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Geometry Filename /// Total Energy (Ha, unless otherwise stated)

- 1_QChem_GeometricAnalysis_Os-Fc.xyz /// N/A (X-ray crystal structure)
- 2_QChem_GeometricAnalysis_Si-Fc.xyz /// N/A (X-ray crystal structure)
- 3_QChem_GeometricAnalysis_C-Fc.xyz /// N/A (X-ray crystal structure)
- 4_QChem_GeometricAnalysis_Os(C8H9)4.xyz /// -1330.54727722953
- 5_QChem_GeometricAnalysis_Si(C8H9)4_fromOs(C8H9)4.xyz /// -1528.84600659461
- 6_QChem_GeometricAnalysis_Si(C6H5)4.xyz /// -1214.75456183905
- 7_QChem_GeometricAnalysis_Si(C8H9)4_fromSi(C6H5)4.xyz /// -1528.84625655137
- 8_QChem_GeometricAnalysis_C(C6H5)4.xyz /// -963.448312892631
- 9_QChem_Model_PBE_Os1h_sim.xyz /// -2205.07520348555
- 10_QChem_Model_PBE_Os1h_diff.xyz /// -2205.07424659267
- 11_QChem_Model_PBE_Si1h_sim.xyz /// -2089.28123404691
- 12_QChem_Model_PBE_Si1h_diff.xyz /// -2089.28140433495
- 13_QChem_Model_PBE_C1h_sim.xyz /// -1837.97255055652
- 14_QChem_Model_PBE_C1h_diff.xyz /// -1837.97297496680
- 15_QChem_Model_PBE_Os1h-Au1_sim.xyz /// -2475.96019868150
- 16_QChem_Model_PBE_Os1h-Au1_diff.xyz /// -2475.96036319345
- 17_QChem_Model_PBE_Si1h-Au1_sim.xyz /// -2360.15678980524
- 18_QChem_Model_PBE_Si1h-Au1_diff.xyz /// -2360.18110871945
- 19_QChem_Model_PBE_C1h-Au1_sim.xyz /// -2108.85135941170
- 20_QChem_Model_PBE_C1h-Au1_diff.xyz /// -2108.84970336778
- 21_QChem_Model_B3LYP_Os1h_sim.xyz /// -2207.18078397311
- 22_QChem_Model_B3LYP_Os1h_diff.xyz /// -2207.17995773226
- 23_QChem_Model_B3LYP_Si1h_sim.xyz /// -2091.13741268375
- 24_QChem_Model_B3LYP_Si1h_diff.xyz /// -2091.13746426853

25_QChem_Model_B3LYP_C1h_sim.xyz /// -1839.70375063244
26_QChem_Model_B3LYP_C1h_diff.xyz /// -1839.70392246166
27_QChem_Model_B3LYP_Os1h-Au1_sim.xyz /// -2478.06722984796
28_QChem_Model_B3LYP_Os1h-Au1_diff.xyz /// -2478.06795840824
29_QChem_Model_B3LYP_Si1h-Au1_sim.xyz /// -2362.01801287426
30_QChem_Model_B3LYP_Si1h-Au1_diff.xyz /// -2362.01893203589
31_QChem_Model_B3LYP_C1h-Au1_sim.xyz /// -2110.58746744725
32_QChem_Model_B3LYP_C1h-Au1_diff.xyz /// -2110.58604061701

33_FHI-aims_Molecule_Os1.xyz /// -566287.731908578 eV
34_FHI-aims_Molecule_Os2.xyz /// -591429.938924243 eV
35_FHI-aims_Molecule_Os3.xyz /// -616572.512776929 eV
36_FHI-aims_Molecule_Si1.xyz /// -80899.498231165 eV
37_FHI-aims_Molecule_Si2.xyz /// -106041.994090932 eV
38_FHI-aims_Molecule_Si3.xyz /// -131184.575636874 eV
39_FHI-aims_Molecule_C1.xyz /// -74034.593620248 eV
40_FHI-aims_Molecule_C2.xyz /// -99177.166157066 eV
41_FHI-aims_Molecule_C3.xyz /// -124319.725560289 eV
42_FHI-aims_Junction_Os1.xyz /// -40204528.015414119 eV
43_FHI-aims_Junction_Os2.xyz /// -40229669.999601454 eV
44_FHI-aims_Junction_Os3.xyz /// -40254812.585844547 eV
45_FHI-aims_Junction_Si1.xyz /// -39719139.529123940 eV
46_FHI-aims_Junction_Si2.xyz /// -39744281.998911940 eV
47_FHI-aims_Junction_Si3.xyz /// -39769424.579884693 eV
48_FHI-aims_Junction_C1.xyz /// -39712274.560149595 eV
49_FHI-aims_Junction_C2.xyz /// -39737417.143819436 eV
50_FHI-aims_Junction_C3.xyz /// -39762559.745518416 eV

51_FHI-aims_Junction_Si2_-2SMe.xyz /// -39720501.768030971 eV
52_FHI-aims_Junction_Si2_-2Ph2SMe.xyz /// -39697497.094350062 eV
53_FHI-aims_Junction_Si2_diMe.xyz /// -39752952.856112286 eV
54_FHI-aims_Junction_Os1h_sim.xyz /// -40180631.634713791 eV
55_FHI-aims_Junction_Os1h_diff.xyz /// -40180631.655162871 eV
56_FHI-aims_Junction_Si1h_sim.xyz /// -39695243.291097976 eV
57_FHI-aims_Junction_Si1h_diff.xyz /// -39695243.277062997 eV
58_FHI-aims_Junction_C1h_sim.xyz /// -39688378.423698835 eV
59_FHI-aims_Junction_C1h_diff.xyz /// -39688378.434473053 eV
60_FHI-aims_Junction_Si2_-2PhSMe_diff.xyz /// -39707929.758849718 eV

XYZ Files:

1_QChem_GeometricAnalysis_Os-Fc.xyz /// N/A (X-ray crystal structure)

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C72H68Fe4Os

Os	8.841250	8.841250	8.593200
Fe	6.830750	2.923625	4.113651
C	8.777593	7.159644	7.506160
C	7.918224	6.137596	7.911759
H	7.376220	6.287738	8.677620
C	7.805056	4.913967	7.263832
C	8.570708	4.698240	6.103750
C	9.438919	5.725593	5.685261
H	9.965857	5.575292	4.908934
C	10.503405	7.983649	5.786661
H	11.074638	8.322233	6.507175
H	9.980993	8.721911	5.409325
H	11.061111	7.586128	5.086255
C	9.573306	6.943918	6.334048
C	6.880261	3.898991	7.865356
H	6.273751	4.341390	8.494224
H	7.404582	3.219630	8.339469
H	6.358645	3.470261	7.154449
C	8.464613	3.494062	5.249586
C	8.020782	2.176716	5.583861
H	7.708085	1.884106	6.487350

C	8.070293	1.359784	4.432373
H	7.820351	0.393294	4.387112
C	8.553025	2.148424	3.353926
H	8.696130	1.838114	2.414096
C	8.782898	3.464002	3.849754
H	9.103375	4.241784	3.309499
C	4.984697	2.118364	3.657266
H	4.757618	1.145578	3.605569
C	4.913967	2.938832	4.807895
H	4.623903	2.637822	5.716386
C	5.350725	4.268556	4.467605
H	5.396840	5.055303	5.084201
C	5.677851	4.259714	3.093552
H	6.009681	5.038063	2.560636
C	5.462124	2.924685	2.600302
H	5.631682	2.617470	1.664391
Fe	10.851750	14.758875	4.113651
C	8.904907	10.522856	7.506160
C	9.764277	11.544904	7.911759
H	10.306280	11.394762	8.677620
C	9.877445	12.768533	7.263832
C	9.111792	12.984260	6.103750
C	8.243581	11.956907	5.685261
H	7.716643	12.107208	4.908934
C	7.179095	9.698851	5.786661
H	6.607862	9.360267	6.507175
H	7.701507	8.960589	5.409325
H	6.621389	10.096372	5.086255
C	8.109195	10.738582	6.334048
C	10.802239	13.783509	7.865356
H	11.408749	13.341110	8.494224
H	10.277918	14.462870	8.339469
H	11.323855	14.212239	7.154449
C	9.217887	14.188438	5.249586
C	9.661718	15.505784	5.583861
H	9.974415	15.798394	6.487350
C	9.612207	16.322716	4.432373
H	9.862149	17.289206	4.387112
C	9.129475	15.534076	3.353926
H	8.986370	15.844386	2.414096
C	8.899602	14.218498	3.849754
H	8.579125	13.440716	3.309499
C	12.697803	15.564137	3.657266
H	12.924882	16.536922	3.605569
C	12.768533	14.743669	4.807895
H	13.058597	15.044678	5.716386

