Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Atom Vacancies and Electronic Transmission Stark Effects in Boron Nanoflake Junctions

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Contents

Ionization energies, electron affinities and reorganization energies

TABLE S1. The energy processes involved for each step per BNF, from the isolated neutral ground states to their charge transfer state (N→CT), involving vertical ionization energy (*IE*v), vertical electron affinity (EA_V), and the hole (λ_h) and electron reorganization energies (λ_e), in eV.

BNF	N→CT	*IE*v	EA_V	λ_h	λ_e
B_{37}	D→S	6.26	2.90	0.33	0.41
	D→T	6.67	2.35	0.18	0.83
B_{36}	S→D	6.73	2.45	0.16	0.23
	T→D	5.89	3.13	0.24	0.39
B_{35}	D→S	6.64	3.29	0.15	0.16
	D→T	7.69	2.77	0.56	0.17

ETSE Shift

Table S2. Electronic transmission Stark effect (ETSE) shifts (ϑ /eV) of the resonance at the Fermi energy for each of the three BNFs with respect to the bias voltage. These ETSE shifts are referenced to the resonance at zero bias.

Bias (V)	ϑ (B_{37})	ϑ (B_{36})	ϑ (B_{35})
0	0	0	0
0.2	-0.052	0.046	-0.052
0.4	-0.136	0.063	-0.141
0.6	-0.221	-0.017	-0.198
0.8	-0.292	-0.011	-0.088
1.0	-0.273	-0.083	-0.057
-0.2	-0.061	0.041	0.069
-0.4	-0.147	0.051	0.146
-0.6	-0.235	-0.032	0.205
-0.8	-0.313	-0.109	0.219
-1.0	-0.310	-0.174	0.210

Dipoles

The electric field numerical values were chosen to be equivalent to the bias voltage in steps of ±0.2 eV between a ±1 eV span. The $B_{35,}$ B_{36} and B_{37} were computed without the sulfur contacts and gold electrodes, in a large box using the Siesta program.

Table S3. B_{37} dipole, in atomic units.

E-field	dipole x	dipole y	dipole z	net dipole
-0.989999	-0.14	0.43	-16.35	-0.14
-0.791999	-0.18	0.50	-13.34	-0.18
-0.593999	-0.23	0.57	-10.33	-0.23
-0.396	-0.28	0.64	-7.31	-0.28
-0.198	-0.34	0.72	-4.04	-0.34
0	-0.43	0.82	-0.21	-0.43
0.198	-0.51	0.91	3.58	-0.51
0.396	-0.59	1.01	7.40	-0.59
0.593999	-0.65	1.10	10.49	-0.65
0.791999	-0.71	1.19	13.50	-0.71
0.989999	-0.77	1.28	16.51	-0.77

Table S4. B_{36} dipoles, in atomic units.

E-field	dipole x	dipole y	dipole z	net dipole
-0.989999	-0.22	0.58	-15.44	-0.22
-0.791999	-0.27	0.64	-12.31	-0.27
-0.593999	-0.33	0.72	-9.21	-0.33
-0.396	-0.39	0.79	-6.13	-0.39
-0.198	-0.44	0.87	-3.06	-0.44
0	-0.50	0.95	0.00	-0.50
0.198	-0.56	1.03	3.06	-0.56
0.396	-0.63	1.12	6.12	-0.63
0.593999	-0.69	1.21	9.20	-0.69
0.791999	-0.76	1.30	12.31	-0.76
0.989999	-0.83	1.40	15.44	-0.83

Table S5. B_{35} dipoles, in atomic units.

E-field	dipole x	dipole y	dipole z	net dipole
-0.989999	-2.13	0.82	14.63	-2.13
-0.791999	-2.07	0.74	11.61	-2.07
-0.593999	-2.01	0.66	8.60	-2.01
-0.396	-1.96	0.57	5.61	-1.96
-0.198	-1.90	0.50	2.62	-1.90
0	-1.83	0.42	-0.37	-1.83
0.198	-1.77	0.35	-3.35	-1.77
0.396	-1.70	0.29	-6.34	-1.70
0.593999	-1.63	0.23	-9.32	-1.63
0.791999	-1.56	0.17	-12.31	-1.56
0.989999	-1.49	0.11	-15.30	-1.49

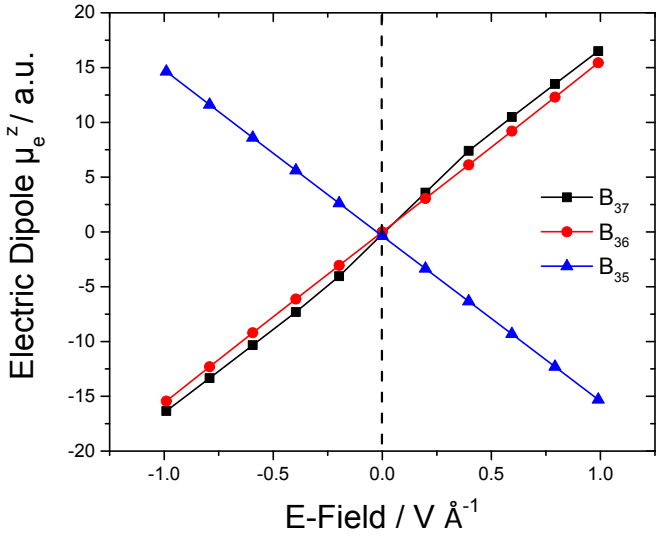

Figure S1. Electric Dipole, z-axis (a.u.) for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

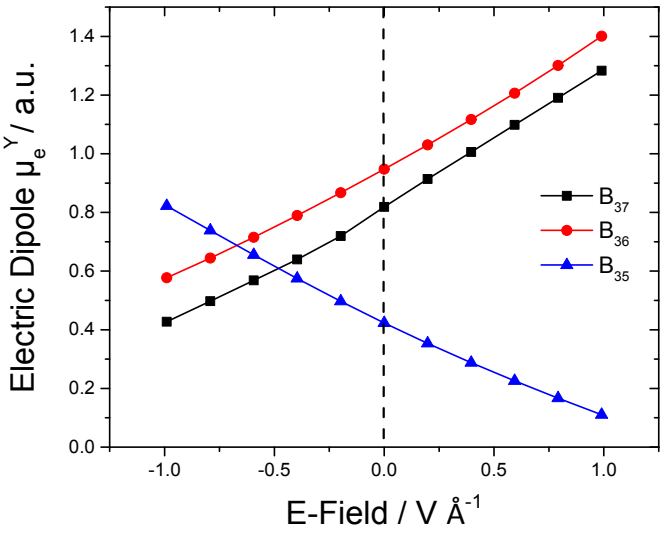

Figure S2. Electric Dipole, y-axis (a.u.) for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

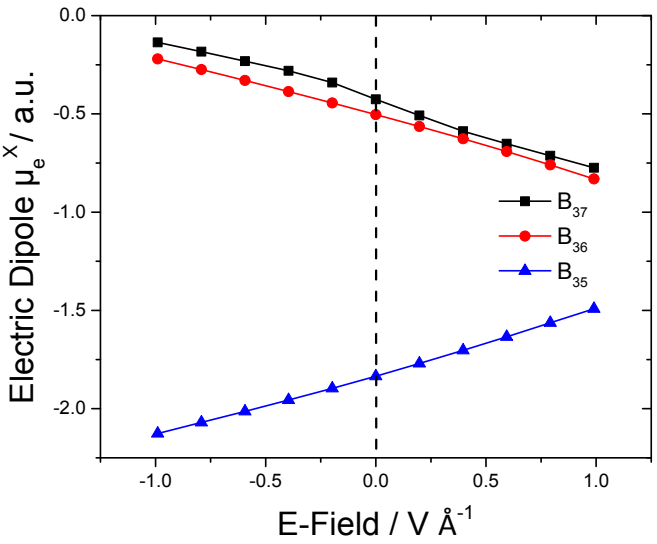

Figure S3. Electric Dipole, x-axis (a.u.) for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

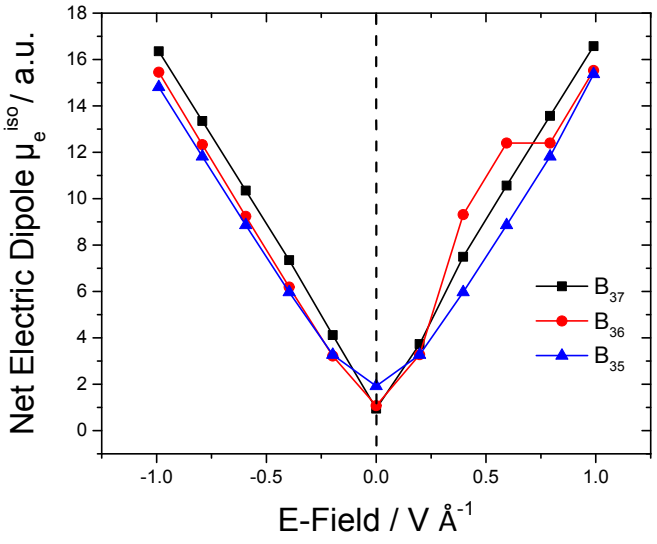

Figure S4. Net Electric Dipole (a.u.) for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

Polarizability and Relative Dielectric Constant

The volumes used were those of the structures, not the volume of the box. The polarizability were computed as the division between the net dipole and E-field. All parameters are in atomic units. The relative dielectric constant were computed for completeness (using the method in reference 54), as a molecular relationship (in radians) between the Bohr volume and the net dipole.

B_{37}

Volume = 345.14 Å^3, 652.23 Bohr^3.

Table S6.

E-field	α_{iso}	ε_{rel}
-0.989999	-16.52	1.46
-0.791999	-16.86	1.35
-0.593999	-17.42	1.25
-0.396	-18.56	1.16
-0.198	-20.81	1.09
0	0	1.02
0.198	18.85	1.08
0.396	18.93	1.17
0.593999	17.79	1.26
0.791999	17.13	1.35
0.989999	16.74	1.47

B_{36}

Volume = 345.37 Å^3, 652.65 Bohr^3.

Table S7.

E-field	α_{iso}	ε_{rel}
-0.989999	-15.61	1.42
-0.791999	-15.57	1.31
-0.593999	-15.55	1.22
-0.396	-15.63	1.14
-0.198	-16.22	1.07
0	0.00	1.02
0.198	16.54	1.07
0.396	23.51	1.22
0.593999	20.88	1.31
0.791999	15.66	1.31
0.989999	15.68	1.43

B_{35}

Volume = 342.79 Å^3, 647.78 Bohr^3.

Table S8.

