junction. d_{mj} is the spacing between two electrode surfaces. The solid rectangle marks the simulation cell of the slab model. The vacuum layer is only considered in the z direction, and d_{vm} is the thickness of this vacuum layer. The dashed rounded rectangles highlight atoms with rigid constraints in optimizing calculations.

S2. Details for plotting Figure 5b in the main text

The explicit equation for plotting Figure 5b is shown in the following:

$$T_{i,j}(E) \approx \left[\frac{(E - \varepsilon_1)s_1}{(E - \varepsilon_1)^2 + \eta^2} + \frac{(E - \varepsilon_2)s_2}{(E - \varepsilon_2)^2 + \eta^2} \right]^2 + \left[\frac{\eta s_1}{(E - \varepsilon_1)^2 + \eta^2} + \frac{\eta s_2}{(E - \varepsilon_2)^2 + \eta^2} \right]^2$$

The parameters used for the plot are:

$s_1 = 0.01$, $s_2 = -0.01$, $\varepsilon_1 = -1.0$ and $\varepsilon_2 = 0.1$ for C1;

$s_1 = 0.01$, $s_2 = 0.003$, $\varepsilon_1 = -0.9$ and $\varepsilon_2 = 0.2$ for C2;

$\eta = 10^{-4}$ is an infinitesimal number.

Some magnitudes of s_n and ε_n are set to be different for C1 and C2 by analyzing the energy levels of their FMOs and the orbital profiles of these FMOs (marked by dashed circles in Fig. 2a). The energy E ranges from -1.5 eV to 1.5 eV with the step of 0.01 eV.

S3. Details for the PDOS of configuration C1 in the junction

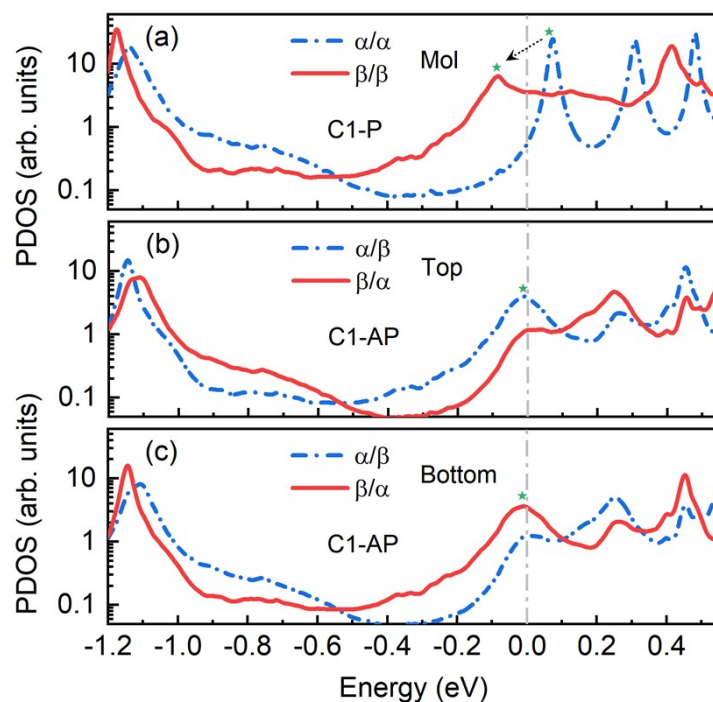


Fig. S2. (a) Projected density of states (PDOS) for the entire supramolecule in the C1-P case. (b) and (c) The PDOS for the top and bottom monomers in the C1-AP case. The green star marks the LUMO of the supramolecule, which is identified by the MPSH calculation. The labels α/α , α/β , etc. have been defined in Fig. 4e.

S4. Transmission spectra calculated by other methods and k samplings

Here, we just take the P scenario as an example to illustrate effects of different methods on the transmission spectra. ‘Co.SZP’ means that the FHI pseudopotential together with the single- ζ plus polarization basis set is used for electrode atoms, while ‘Co.DZP’ means that the FHI pseudopotential together with the double- ζ plus polarization basis set is used for electrode atoms. The PseudoDojo pseudopotential together with the medium basis set is used for atoms of tips and the supramolecule in these four different methods. D2(D3) denotes the dispersion correction.

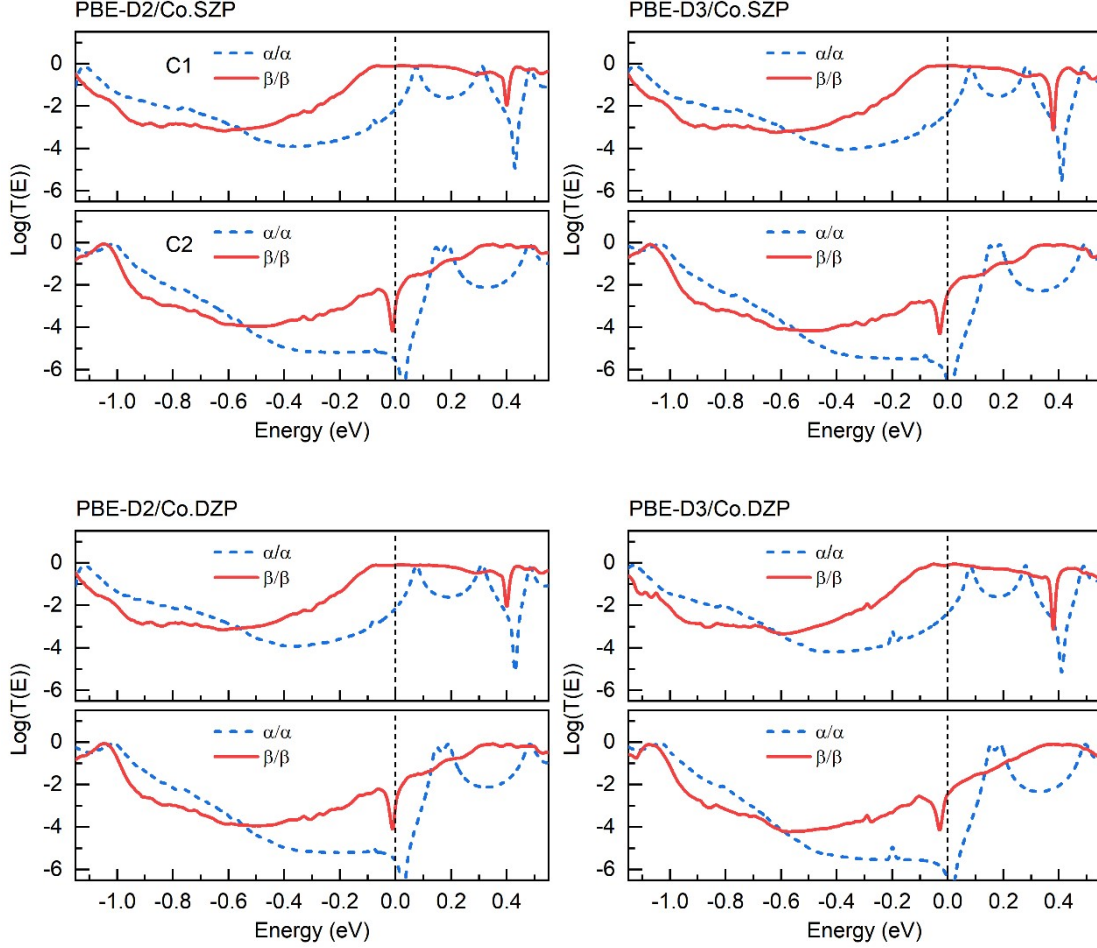


Fig. S3. Transmission spectra of C1 and C2 in the P scenario with considering different calculation methods.

