

Supporting Information for:

The Conformational Dynamics of the Ligands Determines the Electronic Circular Dichroism of the Chiral $\text{Au}_{38}(\text{SC}_2\text{H}_4\text{Ph})_{24}$ Cluster

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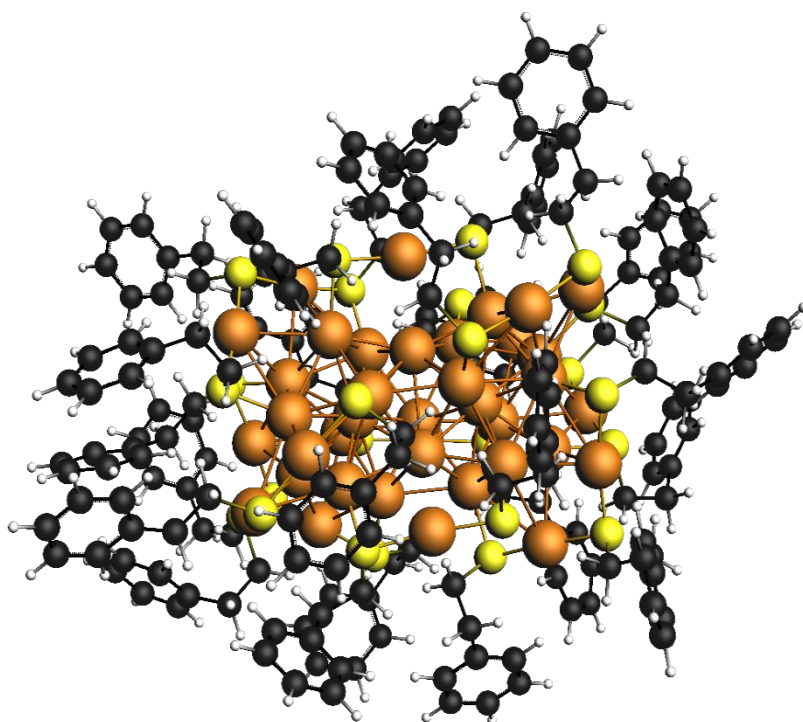


Figure S1. Ball and stick model of the experimental X-ray $\text{Au}_{38}(\text{SC}_2\text{H}_4\text{Ph})_{24}$ structure¹. Au, S, C, and H atoms are reported in orange, yellow, black, and white, respectively.

All-atoms MD vs Au-constrained MD

It is well known the importance of calculating the ECD spectra on realistic geometries to obtain reliable results and in the specific case of gold nanoclusters, the relevance of a reasonable metal-sulphur architecture has proven to be fundamental for the ECD calculation^{1,2}. Therefore, the resolution of several X-ray gold nanostructures has represented a breakthrough for a suitable analysis of the spectral features. Naturally, the X-ray structure is less important when the chirality regards the ligands because of their higher conformational flexibility, which characterizes their ECD in the liquid phase. Hence, the calculation of the ECD on a gas phase nanocluster and its comparison with respect the experimental liquid phase ECD must consider the flexibility of the ligands as well as the necessity of a reliable geometry of the staples (Au-S structures). Starting from these considerations, we constrained the gold atoms to maintain the experimental geometry for the metallic region but without affecting the ligands internal motions. However, we wanted to verify the validity of our choice estimating the effective contribution of the gold atoms to the conformational transitions and to understand if their exclusion in the conformational analysis is justified. Such an estimate was

performed running a 50 ns all-atoms MD simulation with no constraints and calculating the first two total eigenvectors components of the covariance matrix for Au and S (see Figure S2).

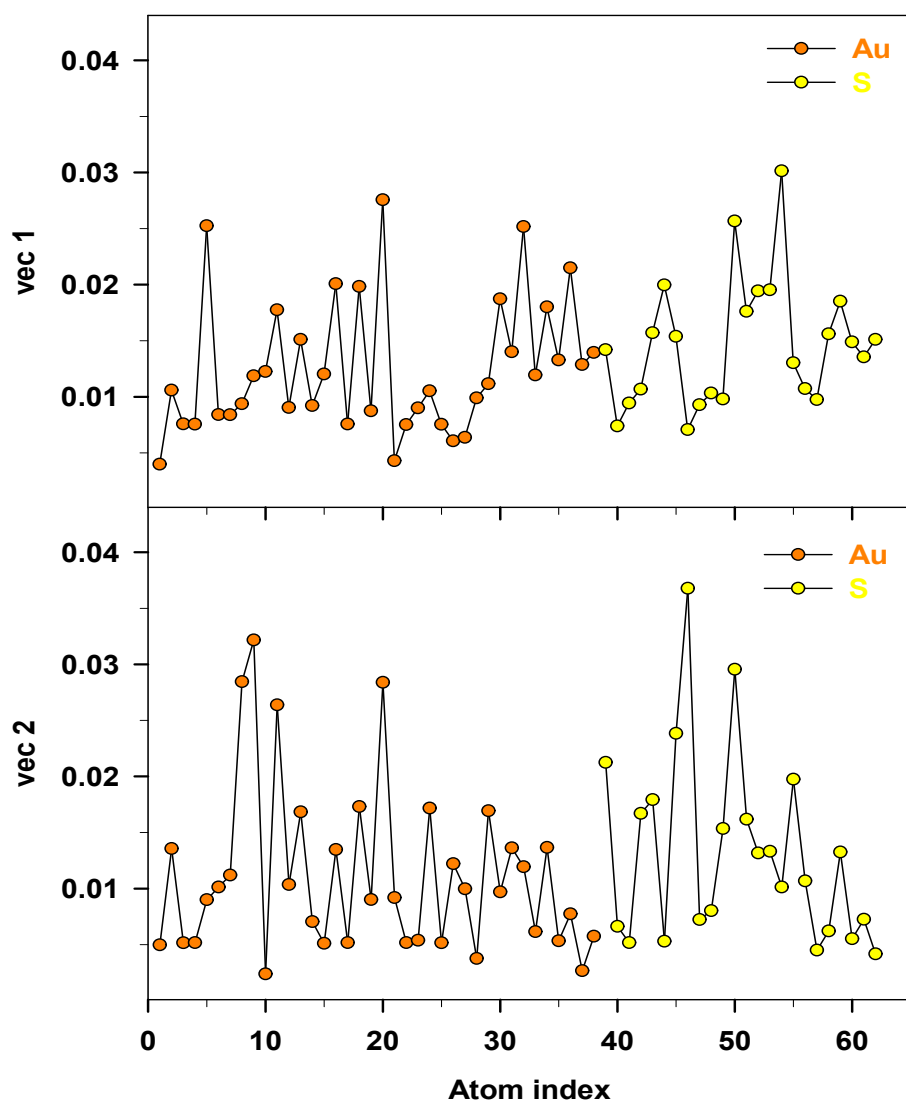


Figure S2. First eigenvector (upper panel) and second eigenvector (lower panel) total components for the gold (orange) and sulphur (yellow) atoms calculated from the 50 ns all atoms free-MD simulation.