E-field	α_{iso}	ε_{rel}
-0.989999	-14.96	1.40
-0.791999	-14.92	1.30
-0.593999	-14.92	1.21
-0.396	-15.07	1.13
-0.198	-16.52	1.07
0	0.00	1.04
0.198	16.52	1.07
0.396	15.07	1.13
0.593999	14.92	1.21
0.791999	14.92	1.30
0.989999	15.53	1.43

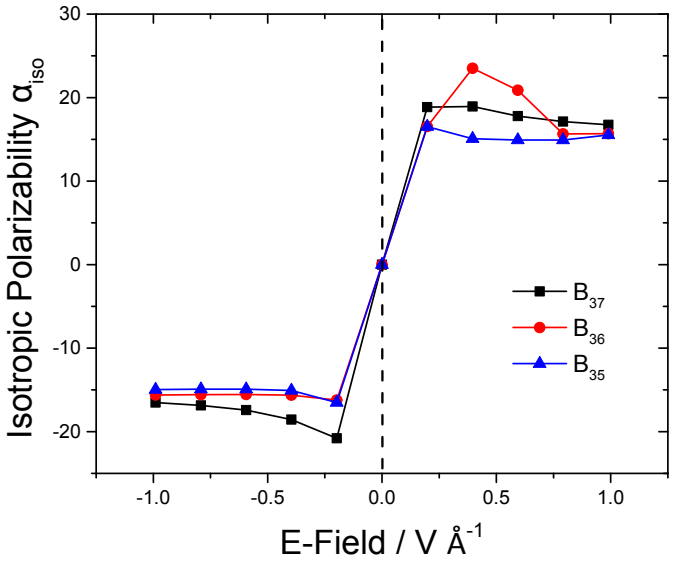

Figure S5. Isotropic polarizability for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

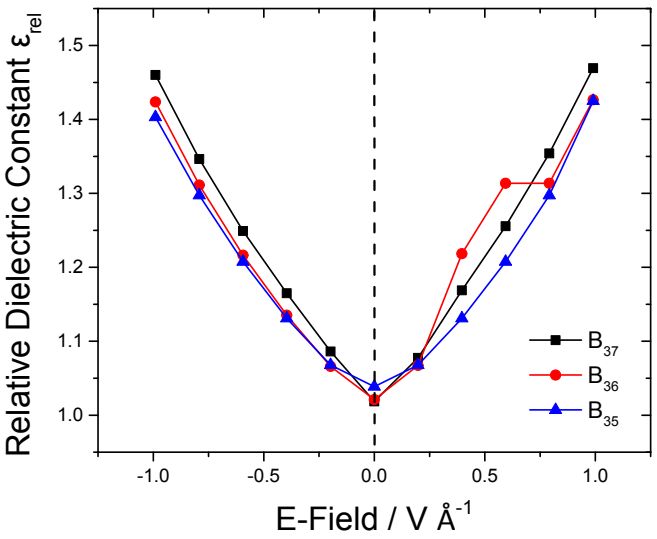

Figure S6. Relative Dielectric Constant for B_{37}, B_{36} and B_{35} across the electric field (V/Å) window.

Electrode Couplings

The coupling was deduced from FWHM analysis.

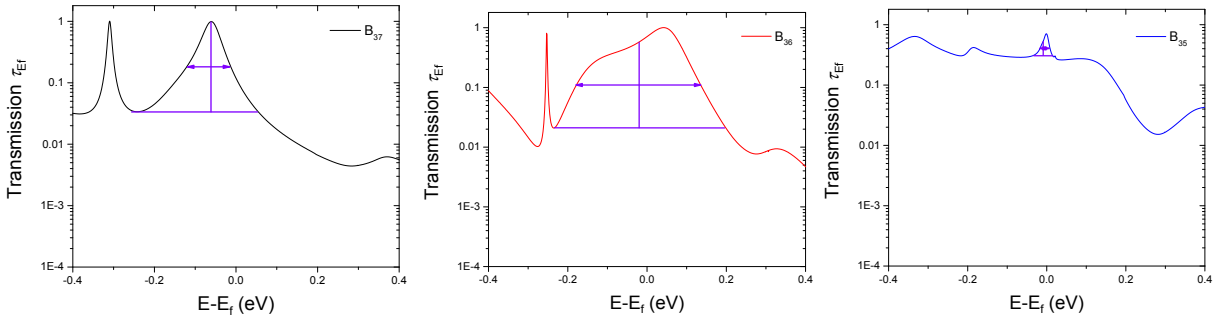

Figure S7. Electrode coupling (eV) from FWHM analysis of the zero-bias resonance at the Fermi energy.

Cartesian Coordinates

Table S9. The Cartesian coordinates of the neutral, ground state isolated molecules.

B_{37} (doublet)				B_{36} (singlet)				B_{35} (doublet)			
B	0.2066981600	-0.1178346500	-4.8080115000	B	0.4380555600	-0.4957833300	-5.0703861100	B	0.5983728200	-0.6386756400	-4.6987572300
B	-1.0625104700	-0.8349147200	-4.1592077000	B	-0.8712444400	-1.1083833300	-4.1811861100	B	-0.7973325000	-1.0917949800	-4.0883604200
B	1.4380816600	0.5984170600	-4.0913597500	B	1.5890555600	0.2754166700	-4.0843861100	B	1.7110316500	0.2450052700	-4.0487932100
B	-2.4603084400	-1.2999769200	-3.3907703700	B	0.0103555600	0.1689166700	-3.4627861100	B	-2.1148647800	-1.7378289600	-3.3276010500
B	2.5271117300	1.5299323100	-3.2498290300	B	-2.1563444400	-1.8210833300	-3.4064861100	B	0.1438492400	0.1085386800	-3.2827679000
B	0.0518449500	0.0709681300	-3.1721465800	B	2.8116555600	1.0299166700	-3.2653861100	B	2.8557219600	1.0359273900	-3.1337107500
B	-3.7569005400	-1.7079760500	-2.5530359300	B	-1.2055444400	-0.5728833300	-2.5867861100	B	-1.2533917600	-0.3867768300	-2.5311929400
B	-0.9278084400	-1.2188258800	-2.5067456200	B	1.2128555600	0.8488166700	-2.5186861100	B	-3.1913194000	-2.5082265100	-2.4626117400
B	1.6009912600	0.2632372600	-2.4050148900	B	-3.2254444400	-2.6104833300	-2.4860861100	B	1.2614815500	1.0068227300	-2.3877507300
B	3.4598634100	2.4325095400	-2.3454376100	B	3.9985555600	1.4949166700	-2.2792861100	B	4.0585289400	1.5433644200	-2.2132570700
B	-2.4061905700	-1.3852627800	-1.6878299400	B	-2.5300444400	-1.2738833300	-1.7621861100	B	-2.4536800500	-1.2209400500	-1.7195550500
B	2.6892452800	1.2010381600	-1.5602494200	B	-0.3175444400	0.6514166700	-1.7527861100	B	-0.2242373100	0.6752197000	-1.6876832900
B	0.1031166100	0.0049786300	-1.5208084400	B	2.4625555600	1.5933166700	-1.6213861100	B	2.5120070800	1.6430585400	-1.5595489400
B	-3.8976652100	-1.7759391400	-0.9686643200	B	-3.5267444400	-2.4109833300	-0.9331861100	B	-3.5005084300	-2.3412188000	-0.9287999800
B	-0.8942156900	-1.3654702600	-0.8335051400	B	-1.4846444400	-0.1695833300	-0.9184861100	B	-1.5155244600	-0.0474595000	-0.8930433700
B	1.7270995300	0.0219817900	-0.7544532700	B	0.9407555600	1.2489166700	-0.8474861100	B	0.9780281500	1.4448631500	-0.8125620600
B	3.5575903600	2.4442545300	-0.7508153300	B	3.9205555600	1.8082166700	-0.7178861100	B	4.0061063300	1.8722446800	-0.7006136700
B	-2.4426818600	-1.6229425900	-0.0614339900	B	-2.6283444400	-1.1092833300	-0.0915861100	B	-2.6667879500	-0.9743370300	-0.0928331600
B	-0.4063196800	0.2259620900	-0.0240595700	B	2.3079555600	1.7012166700	0.0551138900	B	-3.5721455800	-2.3041652200	0.7282460100
B	2.5382309200	1.3383732000	0.0737325100	B	-3.6221444400	-2.3563833300	0.7404138900	B	-1.5866169000	-0.0108357200	0.7615129800
B	-3.9722731600	-1.7279111400	0.7213902500	B	-1.5530444400	-0.1386833300	0.7916138900	B	0.9071462000	1.4814566200	0.8299918100
B	-0.9673700400	-1.3180512500	0.8275819300	B	0.8760555600	1.2596166700	0.8553138900	B	3.9352465600	1.9060082400	0.9567578900
B	1.6544106600	0.0695159000	0.9015661900	B	3.8478555600	1.8378166700	0.9544138900	B	-2.5950318800	-1.1478959900	1.5555506700
B	3.4832878500	2.4924829700	0.9202958100	B	-2.6915444400	-1.1747833300	1.5905138900	B	-0.3673530700	0.7489670500	1.6316290400
B	-0.0306708100	0.0907787600	1.5216397200	B	-0.4448444400	0.7020166700	1.6742138900	B	2.3728689600	1.7130775000	1.6949734400
B	-2.5486547800	-1.2931340100	1.5455982700	B	2.3266555600	1.6442166700	1.7402138900	B	-3.3965270200	-2.4023200400	2.2889361800
B	2.5441358300	1.2955018900	1.7199998200	B	-3.5084444400	-2.4224833300	2.3351138900	B	-1.4673080700	-0.2762851500	2.4296504100
B	-3.9711813100	-1.5694935000	2.3055188700	B	-1.4722444400	-0.3958833300	2.5133138900	B	1.0546867000	1.1121623900	2.4410695600
B	-1.1477086900	-1.0765065200	2.4807738200	B	3.8003555600	1.5961166700	2.5303138900	B	3.8583494600	1.6397006000	2.4807156300
B	3.2448778400	2.5724477200	2.4979686800	B	0.9987555600	0.9653166700	2.5708138900	B	-2.3968332500	-1.5925321400	3.2080398500
B	1.3836805800	0.4045930000	2.5180195900	B	-2.5166444400	-1.5887833300	3.3035138900	B	-0.1381849000	0.2529825300	3.2755350400
B	-0.2274003600	0.2518729100	3.1552058000	B	2.5374555600	1.1595166700	3.4360138900	B	2.5800968600	1.1731278300	3.3168316600
B	-2.7524293400	-1.1111263100	3.2295119100	B	-0.2815444400	0.3242166700	3.4395138900	B	-1.1474928600	-0.9122897900	4.0495689800
B	2.2342319900	1.7206391300	3.3669237600	B	-1.2922444400	-0.8431833300	4.1529138900	B	1.3590254400	0.4229133500	4.1645658900
B	-1.4268168600	-0.5984943400	4.0901473900	B	1.2283555600	0.4825166700	4.1869138900	B	0.1925922700	-0.4318583400	4.7558675300
B	1.0729458200	0.8360539900	4.1611097500	B	0.0207555600	-0.2998833300	5.1162138900				
B	-0.2183382300	0.1583210900	4.8063943400								

Table S10. The Cartesian coordinates of the molecular junctions.