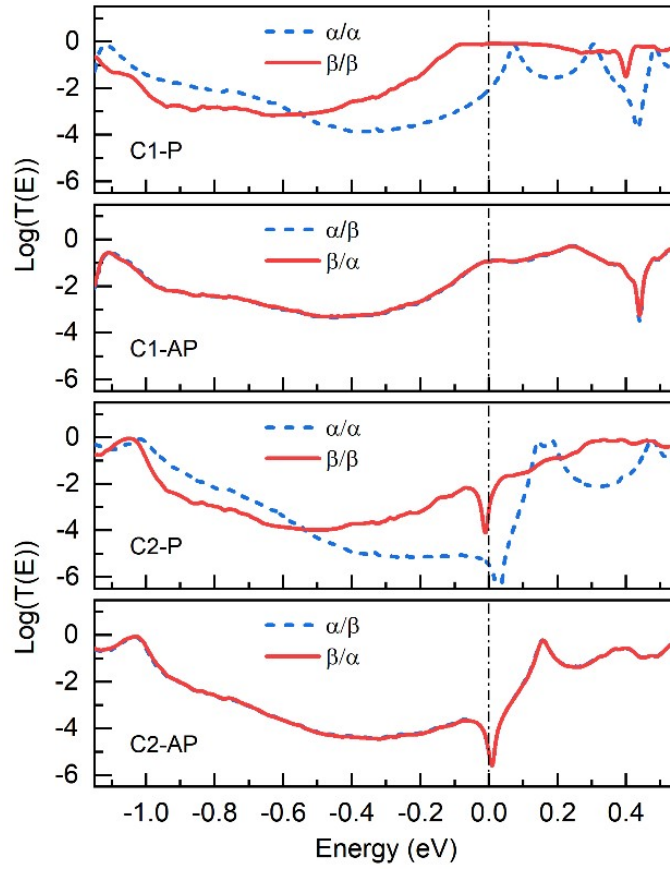


Fig. S4. Transmission spectra calculated by considering a higher k sampling, i.e. $3 \times 3 \times 100$. These spectra are almost the same as those calculated by the sampling of $1 \times 1 \times 100$, shown in Fig. 4a-4d in the main paper.

S5. Cartesian coordinates for supramolecular configurations and junctions

Molecular coordinates of C1 and C2 are listed in the following, which are optimized at PBE-D2/Def2-SVP level using the G16 package. Coordinates of the central scattering region of the junction are also listed in the following, which are optimized using QuantumATK. The lattice parameters are A=15.0426, B=17.3697, C=56.5021 for C1, and A=15.0426, B=17.3697, C=60.0481 for C2.

Coordinates for configuration C1:

C	-0.73926	1.82206	-0.33171
C	-1.25261	1.99057	-1.63094
C	-2.65238	2.08074	-1.65890
C	-3.25537	1.96959	-0.38999
S	-2.02502	1.75261	0.84688
H	-0.60666	2.06421	-2.51700
H	-3.24853	2.22781	-2.57094
C	0.63343	1.71907	0.08418
C	1.16981	1.76783	1.37783
S	1.91048	1.52214	-1.09959
C	2.57406	1.64989	1.41106
H	0.54156	1.88561	2.27242
C	3.14707	1.50441	0.14009
H	3.16890	1.60960	2.33469
C	4.52677	1.31169	-0.21803
C	5.05805	0.87077	-1.43781
S	5.80641	1.58248	0.94445
C	6.46033	0.73010	-1.42171
H	4.42265	0.63060	-2.30213
C	7.03840	1.06327	-0.18985
H	7.05637	0.37523	-2.27481
C	8.41739	0.98007	0.20733
C	8.97718	1.23277	1.47045
S	9.62909	0.43754	-0.92617
C	10.35721	0.98816	1.51381
H	8.37825	1.56435	2.33025
C	10.89289	0.54357	0.28912
H	10.98444	1.11406	2.40759
C	12.26645	0.22743	0.08787
C	12.92301	-0.21292	-1.05486
C	-4.65819	2.02803	-0.15784
H	-5.26201	2.24349	-1.05363
C	-5.37344	1.84648	1.02097
C	14.33144	-0.46958	-1.01864
N	15.48794	-0.67706	-0.98348
C	-6.79837	1.97569	1.03238
C	-4.75263	1.46959	2.25326
N	-4.23872	1.12071	3.25249
N	-7.97032	2.07344	1.04816
C	12.25747	-0.43038	-2.30233
N	11.70611	-0.60653	-3.32625
H	12.89740	0.35386	0.98254
C	-8.41736	-0.96224	0.27450
C	-8.97705	-1.12614	1.55224

C	-10.35704	-0.87897	1.57858
C	-10.89286	-0.52102	0.32588
S	-9.62915	-0.50002	-0.89395
H	-8.37810	-1.39698	2.43305
H	-10.98417	-0.94213	2.47905
C	-7.03843	-1.07322	-0.11604
C	-6.46026	-0.82671	-1.36810
S	-5.80653	-1.51241	1.05171
C	-5.05800	-0.96828	-1.37427
H	-7.05617	-0.53236	-2.24401
C	-4.52685	-1.32342	-0.12680
H	-4.42241	-0.78912	-2.25312
C	-3.14719	-1.49139	0.24371
C	-2.57431	-1.55022	1.52166
S	-1.91045	-1.59306	-0.99179
C	-1.17004	-1.67019	1.49671
H	-3.16935	-1.44732	2.44028
C	-0.63349	-1.70939	0.20280
H	-0.54201	-1.72721	2.39738
C	0.73916	-1.84037	-0.20530
C	1.25207	-2.09645	-1.49034
S	2.02540	-1.69143	0.96538
C	2.65182	-2.18822	-1.51271
H	0.60577	-2.22985	-2.36914
C	3.25529	-1.99123	-0.25450
H	3.24760	-2.39675	-2.41293
C	4.65822	-2.03348	-0.01941
C	5.37395	-1.77134	1.14385
C	-12.26652	-0.22014	0.10312
H	-12.89729	-0.28340	1.00459
C	-12.92343	0.13826	-1.06771
C	6.79885	-1.89977	1.16377
N	7.97077	-1.99655	1.18632
C	-14.33194	0.39632	-1.04942
C	-12.25819	0.26725	-2.32756
N	-11.70704	0.37078	-3.36146
N	-15.48852	0.60530	-1.02878
C	4.75375	-1.31073	2.34767
N	4.24056	-0.89389	3.32088
H	5.26173	-2.30970	-0.89857

Coordinates for configuration C2:

C	1.01569	0.62520	1.59297
C	0.60148	1.96631	1.66644
C	-0.78521	2.10492	1.82606
C	-1.47609	0.87900	1.88361
S	-0.34668	-0.46288	1.75485
H	1.30492	2.80646	1.58350
H	-1.31170	3.06767	1.89212
C	2.34231	0.11139	1.39812
C	2.74642	-1.20667	1.15728
S	3.73562	1.18274	1.42952
C	4.13968	-1.34699	0.99767
H	2.03477	-2.03928	1.06564
C	4.84170	-0.13938	1.10936
H	4.63503	-2.30127	0.77031
C	6.25156	0.09877	0.96230

C	6.93438	1.32170	0.92052
S	7.36121	-1.23325	0.73283
C	8.31694	1.18293	0.69696
H	6.42276	2.28846	1.02986
C	8.72658	-0.15069	0.56254
H	9.01716	2.02655	0.61562
C	10.04760	-0.66392	0.31915
C	10.43874	-1.99504	0.09139
S	11.42422	0.41448	0.27542
C	11.81933	-2.13207	-0.11682
H	9.72148	-2.82761	0.06972
C	12.52736	-0.91542	-0.05517
H	12.32697	-3.08650	-0.31662
C	13.93473	-0.80229	-0.23710
C	14.75302	0.32078	-0.20339
C	-2.88750	0.76680	2.01411
H	-3.41559	1.73186	2.07351
C	-3.69496	-0.36347	2.07442
C	16.16253	0.18646	-0.41766
N	17.31883	0.06905	-0.59394
C	-5.11377	-0.22134	2.19182
C	-3.18515	-1.69687	1.99768
N	-2.77103	-2.79519	1.91928
N	-6.28029	-0.09749	2.27403
C	14.25759	1.64032	0.04049
N	13.84600	2.72355	0.24232
H	14.44521	-1.75902	-0.43397
C	-10.04677	-0.65017	-0.34244
C	-10.43726	-1.98933	-0.16664
C	-11.81769	-2.13495	0.03682
C	-12.52623	-0.91710	0.02311
S	-11.42381	0.42513	-0.25601
H	-9.71965	-2.82180	-0.17775
H	-12.32483	-3.09665	0.19956
C	-8.72610	-0.12721	-0.56620
C	-8.31690	1.21087	-0.64679
S	-7.36068	-1.20163	-0.78169
C	-6.93459	1.35895	-0.86583
H	-9.01723	2.05029	-0.53049
C	-6.25154	0.13890	-0.95781
H	-6.42321	2.32947	-0.93620
C	-4.84177	-0.09262	-1.11577
C	-4.13916	-1.30346	-1.05369
S	-3.73650	1.24188	-1.38314
C	-2.74611	-1.15612	-1.20855
H	-4.63384	-2.26644	-0.86482
C	-2.34276	0.17080	-1.39619
H	-2.03393	-1.99134	-1.15105
C	-1.01636	0.69233	-1.57074
C	-0.60213	2.03532	-1.59090
S	0.34611	-0.38847	-1.77483
C	0.78466	2.18011	-1.74398
H	-1.30569	2.87151	-1.47536
C	1.47554	0.95738	-1.84960
H	1.31119	3.14472	-1.77155
C	2.88698	0.85002	-1.98376
C	3.69398	-0.27725	-2.08959
C	-13.93353	-0.81170	0.21013

