Supplementary Information

A multi-state supramolecular switch realized by a [π···π] dimer

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S1. Details for geometries of supramolecular junctions

For the supramolecular junction, the distance (d_{ssj}) between two electrode surfaces is one of important parameters. It is optimized based on a slab-like model shown in Fig. S1. Rigid constraints are applied for atoms of the electrode surface (marked by red-dashed lines), while other atoms are fully relaxed without any constraints for geometric optimizations. "Rigid constraints" mean that the marked Au 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) d_{ssj} for each conformation of the dimer. If d_{ssj} is optimized for C1, conformations other than C1 will be disfavored in the C1-related SSJ, confirmed by our calculations. Moreover, the semi-infinite electrodes are missing in this slab model, when comparing with the full molecular junction shown in Fig. 1b. However, the optimized geometries of the dimer and the interfaces are quite close to those in the full molecular junction. This is indicated by the fact that the increase of the electrode layers in the slab model has little impact on the finally-optimized geometries of the dimer and the interfaces.

Considering the periodic boundary condition, the thickness of the vacuum layer (d_{vm}) between two electrode surfaces is set to be 12 Å, which is large enough to avoid possible interactions between these two surfaces. The lattice parameters in the x and y directions (L_x, L_y) are 17.8 and 15.4 Å. Other larger supercells, with L_x>17.8 Å and L_y>15.4 Å, are tried as well, but geometries of the dimer and the contact interface are little affected. The force criterion for geometry optimizations is less than 0.04 eV/Å. The binding energy in Table S2 is also based on this slab-like model.

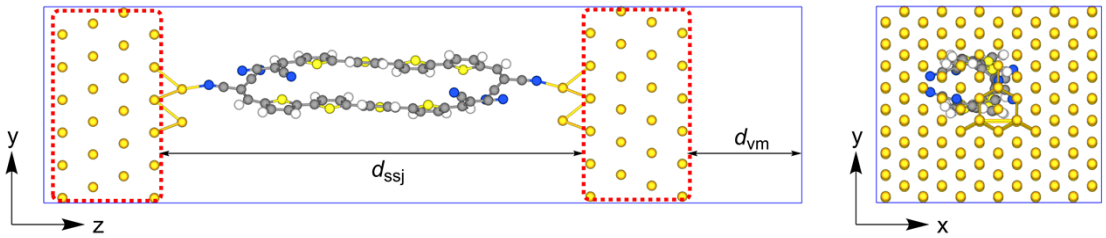

Fig. S1. A typical slab-like model for optimizing the distance between two electrode surfaces of supramolecular junctions. The blue rectangles mark the simulation cell of the slab model. The vacuum layer is only considered in the z direction, and d_{vm} denotes the thickness of this vacuum layer. The red dashed lines mark atoms with rigid constraints for optimizing calculations.

Table S1. The optimized width (d_{ssj}) of the supramolecular junctions with the dimer (Unit=Å).

Conformation	C1	C2	C3	C4	C5
d_{ssj}	34.5	37.2	39.4	43.1	45.4

Table S2. The binding energy (E_b) of the dimer with the electrodes (Unit=eV).

Conformation	C1	C2	C3	C4	C5
E_b	-2.14	-2.03	-1.96	-1.91	-1.85
CP-corrected E_b	-1.55	-1.45	-1.38	-1.33	-1.28

S2. Details for transmission spectra under non-zero gate voltages

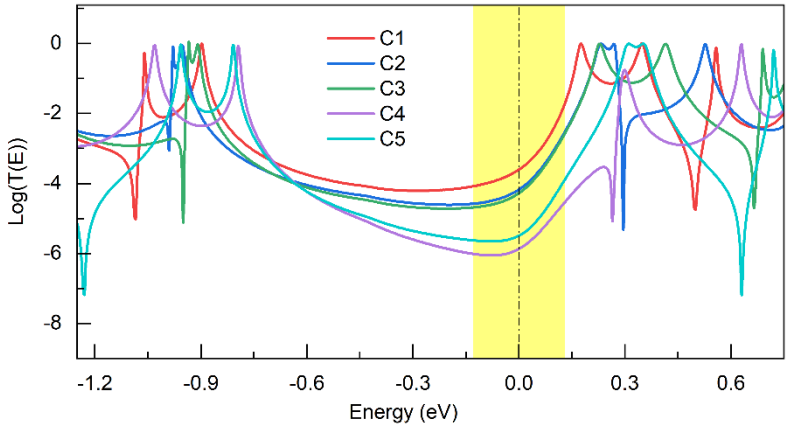

Fig. S2. Transmission spectra for different conformations of the dimer at the gate voltages of -1.0 V. The DQI-induced transmission dip is still present around 0.3 eV for C4, responsible for smallest transmission coefficients of C4 near the Fermi level.

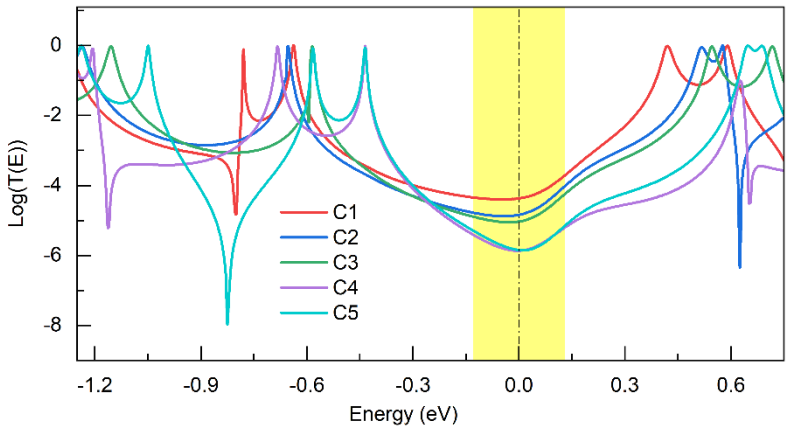

Fig. S3. Transmission spectra for different conformations of the dimer at the gate voltages of -1.5 V. The DQI-induced transmission dip is disrupted by this gate voltage, thus the conductance of C5 is the same as that of C4.

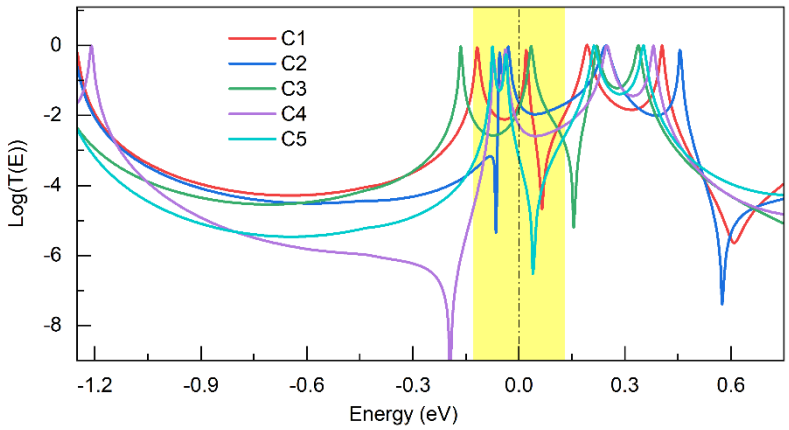

Fig. S4. Transmission spectra for different conformations of the dimer at the gate voltages of +2.5 V. The conductance is generally determined by the transmission peaks related to the LUMO and LUMO+1.