B_{37}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	14.424978	8.328265	14.133500
Au	11.539983	8.328265	14.133500
Au	8.654987	8.328265	14.133500
Au	5.769991	8.328265	14.133500
Au	12.982480	5.829786	14.133500
Au	10.097485	5.829786	14.133500
Au	7.212489	5.829786	14.133500
Au	4.327494	5.829786	14.133500
Au	11.539983	3.331306	14.133500
Au	8.654987	3.331306	14.133500
Au	5.769991	3.331306	14.133500
Au	2.884996	3.331306	14.133500
Au	10.097485	0.832827	14.133500
Au	7.212489	0.832827	14.133500
Au	4.327494	0.832827	14.133500
Au	1.442498	0.832827	14.133500
Au	12.982480	9.161092	16.489100
Au	10.097485	9.161092	16.489100
Au	7.212489	9.161092	16.489100
Au	4.327494	9.161092	16.489100
Au	11.539983	6.662612	16.489100
Au	8.654987	6.662612	16.489100
Au	5.769991	6.662612	16.489100
Au	2.884996	6.662612	16.489100
Au	10.097485	4.164133	16.489100
Au	7.212489	4.164133	16.489100
Au	4.327494	4.164133	16.489100
Au	1.442498	4.164133	16.489100
Au	8.654987	1.665653	16.489100
Au	5.769991	1.665653	16.489100
Au	2.884996	1.665653	16.489100
Au	0.000000	1.665653	16.489100
S	7.120306	5.874894	18.625900
B	7.007159	5.757812	20.482400
B	5.755185	5.097891	21.480400
B	8.166399	6.455891	21.484000
B	6.551915	6.470068	22.063900
B	4.428173	4.383918	22.150000
B	9.420127	7.235009	22.277500
B	5.420302	5.585107	22.977700
B	7.845986	6.941357	23.057100
B	3.345631	3.561939	23.037500
B	10.626599	7.751173	23.225700
B	4.102012	4.841922	23.799000
B	6.208498	6.984032	23.812100
B	9.125644	7.650390	23.938200
B	3.056830	3.687595	24.612300
B	5.355250	5.681775	24.661500
B	7.723788	6.975176	24.735200
B	10.602863	7.974627	24.818900
B	4.246069	4.675617	25.474600
B	5.970827	7.279660	25.454200
B	9.091857	7.528866	25.605300
B	2.963710	3.773478	26.282300
B	5.266554	5.763342	26.317200
B	7.640619	7.057169	26.379500
B	10.527654	8.011275	26.494600
B	3.931634	4.982168	27.108800
B	6.051715	7.102880	27.145400
B	8.975728	7.762500	27.254300
B	3.072166	3.776950	27.884700
B	5.159611	5.795846	28.014000
B	10.416485	7.871768	28.093600
B	7.595346	7.135618	28.065800
B	4.069452	4.641963	28.818300
B	9.124906	7.420905	28.948600
B	6.262066	6.638694	28.988900
B	5.366657	5.337742	29.627500
B	7.818544	6.660800	29.656800
B	6.632025	5.914371	30.618700
S	6.879971	5.849149	32.478100
Au	0.000000	1.665653	34.736100
Au	2.884996	1.665653	34.736100
Au	5.769991	1.665653	34.736100
Au	8.654987	1.665653	34.736100

B_{36}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	1.442498	0.832827	14.133500
Au	4.327494	0.832827	14.133500
Au	7.212489	0.832827	14.133500
Au	10.097485	0.832827	14.133500
Au	2.884996	3.331306	14.133500
Au	5.769991	3.331306	14.133500
Au	8.654987	3.331306	14.133500
Au	11.539983	3.331306	14.133500
Au	4.327494	5.829786	14.133500
Au	7.212489	5.829786	14.133500
Au	10.097485	5.829786	14.133500
Au	12.982480	5.829786	14.133500
Au	5.769991	8.328265	14.133500
Au	8.654987	8.328265	14.133500
Au	11.539983	8.328265	14.133500
Au	14.424978	8.328265	14.133500
Au	0.000000	1.665653	16.489100
Au	2.884996	1.665653	16.489100
Au	5.769991	1.665653	16.489100
Au	8.654987	1.665653	16.489100
Au	1.442498	4.164133	16.489100
Au	4.327494	4.164133	16.489100
Au	7.212489	4.164133	16.489100
Au	10.097485	4.164133	16.489100
Au	2.884996	6.662612	16.489100
Au	5.769991	6.662612	16.489100
Au	8.654987	6.662612	16.489100
Au	11.539983	6.662612	16.489100
Au	4.327494	9.161092	16.489100
Au	7.212489	9.161092	16.489100
Au	10.097485	9.161092	16.489100
Au	12.982480	9.161092	16.489100
S	7.120218	5.875543	18.614500
B	7.029623	5.676245	20.477400
B	5.720299	5.063618	21.366600
B	8.180603	6.447443	21.463400
B	6.601862	6.340870	22.085000
B	4.435157	4.350948	22.141400
B	9.403250	7.201855	22.282500
B	5.385996	5.599083	22.961000
B	7.804448	7.020791	23.029100
B	3.366087	3.561477	23.061700
B	10.590066	7.666890	23.268500
B	4.061530	4.898053	23.785700
B	6.273967	6.823428	23.795000
B	9.054128	7.765287	23.926500
B	3.064813	3.761036	24.614600
B	5.186884	6.002366	24.629400
B	7.532346	7.420868	24.700300
B	10.512082	7.980166	24.830000
B	3.963166	5.062697	25.456300
B	8.899489	7.873167	25.602900
B	2.969401	3.816616	26.302200
B	5.038548	6.033334	26.339400
B	7.467615	7.431566	26.403100
B	10.439449	8.000818	26.502200
B	3.900017	4.997226	27.138300
B	6.146722	6.874009	27.222000
B	8.918242	7.816224	27.280000
B	3.083125	3.749476	27.882900
B	5.119261	5.776143	28.061200
B	10.391855	7.768138	28.072200
B	7.590320	7.137270	28.118700
B	4.074987	4.583150	28.851300
B	9.129040	7.331526	28.983800
B	6.309972	6.496249	28.987300
B	5.299275	5.328816	29.700700
B	7.819945	6.654513	29.734800
B	6.612331	5.872133	30.664000
S	6.862239	5.844230	32.523400
Au	12.982480	9.161092	34.736100
Au	10.097485	9.161092	34.736100
Au	7.212489	9.161092	34.736100
Au	4.327494	9.161092	34.736100
Au	11.539983	6.662612	34.736100

B_{35}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	1.442498	0.832827	14.133900
Au	4.327494	0.832827	14.133900
Au	7.212489	0.832827	14.133900
Au	10.097485	0.832827	14.133900
Au	2.884996	3.331306	14.133900
Au	5.769991	3.331306	14.133900
Au	8.654987	3.331306	14.133900
Au	11.539983	3.331306	14.133900
Au	4.327494	5.829786	14.133900
Au	7.212489	5.829786	14.133900
Au	10.097485	5.829786	14.133900
Au	12.982480	5.829786	14.133900
Au	5.769991	8.328265	14.133900
Au	8.654987	8.328265	14.133900
Au	11.539983	8.328265	14.133900
Au	14.424978	8.328265	14.133900
Au	0.000000	1.665653	16.489400
Au	2.884996	1.665653	16.489400
Au	5.769991	1.665653	16.489400
Au	8.654987	1.665653	16.489400
Au	1.442498	4.164133	16.489400
Au	4.327494	4.164133	16.489400
Au	7.212489	4.164133	16.489400
Au	10.097485	4.164133	16.489400
Au	2.884996	6.662612	16.489400
Au	5.769991	6.662612	16.489400
Au	8.654987	6.662612	16.489400
Au	11.539983	6.662612	16.489400
Au	4.327494	9.161092	16.489400
Au	7.212489	9.161092	16.489400
Au	10.097485	9.161092	16.489400
Au	12.982480	9.161092	16.489400
S	7.133679	5.863145	18.633800
B	7.037419	5.687305	20.510700
B	5.731679	5.079697	21.388800
B	8.194655	6.429540	21.479000
B	6.627757	6.347439	22.130600
B	4.454196	4.359364	22.155300
B	9.397765	7.204407	22.336300
B	5.365451	5.662315	22.979500
B	7.382867	3.559457	23.060300
B	7.811398	7.067515	23.090600
B	10.605576	7.646936	23.304300
B	4.085528	4.897321	23.796800
B	6.267745	6.873240	23.824900
B	9.028956	7.853462	23.940400
B	3.055354	3.747655	24.611800
B	5.052501	6.071883	24.634000
B	7.536047	7.560968	24.712600
B	10.524559	7.997129	24.835600
B	3.932331	5.087868	25.450900
B	2.958445	3.797823	26.278700
B	4.991291	6.061696	26.341000
B	7.501418	7.439272	26.371600
B	10.524837	7.997755	26.489300
B	3.900389	4.988104	27.124200
B	6.197875	6.806949	27.185400
B	8.973995	7.662554	27.190000
B	3.078798	3.734107	27.876600
B	7.618073	7.117677	28.021200
B	5.104746	5.777554	28.029300
B	10.413673	7.789651	28.035900
B	4.069929	4.571737	28.833700
B	9.133212	7.325710	28.932600
B	6.384267	6.595355	28.958600
B	5.271067	5.323884	29.678200
B	7.844721	6.688011	29.732200
B	6.580407	5.878594	30.607400
S	7.011683	5.861964	32.419000
Au	0.000000	1.665653	34.736400
Au	2.884996	1.665653	34.736400
Au	5.769991	1.665653	34.736400
Au	8.654987	1.665653	34.736400
Au	1.442498	4.164133	34.736400
Au	4.327494	4.164133	34.736400