H	-14.44355	-1.77557	0.36989
C	-14.75225	0.31150	0.22067
C	5.11291	-0.13098	-2.20026
N	6.27953	-0.00433	-2.27658
C	-16.16158	0.16841	0.43039
C	-14.25746	1.63973	0.02804
N	-13.84644	2.73018	-0.13173
N	-17.31772	0.04379	0.60266
C	3.18372	-1.61249	-2.06787
N	2.76931	-2.71300	-2.03481
H	3.41553	1.81644	-2.00370

Coordinates for the junction of C1:

Co	0.32306	0.61768	1.01715
Co	2.49427	1.87123	1.01715
Co	4.66548	0.61768	1.01715
Co	6.83669	1.87123	1.01715
Co	9.00791	0.61768	1.01715
Co	11.17912	1.87123	1.01715
Co	13.35033	0.61768	1.01715
Co	15.52154	1.87123	1.01715
Co	1.77053	0.61768	3.05145
Co	3.94174	1.87123	3.05145
Co	6.11296	0.61768	3.05145
Co	8.28417	1.87123	3.05145
Co	10.45538	0.61768	3.05145
Co	12.62659	1.87123	3.05145
Co	14.79781	0.61768	3.05145
Co	16.96902	1.87123	3.05145
Co	0.32306	0.61768	5.08575
Co	2.49427	1.87123	5.08575
Co	4.66548	0.61768	5.08575
Co	6.83669	1.87123	5.08575
Co	9.00791	0.61768	5.08575
Co	11.17912	1.87123	5.08575
Co	13.35033	0.61768	5.08575
Co	15.52154	1.87123	5.08575
Co	1.77053	0.61768	7.12005
Co	3.94174	1.87123	7.12005
Co	6.11296	0.61768	7.12005
Co	8.28417	1.87123	7.12005
Co	10.45538	0.61768	7.12005
Co	12.62659	1.87123	7.12005
Co	14.79781	0.61768	7.12005
Co	16.96902	1.87123	7.12005
Co	0.32306	3.12478	1.01715
Co	2.49427	4.37833	1.01715
Co	4.66548	3.12478	1.01715
Co	6.83669	4.37833	1.01715
Co	9.00791	3.12478	1.01715
Co	11.17912	4.37833	1.01715
Co	13.35033	3.12478	1.01715
Co	15.52154	4.37833	1.01715
Co	1.77053	3.12478	3.05145
Co	3.94174	4.37833	3.05145
Co	6.11296	3.12478	3.05145
Co	8.28417	4.37833	3.05145
Co	10.45538	3.12478	3.05145

Co	12.62659	4.37833	3.05145
Co	14.79781	3.12478	3.05145
Co	16.96902	4.37833	3.05145
Co	0.32306	3.12478	5.08575
Co	2.49427	4.37833	5.08575
Co	4.66548	3.12478	5.08575
Co	6.83669	4.37833	5.08575
Co	9.00791	3.12478	5.08575
Co	11.17912	4.37833	5.08575
Co	13.35033	3.12478	5.08575
Co	15.52154	4.37833	5.08575
Co	1.77053	3.12478	7.12005
Co	3.94174	4.37833	7.12005
Co	6.11296	3.12478	7.12005
Co	8.28417	4.37833	7.12005
Co	10.45538	3.12478	7.12005
Co	12.62659	4.37833	7.12005
Co	14.79781	3.12478	7.12005
Co	16.96902	4.37833	7.12005
Co	0.32306	5.63188	1.01715
Co	2.49427	6.88543	1.01715
Co	4.66548	5.63188	1.01715
Co	6.83669	6.88543	1.01715
Co	9.00791	5.63188	1.01715
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Co	13.35033	5.63188	1.01715
Co	15.52154	6.88543	1.01715
Co	1.77053	5.63188	3.05145
Co	3.94174	6.88543	3.05145
Co	6.11296	5.63188	3.05145
Co	8.28417	6.88543	3.05145
Co	10.45538	5.63188	3.05145
Co	12.62659	6.88543	3.05145
Co	14.79781	5.63188	3.05145
Co	16.96902	6.88543	3.05145
Co	0.32306	5.63188	5.08575
Co	2.49427	6.88543	5.08575
Co	4.66548	5.63188	5.08575
Co	6.83669	6.88543	5.08575
Co	9.00791	5.63188	5.08575
Co	11.17912	6.88543	5.08575
Co	13.35033	5.63188	5.08575
Co	15.52154	6.88543	5.08575
Co	1.77053	5.63188	7.12005
Co	3.94174	6.88543	7.12005
Co	6.11296	5.63188	7.12005
Co	8.28417	6.88543	7.12005
Co	10.45538	5.63188	7.12005
Co	12.62659	6.88543	7.12005
Co	14.79781	5.63188	7.12005
Co	16.96902	6.88543	7.12005
Co	0.32306	8.13898	1.01715
Co	2.49427	9.39253	1.01715
Co	4.66548	8.13898	1.01715
Co	6.83669	9.39253	1.01715
Co	9.00791	8.13898	1.01715
Co	11.17912	9.39253	1.01715
Co	13.35033	8.13898	1.01715

Co	15.52154	9.39253	1.01715
Co	1.77053	8.13898	3.05145
Co	3.94174	9.39253	3.05145
Co	6.11296	8.13898	3.05145
Co	8.28417	9.39253	3.05145
Co	10.45538	8.13898	3.05145
Co	12.62659	9.39253	3.05145
Co	14.79781	8.13898	3.05145
Co	16.96902	9.39253	3.05145
Co	0.32306	8.13898	5.08575
Co	2.49427	9.39253	5.08575
Co	4.66548	8.13898	5.08575
Co	6.83669	9.39253	5.08575
Co	9.00791	8.13898	5.08575
Co	11.17912	9.39253	5.08575
Co	13.35033	8.13898	5.08575
Co	15.52154	9.39253	5.08575
Co	1.77053	8.13898	7.12005
Co	3.94174	9.39253	7.12005
Co	6.11296	8.13898	7.12005
Co	8.28417	9.39253	7.12005
Co	10.45538	8.13898	7.12005
Co	12.62659	9.39253	7.12005
Co	14.79781	8.13898	7.12005
Co	16.96902	9.39253	7.12005
Co	0.32306	10.64608	1.01715
Co	2.49427	11.89963	1.01715
Co	4.66548	10.64608	1.01715
Co	6.83669	11.89963	1.01715
Co	9.00791	10.64608	1.01715
Co	11.17912	11.89963	1.01715
Co	13.35033	10.64608	1.01715
Co	15.52154	11.89963	1.01715
Co	1.77053	10.64608	3.05145
Co	3.94174	11.89963	3.05145
Co	6.11296	10.64608	3.05145
Co	8.28417	11.89963	3.05145
Co	10.45538	10.64608	3.05145
Co	12.62659	11.89963	3.05145
Co	14.79781	10.64608	3.05145
Co	16.96902	11.89963	3.05145
Co	0.32306	10.64608	5.08575
Co	2.49427	11.89963	5.08575
Co	4.66548	10.64608	5.08575
Co	6.83669	11.89963	5.08575
Co	9.00791	10.64608	5.08575
Co	11.17912	11.89963	5.08575
Co	13.35033	10.64608	5.08575
Co	15.52154	11.89963	5.08575
Co	1.77053	10.64608	7.12005
Co	3.94174	11.89963	7.12005
Co	6.11296	10.64608	7.12005
Co	8.28417	11.89963	7.12005
Co	10.45538	10.64608	7.12005
Co	12.62659	11.89963	7.12005
Co	14.79781	10.64608	7.12005
Co	16.96902	11.89963	7.12005
Co	0.32306	13.15318	1.01715

