

## Supplemental Information

# Tunable Charge Transport in Single-Molecule Junctions via Electrolytic Gating

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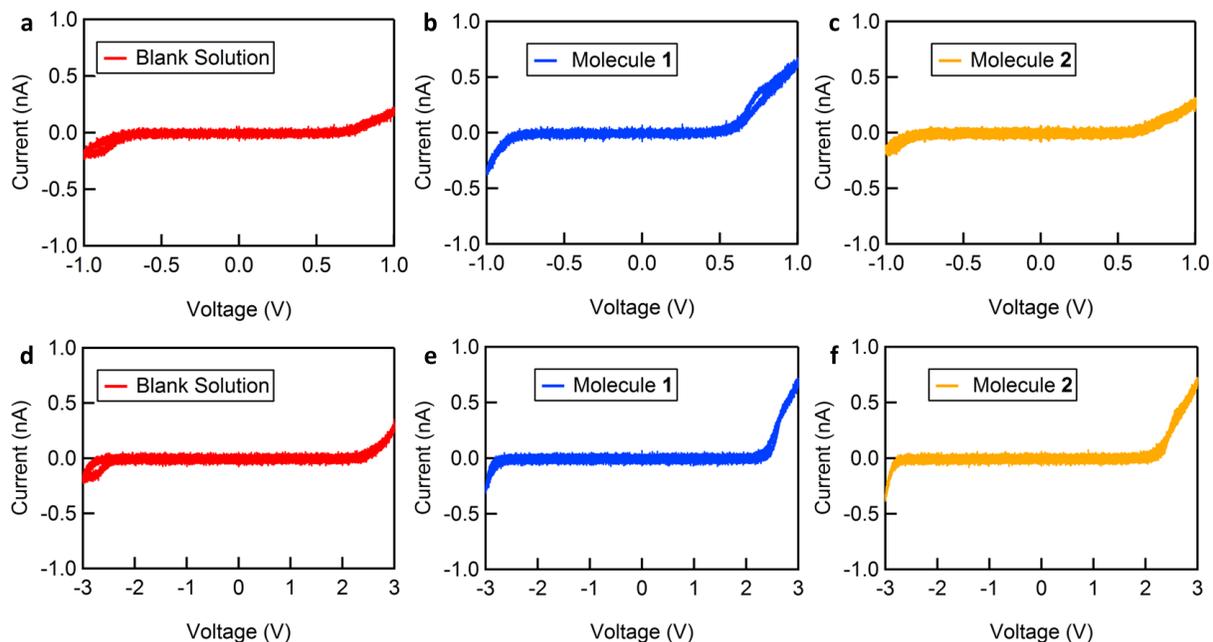
- a. Figure S1. Cyclic voltammograms of blank solution and solution with molecules **1** & **2**
- b. Figure S2. Two dimensional histograms demonstrating gating dependence on step length for molecule **1**
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#### 2. Control Gating Experiment

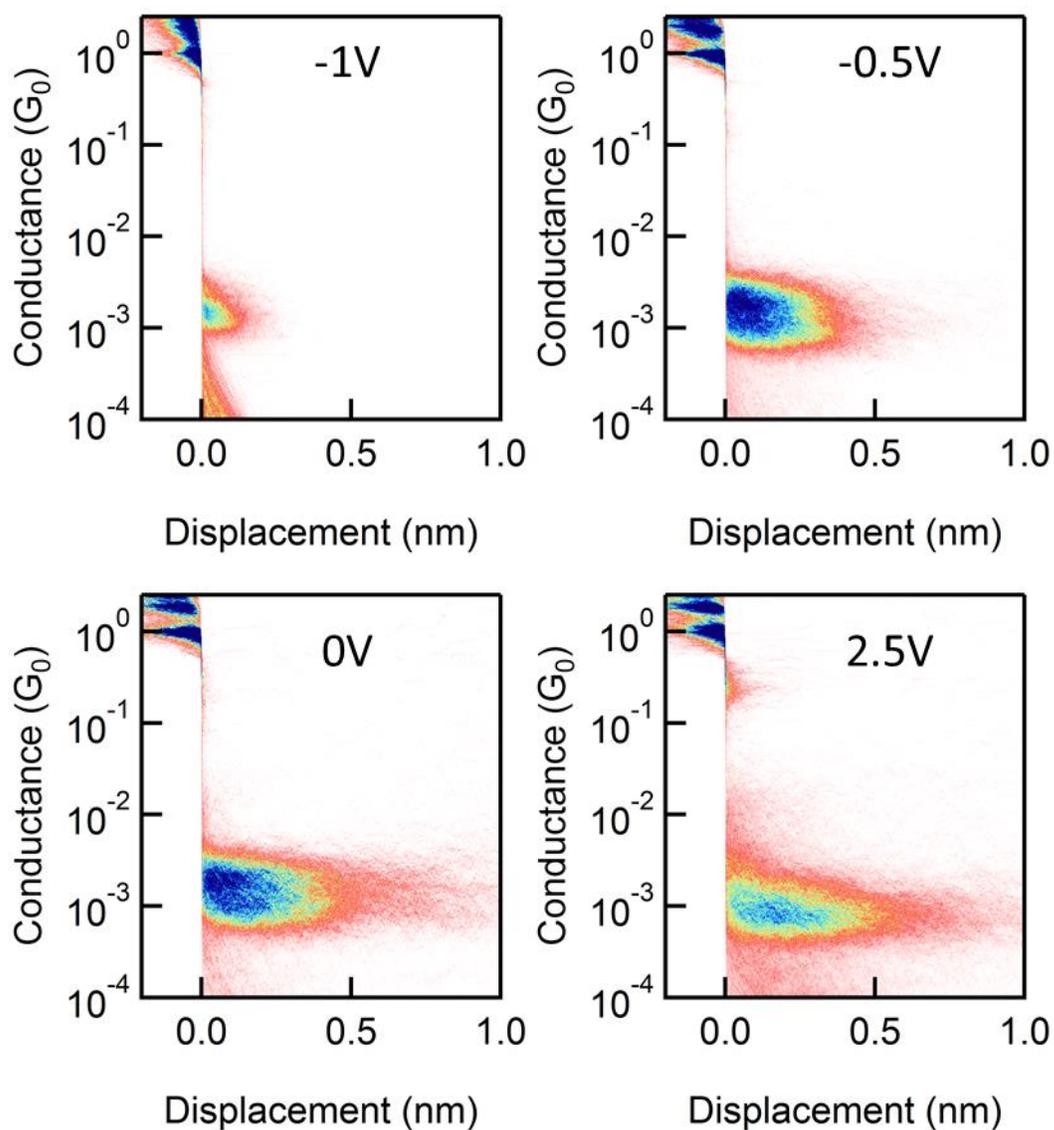
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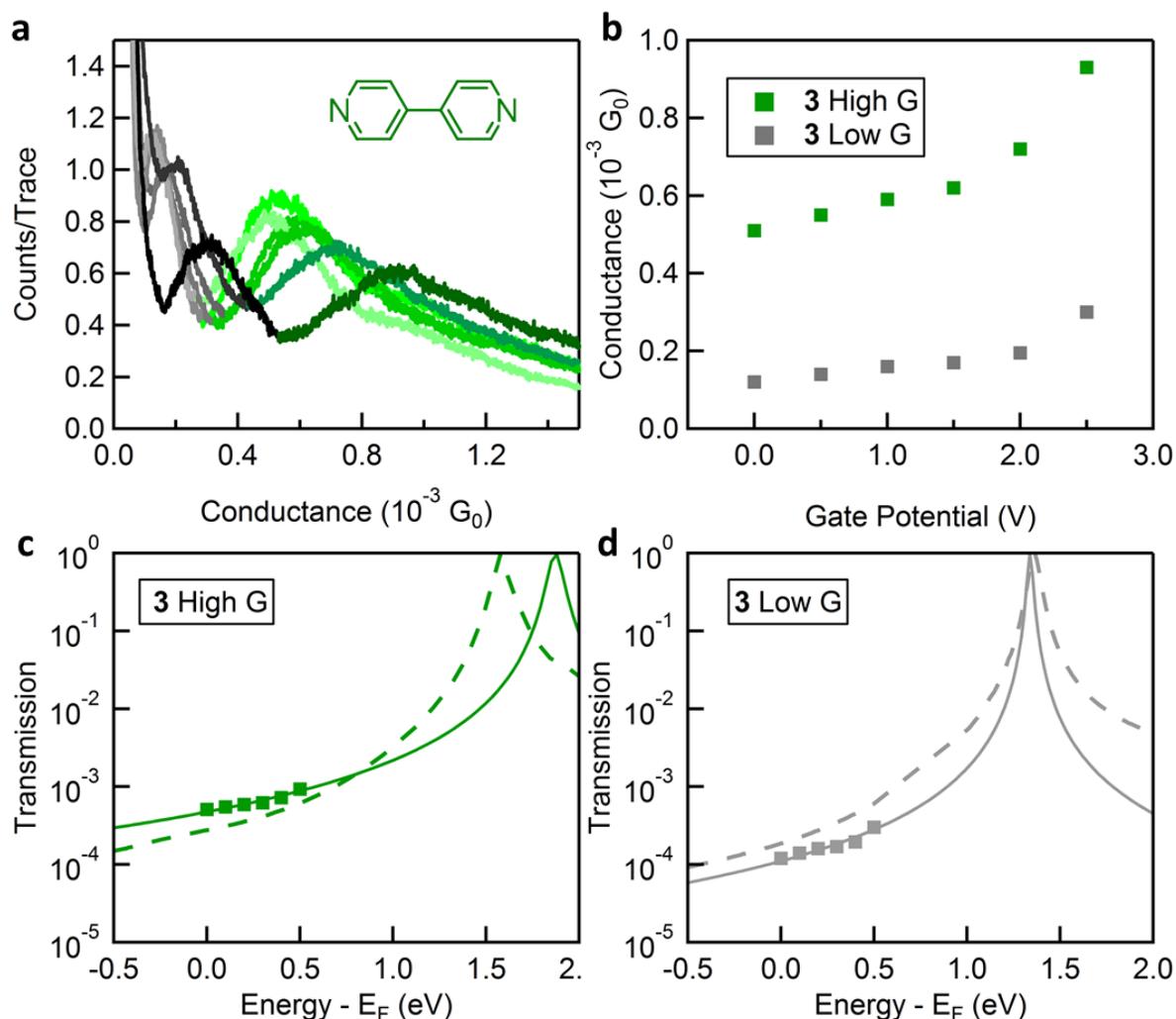
#### 5. Calculated Junction Geometries