S3. Frontier molecular orbitals for the dimer in SSJs and the free monomer

The orbital phase patterns of the end group (S or AS in Fig. 5a) are generated by analyzing the plots presented in Fig. S5a. The schematic orbital distributions in Fig. 6a are derived from the two plots in the upper part of Fig. S5b with some simplifications. The p_z orbitals that are crucial for the interaction between the two monomers have been included in the schematic graphs in Fig. 6a, by carefully comparing the frontier molecular orbitals of the monomer and dimer, especially those in Fig. S5b. The simplifications facilitate a clear understanding of the mechanism for the formation of the OPPs in the end group of the dimer.

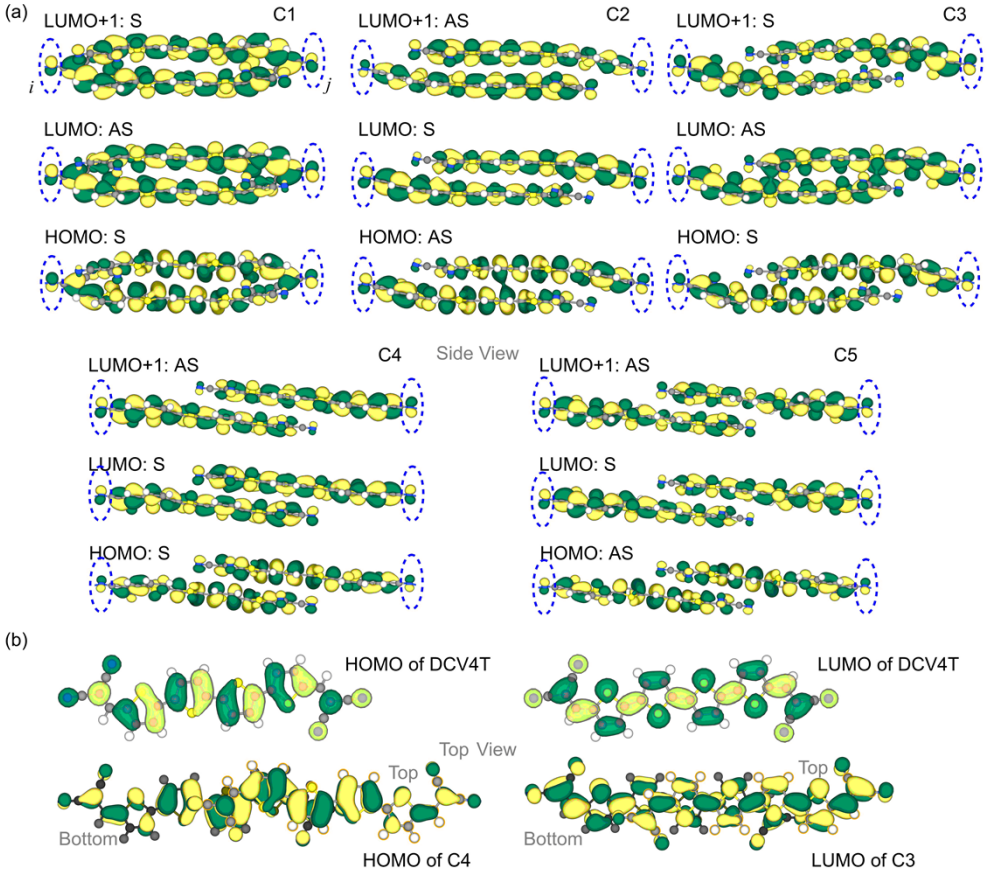

Fig. S5. (a) The frontier molecular orbitals of the dimer in SSJs in the side view. (b) The frontier molecular orbitals of the free DCV4T monomer, C3 and C4 in the top view. The isovalues for plotting these MOs are all the same. The frontier molecular orbitals of the dimer are calculated by the MPSH method at the zero-gate voltage.

S4. Details for plotting Figure 5b and 5c in the main text

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

$$T_{i,j}(E) \approx |g_{ij}(E)|^2 = \left[\frac{(E-\varepsilon_1)s_1}{(E-\varepsilon_1)^2+\eta^2} + \frac{(E-\varepsilon_2)s_2}{(E-\varepsilon_2)^2+\eta^2} + \frac{(E-\varepsilon_3)s_3}{(E-\varepsilon_3)^2+\eta^2}\right]^2 + \left[\frac{\eta s_1}{(E-\varepsilon_1)^2+\eta^2} + \frac{\eta s_2}{(E-\varepsilon_2)^2+\eta^2} + \frac{\eta s_3}{(E-\varepsilon_3)^2+\eta^2}\right]^2$$

The parameters used for the plot are:
$|s_1| = |s_2| = |s_3| = 0.01;\ \varepsilon_1 = -1.0,\ \varepsilon_2 = 0.5,\ \varepsilon_3 = 1.0;\ \eta = 10^{-4}$ is an infinitesimal number. Magnitudes of s_n are set to be the same by noting orbital profiles of FMOs marked by dashed circles in Fig. S5. The energy *E* ranges from -1.25 eV to 1.25 eV with the step of 0.01 eV.

S5. Cartesian coordinates for C1-C5 and central region of a typical junction

Molecular coordinates of C1-C5 are listed in the following, which are optimized at PBE-D2/Def2-SVP level using the G16 package. Before performing calculations for electron transport, these coordinates of C1-C5 are reoptimized in SSJs using the QuantumATK package.

To be more reliable, other methods are also considered for the geometry optimizations using the G16 package, such as PBE-D2/def2SVP with the counterpoise correction (CP) correction, PBE-D3BJ/def2SVP without the CP correction and PBE-D3BJ/def2SVP with the CP correction. By analyzing the FMOs of the dimer (the OPPs and the HOMO-LUMO gap), they are little influenced by the optimization method. This indicates the robustness of our revealed electron transport properties based on the double-zeta basis set level and the D2 dispersion correction. Here, the FMOs of the dimer are calculated using the def2TZVP basis set, and the functional and corrections (e.g. dispersion, CP) are consistent with those for the optimization.