Looking at the value scale of the total first pair of eigenvectors, it is worth noting that the contribution of both gold and sulphur atoms to the most relevant conformational transitions is quite small. Such result justifies the constraints on the gold atoms and thus their exclusion from the conformational analysis we carried out to find the most probable structures. The following Figure S3 underlines how small is the contributions of the staple atoms with respect to the ligand ones, which start from atom index 63.

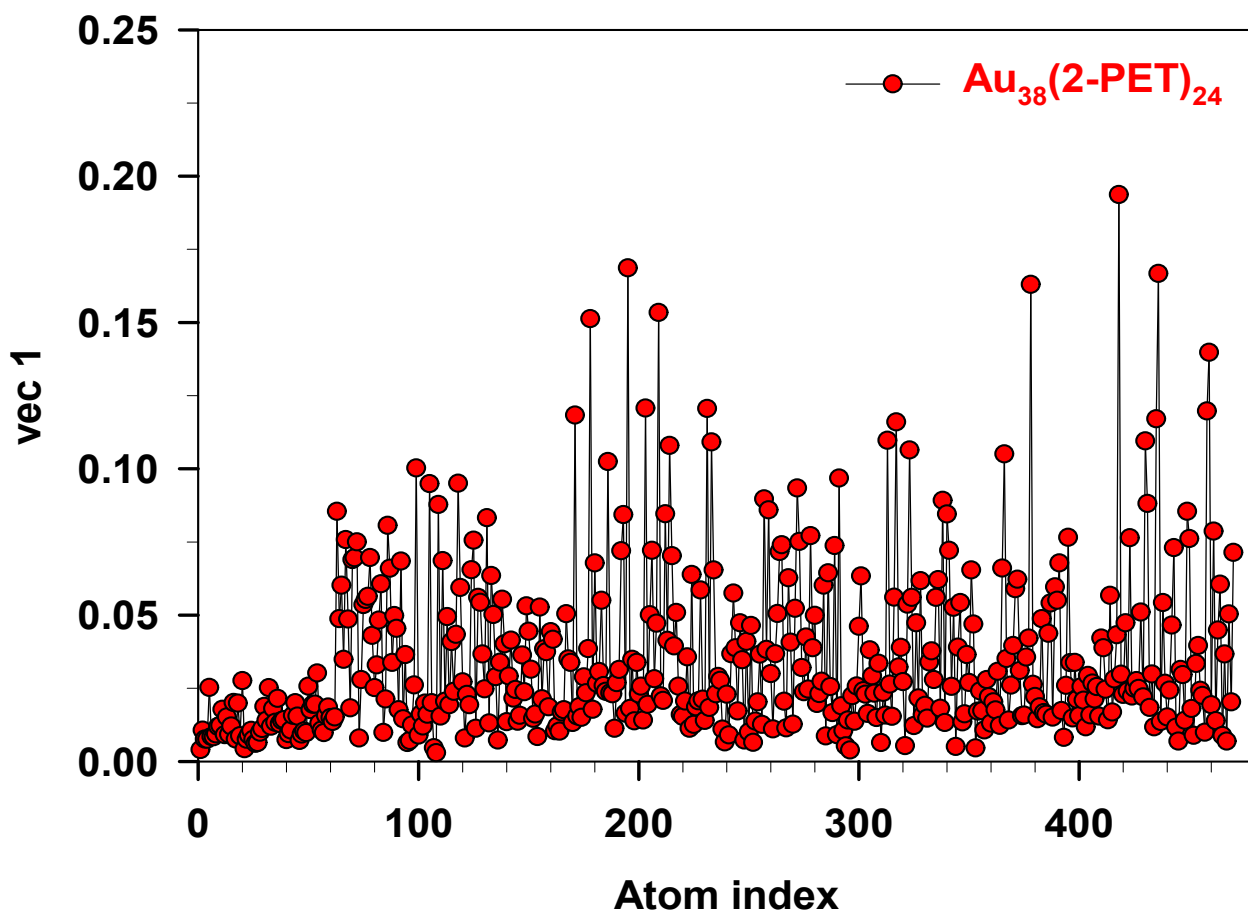


Figure S3. First eigenvector total component for the $\text{Au}_{38}(\text{2-PET})_{24}$ atoms calculated from the 50 ns all atoms free-MD simulation.

As we can see, we obtained that the total component of the first eigenvector, which is directly related to the atomic contribution to the most relevant internal transitions, is on average 10 times larger for the (2-PET) atoms with respect to the values found for the Au/S atoms. This result is easily understood comparing the flexibility, and thus the fluctuations, of the metallic and organic components of the system.