**Figure S1.** Cyclic voltammograms for a blank solution (solvent and electrolyte), a solution with molecule **1** and a solution with molecule **2**, demonstrating the lack of electrochemical activity for all systems in the range -1V to 2.5V. Plots (a), (b), (c) measured using the 2-electrode arrangement as detailed in the text, while plots (d), (e), (f) recorded using the 3-electrode arrangement as detailed in the text. All curves recorded at a scan rate of 100mV/s.



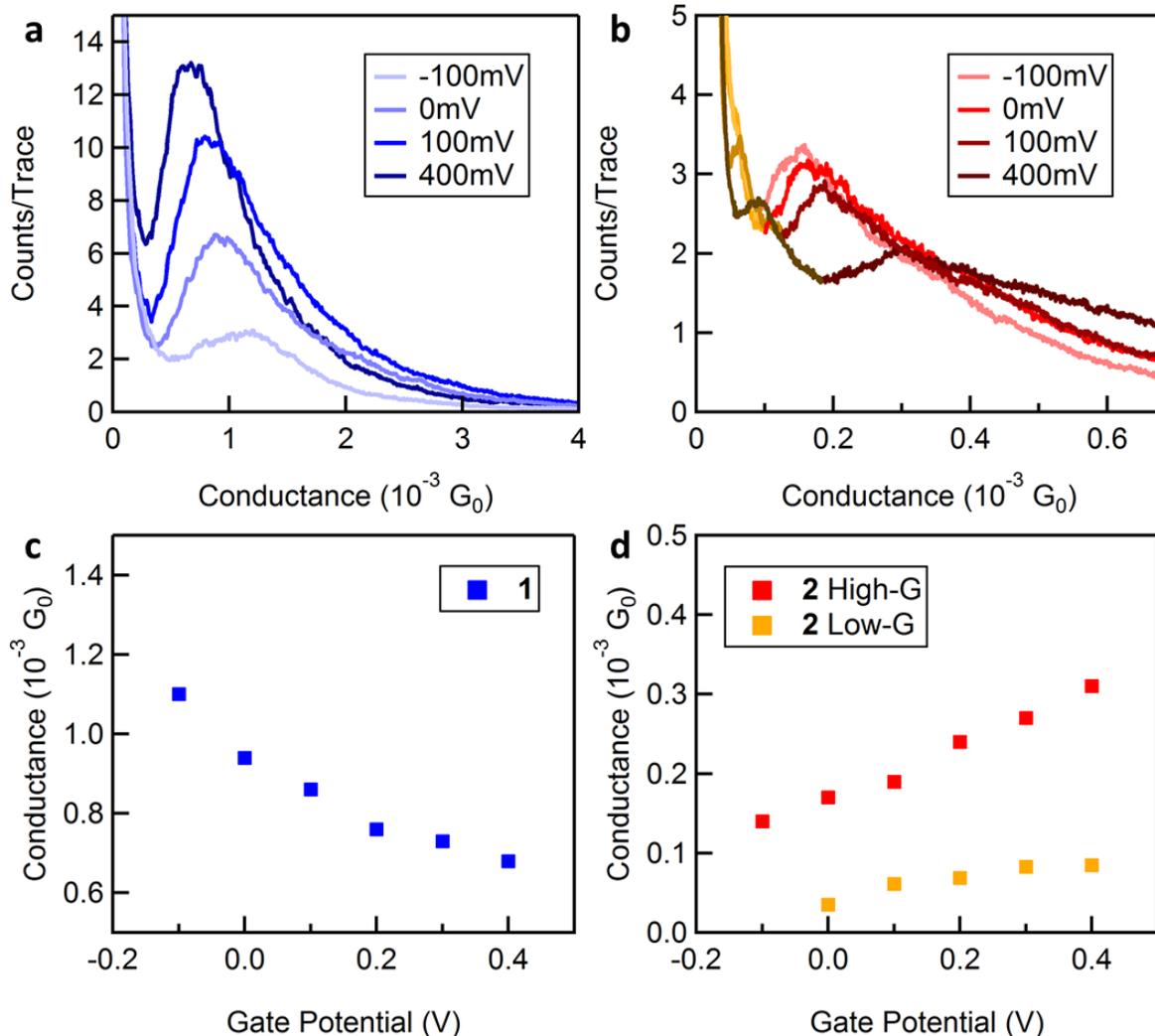
**Figure S2.** Two-dimensional histograms for molecule **1** at selected gate potentials. The histograms were created by aligning each trace just after the  $1G_0$  break (0 displacement is just after this break) and then overlaying all traces at the given gate potential without selection. A systematic decrease in plateau length can be observed as the gate potential is made more negative.



**Figure S3.** Gating data for 4,4'-bipyridine. **(a)** Conductance histograms for 4,4'-bipyridine taken at gate potentials  $V_G = 2.5V, 2V, 1.5V, 1V, 0.5V,$  and  $0V$  darkest to lightest. Note: green shades indicate the high-G feature for this molecule while grey shades indicate the low-G feature. Inset is the molecular structure. **(b)** Peak conductance values vs applied gate potential. **(c)** and **(d)** Conductance data for molecules **3** plotted against the potential drop at the working electrode (markers) fit with a single-Lorentzian transmission model (solid lines) for the high-G and low-G geometries respectively. The DFT+ $\Sigma$  calculated transmission functions are overlaid as dashed lines. For this molecule, we get  $\Gamma$  and  $\epsilon$  of  $0.08$  eV and  $1.83$  eV for the high-G junctions and  $0.028$  eV and  $1.34$  eV for the low-G junctions.

## Control Gating Experiments

Gating measurements for molecules **1** and **2** were also carried out in an arrangement where the Au source and drain electrodes had a much smaller area than the Pt gate electrode. In order to accomplish this, the substrate was also insulated using Apiezon wax, leaving only a small area (~5mm in diameter) exposed in order to carry out the break junction measurements. The Pt wire gate electrode was replaced with a much larger coiled piece of Pt wire in order to increase the surface area relative to the Au. With this arrangement, the majority of the applied gate potential is dropped across the Au electrodes as opposed to the Pt gate electrode. Conductance histograms were collected under applied gate potentials in 100mV intervals from 400mV to -100mV. As can be seen in Figure S4 below, much smaller gate potentials are needed in order to elicit a conductance change in this configuration. The gate potential applied here was also calibrated against oxidation of ferrocene in a similar manner to what is shown in Figure 3 of the manuscript. We found that the ferrocene oxidation peak in this case to be at 0.5 V indicating that the entire gate potential drops at the working electrode.