Co	2.49427	14.40673	1.01715
Co	4.66548	13.15318	1.01715
Co	6.83669	14.40673	1.01715
Co	9.00791	13.15318	1.01715
Co	11.17912	14.40673	1.01715
Co	13.35033	13.15318	1.01715
Co	15.52154	14.40673	1.01715
Co	1.77053	13.15318	3.05145
Co	3.94174	14.40673	3.05145
Co	6.11296	13.15318	3.05145
Co	8.28417	14.40673	3.05145
Co	10.45538	13.15318	3.05145
Co	12.62659	14.40673	3.05145
Co	14.79781	13.15318	3.05145
Co	16.96902	14.40673	3.05145
Co	0.32306	13.15318	5.08575
Co	2.49427	14.40673	5.08575
Co	4.66548	13.15318	5.08575
Co	6.83669	14.40673	5.08575
Co	9.00791	13.15318	5.08575
Co	11.17912	14.40673	5.08575
Co	13.35033	13.15318	5.08575
Co	15.52154	14.40673	5.08575
Co	1.77053	13.15318	7.12005
Co	3.94174	14.40673	7.12005
Co	6.11296	13.15318	7.12005
Co	8.28417	14.40673	7.12005
Co	10.45538	13.15318	7.12005
Co	12.62659	14.40673	7.12005
Co	14.79781	13.15318	7.12005
Co	16.96902	14.40673	7.12005
Co	0.32306	0.61768	9.15435
Co	0.32306	3.12478	9.15435
Co	0.32306	5.63188	9.15435
Co	0.32306	8.13898	9.15435
Co	0.32306	10.64608	9.15435
Co	0.32306	13.15318	9.15435
Co	2.49427	1.87123	9.15435
Co	2.49427	4.37833	9.15435
Co	2.49427	6.88543	9.15435
Co	2.49427	9.39253	9.15435
Co	2.49427	11.89963	9.15435
Co	2.49427	14.40673	9.15435
Co	4.66548	0.61768	9.15435
Co	4.66548	3.12478	9.15435
Co	4.66548	5.63188	9.15435
Co	4.66548	8.13898	9.15435
Co	4.66548	10.64608	9.15435
Co	4.66548	13.15318	9.15435
Co	6.83669	1.87123	9.15435
Co	6.83669	4.37833	9.15435
Co	6.83669	6.88543	9.15435
Co	6.83669	9.39253	9.15435
Co	6.83669	11.89963	9.15435
Co	6.83669	14.40673	9.15435
Co	9.00791	0.61768	9.15435
Co	9.00791	3.12478	9.15435
Co	9.00791	5.63188	9.15435

Co	9.00791	8.13898	9.15435
Co	9.00791	10.64608	9.15435
Co	9.00791	13.15318	9.15435
Co	11.17912	1.87123	9.15435
Co	11.17912	4.37833	9.15435
Co	11.17912	6.88543	9.15435
Co	11.17912	9.39253	9.15435
Co	11.17912	11.89963	9.15435
Co	11.17912	14.40673	9.15435
Co	13.35033	0.61768	9.15435
Co	13.35033	3.12478	9.15435
Co	13.35033	5.63188	9.15435
Co	13.35033	8.13898	9.15435
Co	13.35033	10.64608	9.15435
Co	13.35033	13.15318	9.15435
Co	15.52154	1.87123	9.15435
Co	15.52154	4.37833	9.15435
Co	15.52154	6.88543	9.15435
Co	15.52154	9.39253	9.15435
Co	15.52154	11.89963	9.15435
Co	15.52154	14.40673	9.15435
Co	10.45350	8.12421	10.93123
N	10.56391	7.90549	12.75883
C	10.63406	7.73888	13.93205
C	10.70703	7.53522	15.31486
H	8.72978	6.76343	15.38883
C	11.93129	7.90491	15.94099
C	9.60607	6.99533	16.00764
N	12.94229	8.20641	16.46264
H	7.38799	5.95241	17.31002
C	9.44720	6.71454	17.37221
C	8.26021	6.18275	17.92974
S	10.63616	6.98035	18.63918
C	8.31479	6.00410	19.30422
C	9.54663	6.38754	19.86415
H	7.49100	5.61782	19.91140
N	8.42196	9.32896	20.25063
H	12.00170	7.05389	21.21388
C	9.91808	6.38359	21.23720
C	8.45415	9.30888	21.42687
C	11.14098	6.74476	21.81472
S	8.76471	5.95362	22.48139
C	8.48471	9.28215	22.84973
H	10.53384	9.76414	22.90579
C	11.13758	6.68330	23.21322
C	7.27933	8.90226	23.50012
C	9.65670	9.56927	23.53335
C	9.90915	6.28593	23.75427
H	11.99118	6.95125	23.84310
N	6.29764	8.55609	24.04889
H	12.06188	10.00243	24.85716
C	9.90428	9.64177	24.92218
H	7.35239	6.03984	25.07209
C	9.53447	6.19886	25.13059
C	11.17398	9.86602	25.48207
C	8.25694	6.07815	25.68571
S	8.70934	9.47501	26.19395
S	10.73774	6.32211	26.38984

C	11.17904	9.90620	26.87588
C	8.25663	6.08663	27.08729
C	9.90345	9.73183	27.43439
H	12.06673	10.08848	27.48796
C	9.53153	6.20475	27.64716
H	7.35408	6.00414	27.70010
H	7.35401	9.94932	28.76247
C	9.53168	9.75098	28.81430
H	12.06755	5.86962	28.97355
C	9.90369	6.22394	29.02700
C	8.25682	9.86650	29.37475
C	11.17934	6.04961	29.58548
S	10.73845	9.63233	30.07101
S	8.70919	6.47730	30.26772
C	8.25743	9.87091	30.77619
C	11.17393	6.08664	30.97938
C	9.53538	9.75066	31.33043
H	7.35276	9.90470	31.38984
C	9.90397	6.30886	31.53951
H	12.06159	5.94893	31.60443
N	6.29782	7.39002	32.41201
H	11.99498	9.00534	32.62028
C	9.90952	9.66109	32.70645
C	9.65623	6.37832	32.92850
C	7.27862	7.04348	32.96157
C	11.13871	9.26758	33.24886
H	10.53370	6.18318	33.55555
C	8.48376	6.66297	33.61242
S	8.76167	9.98675	33.97732
C	11.14003	9.20363	34.64733
C	8.45209	6.63325	35.03544
C	9.91423	9.55857	35.22261
H	12.00136	8.89863	35.24966
N	8.41921	6.61232	36.21138
H	7.48047	10.31742	36.53393
C	9.53882	9.55619	36.59407
C	8.30375	9.93952	37.14705
S	10.62777	8.97815	37.82628
C	8.24795	9.77614	38.52301
C	9.43674	9.25728	39.08809
H	7.37497	10.01024	39.13994
N	12.91841	7.73925	40.02356
C	9.59979	9.01179	40.45835
C	11.91659	8.08024	40.53897
H	8.72749	9.26586	41.07390
C	10.70389	8.49194	41.16076
C	10.65085	8.35750	42.55262
N	10.60703	8.25492	43.73429
Co	10.54763	8.12878	45.57308
Co	0.40836	0.61804	47.34774
Co	0.40836	3.12514	47.34774
Co	0.40836	5.63224	47.34774
Co	0.40836	8.13934	47.34774
Co	0.40836	10.64644	47.34774
Co	0.40836	13.15354	47.34774
Co	2.57957	1.87159	47.34774
Co	2.57957	4.37869	47.34774
Co	2.57957	6.88579	47.34774