Au	1.442498	4.164133	34.736100
Au	4.327494	4.164133	34.736100
Au	7.212489	4.164133	34.736100
Au	10.097485	4.164133	34.736100
Au	2.884996	6.662612	34.736100
Au	5.769991	6.662612	34.736100
Au	8.654987	6.662612	34.736100
Au	11.539983	6.662612	34.736100
Au	4.327494	9.161092	34.736100
Au	7.212489	9.161092	34.736100
Au	10.097485	9.161092	34.736100
Au	12.982480	9.161092	34.736100
Au	0.000000	0.000000	37.069700
Au	2.884996	0.000000	37.069700
Au	5.769991	0.000000	37.069700
Au	8.654987	0.000000	37.069700
Au	1.442498	2.498480	37.069700
Au	4.327494	2.498480	37.069700
Au	7.212489	2.498480	37.069700
Au	10.097485	2.498480	37.069700
Au	2.884996	4.996959	37.069700
Au	5.769991	4.996959	37.069700
Au	8.654987	4.996959	37.069700
Au	11.539983	4.996959	37.069700
Au	4.327494	7.495439	37.069700
Au	7.212489	7.495439	37.069700
Au	10.097485	7.495439	37.069700
Au	12.982480	7.495439	37.069700
Au	1.442500	0.832830	39.425300
Au	4.327490	0.832830	39.425300
Au	7.212490	0.832830	39.425300
Au	10.097480	0.832830	39.425300
Au	2.885000	3.331310	39.425300
Au	5.769990	3.331310	39.425300
Au	8.654990	3.331310	39.425300
Au	11.539980	3.331310	39.425300
Au	4.327490	5.829790	39.425300
Au	7.212490	5.829790	39.425300
Au	10.097480	5.829790	39.425300
Au	12.982480	5.829790	39.425300
Au	5.769990	8.328270	39.425300
Au	8.654990	8.328270	39.425300
Au	11.539980	8.328270	39.425300
Au	14.424980	8.328270	39.425300
Au	0.000000	1.665650	41.780900
Au	2.885000	1.665650	41.780900
Au	5.769990	1.665650	41.780900
Au	8.654990	1.665650	41.780900
Au	1.442500	4.164130	41.780900
Au	4.327490	4.164130	41.780900
Au	7.212490	4.164130	41.780900
Au	10.097480	4.164130	41.780900
Au	2.885000	6.662610	41.780900
Au	5.769990	6.662610	41.780900
Au	8.654990	6.662610	41.780900
Au	11.539980	6.662610	41.780900
Au	4.327490	9.161090	41.780900
Au	7.212490	9.161090	41.780900
Au	10.097480	9.161090	41.780900
Au	12.982480	9.161090	41.780900
Au	0.000000	0.000000	44.136500
Au	2.885000	0.000000	44.136500
Au	5.769990	0.000000	44.136500
Au	8.654990	0.000000	44.136500
Au	1.442500	2.498480	44.136500
Au	4.327490	2.498480	44.136500
Au	7.212490	2.498480	44.136500
Au	10.097480	2.498480	44.136500
Au	2.885000	4.996960	44.136500
Au	5.769990	4.996960	44.136500
Au	8.654990	4.996960	44.136500
Au	11.539980	4.996960	44.136500
Au	4.327490	7.495440	44.136500
Au	7.212490	7.495440	44.136500
Au	10.097480	7.495440	44.136500
Au	12.982480	7.495440	44.136500
Au	1.442500	0.832830	46.492100
Au	4.327490	0.832830	46.492100
Au	7.212490	0.832830	46.492100
Au	10.097480	0.832830	46.492100
Au	2.885000	3.331310	46.492100
Au	5.769990	3.331310	46.492100
Au	8.654990	3.331310	46.492100
Au	11.539980	3.331310	46.492100
Au	4.327490	5.829790	46.492100
Au	7.212490	5.829790	46.492100
Au	10.097480	5.829790	46.492100
Au	12.982480	5.829790	46.492100
Au	5.769990	8.328270	46.492100
Au	8.654990	8.328270	46.492100
Au	11.539980	8.328270	46.492100
Au	14.424980	8.328270	46.492100
Au	0.000000	1.665650	48.847700
Au	2.885000	1.665650	48.847700
Au	5.769990	1.665650	48.847700
Au	8.654990	1.665650	48.847700
Au	1.442500	4.164130	48.847700
Au	4.327490	4.164130	48.847700
Au	7.212490	4.164130	48.847700
Au	10.097480	4.164130	48.847700
Au	2.885000	6.662610	48.847700
Au	5.769990	6.662610	48.847700
Au	8.654990	6.662610	48.847700
Au	11.539980	6.662610	48.847700
Au	4.327490	9.161090	48.847700
Au	7.212490	9.161090	48.847700
Au	10.097480	9.161090	48.847700
Au	12.982480	9.161090	48.847700
Au	0.000000	0.000000	51.203300
Au	2.885000	0.000000	51.203300
Au	5.769990	0.000000	51.203300
Au	8.654990	0.000000	51.203300
Au	1.442500	2.498480	51.203300
Au	4.327490	2.498480	51.203300
Au	7.212490	2.498480	51.203300
Au	10.097480	2.498480	51.203300
Au	2.885000	4.996960	51.203300
Au	5.769990	4.996960	51.203300
Au	8.654990	4.996960	51.203300
Au	11.539980	4.996960	51.203300
Au	4.327490	7.495440	51.203300
Au	7.212490	7.495440	51.203300
Au	10.097480	7.495440	51.203300
Au	12.982480	7.495440	51.203300

Au	8.654987	6.662612	34.736100
Au	5.769991	6.662612	34.736100
Au	2.884996	6.662612	34.736100
Au	10.097485	4.164133	34.736100
Au	7.212489	4.164133	34.736100
Au	4.327494	4.164133	34.736100
Au	1.442498	4.164133	34.736100
Au	8.654987	1.665653	34.736100
Au	5.769991	1.665653	34.736100
Au	2.884996	1.665653	34.736100
Au	0.000000	1.665653	34.736100
Au	12.982480	7.495439	37.069700
Au	10.097485	7.495439	37.069700
Au	7.212489	7.495439	37.069700
Au	4.327494	7.495439	37.069700
Au	11.539983	4.996959	37.069700
Au	8.654987	4.996959	37.069700
Au	5.769991	4.996959	37.069700
Au	2.884996	4.996959	37.069700
Au	10.097485	2.498480	37.069700
Au	7.212489	2.498480	37.069700
Au	4.327494	2.498480	37.069700
Au	1.442498	2.498480	37.069700
Au	8.654987	0.000000	37.069700
Au	5.769991	0.000000	37.069700
Au	2.884996	0.000000	37.069700
Au	0.000000	0.000000	37.069700
Au	1.442500	0.832830	39.425300
Au	4.327490	0.832830	39.425300
Au	7.212490	0.832830	39.425300
Au	10.097480	0.832830	39.425300
Au	2.885000	3.331310	39.425300
Au	5.769990	3.331310	39.425300
Au	8.654990	3.331310	39.425300
Au	11.539980	3.331310	39.425300
Au	4.327490	5.829790	39.425300
Au	7.212490	5.829790	39.425300
Au	10.097480	5.829790	39.425300
Au	12.982480	5.829790	39.425300
Au	5.769990	8.328270	39.425300
Au	8.654990	8.328270	39.425300
Au	11.539980	8.328270	39.425300
Au	14.424980	8.328270	39.425300
Au	0.000000	1.665650	41.780900
Au	2.885000	1.665650	41.780900
Au	5.769990	1.665650	41.780900
Au	8.654990	1.665650	41.780900
Au	1.442500	4.164130	41.780900
Au	4.327490	4.164130	41.780900
Au	7.212490	4.164130	41.780900
Au	10.097480	4.164130	41.780900
Au	2.885000	6.662610	41.780900
Au	5.769990	6.662610	41.780900
Au	8.654990	6.662610	41.780900
Au	11.539980	6.662610	41.780900
Au	4.327490	9.161090	41.780900
Au	7.212490	9.161090	41.780900
Au	10.097480	9.161090	41.780900
Au	12.982480	9.161090	41.780900
Au	0.000000	0.000000	44.136500
Au	2.885000	0.000000	44.136500
Au	5.769990	0.000000	44.136500
Au	8.654990	0.000000	44.136500
Au	1.442500	2.498480	44.136500
Au	4.327490	2.498480	44.136500
Au	7.212490	2.498480	44.136500
Au	10.097480	2.498480	44.136500
Au	2.885000	4.996960	44.136500
Au	5.769990	4.996960	44.136500
Au	8.654990	4.996960	44.136500
Au	11.539980	4.996960	44.136500
Au	4.327490	7.495440	44.136500
Au	7.212490	7.495440	44.136500
Au	10.097480	7.495440	44.136500
Au	12.982480	7.495440	44.136500
Au	4.327490	0.832830	46.492100
Au	1.442500	0.832830	46.492100
Au	7.212490	0.832830	46.492100
Au	10.097480	0.832830	46.492100
Au	2.885000	3.331310	46.492100
Au	5.769990	3.331310	46.492100
Au	8.654990	3.331310	46.492100
Au	11.539980	3.331310	46.492100
Au	4.327490	5.829790	46.492100
Au	7.212490	5.829790	46.492100
Au	10.097480	5.829790	46.492100
Au	12.982480	5.829790	46.492100
Au	5.769990	8.328270	46.492100
Au	8.654990	8.328270	46.492100
Au	11.539980	8.328270	46.492100
Au	14.424980	8.328270	46.492100
Au	0.000000	1.665650	48.847700
Au	2.885000	1.665650	48.847700
Au	5.769990	1.665650	48.847700
Au	8.654990	1.665650	48.847700
Au	1.442500	4.164130	48.847700
Au	4.327490	4.164130	48.847700
Au	7.212490	4.164130	48.847700
Au	10.097480	4.164130	48.847700
Au	2.885000	6.662610	48.847700
Au	5.769990	6.662610	48.847700
Au	8.654990	6.662610	48.847700
Au	11.539980	6.662610	48.847700
Au	4.327490	9.161090	48.847700
Au	7.212490	9.161090	48.847700
Au	10.097480	9.161090	48.847700
Au	12.982480	9.161090	48.847700
Au	0.000000	0.000000	51.203300
Au	2.885000	0.000000	51.203300
Au	5.769990	0.000000	51.203300
Au	8.654990	0.000000	51.203300
Au	1.442500	2.498480	51.203300
Au	4.327490	2.498480	51.203300
Au	7.212490	2.498480	51.203300
Au	10.097480	2.498480	51.203300
Au	2.885000	4.996960	51.203300
Au	5.769990	4.996960	51.203300
Au	8.654990	4.996960	51.203300
Au	11.539980	4.996960	51.203300
Au	4.327490	7.495440	51.203300
Au	7.212490	7.495440	51.203300
Au	10.097480	7.495440	51.203300
Au	12.982480	7.495440	51.203300