Coordinates for C1 of the dimer:

C	-3.35036800	0.03371700	1.78733900
C	-3.96757100	1.28244900	1.98285500
C	-5.37020700	1.21182600	1.97937200
C	-5.86450600	-0.08999500	1.76779200
S	-4.54023500	-1.22830300	1.57857400
H	-3.39344600	2.20747300	2.13388900
H	-6.05035700	2.06959300	2.09301000
C	-1.94940700	-0.28770900	1.74464000
C	-1.34614300	-1.55158000	1.70287700
S	-0.72963600	0.97083900	1.75118600
C	0.06192700	-1.50203900	1.67621100
H	-1.93090900	-2.48262200	1.69878800
C	0.57487400	-0.19945600	1.68927300
H	0.71010200	-2.38835600	1.62927000
C	1.94602200	0.23208200	1.64246400
C	2.44581500	1.51910500	1.40746400

S	3.25910800	-0.90659100	1.86573500
C	3.85258200	1.57831300	1.39352000
H	1.78907600	2.38172500	1.22809200
C	4.46781800	0.34161100	1.62793100
H	4.42830800	2.49784000	1.21685600
C	5.87491900	0.04659300	1.66814800
C	6.53108000	-1.14724600	2.01248700
S	7.02432600	1.28496500	1.22460500
C	7.93188300	-1.04626800	1.93709300
H	5.99276900	-2.06128100	2.29940800
C	8.38571700	0.20770600	1.48822800
H	8.62585000	-1.87213900	2.14842000
C	9.74164200	0.53209700	1.18917200
C	10.23148500	1.55739600	0.38763800
C	-7.24643600	-0.40763700	1.64959000
H	-7.92409600	0.44220300	1.83221200
C	-7.84601200	-1.60893400	1.28982600
C	11.64078100	1.73675300	0.21346400
N	12.79709200	1.89551900	0.07684900
C	-9.26571600	-1.68692700	1.13735500
C	-7.10832800	-2.78700400	0.95297400
N	-6.50706300	-3.75173400	0.65014100
N	-10.42758100	-1.73542100	0.96241500
C	9.37221400	2.40181000	-0.38556200
N	8.64235700	3.03130400	-1.06123200
H	10.49337700	-0.16390200	1.59359000
C	-5.87491000	0.03825300	-1.66845300
C	-6.53112300	-1.15726200	-2.00683700
C	-7.93191800	-1.05586900	-1.93189300
C	-8.38569200	0.20032900	-1.48922100
S	-7.02426800	1.27888400	-1.23115400
H	-5.99284900	-2.07272100	-2.28925300
H	-8.62591700	-1.88276100	-2.13907800
C	-4.46779900	0.33341600	-1.62977400
C	-3.85250200	1.57129600	-1.40183700
S	-3.25915000	-0.91607300	-1.86104500
C	-2.44574100	1.51196500	-1.41557900
H	-4.42819000	2.49175800	-1.22998200
C	-1.94599800	0.22373000	-1.64396200
H	-1.78897700	2.37551900	-1.24085000
C	-0.57486700	-0.20804800	-1.68883300
C	-0.06195300	-1.51058300	-1.67006700
S	0.72968500	0.96191400	-1.75587000
C	1.34611500	-1.56028400	-1.69651900
H	-0.71014100	-2.39668100	-1.61931400
C	1.94941100	-0.29662000	-1.74376500
H	1.93085600	-2.49131500	-1.68844300
C	3.35038300	0.02458600	-1.78781600
C	3.96763000	1.27228500	-1.98967700
S	4.54019700	-1.23635100	-1.57234900
C	5.37026700	1.20166500	-1.98560000
H	3.39353400	2.19650900	-2.14563800
C	5.86451500	-0.09905900	-1.76725800
H	6.05042200	2.05884000	-2.10357800
C	7.24641300	-0.41617100	-1.64730700
C	7.84587200	-1.61566400	-1.28138000
C	-9.74159800	0.52625300	-1.19170900
H	-10.49340500	-0.17152700	-1.59291600

C	-10.23136200	1.55531500	-0.39496100
C	9.26555700	-1.69298400	-1.12839900
N	10.42740000	-1.74066800	-0.95309200
C	-11.64064600	1.73564900	-0.22171200
C	-9.37203600	2.40302700	0.37455800
N	-8.64216200	3.03529900	1.04761200
N	-12.79694800	1.89517900	-0.08592200
C	7.10806900	-2.79194100	-0.93858100
N	6.50669000	-3.75504700	-0.63084500
H	7.92419100	0.43261800	-1.83431500

Coordinates for C2 of the dimer:

C	1.78948200	-1.77863700	-0.43309300
C	2.27226600	-1.79300000	-1.75406200
C	3.66942200	-1.88609000	-1.82649800
C	4.30478300	-1.93598700	-0.57029700
S	3.10465800	-1.87119100	0.71555300
H	1.60682800	-1.73983500	-2.62705300
H	4.24363800	-1.91826400	-2.76329100
C	0.42721300	-1.70022900	0.01599800
C	-0.06518100	-1.65193300	1.32621500
S	-0.89775900	-1.65089500	-1.13390100
C	-1.47001700	-1.57556100	1.39811200
H	0.59658100	-1.66734400	2.20385700
C	-2.09290000	-1.56294100	0.14278700
H	-2.03769700	-1.52265300	2.33802100
C	-3.49529800	-1.47506300	-0.16357900
C	-4.12385300	-1.43224100	-1.41478500
S	-4.67998700	-1.37363600	1.12250200
C	-5.52592300	-1.31368500	-1.33358800
H	-3.56253100	-1.47851800	-2.35850200
C	-6.00407800	-1.25948800	-0.01736700
H	-6.19295500	-1.25794000	-2.20586600
C	-7.35433300	-1.08606800	0.44525500
C	-7.81446500	-0.94916800	1.76592000
S	-8.66802800	-0.95799200	-0.70029800
C	-9.20099200	-0.74235600	1.84032400
H	-7.14238200	-0.97152300	2.63548600
C	-9.83783300	-0.70669900	0.58675400
H	-9.75725700	-0.58866700	2.77543200
C	-11.22784700	-0.45566800	0.40483200
C	-11.96689400	-0.35741300	-0.76595300
C	5.71158100	-2.04756800	-0.39568000
H	6.27787800	-2.15024000	-1.33549400
C	6.47486400	-2.05294900	0.76716900
C	-13.37315000	-0.09272500	-0.70905500
N	-14.52800100	0.11971800	-0.65798900
C	7.89320300	-2.22608700	0.69809800
C	5.91885900	-1.84039600	2.06617500
N	5.46727500	-1.62767000	3.13174300
N	9.05932700	-2.36841800	0.64596500
C	-11.38940000	-0.50684900	-2.06637100
N	-10.90714900	-0.63096900	-3.13187900
H	-11.78955500	-0.30977500	1.34122000
C	7.35432400	1.08602400	0.44509800
C	7.81445300	0.94921500	1.76577400
C	9.20099200	0.74249500	1.84020300