**Figure S4.** Gating data for molecules 1 & 2 using a large (with respect to the source drain electrodes) Pt gate electrode. **(A)** and **(B)** Sample conductance histograms at gate potentials  $V_G = 400\text{mV}$ ,  $100\text{mV}$ ,  $0\text{mV}$ ,  $-100\text{mV}$  darkest to lightest for molecule **1** and **2** respectively. Note: for molecule **2**, red shades indicate the high-G conductance feature while orange shades indicate the low-G conductance feature. **(C)** and **(D)** Peak conductance values vs applied gate potential for **1** and **2**, respectively.

### Calculation Details:

We obtain the transmission functions using a parameter-free scattering-state approach based on DFT as implemented in the SCARLET package.<sup>1</sup> For all junctions, the transmission functions are calculated using a  $16 \times 16 k_{//}$ -mesh and a 200-point energy grid in the energy range ( $E_F - 4\text{eV}$ ,  $E_F + 4\text{eV}$ ). The DFT molecular orbital energies in the junctions are corrected using the DFT+ $\Sigma$  method.<sup>2, 3</sup> Specifically, we correct the gas-phase gap with a  $\Delta\text{SCF}$  calculation, and correct for the lack of static nonlocal correlation effects in the junction through an electrostatic “image charge” model. PBE resonance energies are obtained by diagonalizing the junction Hamiltonian projected on the molecular subspace, as defined by the numerical orbitals centered on the atoms of the molecule. The DFT+ $\Sigma$ -corrected frontier orbitals for **1** and **2** LowG/HighG are at  $E_F - 1.52\text{eV}$  ( $\Sigma = -0.61\text{eV}$ ),  $E_F + 1.54\text{eV}$  ( $\Sigma = +1.42\text{eV}$ ) and  $E_F + 1.45\text{eV}$  ( $\Sigma = +1.27\text{eV}$ ) respectively.

### References:

- (1) Choi, H. J.; Marvin, L. C.; Steven, G. L. *Phys. Rev. B*, **2007**, 76, 155420.
- (2) Quek, S. Y.; Choi, H. J.; Louie, S. G.; Neaton, J. B. *Nano Lett.*, **2009**, 9, 3949-3953.
- (3) Quek, S. Y.; Venkataraman, L.; Choi, H. J.; Louie, S. G.; Hybertsen, M. S.; Neaton, J. B. *Nano Letters*, **2007**, 7, 3477-3482.

## Energy Minimized Junction Geometries:

Molecule 1:

284

H	8.581990	17.922396	30.985223
C	8.012243	18.633226	31.514996
C	7.617930	18.220438	32.855324
H	8.663665	16.387718	32.689416
H	6.417811	19.947114	33.402311
C	8.079166	16.972996	33.337014
C	6.812416	19.021684	33.714301
H	10.325120	15.553578	33.987825
H	8.249391	14.297061	33.028117
C	7.841920	16.494836	34.644845
C	6.548831	18.584264	35.007602
C	9.999763	15.260374	34.950433
C	7.966332	14.067193	34.020605
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H	6.898539	13.982295	34.062742
H	10.463048	14.321474	35.197417
H	8.382550	13.108985	34.276905
C	8.455193	15.133651	35.037273
H	5.963572	19.176843	35.680787
C	7.082606	17.354255	35.480844
H	7.607801	13.650988	36.357016
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H	7.768662	15.399615	38.455916
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C	7.797889	24.428777	28.473163
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H	6.796733	24.221923	25.560829
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Au	4.475983	7.752633	7.311627
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Au	5.967979	-0.000001	7.311623

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<b>Au</b>	9.921246	33.414417	55.189132
<b>Au</b>	8.429249	27.384609	50.315358
<b>Au</b>	8.429248	29.107404	52.751804
<b>Au</b>	8.429254	30.830214	55.189129
<b>Au</b>	6.937249	35.137216	50.315368
<b>Au</b>	6.937255	36.860030	52.751813
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Molecule 2 High G:

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N	4.760113	15.738800	25.891487
N	5.872672	19.911252	34.332387
C	5.553254	17.944018	29.492717
C	5.251020	17.176044	28.282905
C	5.820702	17.571714	27.044200
C	5.553113	16.834530	25.882059
C	4.193676	15.352632	27.059793
C	4.406450	16.031808	28.262598
C	5.082241	17.673496	30.749130
C	5.383320	18.449769	31.954352
C	6.246597	19.580139	31.968860
C	6.457777	20.272232	33.164226
C	5.058334	18.831396	34.346103
C	4.791492	18.082067	33.191293
H	6.194864	18.772752	29.362645
H	6.451356	18.417946	27.000662
H	5.970292	17.114119	24.960510
H	3.573021	14.493915	27.036126
H	3.934566	15.674590	29.151899
H	4.438537	16.846674	30.914061
H	6.736180	19.916388	31.113999
H	7.092471	21.120829	33.216126
H	4.623758	18.573805	35.299005
H	4.144795	17.248370	33.272235
Au	6.157639	21.140677	36.162319
Au	4.527260	14.504387	24.046569
Au	4.765985	23.676544	36.108657
Au	5.939997	11.976646	24.093726
Au	7.651517	23.625230	36.098597
Au	3.053746	12.008516	24.099445
Au	12.153438	27.876518	38.197267
Au	0.028026	10.325526	21.983861
Au	10.680521	25.313240	38.215337
Au	1.436022	12.931959	21.965913
Au	9.225483	27.903339	38.212461
Au	2.999063	10.199288	21.943761
Au	7.709399	25.440580	38.255694
Au	4.507447	12.944561	21.769098
Au	6.186558	27.952836	38.234540
Au	6.047583	10.192497	21.938131
Au	4.658315	25.453817	38.268455

Au	7.588118	12.924184	21.978731
Au	3.139445	27.908512	38.207654
Au	9.016834	10.322921	21.985261
Au	1.691213	25.316261	38.214382
Au	10.481781	12.914790	21.994488
Au	12.165125	22.723508	38.206206
Au	0.000002	15.519999	21.979890
Au	10.705757	20.118446	38.218848
Au	1.479460	18.073749	21.986019
Au	9.274515	22.707717	38.231127
Au	2.934382	15.559772	21.932454
Au	7.771041	20.085539	38.264841
Au	4.522637	18.027273	21.968169
Au	6.204187	22.705831	38.436616
Au	6.109691	15.562687	21.916807
Au	4.596642	20.079082	38.298166
Au	7.565630	18.071487	21.993973
Au	3.123526	22.716154	38.222238
Au	9.037025	15.516111	21.985480
Au	1.669149	20.123841	38.215059
Au	10.489069	18.098145	22.001199
Au	12.150457	29.625511	40.724604
Au	0.053103	8.626208	19.488353
Au	10.662298	27.039711	40.714875
Au	1.555394	11.204547	19.494536
Au	9.179933	29.627053	40.724453
Au	3.040622	8.607644	19.488579
Au	7.675837	27.059279	40.713650
Au	4.532023	11.189020	19.489755
Au	6.185676	29.647348	40.738574
Au	6.028431	8.605703	19.485721
Au	4.685974	27.063861	40.718856
Au	7.511086	11.203569	19.495500
Au	3.180518	29.626874	40.737696
Au	9.013360	8.626569	19.488471
Au	1.700150	27.039610	40.716236
Au	10.500626	11.204904	19.499762
Au	12.150477	24.461404	40.704549
Au	0.052417	13.786620	19.499730
Au	10.664063	21.880848	40.703736
Au	1.539606	16.376796	19.475132
Au	9.161255	24.461453	40.708900
Au	3.020390	13.791236	19.452739
Au	7.697356	21.875957	40.754647