Au	7.212489	4.164133	34.736400
Au	10.097485	4.164133	34.736400
Au	2.884996	6.662612	34.736400
Au	5.769991	6.662612	34.736400
Au	8.654987	6.662612	34.736400
Au	11.539983	6.662612	34.736400
Au	4.327494	9.161092	34.736400
Au	7.212489	9.161092	34.736400
Au	10.097485	9.161092	34.736400
Au	12.982480	9.161092	34.736400
Au	0.000000	0.000000	37.070100
Au	2.884996	0.000000	37.070100
Au	5.769991	0.000000	37.070100
Au	8.654987	0.000000	37.070100
Au	1.442498	2.498480	37.070100
Au	4.327494	2.498480	37.070100
Au	7.212489	2.498480	37.070100
Au	10.097485	2.498480	37.070100
Au	2.884996	4.996959	37.070100
Au	5.769991	4.996959	37.070100
Au	8.654987	4.996959	37.070100
Au	11.539983	4.996959	37.070100
Au	4.327494	7.495439	37.070100
Au	7.212489	7.495439	37.070100
Au	10.097485	7.495439	37.070100
Au	12.982480	7.495439	37.070100
Au	1.442500	0.832830	39.425300
Au	4.327490	0.832830	39.425300
Au	7.212490	0.832830	39.425300
Au	10.097480	0.832830	39.425300
Au	2.885000	3.331310	39.425300
Au	5.769990	3.331310	39.425300
Au	8.654990	3.331310	39.425300
Au	11.539980	3.331310	39.425300
Au	4.327490	5.829790	39.425300
Au	7.212490	5.829790	39.425300
Au	10.097480	5.829790	39.425300
Au	12.982480	5.829790	39.425300
Au	5.769990	8.328270	39.425300
Au	8.654990	8.328270	39.425300
Au	11.539980	8.328270	39.425300
Au	14.424980	8.328270	39.425300
Au	0.000000	1.665650	41.780900
Au	2.885000	1.665650	41.780900
Au	5.769990	1.665650	41.780900
Au	8.654990	1.665650	41.780900
Au	1.442500	4.164130	41.780900
Au	4.327490	4.164130	41.780900
Au	7.212490	4.164130	41.780900
Au	10.097480	4.164130	41.780900
Au	2.885000	6.662610	41.780900
Au	5.769990	6.662610	41.780900
Au	8.654990	6.662610	41.780900
Au	11.539980	6.662610	41.780900
Au	4.327490	9.161090	41.780900
Au	7.212490	9.161090	41.780900
Au	10.097480	9.161090	41.780900
Au	12.982480	9.161090	41.780900
Au	0.000000	0.000000	44.136500
Au	2.885000	0.000000	44.136500
Au	5.769990	0.000000	44.136500
Au	8.654990	0.000000	44.136500
Au	1.442500	2.498480	44.136500
Au	4.327490	2.498480	44.136500
Au	7.212490	2.498480	44.136500
Au	10.097480	2.498480	44.136500
Au	2.885000	4.996960	44.136500
Au	5.769990	4.996960	44.136500
Au	8.654990	4.996960	44.136500
Au	11.539980	4.996960	44.136500
Au	4.327490	7.495440	44.136500
Au	7.212490	7.495440	44.136500
Au	10.097480	7.495440	44.136500
Au	12.982480	7.495440	44.136500
Au	4.327490	0.832830	46.492100
Au	1.442500	0.832830	46.492100
Au	7.212490	0.832830	46.492100
Au	10.097480	0.832830	46.492100
Au	2.885000	3.331310	46.492100
Au	5.769990	3.331310	46.492100
Au	8.654990	3.331310	46.492100
Au	11.539980	3.331310	46.492100
Au	4.327490	5.829790	46.492100
Au	7.212490	5.829790	46.492100
Au	10.097480	5.829790	46.492100
Au	12.982480	5.829790	46.492100
Au	5.769990	8.328270	46.492100
Au	8.654990	8.328270	46.492100
Au	11.539980	8.328270	46.492100
Au	14.424980	8.328270	46.492100
Au	0.000000	1.665650	48.847700
Au	2.885000	1.665650	48.847700
Au	5.769990	1.665650	48.847700
Au	8.654990	1.665650	48.847700
Au	1.442500	4.164130	48.847700
Au	4.327490	4.164130	48.847700
Au	7.212490	4.164130	48.847700
Au	10.097480	4.164130	48.847700
Au	2.885000	6.662610	48.847700
Au	5.769990	6.662610	48.847700
Au	8.654990	6.662610	48.847700
Au	11.539980	6.662610	48.847700
Au	4.327490	9.161090	48.847700
Au	7.212490	9.161090	48.847700
Au	10.097480	9.161090	48.847700
Au	12.982480	9.161090	48.847700
Au	0.000000	0.000000	51.203300
Au	2.885000	0.000000	51.203300
Au	5.769990	0.000000	51.203300
Au	8.654990	0.000000	51.203300
Au	1.442500	2.498480	51.203300
Au	4.327490	2.498480	51.203300
Au	7.212490	2.498480	51.203300
Au	10.097480	2.498480	51.203300
Au	2.885000	4.996960	51.203300
Au	5.769990	4.996960	51.203300
Au	8.654990	4.996960	51.203300
Au	11.539980	4.996960	51.203300
Au	4.327490	7.495440	51.203300
Au	7.212490	7.495440	51.203300
Au	10.097480	7.495440	51.203300
Au	12.982480	7.495440	51.203300

Table S11. The Cartesian coordinates of the isomer molecular junctions.

B_{35-i}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	1.442498	0.832827	14.133900
Au	4.327494	0.832827	14.133900
Au	7.212489	0.832827	14.133900
Au	10.097485	0.832827	14.133900
Au	2.884996	3.331306	14.133900
Au	5.769991	3.331306	14.133900
Au	8.654987	3.331306	14.133900
Au	11.539983	3.331306	14.133900
Au	4.327494	5.829786	14.133900
Au	7.212489	5.829786	14.133900
Au	10.097485	5.829786	14.133900
Au	12.982480	5.829786	14.133900
Au	5.769991	8.328265	14.133900
Au	8.654987	8.328265	14.133900
Au	11.539983	8.328265	14.133900
Au	14.424978	8.328265	14.133900
Au	0.000000	1.665653	16.489400
Au	2.884996	1.665653	16.489400
Au	5.769991	1.665653	16.489400
Au	8.654987	1.665653	16.489400
Au	1.442498	4.164133	16.489400
Au	4.327494	4.164133	16.489400
Au	7.212489	4.164133	16.489400
Au	10.097485	4.164133	16.489400
Au	2.884996	6.662612	16.489400
Au	5.769991	6.662612	16.489400
Au	8.654987	6.662612	16.489400
Au	11.539983	6.662612	16.489400
Au	4.327494	9.161092	16.489400
Au	7.212489	9.161092	16.489400
Au	10.097485	9.161092	16.489400
Au	12.982480	9.161092	16.489400
S	7.139222	5.847912	18.639700
B	7.038393	5.689465	20.499700
B	5.745425	5.083881	21.406500
B	8.180305	6.451802	21.489200
B	6.613781	6.353029	22.130500
B	4.457067	4.356792	22.158000
B	9.414618	7.195830	22.301200
B	5.387492	5.636936	22.986900
B	7.805596	7.027477	23.071600
B	3.368372	3.576572	23.053300
B	10.597248	7.673326	23.273700
B	4.103979	4.890218	23.798700
B	6.258681	6.881076	23.813300
B	9.060121	7.747513	23.948500
B	3.062025	3.761254	24.607900
B	5.063398	6.093667	24.657200
B	7.508953	7.488545	24.738700
B	10.532152	7.982387	24.838500
B	3.957253	5.053119	25.451500
B	8.930495	7.870526	25.617000
B	2.923578	3.864272	26.279100
B	5.100428	5.988701	26.359800
B	7.487901	7.432723	26.449400
B	10.462025	8.039051	26.515300
B	4.009865	4.899019	27.106600
B	6.288304	6.665365	27.372000
B	8.958201	7.749088	27.285700
B	3.057132	3.760230	27.872700
B	5.021932	5.849910	28.054200
B	10.420370	7.800001	28.099700
B	7.573143	7.367978	28.149600
B	4.118808	4.531233	28.847700
B	9.154402	7.342635	29.019000
B	5.293066	5.357385	29.643900
B	7.779692	6.781702	29.707600
B	6.569736	5.987007	30.589400
S	6.844614	5.827417	32.410400
Au	12.982480	9.161092	34.736400
Au	10.097485	9.161092	34.736400
Au	7.212489	9.161092	34.736400
Au	4.327494	9.161092	34.736400
Au	11.539983	6.662612	34.736400
Au	8.654987	6.662612	34.736400
Au	5.769991	6.662612	34.736400
Au	2.884996	6.662612	34.736400
Au	10.097485	4.164133	34.736400
Au	7.212489	4.164133	34.736400
Au	4.327494	4.164133	34.736400
Au	1.442498	4.164133	34.736400

B_{35-ii}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	14.424978	8.328265	14.133900
Au	11.539983	8.328265	14.133900
Au	8.654987	8.328265	14.133900
Au	5.769991	8.328265	14.133900
Au	12.982480	5.829786	14.133900
Au	10.097485	5.829786	14.133900
Au	7.212489	5.829786	14.133900
Au	4.327494	5.829786	14.133900
Au	11.539983	3.331306	14.133900
Au	8.654987	3.331306	14.133900
Au	5.769991	3.331306	14.133900
Au	2.884996	3.331306	14.133900
Au	10.097485	0.832827	14.133900
Au	7.212489	0.832827	14.133900
Au	4.327494	0.832827	14.133900
Au	1.442498	0.832827	14.133900
Au	12.982480	9.161092	16.489400
Au	10.097485	9.161092	16.489400
Au	7.212489	9.161092	16.489400
Au	4.327494	9.161092	16.489400
Au	11.539983	6.662612	16.489400
Au	8.654987	6.662612	16.489400
Au	5.769991	6.662612	16.489400
Au	2.884996	6.662612	16.489400
Au	10.097485	4.164133	16.489400
Au	7.212489	4.164133	16.489400
Au	4.327494	4.164133	16.489400
Au	1.442498	4.164133	16.489400
Au	8.654987	1.665653	16.489400
Au	5.769991	1.665653	16.489400
Au	2.884996	1.665653	16.489400
Au	0.000000	1.665653	16.489400
S	7.151309	5.862736	18.629800
B	7.080526	5.648943	20.497700
B	5.780455	5.028912	21.371400
B	8.208127	6.423922	21.486200
B	6.626428	6.335602	22.122900
B	4.468361	4.375432	22.174200
B	9.384400	7.200190	22.370400
B	5.358456	5.641924	22.959500
B	7.821379	7.038720	23.073100
B	3.423893	3.532669	23.091900
B	10.599408	7.666468	23.330400
B	6.235701	6.914426	23.795300
B	4.121521	4.904473	23.817800
B	9.030776	7.756834	24.005300
B	3.092663	3.756365	24.625900
B	5.017592	6.038111	24.639900
B	7.547913	7.545228	24.730600
B	10.522213	7.997259	24.870000
B	6.191916	6.892223	25.528100
B	2.976542	3.820488	26.270200
B	4.923257	6.102886	26.325100
B	7.480973	7.565709	26.412800
B	10.441714	8.018053	26.509700
B	3.932587	5.024921	27.099400
B	6.079639	6.997028	27.250000
B	8.889426	7.798795	27.270900
B	3.083940	3.757147	27.848000
B	5.109271	5.770613	28.054100
B	10.394630	7.764906	28.068600
B	7.599275	7.139424	28.121400
B	4.088438	4.601243	28.810100
B	9.105376	7.318707	28.947400
B	6.335490	6.444843	28.975500
B	5.373411	5.220942	29.685900
B	7.860258	6.539074	29.734400
B	6.665538	5.763559	30.651100
S	6.910422	5.815395	32.521800
Au	0.000000	1.665653	34.736400
Au	2.884996	1.665653	34.736400
Au	5.769991	1.665653	34.736400
Au	8.654987	1.665653	34.736400
Au	1.442498	4.164133	34.736400
Au	4.327494	4.164133	34.736400
Au	7.212489	4.164133	34.736400
Au	10.097485	4.164133	34.736400
Au	2.884996	6.662612	34.736400
Au	5.769991	6.662612	34.736400
Au	8.654987	6.662612	34.736400
Au	11.539983	6.662612	34.736400

