

Supporting information for

Obvious modulation of rectifying performance by conjugation breaking of the bridging fragment in donor-bridge-acceptor molecular diodes

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1. The optimized structure for bare AQ molecule (in .xyz format)

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XYZ file

H	3.029188	5.512366	14.554730
S	1.947984	6.145095	15.075720
H	4.233810	4.826522	16.453130
C	2.364281	5.905419	16.761830
C	3.529445	5.233316	17.195900
H	0.556850	6.948893	17.386370
C	1.465166	6.424781	17.722660
C	3.789758	5.083082	18.559080
H	4.696580	4.558830	18.895500
C	1.726046	6.274480	19.083050
C	2.892797	5.600785	19.526920
H	1.029285	6.676779	19.832670
C	3.130806	5.461817	20.921580
C	3.280572	5.372428	22.143260
H	5.307716	4.215783	23.500080
C	3.412987	5.291869	23.556120
H	1.534848	6.355994	23.974450
C	4.536753	4.651596	24.151760
C	2.419217	5.852867	24.394070
C	4.654620	4.580669	25.538450
C	2.540951	5.779434	25.786860
H	5.511382	4.093306	26.029340
O	0.484656	6.941482	26.120780
C	3.664384	5.140768	26.369210
C	1.462977	6.387958	26.626280
C	3.828368	5.045988	27.839690
C	1.625626	6.295623	28.105120
O	4.802798	4.491714	28.356470
H	-0.222743	7.342803	28.450870
C	2.750410	5.658694	28.680160
C	0.637405	6.856585	28.936970
C	2.879727	5.588411	30.071300
C	0.763324	6.788420	30.324140
H	3.768548	5.085480	30.479710
C	1.891674	6.151120	30.908640
H	-0.002315	7.223771	30.981650
C	2.042858	6.071129	32.321740
C	2.212878	5.980916	33.538970
H	4.340673	4.781910	34.606930
C	2.469667	5.841530	34.931570

C	3.646942	5.177048	35.362300
H	0.660353	6.868594	35.570120
C	1.572271	6.353071	35.902700
C	3.919001	5.027281	36.720910
H	4.830846	4.512128	37.054390
C	1.842735	6.204262	37.262980
C	3.017998	5.539868	37.682040
H	1.148037	6.600202	38.017270
C	3.299730	5.383188	39.082360
N	3.534507	5.251902	40.226700

2. The optimized structure for bare AC molecule (in .xyz format)

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XYZ file

H	1.267409	6.522429	14.845410
S	2.434715	5.847538	14.987970
C	2.409872	5.782840	16.740400
H	4.286283	4.673631	16.763260
H	0.549139	6.874524	17.064260
C	3.484951	5.117239	17.372820
C	1.391197	6.349136	17.539480
C	3.538036	5.019912	18.761160
C	1.445025	6.251638	18.930760
H	4.374200	4.499464	19.249020
H	0.646095	6.696946	19.541470
C	2.520153	5.587430	19.569400
C	2.619912	5.484865	20.983080
C	2.795186	5.364355	22.197780
H	4.921763	4.122951	23.232700
C	3.048922	5.205724	23.585430
C	4.244294	4.511406	24.007540
H	1.263480	6.237585	24.231860
C	2.173534	5.707861	24.550280
C	4.525338	4.342268	25.343880
H	5.439259	3.810978	25.651660
C	2.438681	5.547183	25.939070
C	3.643035	4.847882	26.358280
H	0.649739	6.580555	26.604050
C	1.561582	6.049829	26.921720
C	3.904002	4.689327	27.729900
H	4.817311	4.159029	28.044870
C	1.822023	5.890739	28.291540

C	3.024952	5.191615	28.714830
H	0.023774	6.929880	28.973560
C	0.933220	6.399447	29.295750
C	3.277877	5.036620	30.110040
H	4.186620	4.509180	30.437450
C	1.201394	6.235619	30.635120
C	2.393995	5.542879	31.067410
H	0.517051	6.628806	31.399900
C	2.634233	5.404017	32.465080
C	2.778864	5.329922	33.688840
H	4.832251	4.190140	35.022550
C	2.943643	5.270548	35.102120
H	1.088774	6.332006	35.520250
C	4.079035	4.645331	35.680410
C	1.972585	5.850165	35.960990
C	4.243557	4.610200	37.065150
C	2.135412	5.816064	37.345610
H	5.125770	4.128542	37.509670
C	3.275052	5.198827	37.909760
H	1.383872	6.269634	38.006990
C	3.449415	5.175279	39.335660
N	3.592240	5.160756	40.502760

3. The optimized structure for bare AH molecule (in .xyz format)

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XYZ file

H	3.039839	5.536257	14.683970
S	1.866258	6.130687	15.013800
C	2.282834	6.488910	16.682160
H	4.267126	5.582144	16.704630
H	0.361203	7.470967	16.993880
C	3.506985	6.126324	17.284940
C	1.319775	7.182860	17.450520
C	3.763426	6.451846	18.618520
C	1.576650	7.506402	18.781730
H	4.721461	6.166232	19.077940
H	0.825293	8.049371	19.374100
C	2.803406	7.147678	19.393950
C	3.036855	7.486525	20.755420
C	3.171542	7.805273	21.937840
C	3.336446	8.174443	23.303440
H	5.316662	7.297843	23.463280

H	1.386265	9.125678	23.464660
C	2.315281	8.871782	23.994380
C	4.524820	7.846386	23.996440
C	2.492547	9.223812	25.335460
C	4.701354	8.209658	25.336480
H	6.518102	7.050503	25.578600
H	1.689937	9.762548	25.864420
C	3.678891	8.904091	26.018370
H	6.661184	8.765500	26.024830
C	5.979973	7.881522	26.077910
C	3.904044	9.293854	27.464670
H	4.464189	10.260090	27.492590
C	5.726241	7.554996	27.532750
H	7.271580	6.038093	27.676090
H	2.938281	9.487255	27.974050
C	6.483214	6.587443	28.215800
C	4.706206	8.251660	28.218990
C	6.251839	6.311814	29.565520
C	4.467478	7.973901	29.570710
H	6.847526	5.554416	30.093860
H	3.673390	8.510068	30.113250
C	5.235581	7.007624	30.264190
C	4.985806	6.733643	31.642160
C	4.773462	6.495449	32.833130
C	4.527618	6.220860	34.209080
H	2.879594	7.633733	34.369340
H	6.117538	4.742817	34.372470
C	3.491999	6.895583	34.906020
C	5.314148	5.268431	34.907550
C	3.251128	6.629034	36.253520
C	5.074989	5.000396	36.255080
H	2.448818	7.153810	36.790920
H	5.686254	4.262893	36.793960
C	4.041153	5.678843	36.939760
C	3.794357	5.403432	38.328110
N	3.592370	5.177485	39.464120