Au	4.532818	16.358234	19.468758
Au	6.184032	24.478808	40.714691
Au	6.039890	13.787095	19.462984
Au	4.675364	21.881724	40.746181
Au	7.531689	16.376886	19.474189
Au	3.203000	24.464146	40.710773
Au	9.006339	13.784263	19.505946
Au	1.709699	21.883095	40.699569
Au	10.499325	16.378345	19.477923
Au	12.144672	31.401768	43.145154
Au	0.070022	6.901967	17.051037
Au	10.651936	28.809324	43.158667
Au	1.564807	9.483154	17.060207
Au	9.163961	31.397067	43.161836
Au	3.052755	6.902310	17.054938
Au	7.671131	28.808824	43.153971
Au	4.547318	9.485078	17.060050
Au	6.174167	31.394330	43.171369
Au	6.042276	6.901842	17.055202
Au	4.680654	28.808849	43.156446
Au	7.530839	9.483445	17.058352
Au	3.188076	31.400987	43.160219
Au	9.024908	6.902165	17.050380
Au	1.695189	28.808738	43.161574
Au	10.516155	9.488220	17.051808
Au	12.141230	26.223322	43.158741
Au	0.069517	12.067302	17.062513
Au	10.652834	23.643904	43.148155
Au	1.559530	14.650477	17.048609
Au	9.157338	26.227800	43.149454
Au	3.055762	12.060401	17.042850
Au	7.666993	23.650981	43.167046
Au	4.548246	14.653623	17.040637
Au	6.175434	26.225489	43.148803
Au	6.039289	12.060683	17.045091
Au	4.682926	23.651529	43.165667
Au	7.532969	14.647891	17.052699
Au	3.191020	26.228695	43.152386
Au	9.024789	12.067783	17.063683
Au	1.696808	23.644244	43.148095
Au	10.513374	14.645649	17.064306
Au	13.624901	35.762243	45.595089
Au	0.086765	5.168410	14.622126
Au	12.132916	33.178045	45.595107

Au	1.578763	7.752641	14.622126
Au	13.624898	30.593853	45.595076
Au	0.086763	10.336859	14.622113
Au	12.132917	28.009621	45.595058
Au	1.578763	12.921054	14.622117
Au	10.640930	35.762243	45.595087
Au	3.070764	5.168412	14.622130
Au	9.148932	33.178049	45.595084
Au	4.562760	7.752652	14.622142
Au	10.640929	30.593853	45.595075
Au	3.070762	10.336851	14.622123
Au	9.148931	28.009613	45.595076
Au	4.562760	12.921058	14.622124
Au	7.656935	35.762251	45.595077
Au	6.054756	5.168412	14.622132
Au	6.164938	33.178045	45.595077
Au	7.546759	7.752641	14.622124
Au	7.656933	30.593849	45.595071
Au	6.054759	10.336853	14.622123
Au	6.164937	28.009603	45.595060
Au	7.546759	12.921054	14.622116
Au	4.672939	35.762250	45.595076
Au	9.038759	5.168409	14.622125
Au	3.180938	33.178049	45.595084
Au	10.530741	7.752633	14.622142
Au	4.672943	30.593848	45.595067
Au	9.038757	10.336860	14.622110
Au	3.180939	28.009613	45.595076
Au	10.530741	12.921058	14.622094
Au	0.086766	3.445605	12.185670
Au	0.086772	1.722814	9.749232
Au	0.086773	-0.000002	7.311896
Au	1.578757	6.029815	12.185671
Au	1.578762	4.307015	9.749214
Au	1.578770	2.584212	7.311895
Au	0.086767	8.614053	12.185668
Au	0.086770	6.891229	9.749215
Au	0.086774	5.168422	7.311899
Au	1.578757	11.198256	12.185676
Au	1.578761	9.475453	9.749217
Au	1.578768	7.752627	7.311893
Au	3.070761	3.445609	12.185664
Au	3.070762	1.722813	9.749220
Au	3.070763	0.000001	7.311890

<b>Au</b>	4.562759	6.029819	12.185675
<b>Au</b>	4.562759	4.307014	9.749204
<b>Au</b>	4.562759	2.584213	7.311889
<b>Au</b>	3.070759	8.614052	12.185669
<b>Au</b>	3.070760	6.891227	9.749217
<b>Au</b>	3.070764	5.168420	7.311890
<b>Au</b>	4.562759	11.198259	12.185667
<b>Au</b>	4.562759	9.475448	9.749210
<b>Au</b>	4.562759	7.752627	7.311888
<b>Au</b>	6.054758	3.445609	12.185665
<b>Au</b>	6.054757	1.722812	9.749221
<b>Au</b>	6.054755	0.000001	7.311890
<b>Au</b>	7.546761	6.029815	12.185671
<b>Au</b>	7.546755	4.307014	9.749214
<b>Au</b>	7.546748	2.584213	7.311896
<b>Au</b>	6.054759	8.614052	12.185669
<b>Au</b>	6.054758	6.891226	9.749218
<b>Au</b>	6.054754	5.168420	7.311890
<b>Au</b>	7.546761	11.198257	12.185676
<b>Au</b>	7.546755	9.475453	9.749217
<b>Au</b>	7.546749	7.752628	7.311893
<b>Au</b>	9.038752	3.445604	12.185669
<b>Au</b>	9.038746	1.722814	9.749230
<b>Au</b>	9.038744	-0.000002	7.311897
<b>Au</b>	10.530740	6.029821	12.185660
<b>Au</b>	10.530740	4.307013	9.749225
<b>Au</b>	10.530740	2.584212	7.311902
<b>Au</b>	9.038751	8.614053	12.185666
<b>Au</b>	9.038747	6.891229	9.749214
<b>Au</b>	9.038743	5.168422	7.311900
<b>Au</b>	10.530740	11.198266	12.185664
<b>Au</b>	10.530741	9.475453	9.749228
<b>Au</b>	10.530741	7.752627	7.311896
<b>Au</b>	13.624905	37.485050	48.031524
<b>Au</b>	13.624910	39.207873	50.467976
<b>Au</b>	13.624913	40.930681	52.905295
<b>Au</b>	12.132917	34.900834	48.031525
<b>Au</b>	12.132916	36.623647	50.467964
<b>Au</b>	12.132917	38.346473	52.905298
<b>Au</b>	13.624904	32.316639	48.031520
<b>Au</b>	13.624911	34.039429	50.467960
<b>Au</b>	13.624912	35.762246	52.905297
<b>Au</b>	12.132916	29.732436	48.031530
<b>Au</b>	12.132917	31.455245	50.467966

<b>Au</b>	12.132917	33.178045	52.905292
<b>Au</b>	10.640928	37.485050	48.031521
<b>Au</b>	10.640923	39.207873	50.467975
<b>Au</b>	10.640919	40.930681	52.905295
<b>Au</b>	9.148937	34.900844	48.031512
<b>Au</b>	9.148933	36.623648	50.467973
<b>Au</b>	9.148926	38.346473	52.905301
<b>Au</b>	10.640929	32.316638	48.031519
<b>Au</b>	10.640922	34.039429	50.467959
<b>Au</b>	10.640921	35.762246	52.905298
<b>Au</b>	9.148937	29.732443	48.031518
<b>Au</b>	9.148932	31.455242	50.467976
<b>Au</b>	9.148924	33.178045	52.905299
<b>Au</b>	7.656938	37.485051	48.031519
<b>Au</b>	7.656937	39.207876	50.467972
<b>Au</b>	7.656933	40.930682	52.905304
<b>Au</b>	6.164938	34.900842	48.031522
<b>Au</b>	6.164938	36.623653	50.467980
<b>Au</b>	6.164938	38.346474	52.905305
<b>Au</b>	7.656937	32.316633	48.031525
<b>Au</b>	7.656936	34.039431	50.467970
<b>Au</b>	7.656934	35.762243	52.905304
<b>Au</b>	6.164938	29.732439	48.031515
<b>Au</b>	6.164937	31.455243	50.467988
<b>Au</b>	6.164938	33.178045	52.905305
<b>Au</b>	4.672938	37.485050	48.031520
<b>Au</b>	4.672939	39.207876	50.467972
<b>Au</b>	4.672943	40.930682	52.905304
<b>Au</b>	3.180935	34.900843	48.031513
<b>Au</b>	3.180940	36.623647	50.467973
<b>Au</b>	3.180946	38.346473	52.905301
<b>Au</b>	4.672939	32.316634	48.031524
<b>Au</b>	4.672939	34.039431	50.467969
<b>Au</b>	4.672942	35.762243	52.905304
<b>Au</b>	3.180936	29.732443	48.031518
<b>Au</b>	3.180940	31.455243	50.467976
<b>Au</b>	3.180949	33.178045	52.905298