C	9.83784400	0.70681000	0.58663700
S	8.66803800	0.95798900	-0.70043500
H	7.14235500	0.97155400	2.63532900
H	9.75725800	0.58887200	2.77532100
C	6.00405700	1.25932800	-0.01753200
C	5.52586100	1.31299400	-1.33375600
S	4.68000700	1.37404400	1.12233800
C	4.12379400	1.43159000	-1.41496000
H	6.19286000	1.25680100	-2.20603100
C	3.49528500	1.47497500	-0.16375400
H	3.56244100	1.47744100	-2.35867800
C	2.09289500	1.56300700	0.14260300
C	1.47001500	1.57587900	1.39792700
S	0.89776300	1.65079500	-1.13409800
C	0.06517800	1.65225900	1.32601400
H	2.03769200	1.52310600	2.33784400
C	-0.42721300	1.70027300	0.01578500
H	-0.59658600	1.66781500	2.20365100
C	-1.78948300	1.77847900	-0.43333500
C	-2.27226500	1.79233900	-1.75430900
S	-3.10466400	1.87137300	0.71527900
C	-3.66942800	1.88528400	-1.82678000
H	-1.60682300	1.73889000	-2.62728100
C	-4.30479500	1.93559400	-0.57059900
H	-4.24364800	1.91706800	-2.76358400
C	-5.71159600	2.04718800	-0.39602200
C	-6.47488500	2.05292000	0.76682300
C	11.22787500	0.45585400	0.40473900
H	11.78958300	0.31004000	1.34113900
C	11.96693700	0.35758800	-0.76603600
C	-7.89321800	2.22608600	0.69769900
N	-9.05933000	2.36850100	0.64552300
C	13.37320900	0.09298800	-0.70911500
C	11.38944300	0.50692900	-2.06646500
N	10.90718800	0.63097700	-3.13198000
N	14.52807200	-0.11938500	-0.65803100
C	-5.91889200	1.84075100	2.06589900
N	-5.46733200	1.62831800	3.13153500
H	-6.27789700	2.14954900	-1.33586800

Coordinates for C3 of the dimer:

C	-0.73925600	1.82205700	-0.33171000
C	-1.25261400	1.99057300	-1.63093500
C	-2.65237700	2.08074200	-1.65890300
C	-3.25537300	1.96959400	-0.38999100
S	-2.02502500	1.75261200	0.84688300
H	-0.60665600	2.06421100	-2.51700200
H	-3.24852700	2.22781400	-2.57094300
C	0.63342900	1.71906500	0.08417600
C	1.16980700	1.76782800	1.37782600
S	1.91048400	1.52213900	-1.09959400
C	2.57406400	1.64988900	1.41106000
H	0.54156200	1.88560700	2.27242400
C	3.14707400	1.50441300	0.14009000
H	3.16889600	1.60960000	2.33468700
C	4.52676600	1.31168500	-0.21803200
C	5.05804900	0.87076800	-1.43781100

S	5.80641000	1.58247800	0.94445400
C	6.46032900	0.73009900	-1.42170700
H	4.42264500	0.63060000	-2.30213400
C	7.03839700	1.06327300	-0.18985000
H	7.05637300	0.37523400	-2.27480500
C	8.41739200	0.98006600	0.20733400
C	8.97718300	1.23277200	1.47045100
S	9.62908600	0.43754100	-0.92616600
C	10.35720700	0.98815800	1.51380900
H	8.37824700	1.56434700	2.33025000
C	10.89288800	0.54356600	0.28911600
H	10.98444200	1.11406200	2.40759200
C	12.26645000	0.22742900	0.08787200
C	12.92301300	-0.21292200	-1.05485700
C	-4.65818900	2.02802900	-0.15784100
H	-5.26200600	2.24349000	-1.05362700
C	-5.37343700	1.84648400	1.02096600
C	14.33143500	-0.46958400	-1.01863700
N	15.48793500	-0.67706200	-0.98348400
C	-6.79836900	1.97568900	1.03238400
C	-4.75263300	1.46958600	2.25326300
N	-4.23872400	1.12071400	3.25249100
N	-7.97032300	2.07344100	1.04816300
C	12.25747000	-0.43038200	-2.30232500
N	11.70610900	-0.60653000	-3.32624800
H	12.89740500	0.35386300	0.98254000
C	-8.41736400	-0.96223900	0.27450400
C	-8.97705000	-1.12614200	1.55223800
C	-10.35703900	-0.87896500	1.57857800
C	-10.89285700	-0.52102300	0.32588100
S	-9.62914900	-0.50001600	-0.89394600
H	-8.37810500	-1.39697700	2.43304700
H	-10.98416600	-0.94212800	2.47904800
C	-7.03842800	-1.07321800	-0.11604000
C	-6.46026300	-0.82670700	-1.36809600
S	-5.80653300	-1.51240700	1.05170900
C	-5.05800200	-0.96828000	-1.37427200
H	-7.05617000	-0.53236100	-2.24401200
C	-4.52685100	-1.32342400	-0.12680300
H	-4.42241100	-0.78912000	-2.25312200
C	-3.14719000	-1.49138500	0.24370500
C	-2.57431300	-1.55021600	1.52166300
S	-1.91045300	-1.59306000	-0.99179300
C	-1.17003600	-1.67019000	1.49670700
H	-3.16935300	-1.44732400	2.44028400
C	-0.63349000	-1.70939400	0.20279800
H	-0.54201100	-1.72721100	2.39737800
C	0.73915700	-1.84037300	-0.20530100
C	1.25206700	-2.09645100	-1.49033600
S	2.02540300	-1.69142600	0.96538200
C	2.65181800	-2.18822400	-1.51271000
H	0.60576700	-2.22985000	-2.36913600
C	3.25529500	-1.99123100	-0.25450100
H	3.24760400	-2.39675400	-2.41292700
C	4.65822000	-2.03347700	-0.01940800
C	5.37394500	-1.77134400	1.14385000
C	-12.26651700	-0.22013700	0.10312200
H	-12.89728500	-0.28339500	1.00459300

C	-12.92343200	0.13826100	-1.06770600
C	6.79885100	-1.89977000	1.16376700
N	7.97077500	-1.99654500	1.18631800
C	-14.33194400	0.39632000	-1.04942100
C	-12.25819400	0.26725100	-2.32756000
N	-11.70704000	0.37078400	-3.36146200
N	-15.48852300	0.60530500	-1.02878200
C	4.75375400	-1.31073400	2.34766700
N	4.24056300	-0.89388600	3.32088100
H	5.26173500	-2.30970300	-0.89857300

Coordinates for C4 of the dimer:

C	1.01568900	0.62520200	1.59297200
C	0.60147600	1.96631000	1.66644100
C	-0.78520900	2.10491600	1.82606400
C	-1.47608600	0.87900100	1.88361100
S	-0.34667900	-0.46288500	1.75485300
H	1.30491800	2.80645700	1.58349600
H	-1.31170400	3.06766700	1.89212000
C	2.34230500	0.11139300	1.39811500
C	2.74642400	-1.20666600	1.15727500
S	3.73561700	1.18273600	1.42952400
C	4.13968000	-1.34699300	0.99767300
H	2.03477300	-2.03927600	1.06563800
C	4.84170400	-0.13938400	1.10935600
H	4.63503000	-2.30127100	0.77031500
C	6.25155700	0.09877100	0.96229600
C	6.93437700	1.32169500	0.92051700
S	7.36120500	-1.23325000	0.73282900
C	8.31694100	1.18292600	0.69696500
H	6.42275500	2.28846200	1.02985800
C	8.72658100	-0.15068500	0.56253900
H	9.01715700	2.02655200	0.61562500
C	10.04759600	-0.66392000	0.31915000
C	10.43873800	-1.99503800	0.09139000
S	11.42421700	0.41448400	0.27542100
C	11.81933300	-2.13207200	-0.11681800
H	9.72148500	-2.82761000	0.06971900
C	12.52736200	-0.91541700	-0.05517100
H	12.32697300	-3.08650100	-0.31662400
C	13.93473400	-0.80228500	-0.23709600
C	14.75301700	0.32077800	-0.20338900
C	-2.88749900	0.76679900	2.01410700
H	-3.41558700	1.73186200	2.07351300
C	-3.69496500	-0.36347500	2.07442200
C	16.16253100	0.18646400	-0.41765800
N	17.31882500	0.06904800	-0.59394100
C	-5.11376700	-0.22133600	2.19181600
C	-3.18515200	-1.69687100	1.99767600
N	-2.77103400	-2.79519100	1.91927800
N	-6.28029100	-0.09748600	2.27403200
C	14.25758700	1.64031500	0.04049300
N	13.84600200	2.72354800	0.24232300
H	14.44521500	-1.75901800	-0.43396800
C	-10.04677000	-0.65017000	-0.34243900
C	-10.43725900	-1.98932500	-0.16664100
C	-11.81769000	-2.13494600	0.03682000

C	-12.52622800	-0.91710200	0.02311400
S	-11.42380500	0.42513300	-0.25601100
H	-9.71965200	-2.82179900	-0.17774900
H	-12.32483400	-3.09665000	0.19956200
C	-8.72609700	-0.12721100	-0.56620200
C	-8.31690100	1.21087000	-0.64678600
S	-7.36068100	-1.20163400	-0.78168900
C	-6.93458800	1.35895400	-0.86582800
H	-9.01723400	2.05029300	-0.53048700
C	-6.25154400	0.13890000	-0.95780600
H	-6.42321300	2.32946800	-0.93620300
C	-4.84177200	-0.09261600	-1.11577300
C	-4.13915900	-1.30346000	-1.05368700
S	-3.73650200	1.24187600	-1.38313900
C	-2.74610900	-1.15611700	-1.20855000
H	-4.63383700	-2.26643800	-0.86482000
C	-2.34276100	0.17080300	-1.39619300
H	-2.03393400	-1.99134300	-1.15105500
C	-1.01636100	0.69233200	-1.57074200
C	-0.60213500	2.03531800	-1.59090200
S	0.34610900	-0.38847300	-1.77483200
C	0.78466500	2.18011400	-1.74397500
H	-1.30569200	2.87151100	-1.47536400
C	1.47553500	0.95738100	-1.84960500
H	1.31119400	3.14472000	-1.77155300
C	2.88697700	0.85002300	-1.98376100
C	3.69398200	-0.27725400	-2.08959300
C	-13.93353400	-0.81170300	0.21013500
H	-14.44355000	-1.77557500	0.36988600
C	-14.75224600	0.31150500	0.22067300
C	5.11290800	-0.13098500	-2.20026400
N	6.27953200	-0.00432600	-2.27658100
C	-16.16158000	0.16841100	0.43039400
C	-14.25746200	1.63973500	0.02804400
N	-13.84644300	2.73017800	-0.13173300
N	-17.31772500	0.04379000	0.60266400
C	3.18371800	-1.61249300	-2.06786600
N	2.76931000	-2.71300400	-2.03481100
H	3.41553200	1.81644400	-2.00370100

Coordinates for C5 of the dimer:

C	-2.29428800	0.96412900	-1.44435000
C	-1.98849300	2.33733800	-1.50384500
C	-0.61681700	2.58642100	-1.65145200
C	0.17192700	1.42017500	-1.70649300
S	-0.84898600	-0.00898800	-1.58179100
H	-2.75928900	3.11728500	-1.42843200
H	-0.16857300	3.58836100	-1.71285900
C	-3.57654300	0.34691400	-1.25533800
C	-3.87203500	-0.99900300	-0.99250100
S	-5.04334500	1.30685600	-1.27458600
C	-5.24376700	-1.23729900	-0.78752500
H	-3.09398400	-1.77053000	-0.90325000
C	-6.03264100	-0.08271200	-0.88822000
H	-5.66518000	-2.21959600	-0.53203600
C	-7.45193100	0.05569100	-0.70417600
C	-8.21138400	1.22803500	-0.59196900