C	12.331776	13.413944	4.467605
H	12.285660	12.627197	5.084201
C	12.004649	13.422786	3.093552
H	11.672819	12.644437	2.560636
C	12.220376	14.757815	2.600302
H	12.050818	15.065030	1.664391
Fe	2.923625	10.851750	13.072749
C	7.159644	8.904907	9.680240
C	6.137596	9.764277	9.274641
H	6.287738	10.306280	8.508780
C	4.913967	9.877445	9.922568
C	4.698240	9.111792	11.082650
C	5.725594	8.243581	11.501139
H	5.575292	7.716643	12.277466
C	7.983649	7.179095	11.399739
H	8.322233	6.607862	10.679225
H	8.721911	7.701507	11.777075
H	7.586128	6.621389	12.100145
C	6.943918	8.109195	10.852352
C	3.898991	10.802239	9.321044
H	4.341390	11.408749	8.692176
H	3.219630	10.277918	8.846931
H	3.470261	11.323855	10.031951
C	3.494062	9.217887	11.936814
C	2.176716	9.661718	11.602539
H	1.884106	9.974415	10.699050
C	1.359784	9.612207	12.754027
H	0.393294	9.862149	12.799288
C	2.148424	9.129475	13.832474
H	1.838114	8.986370	14.772304
C	3.464002	8.899602	13.336646
H	4.241784	8.579125	13.876901
C	2.118364	12.697803	13.529134
H	1.145578	12.924882	13.580831
C	2.938832	12.768533	12.378505
H	2.637822	13.058597	11.470014
C	4.268556	12.331776	12.718795
H	5.055303	12.285660	12.102199
C	4.259714	12.004649	14.092848
H	5.038063	11.672819	14.625764
C	2.924686	12.220376	14.586098
H	2.617470	12.050818	15.522009
Fe	14.758875	6.830750	13.072749
C	10.522856	8.777593	9.680240
C	11.544904	7.918224	9.274641
H	11.394762	7.376220	8.508780

C	12.768533	7.805056	9.922568
C	12.984260	8.570708	11.082650
C	11.956907	9.438919	11.501139
H	12.107208	9.965857	12.277466
C	9.698851	10.503405	11.399739
H	9.360267	11.074638	10.679225
H	8.960589	9.980993	11.777075
H	10.096372	11.061111	12.100145
C	10.738582	9.573306	10.852352
C	13.783509	6.880261	9.321044
H	13.341110	6.273751	8.692176
H	14.462870	7.404582	8.846931
H	14.212239	6.358645	10.031951
C	14.188438	8.464613	11.936814
C	15.505784	8.020782	11.602539
H	15.798394	7.708085	10.699050
C	16.322716	8.070293	12.754027
H	17.289206	7.820351	12.799288
C	15.534076	8.553025	13.832474
H	15.844386	8.696130	14.772304
C	14.218498	8.782898	13.336646
H	13.440716	9.103375	13.876901
C	15.564137	4.984697	13.529134
H	16.536922	4.757618	13.580831
C	14.743669	4.913967	12.378505
H	15.044678	4.623903	11.470014
C	13.413944	5.350725	12.718795
H	12.627197	5.396840	12.102199
C	13.422786	5.677851	14.092848
H	12.644437	6.009681	14.625764
C	14.757815	5.462124	14.586098
H	15.065030	5.631682	15.522009

2_QChem_GeometricAnalysis_Si-Fc.xyz /// N/A (X-ray crystal structure)

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C64H52Fe4Si

Fe	17.414371	13.862741	11.958914
Fe	9.311354	12.098934	2.888569
Si	11.118300	16.677450	8.507311
C	10.299771	15.405516	7.396645
C	12.457833	15.944087	9.602195
C	9.017386	13.572331	5.630532
C	14.470690	14.933211	11.330088
C	8.439234	12.621494	4.671605
C	13.789360	16.361913	9.493619

H	14.023868	16.993921	8.824158
C	12.169424	14.999254	10.592686
H	11.275402	14.694546	10.694549
C	14.775776	15.874931	10.340547
H	15.668865	16.184776	10.247355
C	13.156507	14.494038	11.432008
H	12.929560	13.840460	12.082949
C	9.555289	13.156062	6.843879
H	9.491426	12.240737	7.089895
C	9.694935	15.815782	6.200411
H	9.707321	16.739223	5.977498
C	15.493796	14.492482	12.300043
C	10.183473	14.047305	7.704498
H	10.543239	13.725363	8.522770
C	9.086319	14.939882	5.338651
H	8.705807	15.265871	4.531579
C	8.694288	11.216586	4.617032
H	9.237795	10.726580	5.222869
C	16.431513	15.347701	12.958342
H	16.527308	16.281550	12.812630
C	17.716789	13.786914	9.935147
H	17.067391	13.957514	9.263081
C	7.587350	12.935030	3.560369
H	7.263252	13.798989	3.334109
C	17.998304	12.540331	10.509971
H	17.572718	11.719711	10.290785
C	19.024301	12.708662	11.472700
H	19.399966	12.025331	12.015255
C	7.309170	11.721357	2.849778
H	6.760727	11.637680	2.078701
C	18.572675	14.751538	10.532789
H	18.597936	15.680739	10.336212
C	19.386980	14.065761	11.483159
H	20.058347	14.459016	12.027767
C	7.993835	10.674457	3.498760
H	7.989855	9.761556	3.235821
C	17.196897	14.567197	13.867069
H	17.890545	14.888782	14.430864
C	16.747051	13.232111	13.786445
H	17.087626	12.497614	14.283612
C	15.680806	13.177187	12.818202
H	15.190111	12.402730	12.569371
C	11.320653	11.865450	2.694425
H	11.903119	11.477955	3.336961
C	10.989328	13.208540	2.618365
H	11.304776	13.892805	3.197277

C	10.673568	11.176115	1.690434
H	10.722333	10.242867	1.524318
C	10.102087	13.390881	1.534510
H	9.705898	14.208076	1.253963
C	9.924195	12.123394	0.956454
H	9.388515	11.933227	0.195455
C	11.936829	17.949384	7.396645
C	9.778767	17.410813	9.602195
C	13.219214	19.782569	5.630532
C	7.765910	18.421689	11.330088
C	13.797366	20.733406	4.671605
C	8.447240	16.992987	9.493619
H	8.212732	16.360979	8.824158
C	10.067176	18.355646	10.592686
H	10.961198	18.660354	10.694549
C	7.460824	17.479969	10.340547
H	6.567735	17.170124	10.247355
C	9.080093	18.860862	11.432008
H	9.307040	19.514440	12.082949
C	12.681311	20.198838	6.843879
H	12.745174	21.114163	7.089895
C	12.541665	17.539118	6.200411
H	12.529279	16.615677	5.977498
C	6.742804	18.862418	12.300043
C	12.053127	19.307595	7.704498
H	11.693361	19.629537	8.522770
C	13.150281	18.415018	5.338651
H	13.530793	18.089029	4.531579
C	13.542312	22.138314	4.617032
H	12.998805	22.628320	5.222869
C	5.805087	18.007199	12.958342
H	5.709292	17.073350	12.812630
C	14.649250	20.419870	3.560369
H	14.973348	19.555911	3.334109
C	14.927430	21.633543	2.849778
H	15.475873	21.717220	2.078701
C	14.242765	22.680443	3.498760
H	14.246745	23.593344	3.235821
C	5.039703	18.787703	13.867069
H	4.346055	18.466118	14.430864
C	5.489549	20.122789	13.786445
H	5.148974	20.857286	14.283612
C	6.555794	20.177713	12.818202
H	7.046489	20.952170	12.569371
Fe	4.822229	19.492159	11.958914
Fe	12.925246	21.255966	2.888569

C	4.519811	19.567986	9.935147
H	5.169209	19.397386	9.263081
C	4.238296	20.814569	10.509971
H	4.663882	21.635189	10.290785
C	3.212299	20.646238	11.472700
H	2.836634	21.329569	12.015255
C	3.663925	18.603362	10.532789
H	3.638664	17.674161	10.336212
C	2.849620	19.289139	11.483159
H	2.178253	18.895884	12.027767
C	10.915947	21.489450	2.694425
H	10.333481	21.876945	3.336961
C	11.247272	20.146360	2.618365
H	10.931824	19.462095	3.197277
C	11.563032	22.178785	1.690434
H	11.514267	23.112033	1.524318
C	12.134513	19.964019	1.534510
H	12.530702	19.146824	1.253963
C	12.312405	21.231506	0.956454
H	12.848085	21.421673	0.195455

3_QChem_GeometricAnalysis_C-Fc.xyz /// N/A (X-ray crystal structure)

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C65H52Fe4

Fe	4.742234	2.915510	7.273278
C	4.130600	2.355269	9.144271
H	4.481903	1.580422	9.669822
Fe	14.506786	0.869031	13.073046
C	2.877981	3.628774	7.696947
H	2.191750	3.910728	7.026449
Fe	9.919323	12.607667	11.516683
C	3.036255	2.319987	8.227373
H	2.481252	1.519632	8.000431
C	4.635136	3.674025	9.172202
H	5.409016	3.992938	9.719346
Fe	15.808878	7.657967	3.476101
C	3.864742	4.466702	8.281624
H	3.996685	5.440332	8.095102
C	4.846728	2.713479	5.247723
H	4.092106	2.842755	4.604337
C	5.207250	1.493365	5.876177
H	4.744997	0.614562	5.758275
C	6.332535	1.739894	6.718412
H	6.793787	1.065452	7.294938
C	5.751471	3.721454	5.691401