Molecule 2 Low G:

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C	3.275231	14.384737	27.107433
C	5.312536	14.684734	33.081023
C	3.219613	14.347882	28.510073
C	6.519097	14.620079	33.832351
C	4.387506	14.605607	29.281188
C	6.482701	14.635745	35.236675
C	5.575230	14.881220	28.544217
C	4.165337	14.776495	35.242614
C	5.540966	14.902025	27.142511
C	4.109407	14.762388	33.839924
C	4.310683	14.588346	30.748931
C	5.374005	14.678402	31.612655
H	2.414385	14.182163	26.534728
H	7.452348	14.556031	33.355809
H	2.301914	14.124038	28.998784
H	7.377178	14.577205	35.819463
H	6.489387	15.088770	29.043239
H	3.276490	14.833646	35.833869
H	6.416545	15.105913	26.594891
H	3.165850	14.824799	33.386389
H	3.333328	14.483629	31.159319
H	6.352548	14.734628	31.225721
N	4.411689	14.670193	26.429311
N	5.328228	14.721383	35.940164
Au	4.473508	14.515784	24.152130
Au	5.344901	14.534332	38.236034
Au	3.933104	11.961170	38.370821
Au	3.010319	11.971451	24.071059
Au	6.801051	11.984047	38.373522
Au	5.900599	11.962079	24.114617
Au	0.040689	10.321805	21.968546
Au	11.268710	16.286900	40.467169
Au	1.431007	12.934151	21.944476
Au	9.807482	13.715685	40.500117
Au	3.012787	10.176599	21.931370
Au	8.333670	16.329100	40.487330
Au	4.520601	12.948032	21.790877
Au	6.856719	13.823273	40.561900
Au	6.062849	10.198296	21.951023
Au	5.295363	16.385249	40.407222
Au	7.582914	12.925966	22.020345

Au	3.735997	13.829376	40.529297
Au	9.030988	10.327826	21.977589
Au	2.265643	16.342589	40.489431
Au	10.476569	12.920721	21.986241
Au	0.794214	13.722236	40.496508
Au	0.000003	15.515712	21.973671
Au	11.286027	11.123726	40.487199
Au	1.488283	18.053111	21.982063
Au	9.818452	8.518061	40.477881
Au	2.962714	15.541957	21.980798
Au	8.396007	11.074789	40.486516
Au	4.533994	18.022623	21.989057
Au	6.852164	8.503596	40.491894
Au	6.070412	15.544635	22.017967
Au	5.338419	10.976173	40.618724
Au	7.564000	18.064424	21.996021
Au	3.765952	8.523904	40.488944
Au	9.020916	15.515940	21.994031
Au	2.247831	11.095817	40.449965
Au	10.492870	18.096230	22.000795
Au	0.800241	8.531120	40.474218
Au	0.079030	8.600470	19.486562
Au	11.264712	18.039369	42.991338
Au	1.582145	11.176237	19.488605
Au	9.765841	15.453134	42.983224
Au	3.070083	8.573863	19.494990
Au	8.283967	18.040196	42.993671
Au	4.558884	11.174279	19.499987
Au	6.776220	15.468043	42.988729
Au	6.053717	8.596498	19.503874
Au	5.291639	18.037586	42.954185
Au	7.534598	11.201288	19.505800
Au	3.804322	15.463756	42.980152
Au	9.035651	8.616023	19.492806
Au	2.306125	18.044017	42.990225
Au	10.525325	11.193532	19.489532
Au	0.816854	15.453882	42.983763
Au	0.066687	13.768044	19.486803
Au	11.261911	12.867109	42.990972
Au	1.568615	16.339280	19.496191
Au	9.774675	10.288038	42.982547
Au	3.044784	13.763295	19.460912
Au	8.265627	12.873836	42.965822
Au	4.556602	16.333669	19.484762

Au	6.798383	10.288829	43.006038
Au	6.057963	13.776077	19.483701
Au	5.291615	12.875990	42.965776
Au	7.528680	16.358568	19.513478
Au	3.799079	10.295280	42.986011
Au	9.013933	13.776039	19.513902
Au	2.322481	12.875532	42.952915
Au	10.511391	16.363676	19.482551
Au	0.829568	10.294619	42.968188
Au	0.099277	6.875849	17.058170
Au	11.257360	19.816766	45.429204
Au	1.598849	9.453876	17.060829
Au	9.760895	17.228469	45.433184
Au	3.081147	6.876770	17.061277
Au	8.266552	19.813952	45.428787
Au	4.581067	9.464027	17.066585
Au	6.773254	17.227977	45.419764
Au	6.070603	6.888491	17.066114
Au	5.283132	19.806720	45.428765
Au	7.561015	9.472269	17.064783
Au	3.795464	17.226075	45.418716
Au	9.044592	6.887309	17.061211
Au	2.306650	19.814833	45.420607
Au	10.546904	9.467465	17.051069
Au	0.811635	17.228023	45.432578
Au	0.101425	12.045398	17.055306
Au	11.253383	14.641649	45.427173
Au	1.588967	14.627797	17.049951
Au	9.756362	12.062851	45.422898
Au	3.087993	12.034851	17.043922
Au	8.269194	14.644626	45.434085
Au	4.575002	14.634374	17.046619
Au	6.773864	12.064453	45.435954
Au	6.067927	12.046332	17.051400
Au	5.282897	14.640783	45.431328
Au	7.553742	14.640789	17.061891
Au	3.794642	12.062823	45.429268
Au	9.049753	12.057598	17.062742
Au	2.300650	14.642248	45.431212
Au	10.534420	14.631167	17.064683
Au	0.816321	12.062255	45.419423
Au	0.108486	5.168414	14.621835
Au	12.738746	24.181661	47.878943
Au	1.600483	7.752643	14.621836

Au	11.246763	21.597461	47.878947
Au	0.108483	10.336860	14.621829
Au	12.738746	19.013244	47.878925
Au	1.600483	12.921057	14.621829
Au	11.246764	16.429020	47.878923
Au	3.092485	5.168416	14.621848
Au	9.754781	24.181661	47.878940
Au	4.584486	7.752651	14.621848
Au	8.262779	21.597460	47.878926
Au	3.092486	10.336857	14.621841
Au	9.754778	19.013244	47.878921
Au	4.584485	12.921057	14.621832
Au	8.262782	16.429022	47.878928
Au	6.076482	5.168414	14.621844
Au	6.770782	24.181661	47.878930
Au	7.568482	7.752640	14.621832
Au	5.278781	21.597452	47.878921
Au	6.076482	10.336855	14.621837
Au	6.770778	19.013248	47.878924
Au	7.568483	12.921054	14.621823
Au	5.278781	16.429020	47.878914
Au	9.060481	5.168410	14.621834
Au	3.786780	24.181662	47.878932
Au	10.552463	7.752637	14.621849
Au	2.294784	21.597461	47.878927
Au	9.060479	10.336859	14.621821
Au	3.786786	19.013249	47.878925
Au	10.552461	12.921059	14.621809
Au	2.294781	16.429023	47.878930
Au	0.108486	3.445605	12.185389
Au	0.108493	1.722815	9.748950
Au	0.108494	-0.000003	7.311615
Au	1.600479	6.029815	12.185389
Au	1.600484	4.307016	9.748934
Au	1.600492	2.584213	7.311615
Au	0.108488	8.614052	12.185386
Au	0.108492	6.891228	9.748934
Au	0.108497	5.168422	7.311617
Au	1.600480	11.198258	12.185396
Au	1.600483	9.475453	9.748935
Au	1.600489	7.752627	7.311611
Au	3.092482	3.445609	12.185383
Au	3.092484	1.722812	9.748939
Au	3.092485	0.000001	7.311607