4. The optimized structure for the central region of AQ junction (in

.xyz format)

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XYZ file

Au	2.177184	1.011926	1.177289
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Au	5.060942	1.011926	1.177289
Au	7.944700	1.011926	1.177289
Au	10.828460	1.011926	1.177289
Au	13.712220	1.011926	1.177289
Au	0.735304	3.509334	1.177289
Au	3.619063	3.509334	1.177289
Au	6.502821	3.509334	1.177289
Au	9.386579	3.509334	1.177289
Au	12.270340	3.509334	1.177289
Au	-0.706575	6.006742	1.177289
Au	2.177184	6.006742	1.177289
Au	5.060942	6.006742	1.177289
Au	7.944700	6.006742	1.177289
Au	10.828460	6.006742	1.177289
Au	-2.148454	8.504150	1.177289
Au	0.735304	8.504150	1.177289
Au	3.619063	8.504150	1.177289
Au	6.502821	8.504150	1.177289
Au	9.386579	8.504150	1.177289
Au	-3.590333	11.001560	1.177289
Au	-0.706575	11.001560	1.177289
Au	2.177184	11.001560	1.177289
Au	5.060942	11.001560	1.177289
Au	7.944700	11.001560	1.177289
Au	0.735304	1.844395	3.531868
Au	3.619063	1.844395	3.531868
Au	6.502821	1.844395	3.531868
Au	9.386579	1.844395	3.531868
Au	12.270340	1.844395	3.531868
Au	-0.706575	4.341803	3.531868
Au	2.177184	4.341803	3.531868
Au	5.060942	4.341803	3.531868
Au	7.944700	4.341803	3.531868
Au	10.828460	4.341803	3.531868
Au	-2.148454	6.839211	3.531868
Au	0.735304	6.839211	3.531868
Au	3.619063	6.839211	3.531868
Au	6.502821	6.839211	3.531868
Au	9.386579	6.839211	3.531868
Au	-3.590333	9.336619	3.531868
Au	-0.706575	9.336619	3.531868
Au	2.177184	9.336619	3.531868
Au	5.060942	9.336619	3.531868
Au	7.944700	9.336619	3.531868

Au	-5.032212	11.834030	3.531868
Au	-2.148454	11.834030	3.531868
Au	0.735304	11.834030	3.531868
Au	3.619063	11.834030	3.531868
Au	6.502821	11.834030	3.531868
Au	0.735304	0.179457	5.886447
Au	3.619063	0.179457	5.886447
Au	6.502821	0.179457	5.886447
Au	9.386579	0.179457	5.886447
Au	12.270340	0.179457	5.886447
Au	-0.706575	2.676864	5.886447
Au	2.177184	2.676864	5.886447
Au	5.060942	2.676864	5.886447
Au	7.944700	2.676864	5.886447
Au	10.828460	2.676864	5.886447
Au	-2.148454	5.174272	5.886447
Au	0.735304	5.174272	5.886447
Au	3.619063	5.174272	5.886447
Au	6.502821	5.174272	5.886447
Au	9.386579	5.174272	5.886447
Au	-3.590333	7.671680	5.886447
Au	-0.706575	7.671680	5.886447
Au	2.177184	7.671680	5.886447
Au	5.060942	7.671680	5.886447
Au	7.944700	7.671680	5.886447
Au	-5.032212	10.169090	5.886447
Au	-2.148454	10.169090	5.886447
Au	0.735304	10.169090	5.886447
Au	3.619063	10.169090	5.886447
Au	6.502821	10.169090	5.886447
Au	2.177184	1.011926	8.241026
Au	5.060942	1.011926	8.241026
Au	7.944700	1.011926	8.241026
Au	10.828460	1.011926	8.241026
Au	13.712220	1.011926	8.241026
Au	0.735304	3.509334	8.241026
Au	3.619063	3.509334	8.241026
Au	6.502821	3.509334	8.241026
Au	9.386579	3.509334	8.241026
Au	12.270340	3.509334	8.241026
Au	-0.706575	6.006742	8.241026
Au	2.177184	6.006742	8.241026
Au	5.060942	6.006742	8.241026
Au	7.944700	6.006742	8.241026

Au	10.828460	6.006742	8.241026
Au	-2.148454	8.504150	8.241026
Au	0.735304	8.504150	8.241026
Au	3.619063	8.504150	8.241026
Au	6.502821	8.504150	8.241026
Au	9.386579	8.504150	8.241026
Au	-3.590333	11.001560	8.241026
Au	-0.706575	11.001560	8.241026
Au	2.177184	11.001560	8.241026
Au	5.060942	11.001560	8.241026
Au	7.944700	11.001560	8.241026
Au	12.273330	1.835502	10.685130
Au	3.627826	11.834710	10.685670
Au	0.723414	11.833920	10.689330
Au	10.822220	4.352072	10.689490
Au	6.494310	1.841651	10.691130
Au	7.943117	4.349984	10.691580
Au	6.508039	11.831000	10.705990
Au	-3.579154	9.330169	10.706810
Au	-2.138661	6.832598	10.706970
Au	-0.696595	9.332141	10.707110
Au	0.732465	1.853730	10.707290
Au	5.051178	9.334446	10.707370
Au	9.385982	6.845434	10.708360
Au	-2.154206	11.831810	10.708790
Au	3.622952	1.850030	10.709090
Au	6.500022	6.832470	10.709100
Au	7.932184	9.330090	10.709390
Au	-5.032638	11.847880	10.709450
Au	9.383136	1.845270	10.713310
Au	-0.723529	4.330815	10.718050
Au	2.177733	9.355473	10.718780
Au	0.745289	6.834047	10.729180
Au	2.182809	4.352458	10.732500
Au	3.613051	6.829113	10.732530
Au	5.065347	4.339173	10.732920
Au	-5.029868	10.167910	13.113130
Au	2.175632	2.630340	13.138500
Au	5.102046	7.696813	13.138610
Au	-0.731041	7.685896	13.142960
Au	10.820710	2.675461	13.143690
Au	9.383139	0.185587	13.144020
Au	0.607539	5.090908	13.146970
Au	7.944942	2.675599	13.147440