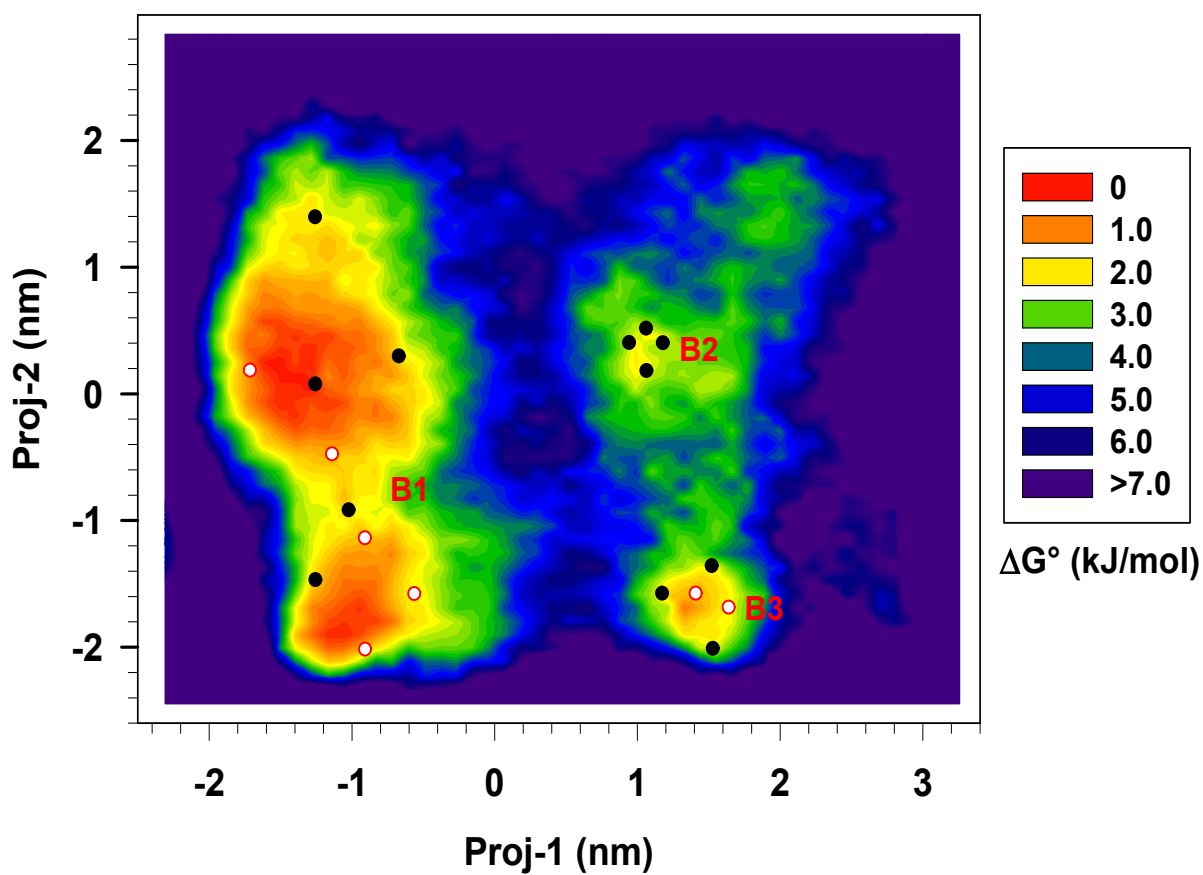


Figure S4. Probability pattern built to represent the ΔG° landscape on the conformational space. The positions of the 19 conformations initially extracted have been marked with dots (i.e., black for the conformations of the final set, white for the conformations discarded in the final analysis).

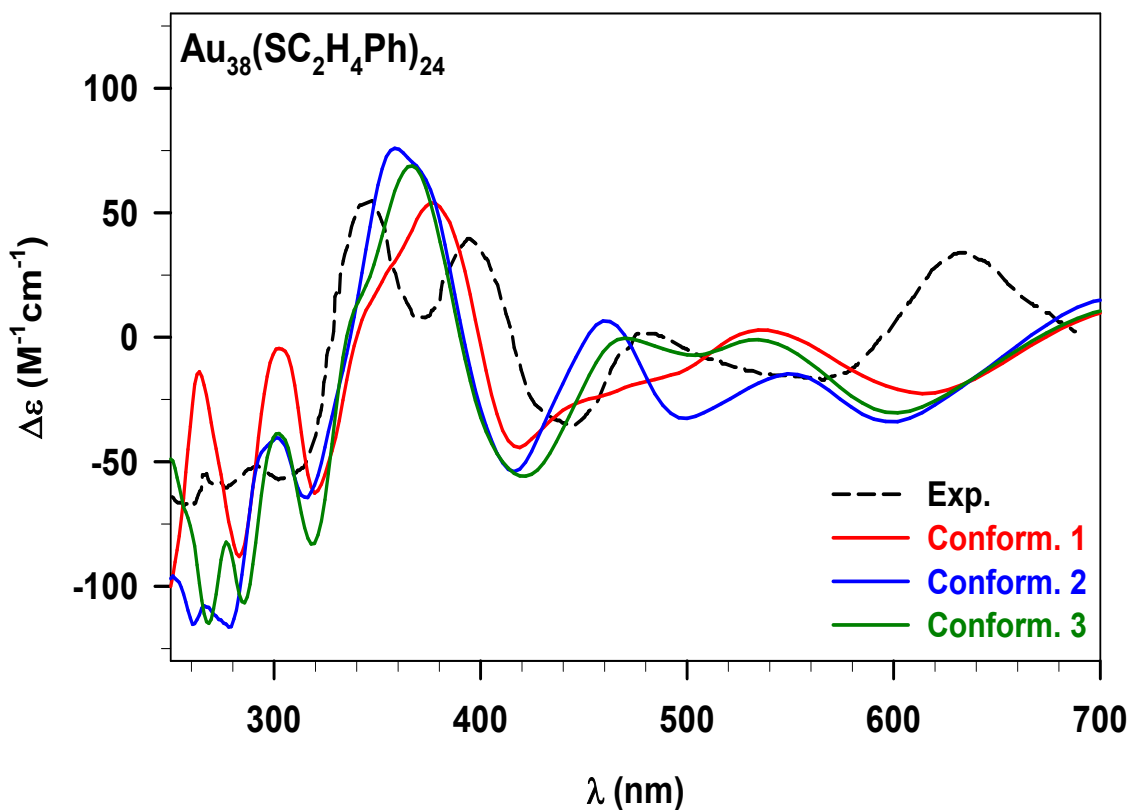


Figure S5. Experimental (Exp., black dashed line) and Calculated ECD spectra of three similar conformations in terms of RMSD values (red, blue, and green solid line). The computational details of the polTDDFT calculations have been reported in the Computational Section.