S	-8.47934600	-1.35671400	-0.57571400
C	-9.58620100	0.98908500	-0.40135700
H	-7.75717600	2.22828100	-0.62423300
C	-9.91512200	-0.37293600	-0.36052400
H	-10.33859100	1.78156100	-0.27911600
C	-11.20464000	-0.98215900	-0.17571600
C	-11.51832800	-2.34927000	-0.07513700
S	-12.64316400	0.00560800	-0.04701600
C	-12.88968400	-2.58511700	0.10449300
H	-10.75436100	-3.13781600	-0.12776700
C	-13.66816500	-1.41160100	0.14672700
H	-13.34141500	-3.58200900	0.20810400
C	-15.08086900	-1.39807700	0.32111400
C	-15.96407600	-0.32636600	0.38083100
C	1.58623400	1.42461400	-1.84348900
H	2.02910600	2.42937900	-1.93434700
C	2.48820500	0.36570300	-1.87639300
C	-17.36449000	-0.56213900	0.56481600
N	-18.51284800	-0.76305800	0.71581100
C	3.88932000	0.61806800	-2.01652600
C	2.09907900	-1.00045500	-1.72538800
N	1.79578000	-2.12682300	-1.57111700
N	5.04184800	0.82767000	-2.12180900
C	-15.54581400	1.03662600	0.26553300
N	-15.19714300	2.15591200	0.16969100
H	-15.53499800	-2.39709200	0.42319700
C	11.20479900	-0.98262600	0.17450400
C	11.51871000	-2.34955200	0.07213800
C	12.89013800	-2.58495200	-0.10753100
C	13.66845300	-1.41126500	-0.14801500
S	12.64320000	0.00552800	0.04743100
H	10.75484900	-3.13828200	0.12354400
H	13.34203900	-3.58163600	-0.21239700
C	9.91515400	-0.37384400	0.35989600
C	9.58601100	0.98807100	0.40242800
S	8.47950700	-1.35812600	0.57366100
C	8.21112300	1.22656200	0.59313500
H	10.33828800	1.78081900	0.28127300
C	7.45185100	0.05395300	0.70372600
H	7.75671500	2.22667800	0.62650000
C	6.03254400	-0.08490300	0.88733600
C	5.24367500	-1.23923600	0.78377900
S	5.04323700	1.30374100	1.27697100
C	3.87192100	-1.00141100	0.98918500
H	5.66510400	-2.22089600	0.52588400
C	3.57642700	0.34386700	1.25527300
H	3.09385400	-1.77268300	0.89789100
C	2.29415700	0.96062100	1.44569600
C	1.98832500	2.33367900	1.50840900
S	0.84888000	-0.01285200	1.58082700
C	0.61664200	2.58237700	1.65661000
H	2.75910100	3.11382100	1.43483200
C	-0.17206800	1.41598300	1.70892400
H	0.16837200	3.58415900	1.72038300
C	-1.58637200	1.42005000	1.84598400
C	-2.48829200	0.36102100	1.87641500
C	15.08119100	-1.39729400	-0.32208900
H	15.53549100	-2.39610400	-0.42542100

C	15.96425000	-0.32537200	-0.38018000
C	-3.88941500	0.61296100	2.01721900
N	-5.04196100	0.82219900	2.12302500
C	17.36473800	-0.56068900	-0.56418700
C	15.54576000	1.03740100	-0.26313700
N	15.19690100	2.15650500	-0.16587400
N	18.51315800	-0.76123300	-0.71521100
C	-2.09911300	-1.00475700	1.72213500
N	-1.79578200	-2.13074600	1.56518200
H	-2.02927900	2.42457900	1.93923900

Coordinates for central region of a typical junction:

The unit cell for the central region is Lx=17.8191, Ly= 15.4318 and Lz= 60.0653

Au	0.744232600	0.386736000	1.212436000
Au	3.714081000	0.386736000	1.212436000
Au	6.683930000	0.386736000	1.212436000
Au	9.653778000	0.386736000	1.212436000
Au	12.623630000	0.386736000	1.212436000
Au	15.593470000	0.386736000	1.212436000
Au	2.229157000	2.958700000	1.212436000
Au	5.199005000	2.958700000	1.212436000
Au	8.168854000	2.958700000	1.212436000
Au	11.138700000	2.958700000	1.212436000
Au	14.108550000	2.958700000	1.212436000
Au	17.078400000	2.958700000	1.212436000
Au	0.744232600	5.530664000	1.212436000
Au	3.714081000	5.530664000	1.212436000
Au	6.683930000	5.530664000	1.212436000
Au	9.653778000	5.530664000	1.212436000
Au	12.623630000	5.530664000	1.212436000
Au	15.593470000	5.530664000	1.212436000
Au	2.229157000	8.102629000	1.212436000
Au	5.199005000	8.102629000	1.212436000
Au	8.168854000	8.102629000	1.212436000
Au	11.138700000	8.102629000	1.212436000
Au	14.108550000	8.102629000	1.212436000
Au	17.078400000	8.102629000	1.212436000
Au	0.744232600	10.674590000	1.212436000
Au	3.714081000	10.674590000	1.212436000
Au	6.683930000	10.674590000	1.212436000
Au	9.653778000	10.674590000	1.212436000
Au	12.623630000	10.674590000	1.212436000
Au	15.593470000	10.674590000	1.212436000
Au	2.229157000	13.246560000	1.212436000
Au	5.199005000	13.246560000	1.212436000
Au	8.168854000	13.246560000	1.212436000
Au	11.138700000	13.246560000	1.212436000
Au	14.108550000	13.246560000	1.212436000
Au	17.078400000	13.246560000	1.212436000
Au	2.229157000	1.244057000	3.637307000
Au	5.199005000	1.244057000	3.637307000
Au	8.168854000	1.244057000	3.637307000
Au	11.138700000	1.244057000	3.637307000
Au	14.108550000	1.244057000	3.637307000
Au	17.078400000	1.244057000	3.637307000
Au	0.744232600	3.816022000	3.637307000
Au	3.714081000	3.816022000	3.637307000

Au	6.683930000	3.816022000	3.637307000
Au	9.653778000	3.816022000	3.637307000
Au	12.623630000	3.816022000	3.637307000
Au	15.593470000	3.816022000	3.637307000
Au	2.229157000	6.387986000	3.637307000
Au	5.199005000	6.387986000	3.637307000
Au	8.168854000	6.387986000	3.637307000
Au	11.138700000	6.387986000	3.637307000
Au	14.108550000	6.387986000	3.637307000
Au	17.078400000	6.387986000	3.637307000
Au	0.744232600	8.959950000	3.637307000
Au	3.714081000	8.959950000	3.637307000
Au	6.683930000	8.959950000	3.637307000
Au	9.653778000	8.959950000	3.637307000
Au	12.623630000	8.959950000	3.637307000
Au	15.593470000	8.959950000	3.637307000
Au	2.229157000	11.531910000	3.637307000
Au	5.199005000	11.531910000	3.637307000
Au	8.168854000	11.531910000	3.637307000
Au	11.138700000	11.531910000	3.637307000
Au	14.108550000	11.531910000	3.637307000
Au	17.078400000	11.531910000	3.637307000
Au	0.744232600	14.103880000	3.637307000
Au	3.714081000	14.103880000	3.637307000
Au	6.683930000	14.103880000	3.637307000
Au	9.653778000	14.103880000	3.637307000
Au	12.623630000	14.103880000	3.637307000
Au	15.593470000	14.103880000	3.637307000
Au	0.744232600	2.101379000	6.062178000
Au	3.714081000	2.101379000	6.062178000
Au	6.683930000	2.101379000	6.062178000
Au	9.653778000	2.101379000	6.062178000
Au	12.623630000	2.101379000	6.062178000
Au	15.593470000	2.101379000	6.062178000
Au	2.229157000	4.673343000	6.062178000
Au	5.199005000	4.673343000	6.062178000
Au	8.168854000	4.673343000	6.062178000
Au	11.138700000	4.673343000	6.062178000
Au	14.108550000	4.673343000	6.062178000
Au	17.078400000	4.673343000	6.062178000
Au	0.744232600	7.245307000	6.062178000
Au	3.714081000	7.245307000	6.062178000
Au	6.683930000	7.245307000	6.062178000
Au	9.653778000	7.245307000	6.062178000
Au	12.623630000	7.245307000	6.062178000
Au	15.593470000	7.245307000	6.062178000
Au	2.229157000	9.817272000	6.062178000
Au	5.199005000	9.817272000	6.062178000
Au	8.168854000	9.817272000	6.062178000
Au	11.138700000	9.817272000	6.062178000
Au	14.108550000	9.817272000	6.062178000
Au	17.078400000	9.817272000	6.062178000
Au	0.744232600	12.389240000	6.062178000
Au	3.714081000	12.389240000	6.062178000
Au	6.683930000	12.389240000	6.062178000
Au	9.653778000	12.389240000	6.062178000
Au	12.623630000	12.389240000	6.062178000
Au	15.593470000	12.389240000	6.062178000