B_{36-i}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	14.424978	8.328265	14.133500
Au	11.539983	8.328265	14.133500
Au	8.654987	8.328265	14.133500
Au	5.769991	8.328265	14.133500
Au	12.982480	5.829786	14.133500
Au	10.097485	5.829786	14.133500
Au	7.212489	5.829786	14.133500
Au	4.327494	5.829786	14.133500
Au	11.539983	3.331306	14.133500
Au	8.654987	3.331306	14.133500
Au	5.769991	3.331306	14.133500
Au	2.884996	3.331306	14.133500
Au	10.097485	0.832827	14.133500
Au	7.212489	0.832827	14.133500
Au	4.327494	0.832827	14.133500
Au	1.442498	0.832827	14.133500
Au	12.982480	9.161092	16.489100
Au	10.097485	9.161092	16.489100
Au	7.212489	9.161092	16.489100
Au	4.327494	9.161092	16.489100
Au	11.539983	6.662612	16.489100
Au	8.654987	6.662612	16.489100
Au	5.769991	6.662612	16.489100
Au	2.884996	6.662612	16.489100
Au	10.097485	4.164133	16.489100
Au	7.212489	4.164133	16.489100
Au	4.327494	4.164133	16.489100
Au	1.442498	4.164133	16.489100
Au	8.654987	1.665653	16.489100
Au	5.769991	1.665653	16.489100
Au	2.884996	1.665653	16.489100
Au	0.000000	1.665653	16.489100
S	7.128967	5.834195	18.658200
B	7.026727	5.681616	20.496900
B	5.728282	5.047245	21.412500
B	8.192446	6.442084	21.483400
B	6.611431	6.329666	22.103900
B	4.418876	4.340803	22.147300
B	9.422698	7.207317	22.277600
B	5.411749	5.540825	22.992700
B	7.871906	6.892871	23.078800
B	3.332470	3.559329	23.047400
B	10.611219	7.688887	23.250800
B	4.059552	4.856394	23.799500
B	6.333756	6.713083	23.841600
B	9.089418	7.760152	23.931000
B	3.036324	3.753745	24.626200
B	5.195036	5.812883	24.707000
B	7.657219	7.221819	24.762400
B	10.534628	8.006396	24.834900
B	3.919615	4.983750	25.492500
B	6.131367	6.993626	25.579900
B	8.998162	7.838142	25.637800
B	2.950589	3.797961	26.298900
B	5.054265	5.977830	26.394400
B	7.535294	7.338092	26.462600
B	10.470576	8.052194	26.504600
B	3.814170	5.053954	27.178000
B	8.918232	7.943854	27.319200
B	3.079617	3.730578	27.891400
B	5.198904	5.642439	28.040200
B	10.407575	7.795357	28.080100
B	7.677808	7.007185	28.096000
B	4.075048	4.588037	28.838900
B	9.122559	7.403304	28.972500
B	6.428436	6.314803	29.024400
B	5.268744	5.337584	29.700900
B	7.824930	6.772862	29.757600
B	6.607048	5.900051	30.659200
S	6.959232	5.785476	32.450800
Au	0.000000	1.665653	34.736100
Au	2.884996	1.665653	34.736100
Au	5.769991	1.665653	34.736100
Au	8.654987	1.665653	34.736100
Au	1.442498	4.164133	34.736100
Au	4.327494	4.164133	34.736100
Au	7.212489	4.164133	34.736100
Au	10.097485	4.164133	34.736100
Au	2.884996	6.662612	34.736100
Au	5.769991	6.662612	34.736100
Au	8.654987	6.662612	34.736100

B_{36-ii}

Au	1.442500	0.832830	0.000000
Au	4.327490	0.832830	0.000000
Au	7.212490	0.832830	0.000000
Au	10.097480	0.832830	0.000000
Au	2.885000	3.331310	0.000000
Au	5.769990	3.331310	0.000000
Au	8.654990	3.331310	0.000000
Au	11.539980	3.331310	0.000000
Au	4.327490	5.829790	0.000000
Au	7.212490	5.829790	0.000000
Au	10.097480	5.829790	0.000000
Au	12.982480	5.829790	0.000000
Au	5.769990	8.328270	0.000000
Au	8.654990	8.328270	0.000000
Au	11.539980	8.328270	0.000000
Au	14.424980	8.328270	0.000000
Au	0.000000	1.665650	2.355590
Au	2.885000	1.665650	2.355590
Au	5.769990	1.665650	2.355590
Au	8.654990	1.665650	2.355590
Au	1.442500	4.164130	2.355590
Au	4.327490	4.164130	2.355590
Au	7.212490	4.164130	2.355590
Au	10.097480	4.164130	2.355590
Au	2.885000	6.662610	2.355590
Au	5.769990	6.662610	2.355590
Au	8.654990	6.662610	2.355590
Au	11.539980	6.662610	2.355590
Au	4.327490	9.161090	2.355590
Au	7.212490	9.161090	2.355590
Au	10.097480	9.161090	2.355590
Au	12.982480	9.161090	2.355590
Au	0.000000	0.000000	4.711180
Au	2.885000	0.000000	4.711180
Au	5.769990	0.000000	4.711180
Au	8.654990	0.000000	4.711180
Au	1.442500	2.498480	4.711180
Au	4.327490	2.498480	4.711180
Au	7.212490	2.498480	4.711180
Au	10.097480	2.498480	4.711180
Au	2.885000	4.996960	4.711180
Au	5.769990	4.996960	4.711180
Au	8.654990	4.996960	4.711180
Au	11.539980	4.996960	4.711180
Au	4.327490	7.495440	4.711180
Au	7.212490	7.495440	4.711180
Au	10.097480	7.495440	4.711180
Au	12.982480	7.495440	4.711180
Au	1.442500	0.832830	7.066770
Au	4.327490	0.832830	7.066770
Au	7.212490	0.832830	7.066770
Au	10.097480	0.832830	7.066770
Au	2.885000	3.331310	7.066770
Au	5.769990	3.331310	7.066770
Au	8.654990	3.331310	7.066770
Au	11.539980	3.331310	7.066770
Au	4.327490	5.829790	7.066770
Au	7.212490	5.829790	7.066770
Au	10.097480	5.829790	7.066770
Au	12.982480	5.829790	7.066770
Au	5.769990	8.328270	7.066770
Au	8.654990	8.328270	7.066770
Au	11.539980	8.328270	7.066770
Au	14.424980	8.328270	7.066770
Au	0.000000	1.665650	9.422360
Au	2.885000	1.665650	9.422360
Au	5.769990	1.665650	9.422360
Au	8.654990	1.665650	9.422360
Au	1.442500	4.164130	9.422360
Au	4.327490	4.164130	9.422360
Au	7.212490	4.164130	9.422360
Au	10.097480	4.164130	9.422360
Au	2.885000	6.662610	9.422360
Au	5.769990	6.662610	9.422360
Au	8.654990	6.662610	9.422360
Au	11.539980	6.662610	9.422360
Au	4.327490	9.161090	9.422360
Au	7.212490	9.161090	9.422360
Au	10.097480	9.161090	9.422360
Au	12.982480	9.161090	9.422360
Au	0.000000	0.000000	11.777950
Au	2.885000	0.000000	11.777950
Au	5.769990	0.000000	11.777950
Au	8.654990	0.000000	11.777950
Au	1.442500	2.498480	11.777950
Au	4.327490	2.498480	11.777950
Au	7.212490	2.498480	11.777950
Au	10.097480	2.498480	11.777950
Au	2.885000	4.996960	11.777950
Au	5.769990	4.996960	11.777950
Au	8.654990	4.996960	11.777950
Au	11.539980	4.996960	11.777950
Au	4.327490	7.495440	11.777950
Au	7.212490	7.495440	11.777950
Au	10.097480	7.495440	11.777950
Au	12.982480	7.495440	11.777950
Au	1.442498	0.832827	14.133900
Au	4.327494	0.832827	14.133900
Au	7.212489	0.832827	14.133900
Au	10.097485	0.832827	14.133900
Au	2.884996	3.331306	14.133900
Au	5.769991	3.331306	14.133900
Au	8.654987	3.331306	14.133900
Au	11.539983	3.331306	14.133900
Au	4.327494	5.829786	14.133900
Au	7.212489	5.829786	14.133900
Au	10.097485	5.829786	14.133900
Au	12.982480	5.829786	14.133900
Au	5.769991	8.328265	14.133900
Au	8.654987	8.328265	14.133900
Au	11.539983	8.328265	14.133900
Au	14.424978	8.328265	14.133900
Au	0.000000	1.665653	16.489400
Au	2.884996	1.665653	16.489400
Au	5.769991	1.665653	16.489400
Au	8.654987	1.665653	16.489400
Au	1.442498	4.164133	16.489400
Au	4.327494	4.164133	16.489400
Au	7.212489	4.164133	16.489400
Au	10.097485	4.164133	16.489400
Au	2.884996	6.662612	16.489400
Au	5.769991	6.662612	16.489400
Au	8.654987	6.662612	16.489400
Au	11.539983	6.662612	16.489400
Au	4.327494	9.161092	16.489400
Au	7.212489	9.161092	16.489400
Au	10.097485	9.161092	16.489400
Au	12.982480	9.161092	16.489400
S	7.120218	5.875543	18.614800
B	7.020103	5.681226	20.434900
B	5.686825	5.100171	21.355700
B	8.174929	6.422381	21.447400
B	6.616915	6.336513	22.072500
B	4.420229	4.360249	22.130200
B	9.402907	7.210764	22.306000
B	5.320005	5.663960	22.912300
B	7.817028	7.055064	22.978900
B	3.336674	3.547902	23.034700
B	10.609413	7.675164	23.289900
B	6.251684	6.865505	23.788600
B	4.088825	4.824717	23.790500
B	9.057589	7.758547	23.923100
B	3.048226	3.724130	24.605100
B	5.094215	5.945644	24.620300
B	7.609409	7.448710	24.683800
B	10.516429	7.972465	24.828400
B	3.936723	5.009528	25.453500
B	6.226862	6.991697	25.498200
B	2.952423	3.784354	26.295300
B	5.014230	5.994096	26.332300
B	7.546958	7.462641	26.402300
B	10.457624	7.994861	26.497300
B	3.910223	4.940771	27.135500
B	6.125030	6.921805	27.204800
B	8.935236	7.771029	27.269200
B	3.055984	3.732547	27.895000
B	10.417319	7.783381	28.052700
B	5.102113	5.794638	28.067900
B	7.608892	7.141170	28.139600
B	4.076040	4.576126	28.845100
B	9.134907	7.345443	28.943400
B	6.346763	6.460263	28.990600
B	5.316462	5.306025	29.673400
B	7.826839	6.633741	29.743300
B	6.624997	5.869047	30.690100
S	6.862239	5.844230	32.523700
Au	12.982480	9.161092	34.736400
Au	10.097485	9.161092	34.736400
Au	7.212489	9.161092	34.736400
Au	4.327494	9.161092	34.736400
Au	11.539983	6.662612	34.736400
Au	8.654987	6.662612	34.736400
Au	5.769991	6.662612	34.736400
Au	2.884996	6.662612	34.736400
Au	10.097485	4.164133	34.736400
Au	7.212489	4.164133	34.736400
Au	4.327494	4.164133	34.736400