Au	4.584483	6.029818	12.185395
Au	4.584483	4.307013	9.748922
Au	4.584483	2.584214	7.311607
Au	3.092482	8.614053	12.185393
Au	3.092482	6.891227	9.748936
Au	3.092487	5.168420	7.311607
Au	4.584484	11.198258	12.185387
Au	4.584483	9.475448	9.748929
Au	4.584483	7.752626	7.311606
Au	6.076485	3.445608	12.185385
Au	6.076482	1.722811	9.748942
Au	6.076480	0.000001	7.311607
Au	7.568486	6.029815	12.185392
Au	7.568480	4.307015	9.748934
Au	7.568472	2.584213	7.311615
Au	6.076484	8.614053	12.185393
Au	6.076483	6.891226	9.748937
Au	6.076478	5.168420	7.311608
Au	7.568484	11.198258	12.185398
Au	7.568480	9.475454	9.748937
Au	7.568474	7.752628	7.311611
Au	9.060475	3.445604	12.185388
Au	9.060469	1.722815	9.748950
Au	9.060469	-0.000003	7.311616
Au	10.552462	6.029822	12.185383
Au	10.552463	4.307013	9.748947
Au	10.552463	2.584212	7.311621
Au	9.060473	8.614052	12.185387
Au	9.060471	6.891229	9.748934
Au	9.060468	5.168422	7.311618
Au	10.552462	11.198267	12.185380
Au	10.552463	9.475452	9.748947
Au	10.552464	7.752627	7.311614
Au	12.738752	25.904458	50.315348
Au	12.738751	27.627274	52.751797
Au	12.738758	29.350089	55.189123
Au	11.246765	23.320256	50.315351
Au	11.246765	25.043059	52.751781
Au	11.246765	26.765877	55.189123
Au	12.738753	20.736053	50.315344
Au	12.738756	22.458852	52.751790
Au	12.738759	24.181662	55.189117
Au	11.246765	18.151827	50.315352
Au	11.246764	19.874640	52.751792

Au	11.246765	21.597450	55.189119
Au	9.754777	25.904457	50.315349
Au	9.754777	27.627274	52.751796
Au	9.754770	29.350088	55.189124
Au	8.262788	23.320260	50.315343
Au	8.262781	25.043058	52.751794
Au	8.262777	26.765877	55.189123
Au	9.754775	20.736053	50.315343
Au	9.754773	22.458851	52.751790
Au	9.754769	24.181662	55.189118
Au	8.262786	18.151834	50.315345
Au	8.262781	19.874644	52.751805
Au	8.262775	21.597451	55.189128
Au	6.770784	25.904457	50.315339
Au	6.770780	27.627274	52.751795
Au	6.770779	29.350087	55.189132
Au	5.278781	23.320253	50.315346
Au	5.278781	25.043063	52.751800
Au	5.278782	26.765877	55.189132
Au	6.770781	20.736053	50.315345
Au	6.770784	22.458852	52.751798
Au	6.770780	24.181661	55.189129
Au	5.278782	18.151835	50.315338
Au	5.278782	19.874645	52.751811
Au	5.278781	21.597451	55.189135
Au	3.786779	25.904457	50.315340
Au	3.786783	27.627275	52.751794
Au	3.786785	29.350087	55.189132
Au	2.294776	23.320260	50.315342
Au	2.294783	25.043058	52.751793
Au	2.294788	26.765877	55.189123
Au	3.786783	20.736054	50.315343
Au	3.786779	22.458853	52.751798
Au	3.786784	24.181661	55.189129
Au	2.294777	18.151834	50.315344
Au	2.294784	19.874645	52.751805
Au	2.294789	21.597451	55.189128

Molecule 3 High G:

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C	7.095750	11.447724	26.747237
C	4.916429	7.259245	30.783528
C	7.158277	10.536758	27.812371
C	4.878095	8.169458	29.715523
C	5.960684	10.040382	28.385841
C	5.977576	9.034653	29.486606
C	4.743847	10.542677	27.857796
C	7.087273	8.896864	30.357497
C	4.769241	11.446356	26.784462
C	7.045905	7.956507	31.400039
H	7.980052	11.816635	26.311549
H	4.096219	6.616257	30.992472
H	8.103480	10.206620	28.160449
H	4.031074	8.185014	29.105345
H	3.812358	10.255330	28.277852
H	7.938247	9.512577	30.279057
H	3.869357	11.816617	26.381498
H	7.860600	7.857284	32.090209
N	5.923646	11.880247	26.223148
N	5.975828	7.154480	31.621398
Au	5.760994	6.129301	33.633245
Au	5.919836	12.502638	24.069407
Au	0.003083	10.551837	21.973878
Au	11.678113	7.760087	35.777733
Au	1.462974	13.144759	21.951054
Au	10.212364	5.175393	35.790594
Au	2.972950	10.553172	21.948074
Au	8.705870	7.764516	35.798750
Au	4.403347	13.199881	21.890314
Au	7.251771	5.130129	35.776280
Au	5.970504	10.522340	21.990039
Au	5.704903	7.867333	35.839761
Au	7.522028	13.189480	21.920523
Au	4.204390	5.152987	35.735846
Au	8.968171	10.552427	21.951474
Au	2.712691	7.770760	35.801983
Au	10.467135	13.142106	21.956451
Au	1.228658	5.178967	35.784567
Au	0.000000	15.734931	21.976594
Au	11.684034	2.587877	35.777742
Au	1.484612	18.317611	21.978096

Au	10.198785	0.000000	35.779723
Au	2.955811	15.762318	21.960499
Au	8.728425	2.571527	35.783292
Au	4.473143	18.301999	21.974464
Au	7.227441	0.038195	35.789840
Au	5.969572	15.735857	21.975904
Au	5.715215	2.578361	35.785090
Au	7.468258	18.301394	21.975949
Au	4.192293	0.047532	35.791135
Au	8.978321	15.755597	21.964941
Au	2.707892	2.588984	35.780093
Au	10.450779	18.316795	21.978677
Au	1.223094	0.007574	35.784131
Au	0.006590	8.786260	19.490967
Au	11.669561	9.500338	38.265753
Au	1.498324	11.369317	19.484790
Au	10.179014	6.914482	38.263900
Au	2.993005	8.780960	19.493461
Au	8.683930	9.503931	38.264753
Au	4.484896	11.366346	19.480873
Au	7.194203	6.918692	38.268210
Au	5.975679	8.800601	19.518524
Au	5.701138	9.509462	38.264211
Au	7.464501	11.367728	19.486531
Au	4.209781	6.918809	38.266836
Au	8.957375	8.781833	19.493141
Au	2.719081	9.505343	38.263929
Au	10.451597	11.369013	19.486157
Au	1.224685	6.915136	38.262073
Au	0.003461	13.958977	19.475711
Au	11.674966	4.330714	38.267599
Au	1.492163	16.542611	19.483162
Au	10.183100	1.748612	38.267901
Au	2.987566	13.954641	19.476435
Au	8.673854	4.341884	38.239375
Au	4.485593	16.533655	19.493947
Au	7.195191	1.764316	38.266175
Au	5.976019	13.958905	19.452317
Au	5.702848	4.342525	38.268523
Au	7.464242	16.534239	19.494995
Au	4.210091	1.766121	38.265982
Au	8.954836	13.950753	19.490710
Au	2.743952	4.350608	38.222714
Au	10.453766	16.541355	19.485615

Au	1.226307	1.752755	38.265965
Au	0.012467	6.994027	17.050469
Au	11.659344	11.261112	40.700889
Au	1.506625	9.576424	17.058591
Au	10.165527	8.672307	40.693191
Au	2.999492	6.995357	17.060503
Au	8.674483	11.258332	40.692209
Au	4.491423	9.573941	17.058804
Au	7.183027	8.674934	40.700604
Au	5.981484	6.999861	17.069835
Au	5.690005	11.256633	40.688568
Au	7.471878	9.575346	17.059617
Au	4.196682	8.675138	40.699989
Au	8.962565	6.995966	17.060488
Au	2.706619	11.258116	40.691818
Au	10.455748	9.576904	17.058625
Au	1.214813	8.672495	40.692552
Au	0.012791	12.160402	17.056660
Au	11.658875	6.089271	40.694503
Au	1.506922	14.746725	17.056013
Au	10.162246	3.508956	40.683890
Au	2.994763	12.158689	17.047007
Au	8.676690	6.087205	40.697089
Au	4.485591	14.750072	17.040944
Au	7.185285	3.507030	40.701717
Au	5.982050	12.157612	17.048050
Au	5.689730	6.091665	40.700176
Au	7.478806	14.749967	17.043753
Au	4.193480	3.508776	40.698189
Au	8.967371	12.159778	17.050429
Au	2.703205	6.087521	40.695631
Au	10.452158	14.745826	17.059525
Au	1.223128	3.509928	40.680236
Au	0.021736	5.191618	14.622464
Au	11.646452	13.025980	43.128532
Au	1.513725	7.775841	14.622447
Au	10.154464	10.441763	43.128534
Au	3.005722	5.191621	14.622451
Au	8.662468	13.025981	43.128533
Au	4.497718	7.775841	14.622462
Au	7.170469	10.441762	43.128518
Au	5.989715	5.191622	14.622454
Au	5.678473	13.025976	43.128525
Au	7.481713	7.775841	14.622461