Table S1. Atomic Coordinates of the 12 selected $\text{Au}_{38}(\text{2-PET})_{24}$ conformations

B1-A	x (Å)	y (Å)	z (Å)
Au	0.098494	-0.071185	0.052891
Au	2.903032	-0.054136	0.10086
Au	1.409987	2.399101	0.019794
Au	1.640136	-1.970445	-1.469053
Au	1.507063	0.263255	2.507801
Au	0.375789	4.77246	1.04364
Au	3.262129	4.467004	0.812334
Au	3.983451	2.250211	-1.128596
Au	-0.691273	2.067122	1.904326
Au	1.607102	0.828972	-2.274374
Au	1.821398	3.028805	2.729325
Au	5.739221	0.001018	0.06139

Au	4.322615	-2.402107	0.018144
Au	4.316982	1.785135	1.689938
Au	1.700332	-2.253163	1.36238
Au	4.166636	-0.535662	-2.332675
Au	4.104844	-0.922612	2.466586
S	6.084377	-1.214399	-3.645056
Au	2.132918	5.754466	3.202088
Au	-0.439934	4.316086	3.689383
Au	4.342627	3.947036	3.577175
Au	0.274268	1.608253	4.615525
Au	3.317134	1.339427	4.37881
Au	2.00762	3.664348	5.425171
S	5.072231	5.934121	-0.00433
S	-0.527771	5.789977	-0.933102
S	5.905406	-1.813162	3.800121
S	-2.138696	-0.887273	0.314693
S	7.906572	1.022775	0.248992
S	6.770719	4.155673	3.545776
S	0.380234	-3.608151	2.870861
S	0.134906	2.035255	-3.697546
S	-1.071683	-0.143769	5.58199
S	3.01467	4.730818	7.387963
S	4.439875	-4.824955	0.34738
Au	-1.021584	-3.095294	-0.313407
C	-2.510567	-1.219685	2.057432
Au	2.148411	-4.77749	-0.239897
C	5.03297	-5.311173	-1.347855
Au	4.803638	6.811594	2.295339
C	6.669195	5.048317	-0.093694
Au	7.206851	2.508967	1.911277
C	8.362756	2.062959	-1.22919
C	7.779455	3.518016	4.962473
Au	-0.133427	3.870667	-2.278788

C	0.6105	7.092465	-1.607025
C	-1.351834	1.168608	-4.340551
Au	-0.216908	-1.7521	4.102174
C	-2.889766	-0.01053	5.27036
C	1.351906	-4.770908	3.938667
Au	3.96159	6.168321	5.727063
C	4.426285	3.538103	7.381467
S	4.793945	7.925932	4.349206
C	6.550741	8.023337	4.927079
S	-0.060968	-5.142005	-0.910326
C	-0.694973	-6.35024	0.341831
S	-2.895396	2.346741	0.973011
S	1.527827	8.072952	3.117833
Au	-2.707728	4.704701	1.630149
C	-2.670168	2.312162	-0.841584
Au	-0.566171	7.348636	2.555394
C	1.263513	8.647932	4.868277
S	-2.79307	6.975622	2.047728
C	-3.423105	7.659453	0.456888
S	0.90785	-2.964547	-3.573696
S	4.221691	3.955649	-2.743562
Au	2.10749	-1.133576	-4.581917
C	-0.876999	-2.496131	-3.6652
Au	3.717947	2.052719	-4.347189
C	2.889685	5.16122	-2.732053
S	3.168551	0.461356	-5.914359
C	4.5569	-0.167801	-6.938706
S	-2.290822	4.758613	5.266902
S	3.710653	-0.173778	6.330097
Au	-0.811877	3.481391	6.751334
C	-3.558882	3.615303	4.581155
Au	1.925916	1.246214	7.331806
C	3.070289	-1.832439	5.868743

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C	-0.823849	1.073503	9.041691
Au	6.899065	-2.222017	-1.804406
C	5.656649	-2.72304	-4.639175
S	8.032857	-3.504063	-0.15484
C	7.700613	5.932615	-0.798582
C	8.02778	7.149334	0.033055
C	8.746859	7.006621	1.228944
C	7.577803	8.423273	-0.330848
C	8.934951	8.09466	2.080902
C	8.37944	9.337878	1.762012
C	7.764291	9.515272	0.520632
C	-3.819103	9.127125	0.609999
C	-3.557867	10.01345	-0.596901
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C	11.301371	-1.059477	-1.207402
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C	3.196178	-6.102569	-3.58351
C	1.592122	-8.189202	-3.17247
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H	14.182042	0.617042	-3.150138
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H	13.271696	-1.601986	-3.887429
H	0.095182	9.718489	-0.23697
H	-3.371503	13.30519	-1.403445
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H	4.286266	1.331375	8.70479
H	1.773775	0.873387	-10.916265
H	0.595304	-2.670716	10.276386
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H	-2.149684	0.420432	11.347148
H	8.651249	9.858755	9.042666
H	7.557674	-3.82284	6.656504

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H	-0.319982	-2.031375	14.427994
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H	-6.558929	6.714381	-2.829986
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H	7.044604	8.553001	-1.275217
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H	9.712594	5.735447	9.429344
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H	9.150709	-3.29243	-4.776875

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H	-0.739209	6.238573	7.607989
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H	1.028205	4.974304	-4.37461
H	10.237854	0.245472	-5.650078
H	-0.808034	-4.762073	-6.883495
H	6.293022	-7.903422	3.675905
H	7.682554	3.511772	-6.803089
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H	4.437433	4.237773	-10.95621
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H	11.694578	4.760046	5.695506

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H	-6.612656	-5.457683	1.964926
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H	3.685674	-5.132576	-3.684742
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Au	6.836659	-2.597803	1.706525
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H	8.538525	3.079604	-0.863834
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Au	1.327414	0.274894	2.502766
Au	0.21627	4.810334	1.110113
Au	3.104855	4.503779	0.90289
Au	3.845707	2.321075	-1.07213
Au	-0.859332	2.090343	1.926189
Au	1.465206	0.921595	-2.258061
Au	1.657983	3.037141	2.774091
Au	5.586324	0.065285	0.080327
Au	4.165357	-2.34097	-0.013632
Au	4.149559	1.818238	1.730247
Au	1.544402	-2.221263	1.325039
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Au	3.938252	-0.903473	2.458634
S	6.09897	-1.037319	-3.518663
Au	1.970395	5.754652	3.297304
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Au	3.140951	1.315572	4.413667
Au	1.827551	3.623733	5.491329
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Au	4.73497	6.80313	2.405604
C	6.271318	5.129624	-0.258165
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C	8.211696	2.144959	-1.291412
C	7.232913	3.272385	5.22508
Au	-0.262968	3.990415	-2.178126
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C	-1.597877	1.435852	-4.092846
Au	-0.392032	-1.782775	4.043137
C	-1.700776	-0.534335	6.938937
C	1.535317	-4.689072	3.902711
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C	4.221707	3.617273	7.725485
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S	-0.227463	-5.108193	-0.752404
C	-0.964909	-6.323682	0.428471
S	-3.06258	2.389764	0.938379
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Au	-2.838597	4.729185	1.70823
C	-2.912621	2.487652	-0.883702
Au	-0.70925	7.340806	2.644184
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S	-3.008739	6.954721	2.363342
C	-3.52139	7.720431	0.761187
S	0.7386	-2.772823	-3.613423
S	3.929188	4.093163	-2.728515
Au	2.135747	-1.107152	-4.613408
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Au	3.607706	2.157666	-4.271406