Co	2.57957	9.39289	47.34774
Co	2.57957	11.89999	47.34774
Co	2.57957	14.40709	47.34774
Co	4.75078	0.61804	47.34774
Co	4.75078	3.12514	47.34774
Co	4.75078	5.63224	47.34774
Co	4.75078	8.13934	47.34774
Co	4.75078	10.64644	47.34774
Co	4.75078	13.15354	47.34774
Co	6.92199	1.87159	47.34774
Co	6.92199	4.37869	47.34774
Co	6.92199	6.88579	47.34774
Co	6.92199	9.39289	47.34774
Co	6.92199	11.89999	47.34774
Co	6.92199	14.40709	47.34774
Co	9.09321	0.61804	47.34774
Co	9.09321	3.12514	47.34774
Co	9.09321	5.63224	47.34774
Co	9.09321	8.13934	47.34774
Co	9.09321	10.64644	47.34774
Co	9.09321	13.15354	47.34774
Co	11.26442	1.87159	47.34774
Co	11.26442	4.37869	47.34774
Co	11.26442	6.88579	47.34774
Co	11.26442	9.39289	47.34774
Co	11.26442	11.89999	47.34774
Co	11.26442	14.40709	47.34774
Co	13.43563	0.61804	47.34774
Co	13.43563	3.12514	47.34774
Co	13.43563	5.63224	47.34774
Co	13.43563	8.13934	47.34774
Co	13.43563	10.64644	47.34774
Co	13.43563	13.15354	47.34774
Co	15.60684	1.87159	47.34774
Co	15.60684	4.37869	47.34774
Co	15.60684	6.88579	47.34774
Co	15.60684	9.39289	47.34774
Co	15.60684	11.89999	47.34774
Co	15.60684	14.40709	47.34774
Co	1.85583	0.61804	49.38204
Co	4.02704	1.87159	49.38204
Co	6.19826	0.61804	49.38204
Co	8.36947	1.87159	49.38204
Co	10.54068	0.61804	49.38204
Co	12.71189	1.87159	49.38204
Co	14.88311	0.61804	49.38204
Co	17.05432	1.87159	49.38204
Co	0.40836	0.61804	51.41634
Co	2.57957	1.87159	51.41634
Co	4.75078	0.61804	51.41634
Co	6.92199	1.87159	51.41634
Co	9.09321	0.61804	51.41634
Co	11.26442	1.87159	51.41634
Co	13.43563	0.61804	51.41634
Co	15.60684	1.87159	51.41634
Co	1.85583	0.61804	53.45064
Co	4.02704	1.87159	53.45064
Co	6.19826	0.61804	53.45064

Co	8.36947	1.87159	53.45064
Co	10.54068	0.61804	53.45064
Co	12.71189	1.87159	53.45064
Co	14.88311	0.61804	53.45064
Co	17.05432	1.87159	53.45064
Co	0.40836	0.61804	55.48494
Co	2.57957	1.87159	55.48494
Co	4.75078	0.61804	55.48494
Co	6.92199	1.87159	55.48494
Co	9.09321	0.61804	55.48494
Co	11.26442	1.87159	55.48494
Co	13.43563	0.61804	55.48494
Co	15.60684	1.87159	55.48494
Co	1.85583	3.12514	49.38204
Co	4.02704	4.37869	49.38204
Co	6.19826	3.12514	49.38204
Co	8.36947	4.37869	49.38204
Co	10.54068	3.12514	49.38204
Co	12.71189	4.37869	49.38204
Co	14.88311	3.12514	49.38204
Co	17.05432	4.37869	49.38204
Co	0.40836	3.12514	51.41634
Co	2.57957	4.37869	51.41634
Co	4.75078	3.12514	51.41634
Co	6.92199	4.37869	51.41634
Co	9.09321	3.12514	51.41634
Co	11.26442	4.37869	51.41634
Co	13.43563	3.12514	51.41634
Co	15.60684	4.37869	51.41634
Co	1.85583	3.12514	53.45064
Co	4.02704	4.37869	53.45064
Co	6.19826	3.12514	53.45064
Co	8.36947	4.37869	53.45064
Co	10.54068	3.12514	53.45064
Co	12.71189	4.37869	53.45064
Co	14.88311	3.12514	53.45064
Co	17.05432	4.37869	53.45064
Co	0.40836	3.12514	55.48494
Co	2.57957	4.37869	55.48494
Co	4.75078	3.12514	55.48494
Co	6.92199	4.37869	55.48494
Co	9.09321	3.12514	55.48494
Co	11.26442	4.37869	55.48494
Co	13.43563	3.12514	55.48494
Co	15.60684	4.37869	55.48494
Co	1.85583	5.63224	49.38204
Co	4.02704	6.88579	49.38204
Co	6.19826	5.63224	49.38204
Co	8.36947	6.88579	49.38204
Co	10.54068	5.63224	49.38204
Co	12.71189	6.88579	49.38204
Co	14.88311	5.63224	49.38204
Co	17.05432	6.88579	49.38204
Co	0.40836	5.63224	51.41634
Co	2.57957	6.88579	51.41634
Co	4.75078	5.63224	51.41634
Co	6.92199	6.88579	51.41634
Co	9.09321	5.63224	51.41634

Co	11.26442	6.88579	51.41634
Co	13.43563	5.63224	51.41634
Co	15.60684	6.88579	51.41634
Co	1.85583	5.63224	53.45064
Co	4.02704	6.88579	53.45064
Co	6.19826	5.63224	53.45064
Co	8.36947	6.88579	53.45064
Co	10.54068	5.63224	53.45064
Co	12.71189	6.88579	53.45064
Co	14.88311	5.63224	53.45064
Co	17.05432	6.88579	53.45064
Co	0.40836	5.63224	55.48494
Co	2.57957	6.88579	55.48494
Co	4.75078	5.63224	55.48494
Co	6.92199	6.88579	55.48494
Co	9.09321	5.63224	55.48494
Co	11.26442	6.88579	55.48494
Co	13.43563	5.63224	55.48494
Co	15.60684	6.88579	55.48494
Co	1.85583	8.13934	49.38204
Co	4.02704	9.39289	49.38204
Co	6.19826	8.13934	49.38204
Co	8.36947	9.39289	49.38204
Co	10.54068	8.13934	49.38204
Co	12.71189	9.39289	49.38204
Co	14.88311	8.13934	49.38204
Co	17.05432	9.39289	49.38204
Co	0.40836	8.13934	51.41634
Co	2.57957	9.39289	51.41634
Co	4.75078	8.13934	51.41634
Co	6.92199	9.39289	51.41634
Co	9.09321	8.13934	51.41634
Co	11.26442	9.39289	51.41634
Co	13.43563	8.13934	51.41634
Co	15.60684	9.39289	51.41634
Co	1.85583	8.13934	53.45064
Co	4.02704	9.39289	53.45064
Co	6.19826	8.13934	53.45064
Co	8.36947	9.39289	53.45064
Co	10.54068	8.13934	53.45064
Co	12.71189	9.39289	53.45064
Co	14.88311	8.13934	53.45064
Co	17.05432	9.39289	53.45064
Co	0.40836	8.13934	55.48494
Co	2.57957	9.39289	55.48494
Co	4.75078	8.13934	55.48494
Co	6.92199	9.39289	55.48494
Co	9.09321	8.13934	55.48494
Co	11.26442	9.39289	55.48494
Co	13.43563	8.13934	55.48494
Co	15.60684	9.39289	55.48494
Co	1.85583	10.64644	49.38204
Co	4.02704	11.89999	49.38204
Co	6.19826	10.64644	49.38204
Co	8.36947	11.89999	49.38204
Co	10.54068	10.64644	49.38204
Co	12.71189	11.89999	49.38204
Co	14.88311	10.64644	49.38204