Au	2.229157000	14.961200000	6.062178000
Au	5.199005000	14.961200000	6.062178000
Au	8.168854000	14.961200000	6.062178000
Au	11.138700000	14.961200000	6.062178000
Au	14.108550000	14.961200000	6.062178000
Au	17.078400000	14.961200000	6.062178000
Au	0.744232600	0.386736000	8.487049000
Au	3.714081000	0.386736000	8.487049000
Au	6.683930000	0.386736000	8.487049000
Au	9.653778000	0.386736000	8.487049000
Au	12.623630000	0.386736000	8.487049000
Au	15.593470000	0.386736000	8.487049000
Au	2.229157000	2.958700000	8.487049000
Au	5.199005000	2.958700000	8.487049000
Au	8.168854000	2.958700000	8.487049000
Au	11.138700000	2.958700000	8.487049000
Au	14.108550000	2.958700000	8.487049000
Au	17.078400000	2.958700000	8.487049000
Au	0.744232600	5.530664000	8.487049000
Au	3.714081000	5.530664000	8.487049000
Au	6.683930000	5.530664000	8.487049000
Au	9.653778000	5.530664000	8.487049000
Au	12.623630000	5.530664000	8.487049000
Au	15.593470000	5.530664000	8.487049000
Au	2.229157000	8.102629000	8.487049000
Au	5.199005000	8.102629000	8.487049000
Au	8.168854000	8.102629000	8.487049000
Au	11.138700000	8.102629000	8.487049000
Au	14.108550000	8.102629000	8.487049000
Au	17.078400000	8.102629000	8.487049000
Au	0.744232600	10.674590000	8.487049000
Au	3.714081000	10.674590000	8.487049000
Au	6.683930000	10.674590000	8.487049000
Au	9.653778000	10.674590000	8.487049000
Au	12.623630000	10.674590000	8.487049000
Au	15.593470000	10.674590000	8.487049000
Au	2.229157000	13.246560000	8.487049000
Au	5.199005000	13.246560000	8.487049000
Au	8.168854000	13.246560000	8.487049000
Au	11.138700000	13.246560000	8.487049000
Au	14.108550000	13.246560000	8.487049000
Au	17.078400000	13.246560000	8.487049000
Au	11.101850000	6.351860000	10.675380000
Au	9.630907000	8.933099000	10.677360000
Au	8.200177000	6.347920000	10.677970000
N	9.756023000	9.315163000	12.805420000
C	9.811817000	9.136445000	13.969080000
C	9.910846000	8.955201000	15.363250000
H	7.883048000	9.495010000	15.686970000
C	11.185490000	8.545082000	15.838010000
C	8.808719000	9.194603000	16.194820000
N	12.242660000	8.200669000	16.224970000
C	8.702640000	9.111399000	17.593170000
H	6.597891000	9.702023000	17.800010000
C	7.515571000	9.387376000	18.308920000
S	9.985962000	8.657730000	18.708990000
C	7.641771000	9.237972000	19.685160000
C	8.933345000	8.849800000	20.087380000

H	6.841902000	9.424072000	20.406800000
H	11.577930000	8.500995000	21.168310000
C	9.405634000	8.616272000	21.413070000
C	10.724130000	8.446721000	21.850590000
S	8.299116000	8.502129000	22.760280000
C	10.830150000	8.244394000	23.231240000
N	9.573479000	11.531920000	23.698550000
H	11.777930000	8.123475000	23.764540000
C	9.597571000	8.247043000	23.892970000
C	9.475456000	11.454050000	24.868130000
C	9.342405000	8.113316000	25.293510000
H	7.211909000	8.574404000	25.480380000
C	8.140735000	8.291622000	25.983970000
C	9.354753000	11.347050000	26.282210000
S	10.629080000	7.722857000	26.409820000
H	11.435840000	11.121820000	26.531780000
C	8.037188000	11.409500000	26.808870000
C	10.482230000	11.171780000	27.070020000
N	6.946507000	11.442300000	27.248050000
C	8.260096000	8.130576000	27.371480000
C	9.554279000	7.814093000	27.788600000
H	7.434278000	8.272212000	28.074540000
C	10.597740000	11.043530000	28.471380000
H	12.768580000	10.812380000	28.601850000
H	12.200570000	7.424663000	28.843030000
C	10.034570000	7.596759000	29.115780000
C	11.817940000	10.857770000	29.142500000
C	11.359060000	7.418428000	29.540210000
S	9.273739000	11.068260000	29.619850000
S	8.934937000	7.544498000	30.468670000
C	11.686680000	10.729510000	30.524200000
C	11.477180000	7.265825000	30.920610000
C	10.356620000	10.806450000	30.961440000
H	12.518370000	10.562130000	31.213090000
H	12.424350000	7.129160000	31.451990000
C	10.250680000	7.314707000	31.604150000
H	7.684914000	10.642160000	32.024630000
C	9.855515000	10.683250000	32.292660000
C	8.528237000	10.620140000	32.720850000
N	6.603218000	7.618956000	32.872190000
C	10.127770000	7.207838000	33.006870000
C	7.685284000	7.441565000	33.297250000
H	11.079350000	7.072835000	33.534060000
S	10.939870000	10.564020000	33.661310000
C	8.996810000	7.249744000	33.808070000
C	8.392252000	10.482070000	34.109190000
H	7.430782000	10.381230000	34.620650000
C	9.611953000	10.425980000	34.788680000
C	9.110696000	7.119343000	35.220760000
C	9.849680000	10.244340000	36.186580000
H	12.015510000	9.954803000	36.295690000
N	9.203770000	7.022712000	36.389800000
C	11.066480000	10.013480000	36.837180000
S	8.536086000	10.236720000	37.330020000
C	10.935690000	9.831756000	38.218440000
C	9.612611000	9.912716000	38.667060000
H	11.768930000	9.614099000	38.893320000
H	6.951690000	9.592434000	39.691730000