Au	8.654987	1.665653	34.736400	Au	4.327494	9.161092	34.736400	Au	11.539983	6.662612	34.736100	Au	1.442498	4.164133	34.736400
Au	5.769991	1.665653	34.736400	Au	7.212489	9.161092	34.736400	Au	4.327494	9.161092	34.736100	Au	8.654987	1.665653	34.736400
Au	2.884996	1.665653	34.736400	Au	10.097485	9.161092	34.736400	Au	7.212489	9.161092	34.736100	Au	5.769991	1.665653	34.736400
Au	0.000000	1.665653	34.736400	Au	12.982480	9.161092	34.736400	Au	10.097485	9.161092	34.736100	Au	2.884996	1.665653	34.736400
Au	12.982480	7.495439	37.070100	Au	0.000000	0.000000	37.070100	Au	12.982480	9.161092	34.736100	Au	0.000000	1.665653	34.736400
Au	10.097485	7.495439	37.070100	Au	2.884996	0.000000	37.070100	Au	0.000000	0.000000	37.069700	Au	12.982480	7.495439	37.070100
Au	7.212489	7.495439	37.070100	Au	5.769991	0.000000	37.070100	Au	2.884996	0.000000	37.069700	Au	10.097485	7.495439	37.070100
Au	4.327494	7.495439	37.070100	Au	8.654987	0.000000	37.070100	Au	5.769991	0.000000	37.069700	Au	7.212489	7.495439	37.070100
Au	11.539983	4.996959	37.070100	Au	1.442498	2.498480	37.070100	Au	8.654987	0.000000	37.069700	Au	4.327494	7.495439	37.070100
Au	8.654987	4.996959	37.070100	Au	4.327494	2.498480	37.070100	Au	1.442498	2.498480	37.069700	Au	11.539983	4.996959	37.070100
Au	5.769991	4.996959	37.070100	Au	7.212489	2.498480	37.070100	Au	4.327494	2.498480	37.069700	Au	8.654987	4.996959	37.070100
Au	2.884996	4.996959	37.070100	Au	10.097485	2.498480	37.070100	Au	7.212489	2.498480	37.069700	Au	5.769991	4.996959	37.070100
Au	10.097485	2.498480	37.070100	Au	2.884996	4.996959	37.070100	Au	10.097485	2.498480	37.069700	Au	2.884996	4.996959	37.070100
Au	7.212489	2.498480	37.070100	Au	5.769991	4.996959	37.070100	Au	2.884996	4.996959	37.069700	Au	10.097485	2.498480	37.070100
Au	4.327494	2.498480	37.070100	Au	8.654987	4.996959	37.070100	Au	5.769991	4.996959	37.069700	Au	7.212489	2.498480	37.070100
Au	1.442498	2.498480	37.070100	Au	11.539983	4.996959	37.070100	Au	8.654987	4.996959	37.069700	Au	4.327494	2.498480	37.070100
Au	8.654987	0.000000	37.070100	Au	4.327494	7.495439	37.070100	Au	11.539983	4.996959	37.069700	Au	1.442498	2.498480	37.070100
Au	5.769991	0.000000	37.070100	Au	7.212489	7.495439	37.070100	Au	4.327494	7.495439	37.069700	Au	8.654987	0.000000	37.070100
Au	2.884996	0.000000	37.070100	Au	10.097485	7.495439	37.070100	Au	7.212489	7.495439	37.069700	Au	5.769991	0.000000	37.070100
Au	0.000000	0.000000	37.070100	Au	12.982480	7.495439	37.070100	Au	10.097485	7.495439	37.069700	Au	2.884996	0.000000	37.070100
Au	1.442500	0.832830	39.425300	Au	1.442500	0.832830	39.425300	Au	12.982480	7.495439	37.069700	Au	0.000000	0.000000	37.070100
Au	4.327490	0.832830	39.425300	Au	4.327490	0.832830	39.425300	Au	1.442500	0.832830	39.425300	Au	1.442500	0.832830	39.425300
Au	7.212490	0.832830	39.425300	Au	7.212490	0.832830	39.425300	Au	4.327490	0.832830	39.425300	Au	4.327490	0.832830	39.425300
Au	10.097480	0.832830	39.425300	Au	10.097480	0.832830	39.425300	Au	7.212490	0.832830	39.425300	Au	7.212490	0.832830	39.425300
Au	2.885000	3.331310	39.425300	Au	2.885000	3.331310	39.425300	Au	10.097480	0.832830	39.425300	Au	10.097480	0.832830	39.425300
Au	5.769990	3.331310	39.425300	Au	5.769990	3.331310	39.425300	Au	2.885000	3.331310	39.425300	Au	2.885000	3.331310	39.425300
Au	8.654990	3.331310	39.425300	Au	8.654990	3.331310	39.425300	Au	5.769990	3.331310	39.425300	Au	5.769990	3.331310	39.425300
Au	11.539980	3.331310	39.425300	Au	11.539980	3.331310	39.425300	Au	8.654990	3.331310	39.425300	Au	8.654990	3.331310	39.425300
Au	4.327490	5.829790	39.425300	Au	4.327490	5.829790	39.425300	Au	11.539980	3.331310	39.425300	Au	11.539980	3.331310	39.425300
Au	7.212490	5.829790	39.425300	Au	7.212490	5.829790	39.425300	Au	4.327490	5.829790	39.425300	Au	4.327490	5.829790	39.425300
Au	10.097480	5.829790	39.425300	Au	10.097480	5.829790	39.425300	Au	7.212490	5.829790	39.425300	Au	7.212490	5.829790	39.425300
Au	12.982480	5.829790	39.425300	Au	12.982480	5.829790	39.425300	Au	10.097480	5.829790	39.425300	Au	10.097480	5.829790	39.425300
Au	5.769990	8.328270	39.425300	Au	5.769990	8.328270	39.425300	Au	12.982480	5.829790	39.425300	Au	12.982480	5.829790	39.425300
Au	8.654990	8.328270	39.425300	Au	8.654990	8.328270	39.425300	Au	5.769990	8.328270	39.425300	Au	5.769990	8.328270	39.425300
Au	11.539980	8.328270	39.425300	Au	11.539980	8.328270	39.425300	Au	8.654990	8.328270	39.425300	Au	8.654990	8.328270	39.425300
Au	14.424980	8.328270	39.425300	Au	14.424980	8.328270	39.425300	Au	11.539980	8.328270	39.425300	Au	11.539980	8.328270	39.425300
Au	0.000000	1.665650	41.780900	Au	0.000000	1.665650	41.780900	Au	14.424980	8.328270	39.425300	Au	14.424980	8.328270	39.425300
Au	2.885000	1.665650	41.780900	Au	2.885000	1.665650	41.780900	Au	0.000000	1.665650	41.780900	Au	0.000000	1.665650	41.780900
Au	5.769990	1.665650	41.780900	Au	5.769990	1.665650	41.780900	Au	2.885000	1.665650	41.780900	Au	2.885000	1.665650	41.780900
Au	8.654990	1.665650	41.780900	Au	8.654990	1.665650	41.780900	Au	5.769990	1.665650	41.780900	Au	5.769990	1.665650	41.780900
Au	1.442500	4.164130	41.780900	Au	1.442500	4.164130	41.780900	Au	8.654990	1.665650	41.780900	Au	8.654990	1.665650	41.780900
Au	4.327490	4.164130	41.780900	Au	4.327490	4.164130	41.780900	Au	1.442500	4.164130	41.780900	Au	1.442500	4.164130	41.780900
Au	7.212490	4.164130	41.780900	Au	7.212490	4.164130	41.780900	Au	4.327490	4.164130	41.780900	Au	4.327490	4.164130	41.780900
Au	10.097480	4.164130	41.780900	Au	10.097480	4.164130	41.780900	Au	7.212490	4.164130	41.780900	Au	7.212490	4.164130	41.780900
Au	2.885000	6.662610	41.780900	Au	2.885000	6.662610	41.780900	Au	10.097480	4.164130	41.780900	Au	10.097480	4.164130	41.780900
Au	5.769990	6.662610	41.780900	Au	5.769990	6.662610	41.780900	Au	2.885000	6.662610	41.780900	Au	2.885000	6.662610	41.780900
Au	8.654990	6.662610	41.780900	Au	8.654990	6.662610	41.780900	Au	5.769990	6.662610	41.780900	Au	5.769990	6.662610	41.780900
Au	11.539980	6.662610	41.780900	Au	11.539980	6.662610	41.780900	Au	8.654990	6.662610	41.780900	Au	8.654990	6.662610	41.780900
Au	4.327490	9.161090	41.780900	Au	4.327490	9.161090	41.780900	Au	11.539980	6.662610	41.780900	Au	11.539980	6.662610	41.780900
Au	7.212490	9.161090	41.780900	Au	7.212490	9.161090	41.780900	Au	4.327490	9.161090	41.780900	Au	4.327490	9.161090	41.780900
Au	10.097480	9.161090	41.780900	Au	10.097480	9.161090	41.780900	Au	7.212490	9.161090	41.780900	Au	7.212490	9.161090	41.780900
Au	12.982480	9.161090	41.780900	Au	12.982480	9.161090	41.780900	Au	10.097480	9.161090	41.780900	Au	10.097480	9.161090	41.780900
Au	0.000000	0.000000	44.136500	Au	0.000000	0.000000	44.136500	Au	12.982480	9.161090	41.780900	Au	12.982480	9.161090	41.780900
Au	2.885000	0.000000	44.136500	Au	2.885000	0.000000	44.136500	Au	0.000000	0.000000	44.136500	Au	0.000000	0.000000	44.136500
Au	5.769990	0.000000	44.136500	Au	5.769990	0.000000	44.136500	Au	2.885000	0.000000	44.136500	Au	2.885000	0.000000	44.136500
Au	8.654990	0.000000	44.136500	Au	8.654990	0.000000	44.136500	Au	5.769990	0.000000	44.136500	Au	5.769990	0.000000	44.136500
Au	1.442500	2.498480	44.136500	Au	1.442500	2.498480	44.136500	Au	8.654990	0.000000	44.136500	Au	8.654990	0.000000	44.136500
Au	4.327490	2.498480	44.136500	Au	4.327490	2.498480	44.136500	Au	1.442500	2.498480	44.136500	Au	1.442500	2.498480	44.136500