Au	2.186251	7.823369	13.149240
Au	12.270850	0.179230	13.169620
Au	6.499466	0.176389	13.171020
Au	9.388128	5.178594	13.171260
Au	-3.591234	7.668739	13.178350
Au	-2.146431	10.171960	13.178690
Au	6.508409	10.181610	13.179820
Au	0.727911	0.169070	13.180080
Au	7.958939	7.665737	13.184090
Au	3.630664	0.171262	13.184420
Au	-0.740841	2.626687	13.194550
Au	3.645610	10.223460	13.194780
Au	-2.197589	5.168363	13.195070
Au	0.715693	10.213530	13.195190
Au	3.724022	5.114251	13.196210
Au	5.086227	2.637304	13.202990
Au	6.551021	5.171915	13.203070
S	2.197759	5.994696	14.956670
H	4.406653	4.729994	16.453650
C	2.533370	5.807366	16.694139
C	3.685745	5.145425	17.176920
H	0.703586	6.860994	17.223801
C	1.597175	6.347274	17.608219
C	3.892868	5.027535	18.554939
H	4.787562	4.513282	18.935511
C	1.807858	6.227140	18.981939
C	2.960067	5.564105	19.483450
H	1.080451	6.646207	19.692610
C	3.152278	5.451702	20.893169
C	3.265588	5.382828	22.122110
H	5.287127	4.226115	23.488991
C	3.392341	5.304558	23.541130
H	1.516109	6.369196	23.976170
C	4.515711	4.662574	24.139450
C	2.402908	5.863435	24.386551
C	4.636007	4.588826	25.526800
C	2.526967	5.787157	25.780720
H	5.494054	4.098846	26.012911
O	0.471418	6.948509	26.127831
C	3.649552	5.147342	26.363180
C	1.451922	6.393568	26.626190
C	3.815933	5.050347	27.837601
C	1.617508	6.298988	28.107491
O	4.790551	4.494297	28.349939

H	-0.230255	7.345501	28.447580
C	2.741426	5.662457	28.684759
C	0.628000	6.860534	28.937410
C	2.868371	5.594246	30.078030
C	0.749482	6.795220	30.324789
H	3.754863	5.092840	30.494940
C	1.877133	6.159124	30.912029
H	-0.018236	7.231565	30.979931
C	2.019052	6.085569	32.326550
C	2.169215	6.007601	33.547180
H	4.305278	4.807254	34.566448
C	2.436537	5.862303	34.935951
C	3.623584	5.193677	35.336689
H	0.632306	6.883358	35.610592
C	1.549932	6.365742	35.923561
C	3.918196	5.030196	36.686310
H	4.833410	4.514207	37.006180
C	1.840144	6.204620	37.277561
C	3.025396	5.535699	37.657940
H	1.163228	6.588291	38.054211
C	3.336878	5.360705	39.035049
N	3.624071	5.198657	40.159710
Au	-0.729261	7.709664	42.260899
Au	3.596967	0.208855	42.265911
Au	7.930718	7.714881	42.265980
Au	-0.725408	2.716742	42.268120
Au	-2.172917	5.210120	42.268341
Au	7.927125	2.712877	42.268360
Au	3.596604	10.204330	42.268501
Au	0.712998	10.210240	42.268688
Au	0.707577	0.212105	42.271069
Au	6.483103	10.216580	42.271320
Au	9.378925	5.209035	42.271351
Au	6.489262	0.206678	42.271450
Au	0.685587	5.212813	42.282429
Au	2.140796	7.734145	42.284340
Au	-5.063008	10.212620	42.292389
Au	10.809120	2.722060	42.295120
Au	9.358398	0.211911	42.296471
Au	-3.609297	7.698734	42.298168
Au	-2.160127	10.209540	42.298790
Au	2.142060	2.682751	42.300999
Au	12.255070	0.214972	42.301819
Au	5.060625	7.738746	42.302711

Au	5.059816	2.679904	42.319309
Au	6.522253	5.212721	42.319759
Au	3.603330	5.209548	42.417728
Au	-3.613579	9.375192	44.740410
Au	-2.168356	6.878766	44.741890
Au	12.249820	1.884648	44.742008
Au	-0.729421	9.371441	44.742088
Au	3.595942	11.870790	44.742111
Au	9.368367	1.880508	44.742580
Au	0.711968	6.877764	44.743099
Au	3.594085	1.880724	44.743179
Au	6.481308	6.880965	44.743309
Au	9.362251	6.877994	44.743790
Au	7.923016	9.373565	44.744061
Au	-5.053036	11.872810	44.744068
Au	-2.172929	11.873790	44.744129
Au	6.484260	11.870830	44.746849
Au	10.809430	4.384894	44.746910
Au	2.139544	4.372811	44.746941
Au	0.709422	11.866820	44.747059
Au	-0.731731	4.377726	44.747471
Au	2.155325	9.378930	44.747791
Au	3.595603	6.894994	44.747952
Au	0.706425	1.880946	44.748402
Au	5.037051	9.382710	44.748562
Au	6.493127	1.877433	44.749691
Au	7.933742	4.371830	44.749809
Au	5.057163	4.369736	44.764721
Au	2.154234	1.050646	47.216160
Au	5.037992	1.050646	47.216160
Au	7.921750	1.050646	47.216160
Au	10.805510	1.050646	47.216160
Au	13.689270	1.050646	47.216160
Au	0.712355	3.548054	47.216160
Au	3.596113	3.548054	47.216160
Au	6.479871	3.548054	47.216160
Au	9.363629	3.548054	47.216160
Au	12.247390	3.548054	47.216160
Au	-0.729525	6.045462	47.216160
Au	2.154234	6.045462	47.216160
Au	5.037992	6.045462	47.216160
Au	7.921750	6.045462	47.216160
Au	10.805510	6.045462	47.216160
Au	-2.171404	8.542870	47.216160

Au	0.712355	8.542870	47.216160
Au	3.596113	8.542870	47.216160
Au	6.479871	8.542870	47.216160
Au	9.363629	8.542870	47.216160
Au	-3.613283	11.040280	47.216160
Au	-0.729525	11.040280	47.216160
Au	2.154234	11.040280	47.216160
Au	5.037992	11.040280	47.216160
Au	7.921750	11.040280	47.216160
Au	0.712355	0.218177	49.570728
Au	3.596113	0.218177	49.570728
Au	6.479871	0.218177	49.570728
Au	9.363629	0.218177	49.570728
Au	12.247390	0.218177	49.570728
Au	-0.729525	2.715585	49.570728
Au	2.154234	2.715585	49.570728
Au	5.037992	2.715585	49.570728
Au	7.921750	2.715585	49.570728
Au	10.805510	2.715585	49.570728
Au	-2.171404	5.212993	49.570728
Au	0.712355	5.212993	49.570728
Au	3.596113	5.212993	49.570728
Au	6.479871	5.212993	49.570728
Au	9.363629	5.212993	49.570728
Au	-3.613283	7.710400	49.570728
Au	-0.729525	7.710400	49.570728
Au	2.154234	7.710400	49.570728
Au	5.037992	7.710400	49.570728
Au	7.921750	7.710400	49.570728
Au	-5.055162	10.207810	49.570728
Au	-2.171404	10.207810	49.570728
Au	0.712355	10.207810	49.570728
Au	3.596113	10.207810	49.570728
Au	6.479871	10.207810	49.570728
Au	0.712355	1.883115	51.925308
Au	3.596113	1.883115	51.925308
Au	6.479871	1.883115	51.925308
Au	9.363629	1.883115	51.925308
Au	12.247390	1.883115	51.925308
Au	-0.729525	4.380523	51.925308
Au	2.154234	4.380523	51.925308
Au	5.037992	4.380523	51.925308
Au	7.921750	4.380523	51.925308
Au	10.805510	4.380523	51.925308