Au	4.186474	10.441763	43.128518
Au	8.973708	5.191621	14.622451
Au	2.694475	13.025981	43.128533
Au	10.465705	7.775841	14.622445
Au	1.202480	10.441763	43.128534
Au	0.021734	10.360046	14.622445
Au	11.646453	7.857556	43.128534
Au	1.513726	12.944255	14.622446
Au	10.154459	5.273343	43.128535
Au	3.005717	10.360049	14.622445
Au	8.662469	7.857553	43.128535
Au	4.497715	12.944258	14.622457
Au	7.170473	5.273341	43.128528
Au	5.989716	10.360045	14.622451
Au	5.678472	7.857555	43.128527
Au	7.481716	12.944258	14.622455
Au	4.186470	5.273341	43.128528
Au	8.973714	10.360049	14.622444
Au	2.694473	7.857553	43.128535
Au	10.465703	12.944255	14.622446
Au	1.202484	5.273343	43.128536
Au	0.021733	3.468819	12.185998
Au	0.021732	1.746016	9.749544
Au	0.021733	0.023203	7.312211
Au	1.513726	6.053033	12.185988
Au	1.513722	4.330225	9.749531
Au	1.513725	2.607415	7.312208
Au	3.005716	3.468819	12.185986
Au	3.005717	1.746016	9.749532
Au	3.005722	0.023203	7.312209
Au	4.497714	6.053037	12.185994
Au	4.497713	4.330227	9.749530
Au	4.497719	2.607415	7.312204
Au	5.989715	3.468819	12.185983
Au	5.989714	1.746011	9.749531
Au	5.989714	0.023205	7.312203
Au	7.481715	6.053036	12.185994
Au	7.481716	4.330226	9.749529
Au	7.481711	2.607415	7.312204
Au	8.973712	3.468819	12.185987
Au	8.973712	1.746016	9.749533
Au	8.973708	0.023203	7.312210
Au	10.465703	6.053033	12.185989
Au	10.465705	4.330225	9.749532

Au	10.465703	2.607415	7.312208
Au	0.021733	8.637254	12.185981
Au	0.021733	6.914440	9.749536
Au	0.021733	5.191629	7.312210
Au	1.513722	11.221456	12.185993
Au	1.513723	9.498651	9.749536
Au	1.513725	7.775838	7.312211
Au	3.005718	8.637250	12.185995
Au	3.005719	6.914441	9.749532
Au	3.005720	5.191628	7.312207
Au	4.497711	11.221456	12.185988
Au	4.497715	9.498649	9.749533
Au	4.497716	7.775839	7.312203
Au	5.989714	8.637248	12.185993
Au	5.989714	6.914439	9.749531
Au	5.989714	5.191627	7.312204
Au	7.481719	11.221456	12.185988
Au	7.481714	9.498649	9.749534
Au	7.481714	7.775839	7.312203
Au	8.973711	8.637251	12.185995
Au	8.973710	6.914441	9.749532
Au	8.973709	5.191628	7.312207
Au	10.465706	11.221456	12.185994
Au	10.465704	9.498652	9.749536
Au	10.465703	7.775838	7.312212
Au	11.646454	14.748783	45.564977
Au	11.646454	16.471588	48.001426
Au	11.646454	18.194401	50.438757
Au	10.154461	12.164570	45.564988
Au	10.154465	13.887378	48.001439
Au	10.154462	15.610187	50.438759
Au	8.662472	14.748785	45.564991
Au	8.662470	16.471588	48.001441
Au	8.662466	18.194401	50.438758
Au	7.170474	12.164568	45.564982
Au	7.170474	13.887376	48.001443
Au	7.170469	15.610188	50.438764
Au	5.678473	14.748783	45.564991
Au	5.678473	16.471592	48.001441
Au	5.678473	18.194399	50.438765
Au	4.186471	12.164568	45.564981
Au	4.186471	13.887376	48.001443
Au	4.186476	15.610188	50.438764
Au	2.694474	14.748785	45.564990

<b>Au</b>	2.694475	16.471588	48.001442
<b>Au</b>	2.694479	18.194401	50.438758
<b>Au</b>	1.202485	12.164571	45.564988
<b>Au</b>	1.202481	13.887378	48.001439
<b>Au</b>	1.202484	15.610187	50.438759
<b>Au</b>	11.646454	9.580352	45.564997
<b>Au</b>	11.646454	11.303166	48.001436
<b>Au</b>	11.646454	13.025977	50.438757
<b>Au</b>	10.154464	6.996145	45.564982
<b>Au</b>	10.154464	8.718951	48.001437
<b>Au</b>	10.154462	10.441766	50.438756
<b>Au</b>	8.662471	9.580355	45.564984
<b>Au</b>	8.662468	11.303165	48.001441
<b>Au</b>	8.662468	13.025977	50.438761
<b>Au</b>	7.170477	6.996145	45.564989
<b>Au</b>	7.170472	8.718954	48.001440
<b>Au</b>	7.170472	10.441764	50.438766
<b>Au</b>	5.678473	9.580357	45.564987
<b>Au</b>	5.678473	11.303168	48.001442
<b>Au</b>	5.678473	13.025978	50.438765
<b>Au</b>	4.186467	6.996145	45.564989
<b>Au</b>	4.186473	8.718954	48.001440
<b>Au</b>	4.186473	10.441764	50.438766
<b>Au</b>	2.694475	9.580355	45.564984
<b>Au</b>	2.694477	11.303165	48.001441
<b>Au</b>	2.694477	13.025977	50.438761
<b>Au</b>	1.202482	6.996145	45.564982
<b>Au</b>	1.202482	8.718951	48.001437
<b>Au</b>	1.202484	10.441766	50.438757

Molecule 3 Low G:

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H	10.458751	14.899054	26.475446
H	10.471217	14.969487	28.932304
H	7.635817	18.186095	28.690539
H	7.710553	17.943929	26.245828
H	7.051021	17.531393	33.188757
H	6.994923	17.394156	30.735553
H	11.060094	16.016154	30.883158
H	10.923417	16.167065	33.332700
C	9.858905	15.596333	26.980724
C	9.870203	15.651931	28.380182
C	9.051524	16.595479	29.050307
C	8.250653	17.443600	28.245060
C	8.296623	17.320422	26.850615
C	7.899301	17.205406	32.625505
C	7.879527	17.135356	31.226974
C	9.030956	16.688402	30.531383
C	10.159308	16.330728	31.311364
C	10.094669	16.427432	32.707049
N	8.986337	16.858839	33.353512
N	9.086709	16.414371	26.229539
Au	9.134125	16.305958	24.024078
Au	8.950118	16.963291	35.544173
Au	9.134868	18.153365	21.915823
Au	8.948978	15.132260	37.655201
Au	12.135788	18.108457	21.945709
Au	5.947607	15.176655	37.624732
Au	15.100747	18.095198	21.969277
Au	2.982644	15.189980	37.601250
Au	18.066715	18.107393	21.948677
Au	0.016960	15.177940	37.621956
Au	7.586178	15.478999	21.886140
Au	10.495886	17.806200	37.683983
Au	10.678658	15.483745	21.884438
Au	7.406835	17.802534	37.685197
Au	13.628752	15.506427	21.947024
Au	4.455168	17.778590	37.623103
Au	16.572112	15.506592	21.947392
Au	1.511093	17.778419	37.622630
Au	9.132073	12.916033	21.960977
Au	8.951352	20.369087	37.611027
Au	12.134330	12.911523	21.945647