Au	7.212490	2.498480	44.136500	Au	7.212490	2.498480	44.136500	Au	4.327490	2.498480	44.136500	Au	4.327490	2.498480	44.136500
Au	10.097480	2.498480	44.136500	Au	10.097480	2.498480	44.136500	Au	7.212490	2.498480	44.136500	Au	7.212490	2.498480	44.136500
Au	2.885000	4.996960	44.136500	Au	2.885000	4.996960	44.136500	Au	10.097480	2.498480	44.136500	Au	10.097480	2.498480	44.136500
Au	5.769990	4.996960	44.136500	Au	5.769990	4.996960	44.136500	Au	2.885000	4.996960	44.136500	Au	2.885000	4.996960	44.136500
Au	8.654990	4.996960	44.136500	Au	8.654990	4.996960	44.136500	Au	5.769990	4.996960	44.136500	Au	5.769990	4.996960	44.136500
Au	11.539980	4.996960	44.136500	Au	11.539980	4.996960	44.136500	Au	8.654990	4.996960	44.136500	Au	8.654990	4.996960	44.136500
Au	4.327490	7.495440	44.136500	Au	4.327490	7.495440	44.136500	Au	11.539980	4.996960	44.136500	Au	11.539980	4.996960	44.136500
Au	7.212490	7.495440	44.136500	Au	7.212490	7.495440	44.136500	Au	4.327490	7.495440	44.136500	Au	4.327490	7.495440	44.136500
Au	10.097480	7.495440	44.136500	Au	10.097480	7.495440	44.136500	Au	7.212490	7.495440	44.136500	Au	7.212490	7.495440	44.136500
Au	12.982480	7.495440	44.136500	Au	12.982480	7.495440	44.136500	Au	10.097480	7.495440	44.136500	Au	10.097480	7.495440	44.136500
Au	1.442500	0.832830	46.492100	Au	1.442500	0.832830	46.492100	Au	12.982480	7.495440	44.136500	Au	12.982480	7.495440	44.136500
Au	4.327490	0.832830	46.492100	Au	4.327490	0.832830	46.492100	Au	1.442500	0.832830	46.492100	Au	1.442500	0.832830	46.492100
Au	7.212490	0.832830	46.492100	Au	7.212490	0.832830	46.492100	Au	4.327490	0.832830	46.492100	Au	4.327490	0.832830	46.492100
Au	10.097480	0.832830	46.492100	Au	10.097480	0.832830	46.492100	Au	7.212490	0.832830	46.492100	Au	7.212490	0.832830	46.492100
Au	2.885000	3.331310	46.492100	Au	2.885000	3.331310	46.492100	Au	10.097480	0.832830	46.492100	Au	10.097480	0.832830	46.492100
Au	5.769990	3.331310	46.492100	Au	5.769990	3.331310	46.492100	Au	2.885000	3.331310	46.492100	Au	2.885000	3.331310	46.492100
Au	8.654990	3.331310	46.492100	Au	8.654990	3.331310	46.492100	Au	5.769990	3.331310	46.492100	Au	5.769990	3.331310	46.492100
Au	11.539980	3.331310	46.492100	Au	11.539980	3.331310	46.492100	Au	8.654990	3.331310	46.492100	Au	8.654990	3.331310	46.492100
Au	4.327490	5.829790	46.492100	Au	4.327490	5.829790	46.492100	Au	11.539980	3.331310	46.492100	Au	11.539980	3.331310	46.492100
Au	7.212490	5.829790	46.492100	Au	7.212490	5.829790	46.492100	Au	4.327490	5.829790	46.492100	Au	4.327490	5.829790	46.492100
Au	10.097480	5.829790	46.492100	Au	10.097480	5.829790	46.492100	Au	7.212490	5.829790	46.492100	Au	7.212490	5.829790	46.492100
Au	12.982480	5.829790	46.492100	Au	12.982480	5.829790	46.492100	Au	10.097480	5.829790	46.492100	Au	10.097480	5.829790	46.492100
Au	5.769990	8.328270	46.492100	Au	5.769990	8.328270	46.492100	Au	12.982480	5.829790	46.492100	Au	12.982480	5.829790	46.492100
Au	8.654990	8.328270	46.492100	Au	8.654990	8.328270	46.492100	Au	5.769990	8.328270	46.492100	Au	5.769990	8.328270	46.492100
Au	11.539980	8.328270	46.492100	Au	11.539980	8.328270	46.492100	Au	8.654990	8.328270	46.492100	Au	8.654990	8.328270	46.492100
Au	14.424980	8.328270	46.492100	Au	14.424980	8.328270	46.492100	Au	11.539980	8.328270	46.492100	Au	11.539980	8.328270	46.492100
Au	0.000000	1.665650	48.847700	Au	0.000000	1.665650	48.847700	Au	14.424980	8.328270	46.492100	Au	14.424980	8.328270	46.492100
Au	2.885000	1.665650	48.847700	Au	2.885000	1.665650	48.847700	Au	0.000000	1.665650	48.847700	Au	0.000000	1.665650	48.847700
Au	5.769990	1.665650	48.847700	Au	5.769990	1.665650	48.847700	Au	2.885000	1.665650	48.847700	Au	2.885000	1.665650	48.847700
Au	8.654990	1.665650	48.847700	Au	8.654990	1.665650	48.847700	Au	5.769990	1.665650	48.847700	Au	5.769990	1.665650	48.847700
Au	1.442500	4.164130	48.847700	Au	1.442500	4.164130	48.847700	Au	8.654990	1.665650	48.847700	Au	8.654990	1.665650	48.847700
Au	4.327490	4.164130	48.847700	Au	4.327490	4.164130	48.847700	Au	1.442500	4.164130	48.847700	Au	1.442500	4.164130	48.847700
Au	7.212490	4.164130	48.847700	Au	7.212490	4.164130	48.847700	Au	4.327490	4.164130	48.847700	Au	4.327490	4.164130	48.847700
Au	10.097480	4.164130	48.847700	Au	10.097480	4.164130	48.847700	Au	7.212490	4.164130	48.847700	Au	7.212490	4.164130	48.847700
Au	2.885000	6.662610	48.847700	Au	2.885000	6.662610	48.847700	Au	10.097480	4.164130	48.847700	Au	10.097480	4.164130	48.847700
Au	5.769990	6.662610	48.847700	Au	5.769990	6.662610	48.847700	Au	2.885000	6.662610	48.847700	Au	2.885000	6.662610	48.847700
Au	8.654990	6.662610	48.847700	Au	8.654990	6.662610	48.847700	Au	5.769990	6.662610	48.847700	Au	5.769990	6.662610	48.847700
Au	11.539980	6.662610	48.847700	Au	11.539980	6.662610	48.847700	Au	8.654990	6.662610	48.847700	Au	8.654990	6.662610	48.847700
Au	4.327490	9.161090	48.847700	Au	4.327490	9.161090	48.847700	Au	11.539980	6.662610	48.847700	Au	11.539980	6.662610	48.847700
Au	7.212490	9.161090	48.847700	Au	7.212490	9.161090	48.847700	Au	4.327490	9.161090	48.847700	Au	4.327490	9.161090	48.847700
Au	10.097480	9.161090	48.847700	Au	10.097480	9.161090	48.847700	Au	7.212490	9.161090	48.847700	Au	7.212490	9.161090	48.847700
Au	12.982480	9.161090	48.847700	Au	12.982480	9.161090	48.847700	Au	10.097480	9.161090	48.847700	Au	10.097480	9.161090	48.847700
Au	0.000000	0.000000	51.203300	Au	0.000000	0.000000	51.203300	Au	12.982480	9.161090	48.847700	Au	12.982480	9.161090	48.847700
Au	2.885000	0.000000	51.203300	Au	2.885000	0.000000	51.203300	Au	0.000000	0.000000	51.203300	Au	0.000000	0.000000	51.203300
Au	5.769990	0.000000	51.203300	Au	5.769990	0.000000	51.203300	Au	2.885000	0.000000	51.203300	Au	2.885000	0.000000	51.203300
Au	8.654990	0.000000	51.203300	Au	8.654990	0.000000	51.203300	Au	5.769990	0.000000	51.203300	Au	5.769990	0.000000	51.203300
Au	1.442500	2.498480	51.203300	Au	1.442500	2.498480	51.203300	Au	8.654990	0.000000	51.203300	Au	8.654990	0.000000	51.203300
Au	4.327490	2.498480	51.203300	Au	4.327490	2.498480	51.203300	Au	1.442500	2.498480	51.203300	Au	1.442500	2.498480	51.203300
Au	7.212490	2.498480	51.203300	Au	7.212490	2.498480	51.203300	Au	4.327490	2.498480	51.203300	Au	4.327490	2.498480	51.203300
Au	10.097480	2.498480	51.203300	Au	10.097480	2.498480	51.203300	Au	7.212490	2.498480	51.203300	Au	7.212490	2.498480	51.203300
Au	2.885000	4.996960	51.203300	Au	2.885000	4.996960	51.203300	Au	10.097480	2.498480	51.203300	Au	10.097480	2.498480	51.203300
Au	5.769990	4.996960	51.203300	Au	5.769990	4.996960	51.203300	Au	2.885000	4.996960	51.203300	Au	2.885000	4.996960	51.203300
Au	8.654990	4.996960	51.203300	Au	8.654990	4.996960	51.203300	Au	5.769990	4.996960	51.203300	Au	5.769990	4.996960	51.203300
Au	11.539980	4.996960	51.203300	Au	11.539980	4.996960	51.203300	Au	8.654990	4.996960	51.203300	Au	8.654990	4.996960	51.203300
Au	4.327490	7.495440	51.203300	Au	4.327490	7.495440	51.203300	Au	11.539980	4.996960	51.203300	Au	11.539980	4.996960	51.203300
Au	7.212490	7.495440	51.203300	Au	7.212490	7.495440	51.203300	Au	4.327490	7.495440	51.203300	Au	4.327490	7.495440	51.203300
Au	10.097480	7.495440	51.203300	Au	10.097480	7.495440	51.203300	Au	7.212490	7.495440	51.203300	Au	7.212490	7.495440	51.203300
Au	12.982480	7.495440	51.203300	Au	12.982480	7.495440	51.203300	Au	10.097480	7.495440	51.203300	Au	10.097480	7.495440	51.203300
								Au	12.982480	7.495440	51.203300	Au	12.982480	7.495440	51.203300