Au	-2.171404	6.877931	51.925308
Au	0.712355	6.877931	51.925308
Au	3.596113	6.877931	51.925308
Au	6.479871	6.877931	51.925308
Au	9.363629	6.877931	51.925308
Au	-3.613283	9.375339	51.925308
Au	-0.729525	9.375339	51.925308
Au	2.154234	9.375339	51.925308
Au	5.037992	9.375339	51.925308
Au	7.921750	9.375339	51.925308
Au	-5.055162	11.872750	51.925308
Au	-2.171404	11.872750	51.925308
Au	0.712355	11.872750	51.925308
Au	3.596113	11.872750	51.925308
Au	6.479871	11.872750	51.925308
Au	2.154234	1.050646	54.279888
Au	5.037992	1.050646	54.279888
Au	7.921750	1.050646	54.279888
Au	10.805510	1.050646	54.279888
Au	13.689270	1.050646	54.279888
Au	0.712355	3.548054	54.279888
Au	3.596113	3.548054	54.279888
Au	6.479871	3.548054	54.279888
Au	9.363629	3.548054	54.279888
Au	12.247390	3.548054	54.279888
Au	-0.729525	6.045462	54.279888
Au	2.154234	6.045462	54.279888
Au	5.037992	6.045462	54.279888
Au	7.921750	6.045462	54.279888
Au	10.805510	6.045462	54.279888
Au	-2.171404	8.542870	54.279888
Au	0.712355	8.542870	54.279888
Au	3.596113	8.542870	54.279888
Au	6.479871	8.542870	54.279888
Au	9.363629	8.542870	54.279888
Au	-3.613283	11.040280	54.279888
Au	-0.729525	11.040280	54.279888
Au	2.154234	11.040280	54.279888
Au	5.037992	11.040280	54.279888
Au	7.921750	11.040280	54.279888

5. The optimized structure for the central region of AC junction (in

.xyz format)

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XYZ file

Au	2.177184	1.011926	1.177289
Au	5.060942	1.011926	1.177289
Au	7.944700	1.011926	1.177289
Au	10.828460	1.011926	1.177289
Au	13.712220	1.011926	1.177289
Au	0.735304	3.509334	1.177289
Au	3.619063	3.509334	1.177289
Au	6.502821	3.509334	1.177289
Au	9.386579	3.509334	1.177289
Au	12.270340	3.509334	1.177289
Au	-0.706575	6.006742	1.177289
Au	2.177184	6.006742	1.177289
Au	5.060942	6.006742	1.177289
Au	7.944700	6.006742	1.177289
Au	10.828460	6.006742	1.177289
Au	-2.148454	8.504150	1.177289
Au	0.735304	8.504150	1.177289
Au	3.619063	8.504150	1.177289
Au	6.502821	8.504150	1.177289
Au	9.386579	8.504150	1.177289
Au	-3.590333	11.001560	1.177289
Au	-0.706575	11.001560	1.177289
Au	2.177184	11.001560	1.177289
Au	5.060942	11.001560	1.177289
Au	7.944700	11.001560	1.177289
Au	0.735304	1.844395	3.531868
Au	3.619063	1.844395	3.531868
Au	6.502821	1.844395	3.531868
Au	9.386579	1.844395	3.531868
Au	12.270340	1.844395	3.531868
Au	-0.706575	4.341803	3.531868
Au	2.177184	4.341803	3.531868
Au	5.060942	4.341803	3.531868
Au	7.944700	4.341803	3.531868
Au	10.828460	4.341803	3.531868
Au	-2.148454	6.839211	3.531868
Au	0.735304	6.839211	3.531868
Au	3.619063	6.839211	3.531868

Au	6.502821	6.839211	3.531868
Au	9.386579	6.839211	3.531868
Au	-3.590333	9.336619	3.531868
Au	-0.706575	9.336619	3.531868
Au	2.177184	9.336619	3.531868
Au	5.060942	9.336619	3.531868
Au	7.944700	9.336619	3.531868
Au	-5.032212	11.834030	3.531868
Au	-2.148454	11.834030	3.531868
Au	0.735304	11.834030	3.531868
Au	3.619063	11.834030	3.531868
Au	6.502821	11.834030	3.531868
Au	0.735304	0.179457	5.886447
Au	3.619063	0.179457	5.886447
Au	6.502821	0.179457	5.886447
Au	9.386579	0.179457	5.886447
Au	12.270340	0.179457	5.886447
Au	-0.706575	2.676864	5.886447
Au	2.177184	2.676864	5.886447
Au	5.060942	2.676864	5.886447
Au	7.944700	2.676864	5.886447
Au	10.828460	2.676864	5.886447
Au	-2.148454	5.174272	5.886447
Au	0.735304	5.174272	5.886447
Au	3.619063	5.174272	5.886447
Au	6.502821	5.174272	5.886447
Au	9.386579	5.174272	5.886447
Au	-3.590333	7.671680	5.886447
Au	-0.706575	7.671680	5.886447
Au	2.177184	7.671680	5.886447
Au	5.060942	7.671680	5.886447
Au	7.944700	7.671680	5.886447
Au	-5.032212	10.169090	5.886447
Au	-2.148454	10.169090	5.886447
Au	0.735304	10.169090	5.886447
Au	3.619063	10.169090	5.886447
Au	6.502821	10.169090	5.886447
Au	2.177184	1.011926	8.241026
Au	5.060942	1.011926	8.241026
Au	7.944700	1.011926	8.241026
Au	10.828460	1.011926	8.241026
Au	13.712220	1.011926	8.241026
Au	0.735304	3.509334	8.241026
Au	3.619063	3.509334	8.241026