Co	17.05432	11.89999	49.38204
Co	0.40836	10.64644	51.41634
Co	2.57957	11.89999	51.41634
Co	4.75078	10.64644	51.41634
Co	6.92199	11.89999	51.41634
Co	9.09321	10.64644	51.41634
Co	11.26442	11.89999	51.41634
Co	13.43563	10.64644	51.41634
Co	15.60684	11.89999	51.41634
Co	1.85583	10.64644	53.45064
Co	4.02704	11.89999	53.45064
Co	6.19826	10.64644	53.45064
Co	8.36947	11.89999	53.45064
Co	10.54068	10.64644	53.45064
Co	12.71189	11.89999	53.45064
Co	14.88311	10.64644	53.45064
Co	17.05432	11.89999	53.45064
Co	0.40836	10.64644	55.48494
Co	2.57957	11.89999	55.48494
Co	4.75078	10.64644	55.48494
Co	6.92199	11.89999	55.48494
Co	9.09321	10.64644	55.48494
Co	11.26442	11.89999	55.48494
Co	13.43563	10.64644	55.48494
Co	15.60684	11.89999	55.48494
Co	1.85583	13.15354	49.38204
Co	4.02704	14.40709	49.38204
Co	6.19826	13.15354	49.38204
Co	8.36947	14.40709	49.38204
Co	10.54068	13.15354	49.38204
Co	12.71189	14.40709	49.38204
Co	14.88311	13.15354	49.38204
Co	17.05432	14.40709	49.38204
Co	0.40836	13.15354	51.41634
Co	2.57957	14.40709	51.41634
Co	4.75078	13.15354	51.41634
Co	6.92199	14.40709	51.41634
Co	9.09321	13.15354	51.41634
Co	11.26442	14.40709	51.41634
Co	13.43563	13.15354	51.41634
Co	15.60684	14.40709	51.41634
Co	1.85583	13.15354	53.45064
Co	4.02704	14.40709	53.45064
Co	6.19826	13.15354	53.45064
Co	8.36947	14.40709	53.45064
Co	10.54068	13.15354	53.45064
Co	12.71189	14.40709	53.45064
Co	14.88311	13.15354	53.45064
Co	17.05432	14.40709	53.45064
Co	0.40836	13.15354	55.48494
Co	2.57957	14.40709	55.48494
Co	4.75078	13.15354	55.48494
Co	6.92199	14.40709	55.48494
Co	9.09321	13.15354	55.48494
Co	11.26442	14.40709	55.48494
Co	13.43563	13.15354	55.48494
Co	15.60684	14.40709	55.48494

Coordinates for the junction of C2:

Co	0.31234	0.62506	1.01715
Co	2.48355	1.87861	1.01715
Co	4.65476	0.62506	1.01715
Co	6.82598	1.87861	1.01715
Co	8.99719	0.62506	1.01715
Co	11.16840	1.87861	1.01715
Co	13.33961	0.62506	1.01715
Co	15.51082	1.87861	1.01715
Co	1.75981	0.62506	3.05145
Co	3.93103	1.87861	3.05145
Co	6.10224	0.62506	3.05145
Co	8.27345	1.87861	3.05145
Co	10.44466	0.62506	3.05145
Co	12.61588	1.87861	3.05145
Co	14.78709	0.62506	3.05145
Co	16.95830	1.87861	3.05145
Co	0.31234	0.62506	5.08575
Co	2.48355	1.87861	5.08575
Co	4.65476	0.62506	5.08575
Co	6.82598	1.87861	5.08575
Co	8.99719	0.62506	5.08575
Co	11.16840	1.87861	5.08575
Co	13.33961	0.62506	5.08575
Co	15.51082	1.87861	5.08575
Co	1.75981	0.62506	7.12005
Co	3.93103	1.87861	7.12005
Co	6.10224	0.62506	7.12005
Co	8.27345	1.87861	7.12005
Co	10.44466	0.62506	7.12005
Co	12.61588	1.87861	7.12005
Co	14.78709	0.62506	7.12005
Co	16.95830	1.87861	7.12005
Co	0.31234	3.13216	1.01715
Co	2.48355	4.38571	1.01715
Co	4.65476	3.13216	1.01715
Co	6.82598	4.38571	1.01715
Co	8.99719	3.13216	1.01715
Co	11.16840	4.38571	1.01715
Co	13.33961	3.13216	1.01715
Co	15.51082	4.38571	1.01715
Co	1.75981	3.13216	3.05145
Co	3.93103	4.38571	3.05145
Co	6.10224	3.13216	3.05145
Co	8.27345	4.38571	3.05145
Co	10.44466	3.13216	3.05145
Co	12.61588	4.38571	3.05145
Co	14.78709	3.13216	3.05145
Co	16.95830	4.38571	3.05145
Co	0.31234	3.13216	5.08575
Co	2.48355	4.38571	5.08575
Co	4.65476	3.13216	5.08575
Co	6.82598	4.38571	5.08575
Co	8.99719	3.13216	5.08575
Co	11.16840	4.38571	5.08575
Co	13.33961	3.13216	5.08575
Co	15.51082	4.38571	5.08575
Co	1.75981	3.13216	7.12005

Co	3.93103	4.38571	7.12005
Co	6.10224	3.13216	7.12005
Co	8.27345	4.38571	7.12005
Co	10.44466	3.13216	7.12005
Co	12.61588	4.38571	7.12005
Co	14.78709	3.13216	7.12005
Co	16.95830	4.38571	7.12005
Co	0.31234	5.63926	1.01715
Co	2.48355	6.89281	1.01715
Co	4.65476	5.63926	1.01715
Co	6.82598	6.89281	1.01715
Co	8.99719	5.63926	1.01715
Co	11.16840	6.89281	1.01715
Co	13.33961	5.63926	1.01715
Co	15.51082	6.89281	1.01715
Co	1.75981	5.63926	3.05145
Co	3.93103	6.89281	3.05145
Co	6.10224	5.63926	3.05145
Co	8.27345	6.89281	3.05145
Co	10.44466	5.63926	3.05145
Co	12.61588	6.89281	3.05145
Co	14.78709	5.63926	3.05145
Co	16.95830	6.89281	3.05145
Co	0.31234	5.63926	5.08575
Co	2.48355	6.89281	5.08575
Co	4.65476	5.63926	5.08575
Co	6.82598	6.89281	5.08575
Co	8.99719	5.63926	5.08575
Co	11.16840	6.89281	5.08575
Co	13.33961	5.63926	5.08575
Co	15.51082	6.89281	5.08575
Co	1.75981	5.63926	7.12005
Co	3.93103	6.89281	7.12005
Co	6.10224	5.63926	7.12005
Co	8.27345	6.89281	7.12005
Co	10.44466	5.63926	7.12005
Co	12.61588	6.89281	7.12005
Co	14.78709	5.63926	7.12005
Co	16.95830	6.89281	7.12005
Co	0.31234	8.14636	1.01715
Co	2.48355	9.39991	1.01715
Co	4.65476	8.14636	1.01715
Co	6.82598	9.39991	1.01715
Co	8.99719	8.14636	1.01715
Co	11.16840	9.39991	1.01715
Co	13.33961	8.14636	1.01715
Co	15.51082	9.39991	1.01715
Co	1.75981	8.14636	3.05145
Co	3.93103	9.39991	3.05145
Co	6.10224	8.14636	3.05145
Co	8.27345	9.39991	3.05145
Co	10.44466	8.14636	3.05145
Co	12.61588	9.39991	3.05145
Co	14.78709	8.14636	3.05145
Co	16.95830	9.39991	3.05145
Co	0.31234	8.14636	5.08575
Co	2.48355	9.39991	5.08575
Co	4.65476	8.14636	5.08575

Co	6.82598	9.39991	5.08575
Co	8.99719	8.14636	5.08575
Co	11.16840	9.39991	5.08575
Co	13.33961	8.14636	5.08575
Co	15.51082	9.39991	5.08575
Co	1.75981	8.14636	7.12005
Co	3.93103	9.39991	7.12005
Co	6.10224	8.14636	7.12005
Co	8.27345	9.39991	7.12005
Co	10.44466	8.14636	7.12005
Co	12.61588	9.39991	7.12005
Co	14.78709	8.14636	7.12005
Co	16.95830	9.39991	7.12005
Co	0.31234	10.65346	1.01715
Co	2.48355	11.90701	1.01715
Co	4.65476	10.65346	1.01715
Co	6.82598	11.90701	1.01715
Co	8.99719	10.65346	1.01715
Co	11.16840	11.90701	1.01715
Co	13.33961	10.65346	1.01715
Co	15.51082	11.90701	1.01715
Co	1.75981	10.65346	3.05145
Co	3.93103	11.90701	3.05145
Co	6.10224	10.65346	3.05145
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Co	12.61588	11.90701	3.05145
Co	14.78709	10.65346	3.05145
Co	16.95830	11.90701	3.05145
Co	0.31234	10.65346	5.08575
Co	2.48355	11.90701	5.08575
Co	4.65476	10.65346	5.08575
Co	6.82598	11.90701	5.08575
Co	8.99719	10.65346	5.08575
Co	11.16840	11.90701	5.08575
Co	13.33961	10.65346	5.08575
Co	15.51082	11.90701	5.08575
Co	1.75981	10.65346	7.12005
Co	3.93103	11.90701	7.12005
Co	6.10224	10.65346	7.12005
Co	8.27345	11.90701	7.12005
Co	10.44466	10.65346	7.12005
Co	12.61588	11.90701	7.12005
Co	14.78709	10.65346	7.12005
Co	16.95830	11.90701	7.12005
Co	0.31234	13.16056	1.01715
Co	2.48355	14.41411	1.01715
Co	4.65476	13.16056	1.01715
Co	6.82598	14.41411	1.01715
Co	8.99719	13.16056	1.01715
Co	11.16840	14.41411	1.01715
Co	13.33961	13.16056	1.01715
Co	15.51082	14.41411	1.01715
Co	1.75981	13.16056	3.05145
Co	3.93103	14.41411	3.05145
Co	6.10224	13.16056	3.05145
Co	8.27345	14.41411	3.05145
Co	10.44466	13.16056	3.05145