H	5.736921	4.682776	5.416506
C	6.681818	3.124390	6.598764
C	7.791847	3.822817	7.272875
C	8.592044	3.203449	8.225627
H	8.411612	2.303376	8.469985
C	9.654104	3.874939	8.830581
H	10.179500	3.426261	9.482561
C	9.159726	5.807587	7.523719
H	9.352821	6.701030	7.264872
C	9.957069	5.189624	8.495674
C	8.100038	5.148808	6.933403
H	7.570774	5.600611	6.286740
C	11.176591	5.962772	9.042617
C	10.759073	7.211162	9.856115
C	11.762475	7.916609	10.530763
H	12.661409	7.615384	10.470845
C	11.476452	9.040350	11.281819
H	12.183647	9.506308	11.712270
C	10.166405	9.503527	11.419193
C	9.164541	8.790254	10.763613
H	8.262698	9.077959	10.843043
C	9.453604	7.667596	9.996040
H	8.747582	7.204904	9.560285
C	9.863833	10.699201	12.231751
C	8.594752	11.329082	12.394102
H	7.731122	11.017520	11.998015
C	8.772468	12.491323	13.203571
H	8.055227	13.135009	13.470543
C	10.140514	12.582903	13.551504
H	10.558898	13.302414	14.105765
C	10.819034	11.489275	12.955547
H	11.799252	11.303312	13.022945
C	10.969245	14.190838	10.770596
H	11.598552	14.773520	11.285418
C	9.585840	14.404499	10.610797
H	9.059338	15.166343	10.988567
C	9.068781	13.337046	9.813816
H	8.114328	13.220090	9.539538
C	10.128598	12.474853	9.490189
H	10.060454	11.638380	8.946469
C	11.315265	12.995340	10.074463
H	12.228531	12.591523	10.014128
C	12.005124	5.096111	10.016586
C	11.464316	4.812745	11.279402
H	10.592069	5.125150	11.489518
C	12.167212	4.090479	12.227051

H	11.764769	3.909552	13.068373
C	13.466243	3.619231	11.968150
C	14.005524	3.913618	10.716614
H	14.883491	3.615720	10.509371
C	13.289290	4.634177	9.760639
H	13.688289	4.812567	8.917208
C	14.234012	2.899433	12.997310
C	13.718346	2.360034	14.222257
H	12.768241	2.417701	14.528776
C	14.774954	1.708155	14.918525
H	14.699776	1.236954	15.797340
C	15.956051	1.843348	14.137255
H	16.857233	1.477659	14.370119
C	15.630153	2.571717	12.954741
H	16.263998	2.804800	12.217235
C	15.317571	-0.851343	12.339313
H	16.278811	-1.120246	12.401044
C	14.726700	-0.080571	11.288533
H	15.198373	0.278610	10.483226
C	13.344920	0.076180	11.592152
H	12.673065	0.571498	11.041382
C	13.088821	-0.601649	12.823276
H	12.207580	-0.654659	13.293005
C	14.307450	-1.167440	13.272460
H	14.434118	-1.687153	14.117341
C	11.994918	6.369174	7.789066
C	12.272549	5.398780	6.818455
H	12.016017	4.497851	6.976535
C	12.912864	5.722189	5.632047
H	13.095254	5.038501	4.998195
C	13.294610	7.037247	5.353271
C	13.050062	7.992114	6.332611
H	13.324975	8.889346	6.184253
C	12.411429	7.665404	7.527345
H	12.258429	8.343718	8.174652
C	13.852126	7.419732	4.047887
C	14.191216	6.544705	2.966355
H	14.140476	5.546134	2.985800
C	14.619198	7.337419	1.854476
H	14.916443	6.992592	0.964126
C	14.552683	8.703416	2.245245
H	14.807056	9.487036	1.678535
C	14.088131	8.763453	3.587289
H	13.962139	9.596621	4.125732
C	17.035777	6.876141	4.910668
H	16.745943	6.335737	5.700613

C	17.165186	8.290270	4.869308
H	16.981728	8.919463	5.624674
C	17.584448	8.654360	3.565804
H	17.754115	9.584653	3.240753
C	17.724941	7.461366	2.801453
H	18.006335	7.408933	1.843303
C	17.384779	6.362928	3.627575
H	17.384627	5.399968	3.357729

4_QChem_GeometricAnalysis_Os(C8H9)4.xyz /// -1330.54727722953

69

C	1.47888	-0.30396	1.30683
C	1.88752	0.69201	2.24800
C	2.93995	0.37978	3.12374
H	3.26477	1.14113	3.84301
C	3.57155	-0.87235	3.11796
H	4.38537	-1.07215	3.82380
C	3.16125	-1.87456	2.22333
C	2.11303	-1.57198	1.33273
H	1.77549	-2.34768	0.63686
C	1.18784	2.02788	2.36271
H	0.20866	1.91339	2.85775
H	0.99017	2.48015	1.37638
H	1.78703	2.74026	2.95249
C	3.84048	-3.22445	2.19244
H	4.14707	-3.54472	3.20149
H	4.75245	-3.19914	1.56897
H	3.18020	-4.00009	1.77306
C	0.49370	1.45746	-1.30452
C	-0.35172	1.86163	-2.38785
C	0.13554	2.83681	-3.27149
H	-0.50198	3.14987	-4.10681
C	1.40862	3.41119	-3.12970
H	1.74669	4.16411	-3.85028
C	2.25529	3.01854	-2.08294
C	1.77911	2.04070	-1.18573
H	2.43412	1.70959	-0.37250
C	-1.72354	1.26879	-2.61814
H	-1.69248	0.16751	-2.59696
H	-2.12751	1.58108	-3.59415
H	-2.44505	1.57936	-1.84266
C	3.62984	3.62093	-1.90394
H	3.66233	4.29834	-1.03216
H	3.93147	4.20424	-2.78815

H	4.39288	2.84307	-1.73324
C	-0.34680	-1.60660	-1.13525
C	0.63689	-2.16286	-2.01075
C	0.29694	-3.31662	-2.73657
H	1.05275	-3.76226	-3.39430
C	-0.97174	-3.90756	-2.65124
H	-1.19024	-4.81059	-3.23212
C	-1.96691	-3.34699	-1.83277
C	-1.63316	-2.20160	-1.08547
H	-2.39823	-1.75067	-0.44516
C	1.99129	-1.52258	-2.21768
H	2.39752	-1.09787	-1.28543
H	1.92465	-0.69024	-2.93970
H	2.72082	-2.24967	-2.60983
C	-3.35803	-3.93513	-1.76948
H	-3.33370	-5.03612	-1.82004
H	-3.97833	-3.58595	-2.61456
H	-3.87777	-3.64669	-0.84198
C	-1.61125	0.48932	1.11017
C	-2.14558	-0.37821	2.11573
C	-3.26771	0.06264	2.83724
H	-3.68650	-0.59856	3.60498
C	-3.85995	1.31411	2.61439
H	-4.73564	1.61347	3.20098
C	-3.33016	2.19144	1.65459
C	-2.21189	1.75905	0.91558
H	-1.78972	2.44189	0.17054
C	-1.54762	-1.73172	2.42618
H	-1.90643	-2.10766	3.39760
H	-0.44780	-1.68285	2.46534
H	-1.80635	-2.48564	1.66186
C	-3.91478	3.56846	1.43857
H	-3.50075	4.29651	2.15929
H	-5.00897	3.56812	1.57208
H	-3.69315	3.94876	0.42851
Os	-0.00808	0.01470	-0.00356

5_QChem_GeometricAnalysis_Si(C8H9)4_fromOs(C8H9)4.xyz /// -1528.84600659461

69

C	1.34452	0.55927	-1.23046
C	1.80878	-0.27061	-2.29221
C	2.78435	0.24086	-3.17027
H	3.14483	-0.39535	-3.98701
C	3.29476	1.53653	-3.03546

H	4.05064	1.89900	-3.74163
C	2.83951	2.37934	-2.00788
C	1.86673	1.86837	-1.12939
H	1.48760	2.53079	-0.34194
C	1.25723	-1.65620	-2.55455
H	0.29459	-1.60442	-3.09307
H	1.06777	-2.21815	-1.62740
H	1.95328	-2.24503	-3.17342
C	3.39121	3.77525	-1.83243
H	3.63953	4.23780	-2.80156
H	4.31784	3.76723	-1.23026
H	2.67289	4.43035	-1.31406
C	0.69541	-1.35325	1.15788
C	-0.00920	-1.84292	2.29741
C	0.59335	-2.84224	3.08454
H	0.05273	-3.22331	3.95857
C	1.86458	-3.34951	2.78898
H	2.30160	-4.12757	3.42510
C	2.58862	-2.86359	1.68909
C	1.98363	-1.86920	0.89708
H	2.55223	-1.47454	0.04656
C	-1.35159	-1.29157	2.73022
H	-1.23253	-0.32362	3.24761
H	-1.85290	-1.98304	3.42647
H	-2.03134	-1.11048	1.88194
C	3.96057	-3.39729	1.34688
H	3.92853	-4.04915	0.45566
H	4.38136	-3.99028	2.17433
H	4.66623	-2.58063	1.11996
C	-0.55669	1.48632	1.08209
C	0.27439	2.07901	2.07638
C	-0.22738	3.17073	2.81223
H	0.41608	3.63800	3.56667
C	-1.51902	3.66798	2.60903
H	-1.87280	4.52224	3.19750
C	-2.36897	3.07808	1.65810
C	-1.86336	1.99754	0.91307
H	-2.52526	1.52969	0.17469
C	1.65424	1.55458	2.41370
H	2.22411	1.24933	1.52226
H	1.58902	0.66385	3.06337
H	2.24343	2.31598	2.94952
C	-3.78345	3.57139	1.45979
H	-3.85016	4.66598	1.57248
H	-4.47050	3.12780	2.20297
H	-4.16770	3.30619	0.46215