Au	6.502821	3.509334	8.241026
Au	9.386579	3.509334	8.241026
Au	12.270340	3.509334	8.241026
Au	-0.706575	6.006742	8.241026
Au	2.177184	6.006742	8.241026
Au	5.060942	6.006742	8.241026
Au	7.944700	6.006742	8.241026
Au	10.828460	6.006742	8.241026
Au	-2.148454	8.504150	8.241026
Au	0.735304	8.504150	8.241026
Au	3.619063	8.504150	8.241026
Au	6.502821	8.504150	8.241026
Au	9.386579	8.504150	8.241026
Au	-3.590333	11.001560	8.241026
Au	-0.706575	11.001560	8.241026
Au	2.177184	11.001560	8.241026
Au	5.060942	11.001560	8.241026
Au	7.944700	11.001560	8.241026
Au	12.277680	1.841054	10.680700
Au	10.822660	4.350571	10.680820
Au	3.628999	11.839480	10.680950
Au	0.722382	11.841650	10.681790
Au	7.937716	4.354247	10.687490
Au	6.487132	1.845618	10.688320
Au	6.511270	11.830740	10.702170
Au	9.385233	6.847016	10.702370
Au	-2.157195	11.832450	10.703270
Au	5.047377	9.335987	10.705470
Au	0.731500	1.858255	10.707170
Au	-0.694527	9.334374	10.708450
Au	-2.141611	6.830489	10.710380
Au	6.495069	6.832700	10.710800
Au	3.619872	1.854590	10.711540
Au	-3.575807	9.328773	10.713020
Au	9.382291	1.847831	10.713030
Au	-5.031895	11.848530	10.713230
Au	7.932463	9.329434	10.713450
Au	2.176485	9.362221	10.715430
Au	-0.718810	4.335887	10.724260
Au	0.743162	6.830839	10.735960
Au	5.058177	4.342826	10.736290
Au	3.610367	6.831018	10.738060
Au	2.181350	4.355754	10.748750
Au	-5.028951	10.168190	13.119290

Au	5.092484	7.696388	13.139360
Au	2.172148	2.636340	13.141500
Au	-0.741688	7.692430	13.143410
Au	7.939899	2.680230	13.145520
Au	10.818100	2.675525	13.146780
Au	9.383054	0.189521	13.147610
Au	2.178533	7.839583	13.152120
Au	9.381628	5.170838	13.163850
Au	12.264610	0.182963	13.164960
Au	6.503446	0.185341	13.166150
Au	0.592514	5.090990	13.174830
Au	6.504957	10.180500	13.174900
Au	0.727211	0.170980	13.176190
Au	-2.149061	10.182370	13.178410
Au	-3.602636	7.667461	13.179790
Au	7.952880	7.665081	13.180580
Au	3.629278	0.175926	13.182150
Au	3.644413	10.230950	13.194910
Au	0.709802	10.227800	13.195540
Au	-0.746992	2.623392	13.198680
Au	-2.212784	5.168152	13.199250
Au	6.543346	5.175056	13.205820
Au	5.081118	2.641191	13.207830
Au	3.721738	5.115191	13.222790
S	2.130363	6.024513	14.960700
H	4.146884	4.735540	16.619221
C	2.276807	5.836216	16.726940
H	0.426318	6.913265	17.137730
C	3.383181	5.160393	17.290239
C	1.287503	6.386706	17.577940
C	3.496272	5.042436	18.677641
C	1.406342	6.264546	18.965380
H	4.357460	4.519441	19.116529
C	2.515085	5.591976	19.546690
H	0.635802	6.695531	19.621290
C	2.663475	5.465946	20.962219
C	2.834914	5.342982	22.181530
H	4.961163	4.101052	23.261320
C	3.080114	5.186719	23.580280
C	4.272891	4.495476	24.022360
H	1.290017	6.216504	24.223970
C	2.200600	5.689471	24.545059
C	4.545439	4.333569	25.363251
H	5.458840	3.805972	25.680460

C	2.456048	5.536842	25.941259
C	3.658615	4.841527	26.372089
H	0.662547	6.571897	26.601990
C	1.574610	6.042757	26.921761
C	3.913991	4.688126	27.746210
H	4.826372	4.160766	28.069340
C	1.828247	5.889392	28.295090
C	3.030066	5.192175	28.725479
H	0.025376	6.929770	28.973330
C	0.934724	6.400267	29.296370
C	3.277910	5.039150	30.121269
H	4.184711	4.513511	30.456560
C	1.197394	6.238305	30.637091
C	2.388240	5.546221	31.072599
H	0.511386	6.630565	31.401131
C	2.625948	5.405266	32.468361
C	2.771893	5.326546	33.691132
H	4.828506	4.186761	35.011799
C	2.937683	5.266075	35.101219
H	1.079616	6.326225	35.514729
C	4.077153	4.640089	35.673050
C	1.963466	5.846563	35.957802
C	4.245502	4.605637	37.055241
C	2.126960	5.814992	37.340530
H	5.127860	4.127167	37.502022
C	3.272864	5.197533	37.894562
H	1.378727	6.266923	38.006641
C	3.453584	5.182463	39.308762
N	3.612544	5.181370	40.470749
Au	-0.724966	7.682553	42.641949
Au	3.606105	10.177030	42.643330
Au	7.934877	2.682639	42.643471
Au	7.942450	7.684906	42.643608
Au	-0.719561	2.684559	42.643620
Au	3.607903	0.177474	42.643749
Au	0.722606	10.184680	42.647091
Au	-2.167296	5.179262	42.647449
Au	6.498907	0.180243	42.647869
Au	0.715712	0.181424	42.649220
Au	9.385276	5.179575	42.649231
Au	6.492647	10.185470	42.649410
Au	-5.053050	10.182510	42.669109
Au	9.371483	0.184644	42.669659
Au	-3.600691	7.669379	42.670872

Au	10.816480	2.688867	42.671780
Au	-2.150155	10.181350	42.673470
Au	12.260530	0.184512	42.674969
Au	0.690912	5.183866	42.677940
Au	2.146790	7.706143	42.681068
Au	2.150884	2.653387	42.683788
Au	5.065437	2.652747	42.686371
Au	5.069021	7.707228	42.687931
Au	6.527435	5.184212	42.689709
Au	3.607685	5.180587	42.735149
Au	-3.602829	9.344474	45.117249
Au	-0.717121	9.341005	45.117401
Au	-2.156813	6.847729	45.117722
Au	12.259770	1.853530	45.118099
Au	3.605677	11.839890	45.118252
Au	2.156752	4.345395	45.118252
Au	3.606594	6.856813	45.118370
Au	-2.161996	11.844960	45.118389
Au	-5.041827	11.844580	45.118469
Au	0.720394	6.848301	45.118801
Au	9.374409	1.850990	45.118839
Au	9.370681	6.846999	45.118980
Au	7.931043	9.341234	45.118980
Au	5.059321	4.343592	45.118999
Au	3.606361	1.849347	45.119110
Au	6.493439	6.849148	45.119251
Au	-0.724478	4.344501	45.122250
Au	2.166071	9.352364	45.122379
Au	0.713711	1.849754	45.123211
Au	6.501266	1.847617	45.123569
Au	0.718000	11.837330	45.123920
Au	5.045630	9.354986	45.124210
Au	10.818450	4.356711	45.124352
Au	7.942619	4.340755	45.124569
Au	6.496805	11.838540	45.124660
Au	2.164889	1.019675	47.590870
Au	5.048647	1.019675	47.590870
Au	7.932405	1.019675	47.590870
Au	10.816160	1.019675	47.590870
Au	13.699920	1.019675	47.590870
Au	0.723010	3.517083	47.590870
Au	3.606768	3.517083	47.590870
Au	6.490526	3.517083	47.590870
Au	9.374284	3.517083	47.590870