Co	12.61588	14.41411	3.05145
Co	14.78709	13.16056	3.05145
Co	16.95830	14.41411	3.05145
Co	0.31234	13.16056	5.08575
Co	2.48355	14.41411	5.08575
Co	4.65476	13.16056	5.08575
Co	6.82598	14.41411	5.08575
Co	8.99719	13.16056	5.08575
Co	11.16840	14.41411	5.08575
Co	13.33961	13.16056	5.08575
Co	15.51082	14.41411	5.08575
Co	1.75981	13.16056	7.12005
Co	3.93103	14.41411	7.12005
Co	6.10224	13.16056	7.12005
Co	8.27345	14.41411	7.12005
Co	10.44466	13.16056	7.12005
Co	12.61588	14.41411	7.12005
Co	14.78709	13.16056	7.12005
Co	16.95830	14.41411	7.12005
Co	0.31234	0.62506	9.15435
Co	0.31234	3.13216	9.15435
Co	0.31234	5.63926	9.15435
Co	0.31234	8.14636	9.15435
Co	0.31234	10.65346	9.15435
Co	0.31234	13.16056	9.15435
Co	2.48355	1.87861	9.15435
Co	2.48355	4.38571	9.15435
Co	2.48355	6.89281	9.15435
Co	2.48355	9.39991	9.15435
Co	2.48355	11.90701	9.15435
Co	2.48355	14.41411	9.15435
Co	4.65476	0.62506	9.15435
Co	4.65476	3.13216	9.15435
Co	4.65476	5.63926	9.15435
Co	4.65476	8.14636	9.15435
Co	4.65476	10.65346	9.15435
Co	4.65476	13.16056	9.15435
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Co	6.82598	4.38571	9.15435
Co	6.82598	6.89281	9.15435
Co	6.82598	9.39991	9.15435
Co	6.82598	11.90701	9.15435
Co	6.82598	14.41411	9.15435
Co	8.99719	0.62506	9.15435
Co	8.99719	3.13216	9.15435
Co	8.99719	5.63926	9.15435
Co	8.99719	8.14636	9.15435
Co	8.99719	10.65346	9.15435
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Co	11.16840	1.87861	9.15435
Co	11.16840	4.38571	9.15435
Co	11.16840	6.89281	9.15435
Co	11.16840	9.39991	9.15435
Co	11.16840	11.90701	9.15435
Co	11.16840	14.41411	9.15435
Co	13.33961	0.62506	9.15435
Co	13.33961	3.13216	9.15435
Co	13.33961	5.63926	9.15435

Co	13.33961	8.14636	9.15435
Co	13.33961	10.65346	9.15435
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Co	15.51082	1.87861	9.15435
Co	15.51082	4.38571	9.15435
Co	15.51082	6.89281	9.15435
Co	15.51082	9.39991	9.15435
Co	15.51082	11.90701	9.15435
Co	15.51082	14.41411	9.15435
Co	10.43747	8.12323	10.92689
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H	8.63539	8.35895	15.65328
C	11.94063	7.39917	15.80966
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N	12.99784	7.05656	16.19744
C	9.44914	7.96554	17.56318
H	7.33404	8.52061	17.77858
C	8.25805	8.22009	18.28263
S	10.73472	7.51488	18.67771
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C	9.67698	7.68235	20.05880
H	7.57631	8.23126	20.37723
H	12.31934	7.30478	21.13113
C	10.14910	7.44448	21.38204
C	11.46713	7.26108	21.81611
S	9.04332	7.34422	22.73089
C	11.57358	7.05849	23.19623
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H	12.52237	6.92528	23.72442
C	10.34300	7.07669	23.86051
C	10.22622	10.29824	24.85806
C	10.08772	6.94887	25.25993
H	7.95411	7.40445	25.44199
C	8.88344	7.12596	25.94677
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S	11.37362	6.56593	26.37904
H	12.17090	9.96460	26.52878
C	8.77070	10.24204	26.78907
C	11.21501	10.00718	27.06398
N	7.67932	10.27282	27.22586
C	8.99971	6.96612	27.33411
C	10.29358	6.65440	27.75433
H	8.17092	7.10234	28.03464
C	11.32820	9.87279	28.46527
H	13.50000	9.64573	28.59737
H	12.93912	6.25703	28.81384
C	10.77072	6.43727	29.08153
C	12.54870	9.68874	29.13630
C	12.09449	6.25631	29.50765
S	10.00494	9.89406	29.61507
S	9.66803	6.38855	30.43266
C	12.42034	9.56025	30.51792
C	12.20858	6.10479	30.88809
C	11.09026	9.63509	30.95633
H	13.25550	9.39694	31.20422
H	13.15507	5.96567	31.41926

C	10.98145	6.15614	31.57005
H	8.42059	9.47946	32.02849
C	10.59254	9.51227	32.28820
C	9.26689	9.45342	32.72091
N	7.33381	6.45594	32.84840
C	10.85796	6.04372	32.97215
C	8.41628	6.27805	33.27282
H	11.80974	5.90223	33.49754
S	11.68214	9.39045	33.65369
C	9.73011	6.08316	33.77674
C	9.13512	9.31691	34.10943
H	8.17432	9.22176	34.62297
C	10.35718	9.25863	34.78510
C	9.85651	5.94132	35.18726
C	10.59591	9.07921	36.18195
H	12.76632	8.82056	36.29800
N	9.96504	5.83229	36.35362
C	11.81382	8.86354	36.83478
S	9.27904	9.05300	37.32290
C	11.68315	8.67666	38.21524
C	10.35782	8.73976	38.66113
H	12.51804	8.47013	38.89163
H	7.69233	8.42956	39.67881
C	9.85841	8.59016	39.98762
C	8.51913	8.45518	40.39476
S	10.93492	8.56794	41.36449
C	8.37200	8.32998	41.77113
H	7.41087	8.20464	42.27988
C	9.59223	8.36956	42.48579
N	13.24976	8.59642	43.84183
C	9.68248	8.28017	43.88330
C	12.14805	8.47086	44.23678
H	8.72090	8.16941	44.40015
C	10.81636	8.32413	44.71789
C	10.68309	8.24012	46.10724
N	10.58394	8.17849	47.28884
Co	10.44309	8.13911	49.12077
Co	0.30980	0.62435	50.89377
Co	0.30980	3.13145	50.89377
Co	0.30980	5.63855	50.89377
Co	0.30980	8.14565	50.89377
Co	0.30980	10.65275	50.89377
Co	0.30980	13.15985	50.89377
Co	2.48102	1.87790	50.89377
Co	2.48102	4.38500	50.89377
Co	2.48102	6.89210	50.89377
Co	2.48102	9.39920	50.89377
Co	2.48102	11.90630	50.89377
Co	2.48102	14.41340	50.89377
Co	4.65223	0.62435	50.89377
Co	4.65223	3.13145	50.89377
Co	4.65223	5.63855	50.89377
Co	4.65223	8.14565	50.89377
Co	4.65223	10.65275	50.89377
Co	4.65223	13.15985	50.89377
Co	6.82344	1.87790	50.89377
Co	6.82344	4.38500	50.89377
Co	6.82344	6.89210	50.89377