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C	5.71755	-2.222119	-4.862822
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C	3.600791	6.866584	-4.793534
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C	5.281199	7.878506	-6.228041
C	5.699093	8.70222	-5.161681
C	7.483835	-0.345111	5.158899
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C	9.463824	-0.436298	3.623792
C	10.251831	-2.840268	4.61153
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S	-0.016396	2.207852	8.415236
C	0.825813	3.374904	9.580187
Au	6.802371	-2.219459	-1.695105
C	5.460639	-2.495713	-4.642865
S	7.799746	-3.550296	0.024814
C	7.426298	6.144816	-0.914744

C	7.8816	7.145146	0.120007
C	8.424036	6.714742	1.341917
C	7.751541	8.523868	-0.075893
C	8.423963	7.561016	2.447241
C	8.370351	8.944188	2.199135
C	8.246814	9.415478	0.881427
C	-2.619001	8.79569	0.228538
C	-3.161428	10.180505	-0.064475
C	-2.366873	11.055144	-0.827802
C	-4.346565	10.694986	0.478842
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C	-4.750574	12.011129	0.225753
C	9.354429	-2.518501	0.12833
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H	5.075922	-7.128879	-1.119172
H	3.968042	-4.665216	-2.497006
B1-E			
Au	0.055062	-0.017184	0.031627
Au	2.849608	0.001345	0.078459
Au	1.365237	2.453985	0.04861
Au	1.59809	-1.882981	-1.529791
Au	1.454795	0.267695	2.492036
Au	0.336964	4.808206	1.121435
Au	3.221264	4.51132	0.883937
Au	3.948351	2.324596	-1.105082
Au	-0.735581	2.088202	1.927367

Au	1.557422	0.930651	-2.277307
Au	1.789473	3.02885	2.769368
Au	5.685695	0.061034	0.038255
Au	4.272193	-2.342577	-0.053092
Au	4.271365	1.821228	1.705499
Au	1.650677	-2.224533	1.295696
Au	4.122179	-0.427597	-2.365941
Au	4.06433	-0.912444	2.42517
S	6.042935	-1.107099	-3.721003
Au	2.09796	5.742477	3.298642
Au	-0.468438	4.301248	3.757934
Au	4.303628	3.922331	3.634666
Au	0.23872	1.583238	4.628876
Au	3.280753	1.31261	4.384645
Au	1.978744	3.60872	5.477523
S	4.795863	6.096918	-0.053754
S	-0.514884	5.756415	-0.905213
S	5.786478	-1.924397	3.757429
S	-2.148677	-0.936631	0.121198
S	7.83717	1.183496	0.234657
S	6.713357	3.940795	3.656493
S	0.349963	-3.610555	2.907676
S	0.174196	2.254132	-3.749248
S	-1.094198	-0.174774	5.562605
S	2.846546	4.73557	7.440009
S	4.402507	-4.701021	-0.009915
Au	-1.035105	-3.072065	-0.380282
C	-2.476806	-1.170115	1.902283
Au	2.171719	-4.716032	-0.3655
C	4.9683	-5.152153	-1.715455
Au	4.887386	6.803943	2.335134
C	6.346402	5.116065	-0.210323
Au	7.215229	2.429186	1.917304

C	8.354107	1.969733	-1.364192
C	7.448606	3.297908	5.216111
Au	-0.13801	3.93663	-2.178931
C	0.389174	7.281417	-1.44014
C	-1.511247	1.634972	-4.149845
Au	-0.256939	-1.747574	4.037992
C	-2.930897	-0.082393	5.509372
C	1.522144	-4.826193	3.692569
Au	3.953537	6.111819	5.809143
C	4.445827	3.73349	7.599813
S	5.103888	7.58255	4.490278
C	4.646552	9.352287	4.623354
S	-0.100991	-5.164155	-0.838266
C	-0.680723	-6.244361	0.552097
S	-2.995339	2.321797	0.999896
S	1.577526	8.151526	3.280395
Au	-2.746853	4.732647	1.722321
C	-2.71865	2.421415	-0.816732
Au	-0.585695	7.364775	2.679448
C	1.033652	8.807903	4.946061
S	-2.848941	6.968747	2.278998
C	-3.284136	7.755764	0.658856
S	0.973978	-2.761629	-3.727039
S	4.170845	4.068733	-2.767007
Au	2.129095	-1.024841	-4.625212
C	-0.670269	-1.890513	-3.865353
Au	3.66873	2.171128	-4.310375
C	2.832778	5.315467	-2.871804
S	3.280735	0.558463	-5.952124
C	1.988159	1.503229	-6.927644
S	-2.236481	4.726764	5.328952
S	3.81999	-0.138523	6.326188
Au	-0.969167	3.415224	6.74991

C	-3.402014	3.356832	4.831839
Au	1.819277	1.19165	7.306909
C	3.025065	-1.742124	5.862985
S	0.033642	2.15472	8.466645
C	0.375479	3.432845	9.757942
Au	6.921952	-2.143059	-1.86889
C	5.273398	-2.525584	-4.650596
S	7.908119	-3.345744	-0.128234
C	7.415032	5.849793	-1.043332
C	8.51362	6.361389	-0.140762
C	9.318523	5.46383	0.577124
C	8.835947	7.721125	-0.082708
C	10.114438	5.926644	1.624078
C	10.073859	7.280473	1.968348
C	9.611904	8.179535	0.995056
C	-3.926414	9.125303	0.876005
C	-3.821066	10.033258	-0.332281
C	-3.443692	11.373094	-0.158074
C	-3.804337	9.521055	-1.63702
C	-3.54915	12.264715	-1.227572
C	-4.107526	11.817192	-2.427038
C	-3.996572	10.437006	-2.687322
C	9.704183	-2.854661	-0.07366
C	10.007625	-1.605005	-0.920872
C	11.437423	-1.113379	-0.776923
C	12.476567	-1.928701	-0.301673
C	11.800208	0.132044	-1.316289
C	13.762379	-1.404153	-0.122513
C	14.032597	-0.071195	-0.436757
C	13.021776	0.720748	-0.99494
C	-4.020724	2.057463	-1.529406
C	-5.08714	3.125909	-1.40328
C	-4.757535	4.482969	-1.542083