Au	12.258040	3.517083	47.590870
Au	-0.718869	6.014491	47.590870
Au	2.164889	6.014491	47.590870
Au	5.048647	6.014491	47.590870
Au	7.932405	6.014491	47.590870
Au	10.816160	6.014491	47.590870
Au	-2.160749	8.511899	47.590870
Au	0.723010	8.511899	47.590870
Au	3.606768	8.511899	47.590870
Au	6.490526	8.511899	47.590870
Au	9.374284	8.511899	47.590870
Au	-3.602628	11.009310	47.590870
Au	-0.718869	11.009310	47.590870
Au	2.164889	11.009310	47.590870
Au	5.048647	11.009310	47.590870
Au	7.932405	11.009310	47.590870
Au	0.723010	0.187206	49.945450
Au	3.606768	0.187206	49.945450
Au	6.490526	0.187206	49.945450
Au	9.374284	0.187206	49.945450
Au	12.258040	0.187206	49.945450
Au	-0.718869	2.684613	49.945450
Au	2.164889	2.684613	49.945450
Au	5.048647	2.684613	49.945450
Au	7.932405	2.684613	49.945450
Au	10.816160	2.684613	49.945450
Au	-2.160749	5.182021	49.945450
Au	0.723010	5.182021	49.945450
Au	3.606768	5.182021	49.945450
Au	6.490526	5.182021	49.945450
Au	9.374284	5.182021	49.945450
Au	-3.602628	7.679429	49.945450
Au	-0.718869	7.679429	49.945450
Au	2.164889	7.679429	49.945450
Au	5.048647	7.679429	49.945450
Au	7.932405	7.679429	49.945450
Au	-5.044507	10.176840	49.945450
Au	-2.160749	10.176840	49.945450
Au	0.723010	10.176840	49.945450
Au	3.606768	10.176840	49.945450
Au	6.490526	10.176840	49.945450
Au	0.723010	1.852144	52.300030
Au	3.606768	1.852144	52.300030
Au	6.490526	1.852144	52.300030

Au	9.374284	1.852144	52.300030
Au	12.258040	1.852144	52.300030
Au	-0.718869	4.349552	52.300030
Au	2.164889	4.349552	52.300030
Au	5.048647	4.349552	52.300030
Au	7.932405	4.349552	52.300030
Au	10.816160	4.349552	52.300030
Au	-2.160749	6.846960	52.300030
Au	0.723010	6.846960	52.300030
Au	3.606768	6.846960	52.300030
Au	6.490526	6.846960	52.300030
Au	9.374284	6.846960	52.300030
Au	-3.602628	9.344368	52.300030
Au	-0.718869	9.344368	52.300030
Au	2.164889	9.344368	52.300030
Au	5.048647	9.344368	52.300030
Au	7.932405	9.344368	52.300030
Au	-5.044507	11.841780	52.300030
Au	-2.160749	11.841780	52.300030
Au	0.723010	11.841780	52.300030
Au	3.606768	11.841780	52.300030
Au	6.490526	11.841780	52.300030
Au	2.164889	1.019675	54.654610
Au	5.048647	1.019675	54.654610
Au	7.932405	1.019675	54.654610
Au	10.816160	1.019675	54.654610
Au	13.699920	1.019675	54.654610
Au	0.723010	3.517083	54.654610
Au	3.606768	3.517083	54.654610
Au	6.490526	3.517083	54.654610
Au	9.374284	3.517083	54.654610
Au	12.258040	3.517083	54.654610
Au	-0.718869	6.014491	54.654610
Au	2.164889	6.014491	54.654610
Au	5.048647	6.014491	54.654610
Au	7.932405	6.014491	54.654610
Au	10.816160	6.014491	54.654610
Au	-2.160749	8.511899	54.654610
Au	0.723010	8.511899	54.654610
Au	3.606768	8.511899	54.654610
Au	6.490526	8.511899	54.654610
Au	9.374284	8.511899	54.654610
Au	-3.602628	11.009310	54.654610
Au	-0.718869	11.009310	54.654610

Au	2.164889	11.009310	54.654610
Au	5.048647	11.009310	54.654610
Au	7.932405	11.009310	54.654610

6. The optimized structure for the central region of AH junction (in

.xyz format)

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XYZ file

Au	2.177184	1.011926	1.177289
Au	5.060942	1.011926	1.177289
Au	7.944700	1.011926	1.177289
Au	10.828460	1.011926	1.177289
Au	13.712220	1.011926	1.177289
Au	0.735304	3.509334	1.177289
Au	3.619063	3.509334	1.177289
Au	6.502821	3.509334	1.177289
Au	9.386579	3.509334	1.177289
Au	12.270340	3.509334	1.177289
Au	-0.706575	6.006742	1.177289
Au	2.177184	6.006742	1.177289
Au	5.060942	6.006742	1.177289
Au	7.944700	6.006742	1.177289
Au	10.828460	6.006742	1.177289
Au	-2.148454	8.504150	1.177289
Au	0.735304	8.504150	1.177289
Au	3.619063	8.504150	1.177289
Au	6.502821	8.504150	1.177289
Au	9.386579	8.504150	1.177289
Au	-3.590333	11.001560	1.177289
Au	-0.706575	11.001560	1.177289
Au	2.177184	11.001560	1.177289
Au	5.060942	11.001560	1.177289
Au	7.944700	11.001560	1.177289
Au	0.735304	1.844395	3.531868
Au	3.619063	1.844395	3.531868
Au	6.502821	1.844395	3.531868
Au	9.386579	1.844395	3.531868
Au	12.270340	1.844395	3.531868
Au	-0.706575	4.341803	3.531868
Au	2.177184	4.341803	3.531868
Au	5.060942	4.341803	3.531868
Au	7.944700	4.341803	3.531868