C	-1.48177	-0.67796	-0.98645
C	-2.08548	0.02589	-2.06765
C	-3.16786	-0.57498	-2.74121
H	-3.64298	-0.03151	-3.56637
C	-3.64431	-1.84284	-2.39287
H	-4.48849	-2.27486	-2.94248
C	-3.04317	-2.56996	-1.35040
C	-1.97142	-1.96593	-0.67099
H	-1.48850	-2.53415	0.13272
C	-1.57806	1.36551	-2.55799
H	-2.32864	1.86022	-3.19534
H	-0.65779	1.24426	-3.15558
H	-1.32472	2.05052	-1.73290
C	-3.53074	-3.95094	-0.97720
H	-3.41285	-4.66106	-1.81447
H	-4.60227	-3.94374	-0.71242
H	-2.97350	-4.35311	-0.11675
Si	-0.00105	0.00612	0.00934

6_QChem_GeometricAnalysis_Si(C6H5)4.xyz /// -1214.75456183905

45

C	-0.05820	-1.54363	1.10019
C	0.68354	-1.61027	2.30315
C	0.68965	-2.77132	3.09042
C	-0.05167	-3.89285	2.69118
C	-0.79886	-3.84619	1.50514
C	-0.80175	-2.68387	0.72078
Si	0.00000	0.00000	0.00000
C	-1.54363	0.05820	-1.10019
C	0.05820	1.54363	1.10019
C	1.54363	-0.05820	-1.10019
C	-1.61027	-0.68354	-2.30315
C	-2.68387	0.80175	-0.72078
C	-0.68354	1.61027	2.30315
C	0.80175	2.68387	0.72078
C	1.61027	0.68354	-2.30315
C	2.68387	-0.80175	-0.72078
C	-2.77132	-0.68965	-3.09042
C	-3.84619	0.79886	-1.50514
C	-0.68965	2.77132	3.09042
C	0.79886	3.84619	1.50514
C	2.77132	0.68965	-3.09042
C	3.84619	-0.79886	-1.50514
C	-3.89285	0.05167	-2.69118

C	0.05167	3.89285	2.69118
C	3.89285	-0.05167	-2.69118
H	1.25667	-0.73781	2.63711
H	1.27074	-2.79842	4.01790
H	-0.05121	-4.79930	3.30488
H	-1.38488	-4.71657	1.19250
H	-1.39778	-2.65966	-0.19815
H	-0.73781	-1.25667	-2.63711
H	-2.65966	1.39778	0.19815
H	-1.25667	0.73781	2.63711
H	1.39778	2.65966	-0.19815
H	0.73781	1.25667	-2.63711
H	2.65966	-1.39778	0.19815
H	-2.79842	-1.27074	-4.01790
H	-4.71657	1.38488	-1.19250
H	-1.27074	2.79842	4.01790
H	1.38488	4.71657	1.19250
H	2.79842	1.27074	-4.01790
H	4.71657	-1.38488	-1.19250
H	-4.79930	0.05121	-3.30488
H	0.05121	4.79930	3.30488
H	4.79930	-0.05121	-3.30488

7_QChem_GeometricAnalysis_Si(C8H9)4_fromSi(C6H5)4.xyz /// -1528.84625655137

69

C	-1.51827	0.26940	-1.12163
C	-1.52474	1.20593	-2.19476
C	-2.67809	1.29835	-2.99932
C	-3.79812	0.48968	-2.78319
C	-3.80725	-0.45568	-1.74221
C	-2.65971	-0.54247	-0.93481
Si	0.00000	0.00000	0.00827
C	-0.26982	-1.52061	1.13492
C	1.51827	-0.26940	-1.12163
C	0.26982	1.52061	1.13492
C	-1.21210	-1.53157	2.20629
C	0.53832	-2.66083	0.94249
C	1.52474	-1.20593	-2.19476
C	2.65971	0.54247	-0.93481
C	1.21210	1.53157	2.20629
C	-0.53832	2.66083	0.94249
C	-1.31314	-2.68941	2.99926
C	0.44226	-3.81648	1.74169
C	2.67809	-1.29835	-2.99932

C	3.80725	0.45568	-1.74221
C	1.31314	2.68941	2.99926
C	-0.44226	3.81648	1.74169
C	-0.50719	-3.81284	2.77517
C	3.79812	-0.48968	-2.78319
C	0.50719	3.81284	2.77517
C	-0.32579	2.06172	-2.54695
H	-2.68969	2.02110	-3.82342
H	-4.67367	0.59292	-3.43476
C	-5.00887	-1.33820	-1.49535
H	-2.64850	-1.28945	-0.13245
C	-2.06394	-0.33064	2.56063
H	1.28749	-2.64461	0.14185
C	0.32579	-2.06172	-2.54695
H	2.64850	1.28945	-0.13245
C	2.06394	0.33064	2.56063
H	-1.28749	2.64461	0.14185
H	-2.03986	-2.70645	3.81969
C	1.33209	-5.01061	1.48433
H	2.68969	-2.02110	-3.82342
C	5.00887	1.33820	-1.49535
H	2.03986	2.70645	3.81969
C	-1.33209	5.01061	1.48433
H	-0.61695	-4.69599	3.41500
H	4.67367	-0.59292	-3.43476
H	0.61695	4.69599	3.41500
H	0.19130	2.45126	-1.65601
H	-0.62458	2.91868	-3.17186
H	0.42142	1.47768	-3.11187
H	-4.80261	-2.08788	-0.71556
H	-5.31149	-1.87544	-2.41046
H	-5.88238	-0.74758	-1.16696
H	-2.91644	-0.62633	3.19294
H	-2.46003	0.18298	1.67038
H	-1.47506	0.41843	3.11792
H	-0.19130	-2.45126	-1.65601
H	0.62458	-2.91868	-3.17186
H	-0.42142	-1.47768	-3.11187
H	2.91644	0.62633	3.19294
H	2.46003	-0.18298	1.67038
H	1.47506	-0.41843	3.11792
H	1.12602	-5.82720	2.19406
H	2.39958	-4.74524	1.57647
H	1.18933	-5.40734	0.46432
H	4.80261	2.08788	-0.71556
H	5.31149	1.87544	-2.41046

H	5.88238	0.74758	-1.16696
H	-1.12602	5.82720	2.19406
H	-2.39958	4.74524	1.57647
H	-1.18933	5.40734	0.46432

8_QChem_GeometricAnalysis_C(C6H5)4.xyz /// -963.448312892631

45

C	1.22995	0.03583	-0.94933
C	1.31293	1.07845	-1.90042
C	2.37657	1.15651	-2.80539
C	3.38080	0.17608	-2.80013
C	3.29859	-0.87725	-1.88351
C	2.23535	-0.94748	-0.96742
C	0.00000	0.00000	0.00000
H	0.51996	1.83238	-1.93619
H	2.41408	1.98032	-3.52516
H	4.21101	0.22938	-3.51105
H	4.06370	-1.66017	-1.87610
H	2.19460	-1.78772	-0.26999
C	0.03583	-1.22995	0.94933
C	-1.22995	-0.03583	-0.94933
C	-0.03583	1.22995	0.94933
C	1.07845	-1.31293	1.90042
C	-0.94748	-2.23535	0.96742
C	-1.31293	-1.07845	-1.90042
C	-2.23535	0.94748	-0.96742
C	-1.07845	1.31293	1.90042
C	0.94748	2.23535	0.96742
C	1.15651	-2.37657	2.80539
H	1.83238	-0.51996	1.93619
C	-0.87725	-3.29859	1.88351
H	-1.78772	-2.19460	0.26999
C	-2.37657	-1.15651	-2.80539
H	-0.51996	-1.83238	-1.93619
C	-3.29859	0.87725	-1.88351
H	-2.19460	1.78772	-0.26999
C	-1.15651	2.37657	2.80539
H	-1.83238	0.51996	1.93619
C	0.87725	3.29859	1.88351
H	1.78772	2.19460	0.26999
C	0.17608	-3.38080	2.80013
H	1.98032	-2.41408	3.52516
H	-1.66017	-4.06370	1.87610
C	-3.38080	-0.17608	-2.80013

H	-2.41408	-1.98032	-3.52516
H	-4.06370	1.66017	-1.87610
C	-0.17608	3.38080	2.80013
H	-1.98032	2.41408	3.52516
H	1.66017	4.06370	1.87610
H	0.22938	-4.21101	3.51105
H	-4.21101	-0.22938	-3.51105
H	-0.22938	4.21101	3.51105

9_QChem_Model_PBE_Os1h_sim.xyz /// -2205.07520348555

77

C	-0.09841	1.20210	2.02381
C	0.90611	2.04039	2.60357
C	0.76280	2.40960	3.95044
H	1.54160	3.03156	4.40774
C	-0.34029	2.01285	4.72134
H	-0.40892	2.32136	5.77033
C	-1.35848	1.22775	4.15706
C	-1.21694	0.83253	2.81195
H	-1.99926	0.21198	2.36156
C	2.07766	2.57301	1.80702
H	1.78686	3.46309	1.22169
H	2.46552	1.83546	1.08525
H	2.90783	2.86748	2.47002
C	-2.58176	0.83044	4.95087
H	-2.38332	0.84830	6.03445
H	-2.92731	-0.18119	4.68250
H	-3.42362	1.52022	4.76015
C	1.60297	-0.64894	-0.10325
C	1.90688	-1.32302	-1.32562
C	3.02474	-2.17084	-1.36859
H	3.23779	-2.68142	-2.31227
C	3.85338	-2.38473	-0.25013
S	5.28289	-3.44894	-0.27603
C	3.55141	-1.74593	0.97924
C	2.43457	-0.89703	1.01901
H	2.19572	-0.41142	1.97059
C	1.06792	-1.15849	-2.57507
H	-0.00516	-1.09732	-2.33140
H	1.21470	-2.00508	-3.26473
H	1.32565	-0.23528	-3.12370
C	4.39795	-1.96800	2.20755
H	5.44826	-1.67286	2.03193
H	4.41425	-3.03293	2.50225