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C	-7.16053	4.935593	-1.586408
C	-5.826263	5.390362	-1.636966
C	7.26316	2.123422	-2.416021
C	7.791729	2.340616	-3.811315
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C	8.700472	1.441444	-4.394708
C	7.716695	3.524656	-5.925267
C	9.16099	1.629933	-5.700068
C	8.778809	2.77026	-6.422983
C	1.572783	7.702735	-0.560711
C	1.710758	9.200161	-0.493478
C	0.682406	10.027936	-0.012351
C	2.912428	9.851889	-0.840553
C	0.686966	11.369504	-0.413475
C	1.926451	12.027258	-0.374474
C	3.059807	11.231559	-0.62104
C	4.882219	10.172967	3.368799
C	4.110847	11.47812	3.322183
C	3.136893	11.85514	4.257037
C	4.350751	12.359201	2.254145
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C	2.935816	14.035396	3.231759
C	3.96226	13.695042	2.338279
C	-2.232922	2.679405	-4.995665
C	-3.518924	2.234405	-5.657493
C	-3.896644	0.892308	-5.785372
C	-4.491526	3.200386	-5.979957
C	-4.973004	0.549741	-6.612833
C	-5.963771	1.495765	-6.877416
C	-5.692111	2.84089	-6.594133
C	-1.353958	-2.167567	-5.218887

C	-2.592886	-3.011783	-5.036895
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C	-3.748414	-2.48657	-4.436989
C	-3.6999	-5.171421	-5.162849
C	-4.781973	-3.332531	-4.033064
C	-4.761912	-4.681632	-4.399591
C	2.903882	-4.778505	3.059394
C	3.921498	-5.765505	3.56109
C	3.641821	-7.135346	3.68518
C	5.235078	-5.34689	3.828711
C	4.635612	-8.017924	4.120584
C	5.968675	-7.58229	4.174066
C	6.285268	-6.259884	3.811897
C	1.012755	7.787788	6.087341
C	-0.238609	7.714312	6.936353
C	-0.142192	7.145569	8.216936
C	-1.48959	8.18609	6.525646
C	-1.287953	6.749834	8.902294
C	-2.538634	6.918938	8.300685
C	-2.616985	7.933578	7.320849
C	6.78374	-0.382991	4.077198
C	3.415967	6.612704	-3.46136
C	3.072211	6.760284	-4.925544
C	1.73566	6.810617	-5.349976
C	4.070325	6.984902	-5.883676
C	1.453522	6.854748	-6.716488
C	3.759703	6.758306	-7.236529
C	2.437258	6.478667	-7.631817
C	7.856639	-0.640423	5.13813
C	9.220938	-0.972368	4.573314
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C	9.621991	-0.594611	3.284002
C	11.244512	-2.236362	4.909444

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C	5.9991	-2.842264	-5.974679
C	4.977195	-3.12986	-7.047038
C	4.549981	-2.131936	-7.935335
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C	3.673914	-2.479154	-8.969907
C	2.784346	-3.538371	-8.797136
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C	-4.778102	3.460079	5.514088
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C	-6.910352	4.204647	4.332768
C	-6.015007	2.052244	3.812569
C	-7.980122	3.920372	3.47374
C	-8.006148	2.720496	2.750271
C	-6.821855	1.944114	2.688139
C	-3.551897	-1.454162	5.803041
C	-4.341087	-1.598094	7.089566
C	-4.94164	-2.840226	7.366347
C	-4.499715	-0.586926	8.050181
C	-5.46718	-3.072073	8.637994
C	-5.997887	-2.001448	9.360052
C	-5.376223	-0.763502	9.134282
C	8.954073	3.512188	5.252081
C	9.422165	4.927225	5.529256
C	8.638454	5.874678	6.198381
C	10.752717	5.261565	5.233711
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C	11.233398	6.552327	5.456876
C	10.379038	7.540525	5.958937
C	0.696533	0.735963	-7.220483
C	0.575822	0.113183	-8.595455
C	1.093682	0.726184	-9.745974

C	-0.071757	-1.12061	-8.750071
C	-0.129279	-1.747872	-9.995619
C	0.788949	0.229784	-11.016093
C	0.180927	-1.0227	-11.148781
C	3.21004	-2.759004	6.988434
C	2.23254	-2.468394	8.107343
C	2.645029	-2.344785	9.43827
C	0.851812	-2.59736	7.878753
C	-0.036006	-2.10983	8.84107
C	1.800354	-1.598616	10.283955
C	0.468214	-1.356597	9.908134
C	4.990027	3.647896	9.034298
C	5.555839	2.264362	9.282141
C	5.279439	1.557936	10.459944
C	6.613824	1.770787	8.50492
C	5.32959	0.165973	10.44959
C	6.258159	-0.378799	9.538114
C	7.100329	0.491255	8.808414
C	1.595013	3.142213	10.616898
C	1.500189	3.680343	12.033847
C	2.623438	3.587929	12.876211
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C	2.435118	3.646795	14.256843
C	0.41243	4.884884	13.795949
C	1.245783	4.237881	14.719008
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C	0.534852	-9.354941	2.381331
C	-0.829529	-8.19865	4.49051
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C	-0.543136	-9.565505	4.527321
C	-3.948984	-1.465356	2.168509

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C	-3.46868	-3.830176	2.870415
C	-5.583554	-4.821097	1.379644
C	-4.549486	-5.691651	1.716507
C	-3.645302	-5.209042	2.687255
C	5.055249	-6.626682	-2.051056
C	6.384997	-6.985733	-2.713813
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H	14.553257	-2.040769	0.278641
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H	10.580087	7.639337	2.864997
H	13.2275	1.750323	-1.293103
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H	0.476732	-2.958082	6.918156
H	-0.19892	-0.784784	10.553846
H	10.73617	8.56354	6.088748
H	4.63662	2.045166	11.199081
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H	-1.110486	-2.128246	8.644813
H	6.463846	-1.451573	9.537447
H	4.814117	-0.446236	11.187944
H	9.215922	4.387788	0.417671
H	2.828068	11.152382	5.043225
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H	12.200533	-2.837957	3.047106
H	0.921825	6.852129	-4.623059
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H	-1.77725	-4.735294	-6.047877
H	4.389441	-9.059695	4.332994
H	9.891666	0.934937	-6.119255
H	-4.764345	-3.680322	6.689138
H	-8.823556	2.536991	2.049086
H	9.149484	2.931608	-7.436596
H	-3.772114	-1.439442	-4.128002
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H	1.624771	1.677227	-9.668072
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H	1.109318	-9.802212	1.565548
H	-1.29522	-7.714149	5.350989
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H	-6.447196	-5.196245	0.823765
H	-2.63824	-3.455043	3.48645
H	-6.093891	-2.75123	0.996759
H	-2.973101	-5.908584	3.186193
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H	7.3991	-5.042127	-2.551612
H	5.852189	-9.069765	-2.825988
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H	7.666863	-9.62197	-4.438214
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H	-4.983957	8.993091	1.156928
H	6.96483	6.671619	-1.617066
H	6.718551	4.875306	0.790278
H	9.780969	-1.805489	-1.981786
H	-1.924657	1.697713	-1.046533
H	9.332069	-0.794979	-0.602341
H	9.12678	1.277134	-1.718783
H	2.509011	7.24608	-0.898404
H	9.97353	-2.562201	0.954022
H	-3.442402	9.62413	1.731345
H	7.826116	5.13639	-1.777717
H	8.842354	2.925082	-1.131904
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H	-3.189904	0.675139	6.256681
H	-1.53547	3.026369	-5.778838
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H	-2.899217	2.403098	4.988283
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B2-A			