Au	10.828460	4.341803	3.531868
Au	-2.148454	6.839211	3.531868
Au	0.735304	6.839211	3.531868
Au	3.619063	6.839211	3.531868
Au	6.502821	6.839211	3.531868
Au	9.386579	6.839211	3.531868
Au	-3.590333	9.336619	3.531868
Au	-0.706575	9.336619	3.531868
Au	2.177184	9.336619	3.531868
Au	5.060942	9.336619	3.531868
Au	7.944700	9.336619	3.531868
Au	-5.032212	11.834030	3.531868
Au	-2.148454	11.834030	3.531868
Au	0.735304	11.834030	3.531868
Au	3.619063	11.834030	3.531868
Au	6.502821	11.834030	3.531868
Au	0.735304	0.179457	5.886447
Au	3.619063	0.179457	5.886447
Au	6.502821	0.179457	5.886447
Au	9.386579	0.179457	5.886447
Au	12.270340	0.179457	5.886447
Au	-0.706575	2.676864	5.886447
Au	2.177184	2.676864	5.886447
Au	5.060942	2.676864	5.886447
Au	7.944700	2.676864	5.886447
Au	10.828460	2.676864	5.886447
Au	-2.148454	5.174272	5.886447
Au	0.735304	5.174272	5.886447
Au	3.619063	5.174272	5.886447
Au	6.502821	5.174272	5.886447
Au	9.386579	5.174272	5.886447
Au	-3.590333	7.671680	5.886447
Au	-0.706575	7.671680	5.886447
Au	2.177184	7.671680	5.886447
Au	5.060942	7.671680	5.886447
Au	7.944700	7.671680	5.886447
Au	-5.032212	10.169090	5.886447
Au	-2.148454	10.169090	5.886447
Au	0.735304	10.169090	5.886447
Au	3.619063	10.169090	5.886447
Au	6.502821	10.169090	5.886447
Au	2.177184	1.011926	8.241026
Au	5.060942	1.011926	8.241026
Au	7.944700	1.011926	8.241026

Au	10.828460	1.011926	8.241026
Au	13.712220	1.011926	8.241026
Au	0.735304	3.509334	8.241026
Au	3.619063	3.509334	8.241026
Au	6.502821	3.509334	8.241026
Au	9.386579	3.509334	8.241026
Au	12.270340	3.509334	8.241026
Au	-0.706575	6.006742	8.241026
Au	2.177184	6.006742	8.241026
Au	5.060942	6.006742	8.241026
Au	7.944700	6.006742	8.241026
Au	10.828460	6.006742	8.241026
Au	-2.148454	8.504150	8.241026
Au	0.735304	8.504150	8.241026
Au	3.619063	8.504150	8.241026
Au	6.502821	8.504150	8.241026
Au	9.386579	8.504150	8.241026
Au	-3.590333	11.001560	8.241026
Au	-0.706575	11.001560	8.241026
Au	2.177184	11.001560	8.241026
Au	5.060942	11.001560	8.241026
Au	7.944700	11.001560	8.241026
Au	0.725397	11.830620	10.681580
Au	10.811320	4.345786	10.684260
Au	12.261730	1.827765	10.687060
Au	6.500106	1.838451	10.687130
Au	3.621722	11.825800	10.687710
Au	0.725966	1.855789	10.692600
Au	7.942184	4.348103	10.693030
Au	-0.738315	4.322762	10.694980
Au	3.626636	1.856816	10.696510
Au	5.052179	9.334239	10.698740
Au	-2.156041	11.831550	10.699090
Au	9.384617	6.844970	10.699140
Au	6.509838	11.830250	10.701620
Au	7.935261	9.329471	10.703820
Au	6.493745	6.830036	10.703960
Au	-2.135112	6.829115	10.704350
Au	-0.697063	9.331283	10.704590
Au	-3.576278	9.328752	10.705070
Au	-5.031036	11.855330	10.706810
Au	9.380854	1.842990	10.715940
Au	5.070434	4.336573	10.723440
Au	2.175216	9.337390	10.725770

Au	0.744558	6.836109	10.728600
Au	3.603702	6.837721	10.731460
Au	2.178820	4.355140	10.737150
Au	0.596493	5.105421	13.107140
Au	-5.033571	10.173440	13.111300
Au	2.178359	2.638565	13.123900
Au	5.102294	7.698592	13.127030
Au	-0.747993	7.700899	13.145480
Au	10.823460	2.672675	13.147720
Au	9.383927	0.178774	13.148030
Au	7.949513	2.672977	13.152190
Au	-3.603082	7.668050	13.164880
Au	6.507853	0.182141	13.166530
Au	6.505591	10.184890	13.167380
Au	0.722853	0.176747	13.167790
Au	3.761212	5.104531	13.168370
Au	3.631446	0.174952	13.169510
Au	12.270530	0.182348	13.170190
Au	-2.150214	10.189790	13.170400
Au	7.956607	7.668753	13.170730
Au	9.386725	5.174398	13.172760
Au	-0.735109	2.637760	13.184440
Au	3.643488	10.215430	13.185110
Au	0.713144	10.209800	13.188260
Au	-2.207893	5.171210	13.188760
Au	5.091536	2.634373	13.190770
Au	2.177420	7.794379	13.192490
Au	6.564329	5.171689	13.202270
S	2.217525	6.009246	14.937020
C	2.486243	6.499921	16.626289
H	4.471044	5.624685	16.740191
H	0.533779	7.446477	16.787470
C	3.676760	6.144906	17.297750
C	1.455793	7.171583	17.322969
C	3.834350	6.463013	18.649460
C	1.618076	7.485671	18.673559
H	4.760845	6.189975	19.175400
H	0.819251	8.008995	19.219000
C	2.811101	7.140921	19.363800
C	2.979586	7.484190	20.739901
C	3.122866	7.800301	21.925091
C	3.302321	8.173193	23.293570
H	5.284668	7.294945	23.443199
H	1.357270	9.133471	23.480410

C	4.498320	7.846826	23.979750
C	2.292844	8.877031	23.996920
C	4.690716	8.215769	25.317350
C	2.484502	9.234501	25.334591
H	6.519335	7.065783	25.552731
H	1.689163	9.776235	25.871031
H	6.651312	8.779996	26.002720
C	3.676805	8.915205	26.007660
C	5.976336	7.891980	26.053120
C	3.911829	9.305227	27.452650
H	4.476233	10.268340	27.481911
C	5.730059	7.561323	27.509140
H	7.276846	6.042829	27.644911
H	2.949975	9.499342	27.968571
C	6.489758	6.590493	28.186609
C	4.712921	8.258100	28.199970
C	6.260291	6.310771	29.535339
C	4.474192	7.975107	29.549641
H	6.854020	5.551569	30.064159
H	3.680849	8.506204	30.097309
C	5.244913	7.005800	30.234751
C	4.998647	6.733833	31.609421
C	4.788488	6.505715	32.801960
C	4.544608	6.236968	34.173710
H	2.902985	7.657801	34.325611
H	6.141114	4.766598	34.332581
C	3.507560	6.916472	34.864521
C	5.334800	5.284457	34.868469
C	3.255413	6.643534	36.205669
C	5.088854	5.006115	36.209610
H	2.452061	7.163309	36.746269
H	5.694760	4.267846	36.753281
C	4.041240	5.679879	36.879711
C	3.756279	5.364443	38.235760
N	3.482988	5.062875	39.336559
Au	-0.724275	7.688813	41.453079
Au	7.933587	2.684952	41.453541
Au	3.609183	0.176419	41.453819
Au	3.604699	10.177230	41.454300
Au	-0.725702	2.683494	41.455441
Au	9.379328	5.178899	41.458881
Au	-2.174950	5.177971	41.459332
Au	7.934064	7.680178	41.459412
Au	0.719449	10.184060	41.461170