H	4.01831	-1.38536	3.06078
C	-1.59189	-0.55740	-0.32341
C	-1.87253	-1.80421	0.31675
C	-3.03869	-2.49897	-0.03944
H	-3.24070	-3.44652	0.46827
C	-3.93058	-2.02460	-1.02082
S	-5.42133	-2.87594	-1.49726
C	-3.64866	-0.80999	-1.69542
C	-2.48564	-0.11216	-1.33154
H	-2.26939	0.82219	-1.86072
C	-0.93302	-2.41660	1.33142
H	-0.57837	-1.67057	2.06204
H	-0.03425	-2.82458	0.83934
H	-1.41862	-3.23426	1.88814
C	-4.56576	-0.27897	-2.76846
H	-5.58294	-0.09702	-2.37674
H	-4.67141	-0.99798	-3.60069
H	-4.18705	0.66751	-3.18355
C	0.14253	2.20154	-1.00267
C	-0.83043	3.24826	-0.95828
C	-0.65545	4.34799	-1.81353
H	-1.40800	5.14549	-1.79980
C	0.44746	4.46040	-2.67280
H	0.54024	5.33816	-3.32197
C	1.43644	3.46330	-2.69769
C	1.26297	2.34567	-1.85858
H	2.02921	1.56257	-1.86495
C	-2.00264	3.22199	-0.00322
H	-2.73554	4.00551	-0.25388
H	-1.66807	3.38715	1.03520
H	-2.52419	2.25085	-0.01329
C	2.66133	3.59217	-3.57397
H	3.41421	4.25772	-3.11458
H	2.41137	4.01999	-4.55892
H	3.14462	2.61618	-3.73926
Os	0.01536	0.55322	0.12857
C	-5.45741	-4.33205	-0.40395
C	5.37878	-3.99023	-2.01230
H	-6.38437	-4.86505	-0.66144
H	-5.49704	-4.04173	0.65715
H	-4.60164	-5.00147	-0.58236
H	6.28443	-4.61103	-2.07641
H	5.48424	-3.13296	-2.69472
H	4.50888	-4.60027	-2.30023

10_QChem_Model_PBE_Os1h_diff.xyz /// -2205.07424659267

C	1.51716	-0.70064	0.42909
C	2.85524	-0.25755	0.65260
C	3.83640	-1.20332	0.98715
H	4.85775	-0.84071	1.14004
C	3.54250	-2.57299	1.13691
S	4.76273	-3.80030	1.56086
C	2.21269	-3.02810	0.94908
C	1.23662	-2.08105	0.60182
H	0.21020	-2.43685	0.46088
C	3.23448	1.20622	0.58873
H	2.97606	1.72031	1.53059
H	2.69569	1.73563	-0.21480
H	4.31567	1.33348	0.41719
C	1.84815	-4.48329	1.10918
H	2.08036	-4.84947	2.12557
H	2.41198	-5.12263	0.40583
H	0.77446	-4.64099	0.92660
C	0.31862	1.42085	-1.85778
C	-0.63661	2.31147	-2.44558
C	-0.34864	2.84271	-3.71292
H	-1.07691	3.52263	-4.17077
C	0.82299	2.52130	-4.41438
C	1.76136	1.63451	-3.86342
C	1.48777	1.09577	-2.59071
H	2.20537	0.38944	-2.15961
C	-1.93892	2.67198	-1.76680
H	-2.49014	1.76845	-1.45746
H	-2.58600	3.25344	-2.44264
H	-1.77942	3.27413	-0.85526
C	3.03657	1.28228	-4.59434
H	3.85004	1.98761	-4.34541
H	2.89809	1.31911	-5.68697
H	3.38980	0.27300	-4.32820
C	-1.67541	-0.47986	-0.24940
C	-1.87154	-1.48614	-1.24397
C	-3.09406	-2.17484	-1.27655
H	-3.21964	-2.95010	-2.03791
C	-4.14392	-1.89002	-0.38166
S	-5.70563	-2.74890	-0.39143
C	-3.98300	-0.86602	0.58693
C	-2.75500	-0.18703	0.62301
H	-2.63252	0.61110	1.36199
C	-0.83031	-1.78890	-2.29917

H	0.19604	-1.69639	-1.90783
H	-0.91097	-1.07879	-3.14050
H	-0.95168	-2.80708	-2.70386
C	-5.08995	-0.51821	1.54997
H	-5.36558	-1.38406	2.17885
H	-6.00739	-0.21094	1.01624
H	-4.79264	0.30467	2.21810
C	-0.04245	1.88347	1.41931
C	-0.21883	1.54215	2.79897
C	-0.23671	2.58832	3.73693
H	-0.38090	2.33695	4.79439
C	-0.07438	3.93252	3.37100
H	-0.10096	4.71146	4.14114
C	0.13625	4.28333	2.02789
C	0.14973	3.24651	1.07539
H	0.32493	3.50677	0.02633
C	-0.37290	0.11667	3.28324
H	-0.30378	0.07055	4.38176
H	0.40695	-0.53941	2.86332
H	-1.34494	-0.31940	2.99426
C	0.36796	5.71886	1.61502
H	1.42406	6.01255	1.75502
H	-0.24237	6.41330	2.21528
H	0.12232	5.87837	0.55323
Os	0.03227	0.54591	-0.07123
C	-5.54095	-3.92295	-1.77254
H	-6.50088	-4.45817	-1.81615
H	-4.73580	-4.65273	-1.59582
H	-5.37963	-3.40336	-2.72949
C	6.29015	-2.82865	1.75982
H	0.99964	2.95579	-5.40454
H	7.06547	-3.55573	2.04216
H	6.19134	-2.08232	2.56282
H	6.58619	-2.33898	0.81946

11_QChem_Model_PBE_Si1h_sim.xyz /// -2089.28123404691

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C	1.53648	0.37700	-0.03734
C	1.55720	1.57421	-0.79412
C	2.70217	2.37010	-0.88095
C	3.88252	1.99680	-0.20128
C	3.88075	0.81629	0.56623
C	2.72368	0.02765	0.63994
Si	0.00001	-0.72693	-0.00000

C	0.04590	-1.83542	1.53929
C	-1.53646	0.37699	0.03726
C	-0.04589	-1.83553	-1.53921
C	0.80589	-3.02875	1.54854
C	-0.63272	-1.47812	2.72596
C	-1.55719	1.57423	0.79401
C	-2.72367	0.02761	-0.63999
C	-0.80577	-3.02893	-1.54833
C	0.63260	-1.47824	-2.72596
C	0.89352	-3.82664	2.69899
C	-0.55004	-2.27413	3.87772
C	-2.70217	2.37010	0.88084
C	-3.88075	0.81624	-0.56628
C	-0.89343	-3.82689	-2.69873
C	0.54990	-2.27432	-3.87767
C	0.21554	-3.44919	3.86718
C	-3.88252	1.99676	0.20121
C	-0.21558	-3.44945	-3.86700
H	0.65404	1.90135	-1.32170
H	2.68475	3.28987	-1.47521
S	5.27943	3.08155	-0.38376
H	4.77325	0.50359	1.11399
H	2.75174	-0.88267	1.24913
H	1.32746	-3.34790	0.63893
H	-1.24023	-0.56667	2.74751
H	-0.65403	1.90140	1.32156
H	-2.75173	-0.88273	-1.24915
H	-1.32724	-3.34807	-0.63866
H	1.24003	-0.56674	-2.74761
H	1.48704	-4.74652	2.68131
H	-1.08796	-1.97868	4.78439
H	-2.68475	3.28989	1.47508
H	-4.77326	0.50351	-1.11402
H	-1.48687	-4.74683	-2.68095
H	1.08772	-1.97887	-4.78440
H	0.27908	-4.07175	4.76535
S	-5.27945	3.08149	0.38370
C	-6.58120	2.26532	-0.59341
H	-7.47311	2.89924	-0.48278
H	-6.80867	1.26075	-0.20514
H	-6.31568	2.21007	-1.66031
C	6.58121	2.26533	0.59325
H	-0.27913	-4.07206	-4.76513
H	7.47308	2.89934	0.48275
H	6.80877	1.26084	0.20482
H	6.31567	2.20988	1.66014