C	9.115955000	9.763354000	39.995640000
C	7.777910000	9.618491000	40.406980000
S	10.197530000	9.744456000	41.364570000
C	7.637573000	9.481539000	41.782840000
H	6.681389000	9.345289000	42.299840000
C	8.861349000	9.525659000	42.488600000
N	12.511000000	9.767555000	43.826600000
C	8.957764000	9.430351000	43.886620000
C	11.413550000	9.639692000	44.232540000
H	7.994871000	9.307851000	44.399320000
C	10.086400000	9.485945000	44.715610000
C	9.937362000	9.424689000	46.116440000
N	9.803637000	9.402571000	47.286280000
Au	8.202112000	6.349675000	49.386670000
Au	9.636991000	8.933738000	49.388250000
Au	11.103750000	6.351682000	49.390490000
Au	0.745365000	0.386117200	51.578220000
Au	3.715213000	0.386117200	51.578220000
Au	6.685062000	0.386117200	51.578220000
Au	9.654910000	0.386117200	51.578220000
Au	12.624760000	0.386117200	51.578220000
Au	15.594610000	0.386117200	51.578220000
Au	2.230289000	2.958081000	51.578220000
Au	5.200138000	2.958081000	51.578220000
Au	8.169986000	2.958081000	51.578220000
Au	11.139830000	2.958081000	51.578220000
Au	14.109680000	2.958081000	51.578220000
Au	17.079530000	2.958081000	51.578220000
Au	0.745365000	5.530046000	51.578220000
Au	3.715213000	5.530046000	51.578220000
Au	6.685062000	5.530046000	51.578220000
Au	9.654910000	5.530046000	51.578220000
Au	12.624760000	5.530046000	51.578220000
Au	15.594610000	5.530046000	51.578220000
Au	2.230289000	8.102010000	51.578220000
Au	5.200138000	8.102010000	51.578220000
Au	8.169986000	8.102010000	51.578220000
Au	11.139830000	8.102010000	51.578220000
Au	14.109680000	8.102010000	51.578220000
Au	17.079530000	8.102010000	51.578220000
Au	0.745365000	10.673970000	51.578220000
Au	3.715213000	10.673970000	51.578220000
Au	6.685062000	10.673970000	51.578220000
Au	9.654910000	10.673970000	51.578220000
Au	12.624760000	10.673970000	51.578220000
Au	15.594610000	10.673970000	51.578220000
Au	2.230289000	13.245940000	51.578220000
Au	5.200138000	13.245940000	51.578220000
Au	8.169986000	13.245940000	51.578220000
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Au	14.109680000	13.245940000	51.578220000
Au	17.079530000	13.245940000	51.578220000
Au	0.745365000	2.100760000	54.003100000
Au	3.715213000	2.100760000	54.003100000
Au	6.685062000	2.100760000	54.003100000
Au	9.654910000	2.100760000	54.003100000
Au	12.624760000	2.100760000	54.003100000
Au	15.594610000	2.100760000	54.003100000

Au	2.230289000	4.672724000	54.003100000
Au	5.200138000	4.672724000	54.003100000
Au	8.169986000	4.672724000	54.003100000
Au	11.139830000	4.672724000	54.003100000
Au	14.109680000	4.672724000	54.003100000
Au	17.079530000	4.672724000	54.003100000
Au	0.745365000	7.244688000	54.003100000
Au	3.715213000	7.244688000	54.003100000
Au	6.685062000	7.244688000	54.003100000
Au	9.654910000	7.244688000	54.003100000
Au	12.624760000	7.244688000	54.003100000
Au	15.594610000	7.244688000	54.003100000
Au	2.230289000	9.816653000	54.003100000
Au	5.200138000	9.816653000	54.003100000
Au	8.169986000	9.816653000	54.003100000
Au	11.139830000	9.816653000	54.003100000
Au	14.109680000	9.816653000	54.003100000
Au	17.079530000	9.816653000	54.003100000
Au	0.745365000	12.388620000	54.003100000
Au	3.715213000	12.388620000	54.003100000
Au	6.685062000	12.388620000	54.003100000
Au	9.654910000	12.388620000	54.003100000
Au	12.624760000	12.388620000	54.003100000
Au	15.594610000	12.388620000	54.003100000
Au	2.230289000	14.960580000	54.003100000
Au	5.200138000	14.960580000	54.003100000
Au	8.169986000	14.960580000	54.003100000
Au	11.139830000	14.960580000	54.003100000
Au	14.109680000	14.960580000	54.003100000
Au	17.079530000	14.960580000	54.003100000
Au	2.230289000	1.243439000	56.427970000
Au	5.200138000	1.243439000	56.427970000
Au	8.169986000	1.243439000	56.427970000
Au	11.139830000	1.243439000	56.427970000
Au	14.109680000	1.243439000	56.427970000
Au	17.079530000	1.243439000	56.427970000
Au	0.745365000	3.815403000	56.427970000
Au	3.715213000	3.815403000	56.427970000
Au	6.685062000	3.815403000	56.427970000
Au	9.654910000	3.815403000	56.427970000
Au	12.624760000	3.815403000	56.427970000
Au	15.594610000	3.815403000	56.427970000
Au	2.230289000	6.387367000	56.427970000
Au	5.200138000	6.387367000	56.427970000
Au	8.169986000	6.387367000	56.427970000
Au	11.139830000	6.387367000	56.427970000
Au	14.109680000	6.387367000	56.427970000
Au	17.079530000	6.387367000	56.427970000
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Au	3.715213000	8.959331000	56.427970000
Au	6.685062000	8.959331000	56.427970000
Au	9.654910000	8.959331000	56.427970000
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Au	15.594610000	8.959331000	56.427970000
Au	2.230289000	11.531300000	56.427970000
Au	5.200138000	11.531300000	56.427970000
Au	8.169986000	11.531300000	56.427970000
Au	11.139830000	11.531300000	56.427970000

Au	14.109680000	11.531300000	56.427970000
Au	17.079530000	11.531300000	56.427970000
Au	0.745365000	14.103260000	56.427970000
Au	3.715213000	14.103260000	56.427970000
Au	6.685062000	14.103260000	56.427970000
Au	9.654910000	14.103260000	56.427970000
Au	12.624760000	14.103260000	56.427970000
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Au	6.685062000	0.386117200	58.852840000
Au	9.654910000	0.386117200	58.852840000
Au	12.624760000	0.386117200	58.852840000
Au	15.594610000	0.386117200	58.852840000
Au	2.230289000	2.958081000	58.852840000
Au	5.200138000	2.958081000	58.852840000
Au	8.169986000	2.958081000	58.852840000
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Au	14.109680000	2.958081000	58.852840000
Au	17.079530000	2.958081000	58.852840000
Au	0.745365000	5.530046000	58.852840000
Au	3.715213000	5.530046000	58.852840000
Au	6.685062000	5.530046000	58.852840000
Au	9.654910000	5.530046000	58.852840000
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