Au	5.948735	20.373705	37.625626
Au	15.099730	12.918407	21.972102
Au	2.983565	20.366456	37.599130
Au	18.064850	12.909220	21.944679
Au	0.018758	20.375647	37.626161
Au	7.629936	10.360883	21.954657
Au	10.453589	22.923521	37.617231
Au	10.634334	10.363300	21.953162
Au	7.448915	22.921522	37.618293
Au	13.614211	10.339586	21.967166
Au	4.469078	22.945694	37.603892
Au	16.586037	10.338316	21.968308
Au	1.497407	22.946871	37.602968
Au	9.131598	16.377472	19.440016
Au	8.951581	16.907562	40.131290
Au	12.121045	16.373560	19.472985
Au	5.962173	16.911804	40.097358
Au	15.100085	16.380771	19.475648
Au	2.983134	16.904375	40.095305
Au	18.079404	16.373589	19.474923
Au	0.003970	16.911763	40.095799
Au	7.639148	13.784961	19.473332
Au	10.444235	19.500379	40.097441
Au	10.624426	13.785478	19.473546
Au	7.458599	19.499997	40.097359
Au	13.610656	13.789805	19.482927
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Au	16.588901	13.789920	19.483284
Au	1.494388	19.495269	40.087629
Au	9.131521	11.208914	19.484681
Au	8.951684	22.076588	40.085890
Au	12.121886	11.201479	19.477446
Au	5.961057	22.084000	40.093206
Au	15.100043	11.207580	19.490248
Au	2.983206	22.077648	40.080784
Au	18.077641	11.201158	19.477502
Au	0.005860	22.084251	40.093077
Au	7.641457	8.623937	19.482214
Au	10.441848	24.661187	40.088437
Au	10.622661	8.624417	19.480667
Au	7.460690	24.660799	40.089755
Au	13.609734	8.621979	19.483608
Au	4.473420	24.663374	40.087375
Au	16.590525	8.621861	19.483415

Au	1.492748	24.663459	40.087325
Au	9.131518	14.645351	17.042467
Au	8.951742	18.638497	42.526897
Au	12.117533	14.649757	17.048077
Au	5.965645	18.635130	42.522921
Au	15.099671	14.652062	17.056845
Au	2.983604	18.632838	42.514444
Au	18.081709	14.649973	17.048586
Au	0.001685	18.634961	42.522482
Au	7.638947	12.066754	17.054678
Au	10.445062	21.218722	42.515418
Au	10.624224	12.066732	17.054822
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Au	13.608217	12.067908	17.055503
Au	4.475041	21.217044	42.515757
Au	16.591066	12.067980	17.055249
Au	1.492250	21.217004	42.515883
Au	9.131451	9.485533	17.052001
Au	8.951806	23.799318	42.519079
Au	12.116288	9.483796	17.055252
Au	5.966955	23.801236	42.515831
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Au	2.983660	23.798853	42.515161
Au	18.083216	9.483813	17.055685
Au	0.000220	23.801248	42.515524
Au	7.634199	6.903914	17.044557
Au	10.449242	26.380716	42.526506
Au	10.628821	6.903919	17.044318
Au	7.454297	26.380734	42.526777
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Au	4.475280	26.383812	42.518277
Au	16.591677	6.900956	17.053250
Au	1.491629	26.383935	42.517909
Au	9.131554	12.919570	14.615139
Au	8.952000	20.363137	44.948865
Au	12.115630	12.921531	14.623318
Au	5.967992	20.363132	44.948870
Au	15.099571	12.921528	14.623307
Au	2.984000	20.363133	44.948877
Au	18.083512	12.921532	14.623318
Au	0.000008	20.363132	44.948870
Au	7.639539	10.336592	14.623333
Au	10.444002	22.948023	44.948857
Au	10.623604	10.336593	14.623333

Au	7.459998	22.948023	44.948857
Au	13.607580	10.336627	14.623309
Au	4.475999	22.948029	44.948875
Au	16.591562	10.336627	14.623308
Au	1.492001	22.948029	44.948875
Au	9.131571	7.752649	14.623311
Au	8.952000	25.532009	44.948869
Au	12.115583	7.752654	14.623308
Au	5.967993	25.532008	44.948873
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Au	2.984000	25.532013	44.948865
Au	18.083559	7.752654	14.623308
Au	0.000007	25.532008	44.948873
Au	7.639543	5.168698	14.623324
Au	10.444005	28.116004	44.948862
Au	10.623598	5.168698	14.623325
Au	7.459995	28.116003	44.948862
Au	13.607582	5.168661	14.623307
Au	4.475996	28.116006	44.948876
Au	16.591560	5.168661	14.623308
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Au	9.131571	11.198566	12.186295
Au	9.131571	9.475804	9.749885
Au	9.131571	7.752997	7.312569
Au	12.115600	11.198604	12.186346
Au	12.115581	9.475806	9.749886
Au	12.115576	7.752998	7.312572
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Au	18.083542	11.198604	12.186346
Au	18.083561	9.475806	9.749886
Au	18.083565	7.752998	7.312573
Au	7.639557	8.614608	12.186346
Au	7.639562	6.891810	9.749884
Au	7.639568	5.168997	7.312567
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Au	10.623580	6.891810	9.749884
Au	10.623573	5.168997	7.312567
Au	13.607579	8.614609	12.186347
Au	13.607581	6.891808	9.749893
Au	13.607574	5.168996	7.312571
Au	16.591563	8.614609	12.186348
Au	16.591561	6.891808	9.749893

Au	16.591567	5.168996	7.312571
Au	9.131571	6.029637	12.186332
Au	9.131571	4.306813	9.749871
Au	9.131570	2.583997	7.312562
Au	12.115589	6.029626	12.186342
Au	12.115584	4.306812	9.749888
Au	12.115575	2.583996	7.312567
Au	15.099571	6.029620	12.186358
Au	15.099571	4.306814	9.749896
Au	15.099571	2.583995	7.312574
Au	18.083553	6.029626	12.186342
Au	18.083558	4.306812	9.749888
Au	18.083566	2.583996	7.312567
Au	7.639521	3.445641	12.186294
Au	7.639559	1.722805	9.749874
Au	7.639567	-0.000004	7.312564
Au	10.623620	3.445641	12.186294
Au	10.623583	1.722805	9.749874
Au	10.623574	-0.000004	7.312564
Au	13.607591	3.445620	12.186341
Au	13.607579	1.722808	9.749890
Au	13.607575	-0.000003	7.312574
Au	16.591552	3.445620	12.186341
Au	16.591563	1.722808	9.749890
Au	16.591567	-0.000003	7.312574
Au	8.952000	22.086046	47.393654
Au	8.952000	23.808853	49.830093
Au	8.952000	25.531664	52.267386
Au	5.967993	22.086047	47.393649
Au	5.967993	23.808853	49.830095
Au	5.967996	25.531663	52.267382
Au	2.984000	22.086044	47.393663
Au	2.984000	23.808855	49.830089
Au	2.984000	25.531662	52.267377
Au	0.000007	22.086047	47.393649
Au	0.000007	23.808853	49.830095
Au	0.000005	25.531663	52.267382
Au	10.444009	24.670046	47.393657
Au	10.444009	26.392854	49.830097
Au	10.444002	28.115666	52.267387
Au	7.459991	24.670046	47.393657
Au	7.459991	26.392854	49.830097
Au	7.459998	28.115666	52.267387
Au	4.475995	24.670052	47.393662

Au	4.475991	26.392855	49.830088
Au	4.475997	28.115667	52.267382
Au	1.492005	24.670052	47.393662
Au	1.492009	26.392855	49.830088
Au	1.492003	28.115667	52.267382
Au	8.952000	27.255044	47.393667
Au	8.952000	28.977856	49.830097
Au	8.952000	30.700667	52.267390
Au	5.967990	27.255044	47.393663
Au	5.967991	28.977853	49.830090
Au	5.967996	30.700667	52.267386
Au	2.984000	27.255045	47.393651
Au	2.984000	28.977850	49.830085
Au	2.984000	30.700668	52.267380
Au	0.000010	27.255044	47.393663
Au	0.000009	28.977853	49.830090
Au	0.000004	30.700667	52.267386
Au	10.444008	29.839049	47.393664
Au	10.444006	31.561855	49.830094
Au	10.444003	33.284665	52.267389
Au	7.459992	29.839049	47.393664
Au	7.459994	31.561855	49.830094
Au	7.459997	33.284665	52.267390
Au	4.475991	29.839045	47.393665
Au	4.475996	31.561854	49.830092
Au	4.475997	33.284665	52.267380
Au	1.492009	29.839045	47.393664
Au	1.492004	31.561854	49.830092
Au	1.492003	33.284665	52.267380