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Au	3.177217	4.514194	0.8369
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Au	2.06171	5.725892	3.265025
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S	4.904075	6.015105	-0.093137
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C	6.503586	5.14471	-0.36836
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S	-0.170822	-5.202984	-0.905884
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S	-3.021534	2.335965	0.92378
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Au	-0.634668	7.315788	2.690267
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C	-3.800786	7.200961	3.731827
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C	4.664776	0.277353	-6.701475
S	-2.30346	4.60427	5.394816
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C	0.633802	3.210077	9.735035
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C	10.144121	7.876166	1.604128
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S	4.80612	6.030222	-0.027703
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C	2.654302	5.114993	-2.989626
S	3.259412	0.365442	-6.008454
C	2.121476	0.984125	-7.332995

S	-2.16456	4.802	5.250894
S	3.791818	0.122055	6.229134
Au	-0.982329	3.624466	6.627235
C	-3.795631	3.932853	5.258867
Au	1.912856	1.427477	7.224324
C	3.065598	-1.520531	5.884753
S	0.085224	2.371918	8.315965
C	0.724874	3.560169	9.574509
Au	6.862521	-2.150854	-1.888145
C	5.886746	-2.255252	-5.085707
S	7.874961	-3.423476	-0.194644
C	7.394735	6.176578	-1.257518
C	8.18877	6.89012	-0.187182
C	9.002949	6.153659	0.686648
C	8.362817	8.277113	-0.232573
C	9.586064	6.776726	1.787959
C	9.384375	8.148682	1.974349
C	8.997494	8.903326	0.852964
C	-3.942784	8.77139	3.780921
C	-4.208874	8.955125	5.260396
C	-4.025921	10.208677	5.870717
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C	-4.940382	8.103187	7.410146
C	9.596434	-2.745332	-0.036624
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C	11.24502	-1.187182	-1.233654
C	12.18081	-2.170402	-1.593116
C	11.708992	0.138799	-1.167108
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H	0.597574	-7.686992	0.85227
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H	-1.456633	-7.104919	-0.408881
H	-1.859334	-5.834142	0.773316
H	-4.664876	-1.130532	2.874252
H	-2.656363	-0.074931	2.290849
H	-2.094437	-1.760609	2.36995
H	-4.827986	-1.103413	1.125442
H	3.671992	-4.00896	-2.626791
H	3.995989	-6.514118	-1.515166

H	5.338545	-4.306957	-3.112041
H	5.680256	-5.975814	-1.534054
B3-A			
Au	0.026667	0.159251	-0.031944
Au	2.820731	0.148886	0.039666
Au	1.362774	2.626625	0.011425
Au	1.564428	-1.714185	-1.589407
Au	1.407318	0.417091	2.442192
Au	0.35206	4.977084	1.085865
Au	3.234706	4.649018	0.871988
Au	3.955419	2.4652	-1.121576
Au	-0.757124	2.264423	1.867798
Au	1.560603	1.103553	-2.322574
Au	1.770567	3.173085	2.737446
Au	5.66751	0.180881	0.02446
Au	4.22043	-2.208793	-0.091552
Au	4.246475	1.945695	1.688713
Au	1.598563	-2.06918	1.234023
Au	4.110527	-0.280489	-2.395613
Au	4.005163	-0.78938	2.392195
S	6.108447	-0.87202	-3.726773
Au	2.11313	5.881697	3.283074
Au	-0.482258	4.465361	3.712434
Au	4.286517	4.034473	3.62965
Au	0.187655	1.734945	4.575527
Au	3.228563	1.432246	4.356781
Au	1.942027	3.73683	5.450188
S	4.902679	6.146671	-0.026351
S	-0.460866	6.029347	-0.917964
S	5.809371	-1.623894	3.773795
S	-2.19349	-0.85549	-0.066362
S	7.878056	1.124289	0.262878
S	6.673352	4.285109	3.549606

S	0.655649	-3.346853	3.04735
S	0.174461	2.386258	-3.800583
S	-1.52341	0.167483	5.119618
S	2.932851	4.828906	7.371427
S	4.324831	-4.620076	-0.160787
Au	-1.083677	-2.882889	-0.468461
C	-2.849863	-1.014749	1.64819
Au	2.085679	-4.558858	-0.429091
C	5.02642	-5.402807	-1.678731
Au	4.917685	6.892707	2.350261
C	6.328095	5.061385	-0.421454
Au	7.157203	2.598669	1.944863
C	8.486398	1.981034	-1.266993
C	7.448418	3.790524	5.146305
Au	-0.092028	4.107578	-2.222825
C	0.632059	7.451406	-1.385337
C	-1.441976	1.539446	-4.052624
Au	-0.310372	-1.53183	3.98789
C	-1.68751	-0.492917	6.834047
C	1.767304	-4.449687	4.030951
Au	3.952759	6.223589	5.793374
C	4.272161	3.558391	7.543776
S	5.088964	7.787506	4.475029
C	4.622524	9.56561	4.552736
S	-0.170904	-4.99294	-0.831564
C	-0.875031	-6.147909	0.443814
S	-3.017366	2.456156	0.9306
S	1.644559	8.378136	3.335417
Au	-2.680339	4.945163	1.598476
C	-2.856136	2.654823	-0.888191
Au	-0.558205	7.464392	2.703761
C	1.15258	8.937424	5.025087
S	-2.818688	7.208018	2.087624