Co	6.82344	9.39920	50.89377
Co	6.82344	11.90630	50.89377
Co	6.82344	14.41340	50.89377
Co	8.99465	0.62435	50.89377
Co	8.99465	3.13145	50.89377
Co	8.99465	5.63855	50.89377
Co	8.99465	8.14565	50.89377
Co	8.99465	10.65275	50.89377
Co	8.99465	13.15985	50.89377
Co	11.16586	1.87790	50.89377
Co	11.16586	4.38500	50.89377
Co	11.16586	6.89210	50.89377
Co	11.16586	9.39920	50.89377
Co	11.16586	11.90630	50.89377
Co	11.16586	14.41340	50.89377
Co	13.33708	0.62435	50.89377
Co	13.33708	3.13145	50.89377
Co	13.33708	5.63855	50.89377
Co	13.33708	8.14565	50.89377
Co	13.33708	10.65275	50.89377
Co	13.33708	13.15985	50.89377
Co	15.50829	1.87790	50.89377
Co	15.50829	4.38500	50.89377
Co	15.50829	6.89210	50.89377
Co	15.50829	9.39920	50.89377
Co	15.50829	11.90630	50.89377
Co	15.50829	14.41340	50.89377
Co	1.75728	0.62435	52.92807
Co	3.92849	1.87790	52.92807
Co	6.09970	0.62435	52.92807
Co	8.27091	1.87790	52.92807
Co	10.44213	0.62435	52.92807
Co	12.61334	1.87790	52.92807
Co	14.78455	0.62435	52.92807
Co	16.95576	1.87790	52.92807
Co	0.30980	0.62435	54.96237
Co	2.48102	1.87790	54.96237
Co	4.65223	0.62435	54.96237
Co	6.82344	1.87790	54.96237
Co	8.99465	0.62435	54.96237
Co	11.16586	1.87790	54.96237
Co	13.33708	0.62435	54.96237
Co	15.50829	1.87790	54.96237
Co	1.75728	0.62435	56.99667
Co	3.92849	1.87790	56.99667
Co	6.09970	0.62435	56.99667
Co	8.27091	1.87790	56.99667
Co	10.44213	0.62435	56.99667
Co	12.61334	1.87790	56.99667
Co	14.78455	0.62435	56.99667
Co	16.95576	1.87790	56.99667
Co	0.30980	0.62435	59.03097
Co	2.48102	1.87790	59.03097
Co	4.65223	0.62435	59.03097
Co	6.82344	1.87790	59.03097
Co	8.99465	0.62435	59.03097
Co	11.16586	1.87790	59.03097
Co	13.33708	0.62435	59.03097

Co	15.50829	1.87790	59.03097
Co	1.75728	3.13145	52.92807
Co	3.92849	4.38500	52.92807
Co	6.09970	3.13145	52.92807
Co	8.27091	4.38500	52.92807
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Co	12.61334	4.38500	52.92807
Co	14.78455	3.13145	52.92807
Co	16.95576	4.38500	52.92807
Co	0.30980	3.13145	54.96237
Co	2.48102	4.38500	54.96237
Co	4.65223	3.13145	54.96237
Co	6.82344	4.38500	54.96237
Co	8.99465	3.13145	54.96237
Co	11.16586	4.38500	54.96237
Co	13.33708	3.13145	54.96237
Co	15.50829	4.38500	54.96237
Co	1.75728	3.13145	56.99667
Co	3.92849	4.38500	56.99667
Co	6.09970	3.13145	56.99667
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Co	12.61334	4.38500	56.99667
Co	14.78455	3.13145	56.99667
Co	16.95576	4.38500	56.99667
Co	0.30980	3.13145	59.03097
Co	2.48102	4.38500	59.03097
Co	4.65223	3.13145	59.03097
Co	6.82344	4.38500	59.03097
Co	8.99465	3.13145	59.03097
Co	11.16586	4.38500	59.03097
Co	13.33708	3.13145	59.03097
Co	15.50829	4.38500	59.03097
Co	1.75728	5.63855	52.92807
Co	3.92849	6.89210	52.92807
Co	6.09970	5.63855	52.92807
Co	8.27091	6.89210	52.92807
Co	10.44213	5.63855	52.92807
Co	12.61334	6.89210	52.92807
Co	14.78455	5.63855	52.92807
Co	16.95576	6.89210	52.92807
Co	0.30980	5.63855	54.96237
Co	2.48102	6.89210	54.96237
Co	4.65223	5.63855	54.96237
Co	6.82344	6.89210	54.96237
Co	8.99465	5.63855	54.96237
Co	11.16586	6.89210	54.96237
Co	13.33708	5.63855	54.96237
Co	15.50829	6.89210	54.96237
Co	1.75728	5.63855	56.99667
Co	3.92849	6.89210	56.99667
Co	6.09970	5.63855	56.99667
Co	8.27091	6.89210	56.99667
Co	10.44213	5.63855	56.99667
Co	12.61334	6.89210	56.99667
Co	14.78455	5.63855	56.99667
Co	16.95576	6.89210	56.99667
Co	0.30980	5.63855	59.03097

Co	2.48102	6.89210	59.03097
Co	4.65223	5.63855	59.03097
Co	6.82344	6.89210	59.03097
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Co	12.61334	9.39920	52.92807
Co	14.78455	8.14565	52.92807
Co	16.95576	9.39920	52.92807
Co	0.30980	8.14565	54.96237
Co	2.48102	9.39920	54.96237
Co	4.65223	8.14565	54.96237
Co	6.82344	9.39920	54.96237
Co	8.99465	8.14565	54.96237
Co	11.16586	9.39920	54.96237
Co	13.33708	8.14565	54.96237
Co	15.50829	9.39920	54.96237
Co	1.75728	8.14565	56.99667
Co	3.92849	9.39920	56.99667
Co	6.09970	8.14565	56.99667
Co	8.27091	9.39920	56.99667
Co	10.44213	8.14565	56.99667
Co	12.61334	9.39920	56.99667
Co	14.78455	8.14565	56.99667
Co	16.95576	9.39920	56.99667
Co	0.30980	8.14565	59.03097
Co	2.48102	9.39920	59.03097
Co	4.65223	8.14565	59.03097
Co	6.82344	9.39920	59.03097
Co	8.99465	8.14565	59.03097
Co	11.16586	9.39920	59.03097
Co	13.33708	8.14565	59.03097
Co	15.50829	9.39920	59.03097
Co	1.75728	10.65275	52.92807
Co	3.92849	11.90630	52.92807
Co	6.09970	10.65275	52.92807
Co	8.27091	11.90630	52.92807
Co	10.44213	10.65275	52.92807
Co	12.61334	11.90630	52.92807
Co	14.78455	10.65275	52.92807
Co	16.95576	11.90630	52.92807
Co	0.30980	10.65275	54.96237
Co	2.48102	11.90630	54.96237
Co	4.65223	10.65275	54.96237
Co	6.82344	11.90630	54.96237
Co	8.99465	10.65275	54.96237
Co	11.16586	11.90630	54.96237
Co	13.33708	10.65275	54.96237
Co	15.50829	11.90630	54.96237
Co	1.75728	10.65275	56.99667
Co	3.92849	11.90630	56.99667
Co	6.09970	10.65275	56.99667

Co	8.27091	11.90630	56.99667
Co	10.44213	10.65275	56.99667
Co	12.61334	11.90630	56.99667
Co	14.78455	10.65275	56.99667
Co	16.95576	11.90630	56.99667
Co	0.30980	10.65275	59.03097
Co	2.48102	11.90630	59.03097
Co	4.65223	10.65275	59.03097
Co	6.82344	11.90630	59.03097
Co	8.99465	10.65275	59.03097
Co	11.16586	11.90630	59.03097
Co	13.33708	10.65275	59.03097
Co	15.50829	11.90630	59.03097
Co	1.75728	13.15985	52.92807
Co	3.92849	14.41340	52.92807
Co	6.09970	13.15985	52.92807
Co	8.27091	14.41340	52.92807
Co	10.44213	13.15985	52.92807
Co	12.61334	14.41340	52.92807
Co	14.78455	13.15985	52.92807
Co	16.95576	14.41340	52.92807
Co	0.30980	13.15985	54.96237
Co	2.48102	14.41340	54.96237
Co	4.65223	13.15985	54.96237
Co	6.82344	14.41340	54.96237
Co	8.99465	13.15985	54.96237
Co	11.16586	14.41340	54.96237
Co	13.33708	13.15985	54.96237
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Co	16.95576	14.41340	56.99667
Co	0.30980	13.15985	59.03097
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Co	4.65223	13.15985	59.03097
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Co	8.99465	13.15985	59.03097
Co	11.16586	14.41340	59.03097
Co	13.33708	13.15985	59.03097
Co	15.50829	14.41340	59.03097