Au	6.485388	10.183560	41.461578
Au	0.706844	0.177651	41.461739
Au	6.495777	0.177807	41.462780
Au	-2.154974	10.181220	41.477249
Au	5.063005	7.704872	41.477989
Au	2.145758	7.706596	41.479382
Au	10.814480	2.688063	41.480122
Au	6.520823	5.180980	41.481628
Au	12.255800	0.187429	41.483589
Au	5.063015	2.651833	41.491211
Au	-5.057354	10.184070	41.495640
Au	-3.601952	7.669180	41.496181
Au	9.367071	0.184912	41.496521
Au	0.684290	5.183219	41.507252
Au	2.144824	2.648389	41.513279
Au	3.607324	5.183095	41.587421
Au	-3.603359	9.346104	43.928310
Au	0.721516	6.849962	43.929619
Au	3.608468	1.850654	43.930038
Au	3.601791	6.856511	43.931438
Au	3.605022	11.838400	43.931511
Au	9.371371	1.855978	43.931671
Au	-2.157850	6.847232	43.931740
Au	7.927765	9.340732	43.931820
Au	9.367847	6.846711	43.932381
Au	-5.044918	11.846720	43.932529
Au	12.250510	1.850205	43.932739
Au	-0.719453	9.342243	43.933262
Au	6.485506	6.846103	43.933300
Au	5.055558	4.342436	43.933460
Au	7.932442	4.347576	43.933472
Au	-2.164269	11.843410	43.934422
Au	5.043424	9.346620	43.934509
Au	2.163964	9.350228	43.935619
Au	10.809980	4.356187	43.936611
Au	6.497879	1.849990	43.936840
Au	0.716535	11.838390	43.937191
Au	6.489827	11.834460	43.938042
Au	-0.734508	4.341495	43.938141
Au	0.703986	1.844576	43.940620
Au	2.141971	4.338135	43.955742
Au	2.162493	1.019936	46.404781
Au	5.046251	1.019936	46.404781
Au	7.930009	1.019936	46.404781

Au	10.813770	1.019936	46.404781
Au	13.697530	1.019936	46.404781
Au	0.720614	3.517344	46.404781
Au	3.604372	3.517344	46.404781
Au	6.488130	3.517344	46.404781
Au	9.371888	3.517344	46.404781
Au	12.255650	3.517344	46.404781
Au	-0.721266	6.014751	46.404781
Au	2.162493	6.014751	46.404781
Au	5.046251	6.014751	46.404781
Au	7.930009	6.014751	46.404781
Au	10.813770	6.014751	46.404781
Au	-2.163145	8.512159	46.404781
Au	0.720614	8.512159	46.404781
Au	3.604372	8.512159	46.404781
Au	6.488130	8.512159	46.404781
Au	9.371888	8.512159	46.404781
Au	-3.605024	11.009570	46.404781
Au	-0.721266	11.009570	46.404781
Au	2.162493	11.009570	46.404781
Au	5.046251	11.009570	46.404781
Au	7.930009	11.009570	46.404781
Au	0.720614	0.187466	48.759361
Au	3.604372	0.187466	48.759361
Au	6.488130	0.187466	48.759361
Au	9.371888	0.187466	48.759361
Au	12.255650	0.187466	48.759361
Au	-0.721266	2.684874	48.759361
Au	2.162493	2.684874	48.759361
Au	5.046251	2.684874	48.759361
Au	7.930009	2.684874	48.759361
Au	10.813770	2.684874	48.759361
Au	-2.163145	5.182282	48.759361
Au	0.720614	5.182282	48.759361
Au	3.604372	5.182282	48.759361
Au	6.488130	5.182282	48.759361
Au	9.371888	5.182282	48.759361
Au	-3.605024	7.679690	48.759361
Au	-0.721266	7.679690	48.759361
Au	2.162493	7.679690	48.759361
Au	5.046251	7.679690	48.759361
Au	7.930009	7.679690	48.759361
Au	-5.046903	10.177100	48.759361
Au	-2.163145	10.177100	48.759361

Au	0.720614	10.177100	48.759361
Au	3.604372	10.177100	48.759361
Au	6.488130	10.177100	48.759361
Au	0.720614	1.852405	51.113941
Au	3.604372	1.852405	51.113941
Au	6.488130	1.852405	51.113941
Au	9.371888	1.852405	51.113941
Au	12.255650	1.852405	51.113941
Au	-0.721266	4.349813	51.113941
Au	2.162493	4.349813	51.113941
Au	5.046251	4.349813	51.113941
Au	7.930009	4.349813	51.113941
Au	10.813770	4.349813	51.113941
Au	-2.163145	6.847221	51.113941
Au	0.720614	6.847221	51.113941
Au	3.604372	6.847221	51.113941
Au	6.488130	6.847221	51.113941
Au	9.371888	6.847221	51.113941
Au	-3.605024	9.344629	51.113941
Au	-0.721266	9.344629	51.113941
Au	2.162493	9.344629	51.113941
Au	5.046251	9.344629	51.113941
Au	7.930009	9.344629	51.113941
Au	-5.046903	11.842040	51.113941
Au	-2.163145	11.842040	51.113941
Au	0.720614	11.842040	51.113941
Au	3.604372	11.842040	51.113941
Au	6.488130	11.842040	51.113941
Au	2.162493	1.019936	53.468510
Au	5.046251	1.019936	53.468510
Au	7.930009	1.019936	53.468510
Au	10.813770	1.019936	53.468510
Au	13.697530	1.019936	53.468510
Au	0.720614	3.517344	53.468510
Au	3.604372	3.517344	53.468510
Au	6.488130	3.517344	53.468510
Au	9.371888	3.517344	53.468510
Au	12.255650	3.517344	53.468510
Au	-0.721266	6.014751	53.468510
Au	2.162493	6.014751	53.468510
Au	5.046251	6.014751	53.468510
Au	7.930009	6.014751	53.468510
Au	10.813770	6.014751	53.468510
Au	-2.163145	8.512159	53.468510

Au	0.720614	8.512159	53.468510
Au	3.604372	8.512159	53.468510
Au	6.488130	8.512159	53.468510
Au	9.371888	8.512159	53.468510
Au	-3.605024	11.009570	53.468510
Au	-0.721266	11.009570	53.468510
Au	2.162493	11.009570	53.468510
Au	5.046251	11.009570	53.468510
Au	7.930009	11.009570	53.468510