12_QChem_Model_PBE_Si1h_diff.xyz /// -2089.28140433495

53

C	-0.11511	1.97521	1.55779
C	0.18923	1.44020	2.83183
C	0.06574	2.21581	3.99392
C	-0.35831	3.54997	3.90549
C	-0.65538	4.10325	2.65164
C	-0.53448	3.32284	1.49274
Si	-0.00836	0.89453	0.00206
C	0.07818	1.99288	-1.54208
C	1.54443	-0.18115	0.12558
C	-1.54605	-0.20400	-0.12796
C	-1.09313	2.57901	-2.07700
C	1.30854	2.28426	-2.17266
C	2.73251	0.30757	0.72135
C	1.58179	-1.48954	-0.40064
C	-1.96446	-0.73150	-1.37400
C	-2.29636	-0.57167	1.00867
C	-1.03685	3.42831	-3.19165
C	1.36927	3.13174	-3.28840
C	3.89532	-0.46469	0.78244
C	2.73932	-2.27811	-0.34724
C	-3.06206	-1.58971	-1.47718
C	-3.40214	-1.42939	0.92260
C	0.19644	3.70656	-3.79914
C	3.91153	-1.77075	0.24557
C	-3.79336	-1.95198	-0.32487
H	0.54353	0.40637	2.91564
H	0.30718	1.78054	4.96915
H	-0.45105	4.15762	4.81125
H	-0.97826	5.14654	2.57504
H	-0.76222	3.77133	0.51957
H	-2.06590	2.35908	-1.62260
H	2.23152	1.83612	-1.78844
H	2.74651	1.31041	1.16267
H	0.68151	-1.91466	-0.85866
H	-1.42797	-0.45692	-2.28926
H	-2.01981	-0.17492	1.99196
H	-1.95667	3.86919	-3.58943
H	2.33365	3.34103	-3.76259
H	4.79723	-0.05952	1.25333
H	2.71536	-3.28738	-0.76549
H	-3.36050	-1.98115	-2.45548

H	-3.95442	-1.68103	1.83137
H	0.24258	4.36639	-4.67142
S	5.44133	-2.67008	0.37851
S	-5.16724	-3.05360	-0.57316
C	5.05735	-4.27239	-0.39478
C	-5.81585	-3.31212	1.10872
H	5.98428	-4.86101	-0.33025
H	4.78424	-4.15650	-1.45492
H	4.26044	-4.80374	0.14793
H	-6.65261	-4.01686	0.99614
H	-6.19589	-2.37679	1.54746
H	-5.05784	-3.76184	1.76822

13_QChem_Model_PBE_C1h_sim.xyz /// -1837.97255055652

53

C	1.21844	0.00396	-0.13934
C	1.48872	0.91933	0.89950
C	2.52933	1.85028	0.81713
C	3.33236	1.91511	-0.33882
C	3.05642	1.02616	-1.39554
C	2.02054	0.08985	-1.29305
C	0.00006	-0.94896	-0.00000
H	0.85758	0.91560	1.79374
H	2.69825	2.53026	1.65522
S	4.68035	3.05448	-0.57238
H	3.65367	1.06773	-2.31232
H	1.83349	-0.57624	-2.13858
C	-0.13342	-1.90468	-1.21896
C	-1.21834	0.00392	0.13938
C	0.13358	-1.90465	1.21896
C	0.91854	-2.81084	-1.48273
C	-1.28402	-1.98313	-2.02368
C	-1.48875	0.91922	-0.89949
C	-2.02036	0.08982	1.29314
C	-0.91833	-2.81088	1.48270
C	1.28416	-1.98300	2.02371
C	0.83887	-3.73154	-2.53248
H	1.80564	-2.80059	-0.84192
C	-1.37130	-2.91561	-3.07119
H	-2.12888	-1.31815	-1.82966
C	-2.52938	1.85015	-0.81707
H	-0.85770	0.91547	-1.79379
C	-3.05629	1.02608	1.39566
H	-1.83324	-0.57625	2.13867

C	-0.83862	-3.73158	2.53246
H	-1.80541	-2.80071	0.84187
C	1.37149	-2.91548	3.07122
H	2.12898	-1.31796	1.82971
C	-0.31029	-3.78795	-3.33696
H	1.67303	-4.41632	-2.71522
H	-2.28180	-2.95609	-3.67758
C	-3.33233	1.91500	0.33894
H	-2.69838	2.53011	-1.65516
H	-3.65353	1.06758	2.31245
C	0.31053	-3.78790	3.33697
H	-1.67273	-4.41642	2.71518
H	2.28197	-2.95587	3.67763
H	-0.37884	-4.51192	-4.15459
S	-4.68025	3.05443	0.57264
H	0.37912	-4.51185	4.15461
C	4.64567	4.06431	0.94215
C	-4.64629	4.06365	-0.94233
H	5.45275	4.80189	0.82274
H	4.84798	3.46017	1.83996
H	3.68912	4.59833	1.05006
H	-5.45379	4.80081	-0.82316
H	-4.84832	3.45897	-1.83984
H	-3.69006	4.59818	-1.05057

14_QChem_Model_PBE_C1h_diff.xyz /// -1837.97297496680

53

C	-0.12501	-1.48658	1.38281
C	-1.27547	-2.27758	1.60675
C	-1.46162	-2.97198	2.80694
C	-0.50609	-2.88069	3.83067
C	0.62858	-2.08671	3.63246
C	0.81837	-1.39848	2.42197
C	0.01596	-0.74925	0.01985
H	-2.03952	-2.34095	0.82579
H	-2.36191	-3.57908	2.94541
H	1.37807	-1.99162	4.42467
H	1.71112	-0.77996	2.30146
C	1.20887	0.24524	0.04053
C	-1.32946	-0.00677	-0.21549
C	0.30487	-1.75654	-1.13203
C	2.52375	-0.26617	0.01869
C	1.06512	1.64512	0.05828
C	-1.86335	0.78599	0.82313

C	-2.07977	-0.09354	-1.40304
C	0.65063	-1.24768	-2.40511
C	0.26707	-3.15317	-0.97442
C	3.64644	0.56913	0.03705
H	2.67255	-1.34960	-0.02312
C	2.17850	2.49350	0.06557
H	0.06771	2.08960	0.04841
C	-3.06872	1.48364	0.68286
H	-1.32855	0.84945	1.77596
C	-3.29205	0.58983	-1.55369
H	-1.72656	-0.71339	-2.23035
C	0.91575	-2.10013	-3.48268
H	0.72100	-0.16449	-2.54456
C	0.54280	-4.01130	-2.05249
H	0.03038	-3.58537	0.00061
C	3.48543	1.96845	0.06041
H	4.64216	0.11942	0.02397
H	2.02857	3.57806	0.06478
C	-3.80221	1.39404	-0.51592
H	-3.43111	2.08446	1.52048
H	-3.85095	0.49177	-2.49020
C	0.86161	-3.49212	-3.31202
H	1.17437	-1.67415	-4.45731
H	0.51005	-5.09427	-1.89632
S	4.82622	3.13987	0.08213
S	-5.35033	2.21730	-0.82038
H	1.07469	-4.16151	-4.15105
C	-5.66433	3.11198	0.73450
H	-6.62432	3.62835	0.58854
H	-4.88544	3.86361	0.93613
H	-5.75847	2.42288	1.58777
C	6.30412	2.09200	-0.10086
H	-0.65154	-3.41604	4.77391
H	7.15454	2.78793	-0.14812
H	6.27040	1.50791	-1.03334
H	6.44377	1.42293	0.76221

15_QChem_Model_PBE_Os1h-Au1_sim.xyz /// -2475.96019868150

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C	0.19568	-2.08819	1.74610
C	-0.68747	-3.16336	2.07482
C	-0.47995	-3.83334	3.29020
H	-1.16273	-4.64681	3.56255
C	0.57200	-3.49771	4.15649

H	0.69368	-4.04540	5.09726
C	1.47814	-2.47848	3.82370
C	1.27476	-1.78917	2.61121
H	1.98011	-1.00440	2.32162
C	-1.77750	-3.63389	1.13576
H	-1.36033	-4.29000	0.35169
H	-2.27823	-2.80317	0.61041
H	-2.54812	-4.20680	1.67590
C	2.65310	-2.14447	4.71305
H	2.49185	-2.50168	5.74240
H	2.83746	-1.05875	4.75301
H	3.58064	-2.61533	4.34177
C	-1.66423	0.13698	0.21933
C	-1.97451	1.21784	-0.67454
C	-3.19443	1.88616	-0.51701
H	-3.42700	2.68755	-1.22496
C	-4.10342	1.56889	0.51597
S	-5.67786	2.34456	0.71004
C	-3.79503	0.53333	1.43878
C	-2.58134	-0.14231	1.27054
H	-2.33743	-0.92729	1.99343
C	-1.04005	1.66998	-1.77682
H	-0.07086	2.00201	-1.36967
H	-1.47986	2.50856	-2.33880
H	-0.82220	0.86277	-2.49698
C	-4.75149	0.14644	2.53787
H	-5.72529	-0.16961	2.11840
H	-4.95434	0.99073	3.22068
H	-4.34664	-0.68518	3.13333
C	1.56249	0.15798	-0.10589
C	1.87325	1.25661	0.76578
C	3.09092	1.92383	0.58928
H	3.32641	2.73885	1.28055
C	3.99447	1.58939	-0.44362
S	5.56940	2.35852	-0.65867
C	3.68020	0.54130	-1.35039
C	2.46846	-0.13300	-1.16272
H	2.21036	-0.92375	-1.87432
C	0.93868	1.72606	1.86040
H	0.72691	0.93147	2.59607
H	-0.03364	2.04256	1.44788
H	1.37309	2.57902	2.40467
C	4.62785	0.14174	-2.45261
H	5.60564	-0.16755	-2.03713
H	4.82394	0.97760	-3.14758
H	4.21965	-0.69812	-3.03408