C	-3.677925	7.387227	3.713135
S	1.006973	-2.745379	-3.713267
S	4.325212	4.221943	-2.920656
Au	2.180831	-0.891274	-4.694882
C	-0.749385	-2.155518	-3.737396
Au	3.670539	2.297642	-4.336283
C	2.896486	5.370326	-3.01107
S	3.177395	0.765572	-5.970813
C	1.958349	1.386293	-7.229687
S	-2.122981	4.962715	5.499734
S	3.743595	0.008965	6.259479
Au	-0.921321	3.551393	6.732317
C	-3.23342	3.629709	4.820182
Au	1.834847	1.243036	7.29811
C	3.016335	-1.637706	5.854656
S	0.065393	2.19552	8.401664
C	0.46309	3.308578	9.817911
Au	6.875078	-2.020516	-1.83021
C	5.123985	-2.187188	-4.608447
S	7.762159	-3.256021	-0.049379
C	7.400436	5.849558	-1.161352
C	8.106195	6.748952	-0.170044
C	8.442568	8.080863	-0.459305
C	8.727874	6.215651	0.979464
C	8.559187	8.952457	0.635987
C	9.033311	8.453811	1.855627
C	9.088201	7.063712	2.034315
C	-3.705335	8.851844	4.153178
C	-4.212818	8.985048	5.569257
C	-5.551915	9.300784	5.838945
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C	-5.088107	9.392713	8.176825

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C	11.211986	-2.119719	-1.705631
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C	-4.214788	2.332181	-1.538187
C	-5.034299	3.583194	-1.729641
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C	-5.250008	5.820834	-2.590028
C	-6.527669	5.976295	-2.040747
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C	7.485961	2.211557	-2.393461
C	8.056914	2.163651	-3.79472
C	7.205542	2.45901	-4.873315
C	9.392885	1.881867	-4.08984
C	7.516302	2.04194	-6.161208
C	9.783655	1.745418	-5.431562
C	8.785508	1.48893	-6.393806
C	1.787872	7.707924	-0.423508
C	2.549701	8.973905	-0.73277
C	2.086964	10.20527	-0.242954
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C	4.110485	11.287674	-0.978111
C	4.542883	10.076319	-1.536154
C	5.78033	10.446264	4.074756
C	5.426019	11.558645	3.118212
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C	-2.338537	2.342414	-5.002626
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C	-4.098213	-0.101051	-7.336695
C	-5.23884	-0.401083	-6.57445
C	-5.579283	0.489369	-5.537746
C	-1.587453	-2.613516	-4.945812
C	-2.924887	-3.066095	-4.422447
C	-3.304589	-4.413798	-4.374878
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C	4.912073	-8.407828	4.481151
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C	0.590192	7.853767	5.943315
C	0.930768	7.940024	7.413746
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C	1.753858	8.922167	7.980097
C	0.675176	6.959997	9.616044
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C	2.27139	8.728419	9.269085
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C	1.872533	6.17749	-5.146168
C	1.936751	5.356403	-6.284957
C	0.726802	6.980146	-5.020887
C	0.760337	5.055807	-6.984381
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C	-0.428845	5.740827	-6.720326
C	7.7717	-0.270027	5.174625
C	8.967977	-1.119843	4.831443
C	10.014613	-0.571594	4.070087
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C	-7.731885	1.240641	4.167156
C	-6.479675	0.994454	3.588204
C	-2.452501	-1.812185	6.899318
C	-3.487931	-1.938281	7.994823
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C	-3.75336	-0.946686	8.949176
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C	11.59138	6.704986	6.512788
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C	1.920642	-0.597207	-9.560861
C	0.467081	-1.951113	-8.247467
C	0.609743	-2.965788	-9.202031
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C	1.301858	-2.731033	-10.397108
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C	1.121823	4.358451	12.512868

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H	1.159691	10.24469	0.335709
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H	4.846816	-3.314559	9.100698
H	1.309756	-3.729508	11.528142
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H	7.923218	3.719054	9.49508
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H	0.214754	4.686971	12.000584
H	8.532178	10.031962	0.465507
H	3.447398	1.926801	12.391901
H	7.085197	13.883305	1.297862
H	3.800752	-3.802381	11.300582
H	7.773053	-0.279325	10.972895
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H	8.151829	8.495862	-1.430428
H	7.413066	11.643735	2.279542
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H	2.869891	13.612567	2.117788
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H	4.506173	-5.721043	-4.664499
H	5.5348	9.994663	-1.987285
H	-3.886704	-0.674679	-8.242209
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H	0.710453	7.756055	-4.251584
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H	-6.393209	0.335216	2.722044
H	8.467433	5.457174	7.066955
H	-4.933687	-5.743872	-3.921887
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H	11.314645	4.434634	4.009475
H	4.361281	1.347377	8.948757
H	-6.544314	0.419682	-5.033934
H	-5.281922	-1.763784	-2.390416
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H	5.207875	-8.594315	2.326496
H	-1.388145	7.179308	-5.407982
H	3.036641	9.406022	9.65218
H	2.156746	7.543994	11.082149
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H	-5.842402	-4.220271	-2.146562
H	10.013888	7.170082	7.91092
H	-0.124225	-2.127138	-7.347532
H	5.620488	-0.6111	9.702213
H	1.335656	-3.507922	-11.164192
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H	-6.826196	-2.204721	9.816688
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H	-5.503007	-3.377199	5.885916
H	-2.223902	-3.845652	2.280269
H	-5.860042	-2.115869	3.777887
H	-2.575725	-5.787034	3.812175
H	-4.151506	-5.491281	5.748375
H	4.566451	-9.529307	-0.879132
H	7.360548	-6.263471	-0.806887
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H	8.353195	-9.884613	1.162155
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H	-2.676651	9.248626	4.102707
H	6.952932	6.437913	-1.975303
H	6.713932	4.60872	0.501112
H	11.040185	-4.000788	-0.730334
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H	6.94049	3.153691	-2.246073

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H	6.266668	10.909821	4.951804
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H	-1.18128	-2.586525	-2.820312
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S	-0.628605	6.006935	-0.956161
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C	-1.746623	1.399398	-3.475414
Au	-0.275267	-1.600928	4.081143
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Au	1.656325	-2.20269	1.33982
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S	4.771144	6.163509	-0.2276
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S	-2.249014	-0.920684	0.012938
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C	6.314361	5.282762	-0.70598
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