C	-0.24356	-2.16794	-1.55158
C	0.63662	-3.25683	-1.84471
C	0.40631	-3.97834	-3.02861
H	1.08116	-4.80809	-3.26995
C	-0.65105	-3.67824	-3.89948
H	-0.78561	-4.27080	-4.81092
C	-1.54652	-2.63797	-3.60423
C	-1.32723	-1.90116	-2.42427
H	-2.03345	-1.10555	-2.16756
C	1.76705	-3.68208	-0.93039
H	2.33239	-4.51402	-1.37856
H	1.38880	-4.02003	0.04916
H	2.48254	-2.86656	-0.72748
C	-2.72770	-2.33581	-4.49687
H	-3.55191	-3.05033	-4.32376
H	-2.45580	-2.40758	-5.56277
H	-3.12588	-1.32605	-4.31107
Os	-0.04065	-1.00253	0.07349
C	5.60875	3.64968	0.62805
C	-5.70062	3.62473	-0.58797
H	6.60950	4.09756	0.55033
H	5.49479	3.20623	1.62679
H	4.83584	4.40728	0.43122
H	-6.69850	4.08051	-0.51986
H	-5.58437	3.17202	-1.58224
H	-4.92329	4.37833	-0.39313
Au	-7.58968	0.83365	-0.32664
Au	7.48637	0.84776	0.37082

16_QChem_Model_PBE_Os1h-Au1_diff.xyz /// -2475.96036319345

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C	1.71656	0.60854	-0.51354
C	2.90909	1.39609	-0.63795
C	4.09894	0.76187	-1.01123
H	5.00024	1.37687	-1.09090
C	4.15916	-0.62087	-1.29174
S	5.63562	-1.45478	-1.78712
C	2.99589	-1.42711	-1.14707
C	1.81255	-0.79063	-0.75810
H	0.91881	-1.41167	-0.63744
C	2.93722	2.87618	-0.32566
H	2.95134	3.05014	0.76445
H	2.04954	3.39652	-0.72158
H	3.83167	3.35639	-0.75378

C	3.03711	-2.91549	-1.38077
H	3.79544	-3.39647	-0.73462
H	3.30595	-3.15939	-2.42429
H	2.06081	-3.37431	-1.16413
C	-0.71155	2.78768	-1.24579
C	-1.93983	3.49136	-1.04998
C	-2.32063	4.43133	-2.02152
H	-3.25917	4.97944	-1.87907
C	-1.55087	4.67397	-3.16842
C	-0.35501	3.97149	-3.39167
C	0.04281	3.03362	-2.41929
H	0.96877	2.47003	-2.57701
C	-2.85238	3.21991	0.12467
H	-3.32905	2.22863	0.03108
H	-3.65360	3.97297	0.18587
H	-2.30855	3.22405	1.08426
C	0.49487	4.23050	-4.61415
H	1.21208	5.05186	-4.43590
H	-0.12275	4.52157	-5.47896
H	1.08066	3.34087	-4.89542
C	-1.45346	0.00364	0.02393
C	-1.84939	-0.72737	-1.14652
C	-2.84998	-1.69632	-1.02415
H	-3.14592	-2.24097	-1.92519
C	-3.47660	-1.98057	0.20966
S	-4.76485	-3.17259	0.39814
C	-3.14305	-1.22780	1.37053
C	-2.14816	-0.25286	1.23984
H	-1.88738	0.33013	2.12919
C	-1.26840	-0.43233	-2.50992
H	-0.16678	-0.39659	-2.48845
H	-1.60901	0.55290	-2.87241
H	-1.57211	-1.19094	-3.24830
C	-3.84084	-1.45151	2.68823
H	-3.74629	-2.49790	3.02887
H	-4.92315	-1.23467	2.61076
H	-3.42033	-0.80130	3.46999
C	0.36221	2.07715	1.87529
C	0.81459	1.27451	2.97043
C	1.05066	1.91971	4.19567
H	1.38957	1.31630	5.04570
C	0.87253	3.30099	4.36643
H	1.06568	3.75448	5.34462
C	0.45773	4.10721	3.29533
C	0.21085	3.47470	2.06037
H	-0.10759	4.09298	1.21292

C	1.07280	-0.21057	2.85186
H	1.40265	-0.62753	3.81614
H	1.85726	-0.42038	2.10528
H	0.17385	-0.76656	2.53480
C	0.29887	5.60288	3.43995
H	1.17940	6.13932	3.04329
H	0.18527	5.89562	4.49562
H	-0.58000	5.97113	2.88612
Os	-0.03084	1.38587	0.03244
C	-4.85797	-3.99406	-1.22727
H	-5.66890	-4.72966	-1.12949
H	-3.90802	-4.50427	-1.44476
H	-5.12001	-3.27633	-2.01665
C	6.89731	-0.13915	-1.80103
H	-1.89193	5.41293	-3.90186
H	7.83451	-0.64720	-2.06802
H	7.00409	0.30197	-0.80029
H	6.65048	0.62222	-2.55567
Au	-7.06627	-1.94033	0.31659
Au	6.72132	-2.91286	0.15469

17_QChem_Model_PBE_Si1h-Au1_sim.xyz /// -2360.15678980524

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C	1.44967	-0.49708	0.53351
C	1.70146	0.74482	-0.09786
C	2.86130	1.47754	0.16404
C	3.80861	0.98129	1.08373
C	3.57123	-0.23561	1.74721
C	2.39952	-0.95426	1.47121
Si	-0.05915	-1.53309	0.03427
C	-0.49372	-2.78237	1.39044
C	-1.51380	-0.35149	-0.25488
C	0.32179	-2.46916	-1.56819
C	0.25912	-3.97134	1.53984
C	-1.56123	-2.55834	2.28868
C	-1.82931	0.67375	0.67004
C	-2.34682	-0.48268	-1.38701
C	-0.42105	-3.62534	-1.90371
C	1.30748	-2.02685	-2.47830
C	-0.03552	-4.89304	2.55510
C	-1.86148	-3.48013	3.30170
C	-2.93123	1.51277	0.48667
C	-3.45564	0.34921	-1.59032
C	-0.19466	-4.30740	-3.10795

C	1.53866	-2.70820	-3.68197
C	-1.09723	-4.64768	3.43847
C	-3.75120	1.35316	-0.65100
C	0.78584	-3.84827	-3.99947
H	0.97600	1.14977	-0.81209
H	3.04601	2.42383	-0.35450
S	5.28576	1.96178	1.27274
H	4.28838	-0.63444	2.46885
H	2.22854	-1.90053	1.99593
H	1.07407	-4.18859	0.83992
H	-2.17661	-1.65738	2.19133
H	-1.19600	0.82570	1.55118
H	-2.13079	-1.25551	-2.13245
H	-1.17752	-4.00530	-1.20778
H	1.90804	-1.14225	-2.23992
H	0.55835	-5.80768	2.65062
H	-2.69783	-3.28911	3.98156
H	-3.16062	2.28990	1.22298
H	-4.07820	0.20823	-2.47615
H	-0.77959	-5.20110	-3.34785
H	2.31098	-2.35085	-4.37044
H	-1.33288	-5.36956	4.22676
S	-5.13881	2.46345	-0.77053
C	-5.84767	2.10786	-2.41165
H	-6.70335	2.79049	-2.51137
H	-6.21014	1.07228	-2.46433
H	-5.10613	2.31799	-3.19660
C	6.25812	1.05454	2.52080
H	0.96706	-4.38113	-4.93830
H	7.18685	1.63017	2.64039
H	6.50621	0.04509	2.16324
H	5.71345	1.02228	3.47621
Au	-7.05163	1.37538	0.67727
Au	6.69130	1.27981	-0.84504

18_QChem_Model_PBE_Si1h-Au1_diff.xyz /// -2360.18110871945

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C	-0.28461	3.03534	1.41219
C	-0.10624	2.85848	2.80471
C	-0.30623	3.91831	3.70125
C	-0.68545	5.18043	3.22048
C	-0.86348	5.37735	1.84361
C	-0.66412	4.31530	0.94976
Si	-0.06226	1.59117	0.21123

C	0.10653	2.21140	-1.56832
C	1.50183	0.62436	0.67679
C	-1.56255	0.43586	0.30518
C	-1.03289	2.57902	-2.32271
C	1.37671	2.35131	-2.17218
C	2.59505	1.25156	1.32105
C	1.65288	-0.73323	0.31719
C	-1.85853	-0.44475	-0.76368
C	-2.40446	0.38784	1.43906
C	-0.90648	3.07570	-3.62808
C	1.50558	2.84452	-3.47842
C	3.78615	0.56618	1.57497
C	2.84078	-1.43549	0.55500
C	-2.92884	-1.34088	-0.69974
C	-3.49117	-0.49199	1.51615
C	0.36412	3.20845	-4.20738
C	3.91580	-0.78383	1.18758
C	-3.74838	-1.37197	0.44769
H	0.20524	1.88153	3.19288
H	-0.16080	3.76088	4.77475
H	-0.83807	6.00991	3.91810
H	-1.15465	6.36189	1.46407
H	-0.79971	4.48279	-0.12425
H	-2.03327	2.46487	-1.88942
H	2.27675	2.06463	-1.61715
H	2.51541	2.29894	1.63109
H	0.82534	-1.26360	-0.16684
H	-1.24816	-0.42296	-1.67336
H	-2.22217	1.06898	2.27754
H	-1.80055	3.35309	-4.19548
H	2.49830	2.94053	-3.92941
H	4.62314	1.07923	2.05957
H	2.91755	-2.48048	0.24587
H	-3.13716	-2.01288	-1.53853
H	-4.13571	-0.47581	2.39855
H	0.46387	3.59047	-5.22831
S	5.49925	-1.53415	1.50588
S	-5.12002	-2.50411	0.39189
C	5.26576	-3.26879	0.99494
C	-5.59859	-2.70210	2.14206
H	6.23289	-3.75879	1.17430
H	5.02819	-3.32713	-0.07647
H	4.48590	-3.74241	1.60960
H	-6.36665	-3.48862	2.14496
H	-6.03767	-1.77943	2.54488
H	-4.72612	-3.02418	2.72940

Au	-7.17975	-1.09224	-0.37983
Au	7.00150	-0.77984	-0.51003

19_QChem_Model_PBE_C1h-Au1_sim.xyz /// -2108.85135941170

55

C	-1.15861	-0.70795	0.19755
C	-1.55928	0.13637	-0.86356
C	-2.57601	1.08032	-0.71233
C	-3.20226	1.23978	0.54070
C	-2.79866	0.42721	1.61802
C	-1.79344	-0.52922	1.44314
C	0.02492	-1.68494	-0.01808
H	-1.06352	0.04942	-1.83510
H	-2.86894	1.69036	-1.56967
S	-4.54490	2.35932	0.85336
H	-3.27128	0.54305	2.59844
H	-1.50123	-1.14646	2.29591
C	0.24044	-2.63907	1.18855
C	1.22251	-0.72410	-0.23361
C	-0.20183	-2.64172	-1.21997
C	-0.82387	-3.47437	1.59505
C	1.48238	-2.79434	1.83105
C	1.61980	0.12559	0.82579
C	1.88039	-0.57218	-1.46971
C	0.85201	-3.49211	-1.62286
C	-1.44628	-2.78710	-1.85999
C	-0.66218	-4.40084	2.63075
H	-1.78828	-3.40514	1.08199
C	1.64888	-3.73140	2.86388
H	2.33701	-2.18563	1.52559
C	2.65805	1.04545	0.68182
H	1.10861	0.05539	1.79052
C	2.91321	0.35878	-1.63570
H	1.58720	-1.18953	-2.32203
C	0.67876	-4.42189	-2.65372
H	1.81705	-3.43277	-1.10983
C	-1.62465	-3.72756	-2.88774
H	-2.29404	-2.16862	-1.55504
C	0.57801	-4.53274	3.27471
H	-1.50668	-5.03042	2.92767
H	2.62746	-3.83049	3.34373
C	3.31381	1.17244	-0.56017
H	2.96059	1.65403	1.53754
H	3.40767	0.45456	-2.60731

C	-0.56335	-4.54279	-3.29604
H	1.51554	-5.06309	-2.94765
H	-2.60518	-3.81905	-3.36518
H	0.70784	-5.26050	4.08122
S	4.71055	2.23915	-0.82578
H	-0.70231	-5.27333	-4.09852
C	-4.40407	3.58584	-0.49027
C	4.34965	3.67717	0.24532
H	-5.17688	4.33908	-0.28055
H	-4.60757	3.13444	-1.47071
H	-3.40655	4.04833	-0.46143
H	5.15380	4.40089	0.04873
H	4.37504	3.40414	1.30932
H	3.37624	4.10549	-0.03508
Au	6.64032	1.24315	0.64835
Au	-6.73651	1.19955	0.06769

20_QChem_Model_PBE_C1h-Au1_diff.xyz /// -2108.84970336778

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C	0.04504	1.74153	1.71905
C	1.26777	2.04486	2.36111
C	1.34226	2.18977	3.75122
C	0.19427	2.02329	4.54060
C	-1.02015	1.70850	3.92106
C	-1.09417	1.56891	2.52518
C	0.02570	1.61457	0.16883
H	2.17415	2.16069	1.75898
H	2.30320	2.42652	4.21842
H	-1.92273	1.56068	4.52203
H	-2.05317	1.30932	2.07108
C	-1.31092	0.98762	-0.32094
C	1.22239	0.71117	-0.23936
C	0.14032	3.01353	-0.50620
C	-2.48185	1.77836	-0.31139
C	-1.42634	-0.33169	-0.79954
C	1.45957	-0.47923	0.48572
C	2.09696	1.00231	-1.30419
C	-0.12048	3.12571	-1.89162
C	0.48785	4.18402	0.19150
C	-3.71606	1.27956	-0.73842
H	-2.42432	2.81328	0.03792
C	-2.64880	-0.84119	-1.25021
H	-0.54681	-0.97724	-0.84030
C	2.50402	-1.35028	0.16206

H	0.81946	-0.72336	1.33914
C	3.14304	0.13859	-1.64638
H	1.97672	1.92214	-1.88044
C	-0.01360	4.35316	-2.55587
H	-0.42153	2.23527	-2.45240
C	0.58769	5.41834	-0.47186
H	0.67379	4.14198	1.26668
C	-3.80426	-0.03712	-1.22866
H	-4.59619	1.92476	-0.69539
H	-2.70371	-1.86902	-1.62234
C	3.34817	-1.05136	-0.92370
H	2.65229	-2.25034	0.76353
H	3.80633	0.39523	-2.47837
C	0.34394	5.50988	-1.84661
H	-0.21799	4.40614	-3.62979
H	0.85449	6.31273	0.09965
S	-5.30070	-0.78782	-1.83399
S	4.72535	-2.05837	-1.43541
H	0.42288	6.47226	-2.36115
C	4.45807	-3.63531	-0.55596
H	5.25685	-4.30387	-0.90738
H	3.47531	-4.04973	-0.82570
H	4.55585	-3.50694	0.53130
C	-6.51782	0.56742	-1.78384
H	0.25088	2.12917	5.62812
H	-7.45612	0.12563	-2.14783
H	-6.20450	1.38629	-2.44852
H	-6.66710	0.91713	-0.75303
Au	-6.34406	-2.22576	0.12214
Au	6.82210	-1.26471	-0.11134

21_QChem_Model_B3LYP_Os1h_sim.xyz /// -2207.18078397311

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C	-0.07521	1.23229	2.07113
C	0.92079	2.07612	2.63947
C	0.77123	2.47571	3.96958
H	1.53554	3.11041	4.41338
C	-0.33112	2.09593	4.73988
H	-0.40841	2.43130	5.77140
C	-1.33420	1.29499	4.19286
C	-1.18631	0.87744	2.86077
H	-1.96345	0.25405	2.42734
C	2.09948	2.59824	1.84549
H	1.81946	3.48212	1.26058

H	2.48735	1.86130	1.13704
H	2.92041	2.88813	2.50916
C	-2.53787	0.86785	5.00093
H	-2.55436	1.35658	5.97926
H	-2.54108	-0.21552	5.17135
H	-3.47357	1.11369	4.48631
C	1.59607	-0.65745	-0.11985
C	1.88149	-1.32885	-1.34007
C	2.99389	-2.17355	-1.39862
H	3.19655	-2.67380	-2.33945
C	3.83179	-2.39529	-0.29680
S	5.25723	-3.46929	-0.34905
C	3.55237	-1.75590	0.92704
C	2.44328	-0.90570	0.97940
H	2.23011	-0.41844	1.92582
C	1.01491	-1.19170	-2.57431
H	0.00459	-1.57274	-2.39495
H	1.43950	-1.75045	-3.41358
H	0.90987	-0.14892	-2.89059
C	4.41236	-1.96916	2.14836
H	5.45433	-1.68148	1.96190
H	4.42494	-3.02261	2.45423
H	4.04534	-1.37861	2.99183
C	-1.60181	-0.57168	-0.29724
C	-1.89282	-1.81076	0.33404
C	-3.03342	-2.51721	-0.05783
H	-3.24246	-3.45615	0.44339
C	-3.89143	-2.06032	-1.06741
S	-5.35572	-2.93917	-1.58660
C	-3.60005	-0.85147	-1.73134
C	-2.46442	-0.14225	-1.32733
H	-2.24736	0.78737	-1.84526
C	-0.98920	-2.41707	1.38576
H	-0.66252	-1.67672	2.12137
H	-0.08289	-2.83292	0.93262
H	-1.49478	-3.22359	1.92572
C	-4.48054	-0.32548	-2.83795
H	-5.50393	-0.14618	-2.48603
H	-4.55195	-1.03827	-3.66860
H	-4.09112	0.61529	-3.23564
C	0.12488	2.22290	-0.97819
C	-0.84326	3.26449	-0.95202
C	-0.65580	4.36282	-1.79642
H	-1.40127	5.15549	-1.79572
C	0.45651	4.47713	-2.63273
H	0.55880	5.35055	-3.27275

C	1.43916	3.48445	-2.64417
C	1.25044	2.37023	-1.81422
H	2.00905	1.59275	-1.81423
C	-2.03704	3.24264	-0.02284
H	-2.75124	4.02867	-0.28579
H	-1.72998	3.40257	1.01635
H	-2.56679	2.28631	-0.05207
C	2.67765	3.61305	-3.50079
H	3.42840	4.25360	-3.02091
H	2.44805	4.05949	-4.47389
H	3.14505	2.63988	-3.67754
Os	0.00742	0.56058	0.16401
C	-5.43702	-4.36511	-0.45573
C	5.29432	-4.06296	-2.07121
H	-6.34767	-4.90046	-0.73264
H	-5.51647	-4.04642	0.58624
H	-4.58245	-5.03439	-0.58061
H	6.17476	-4.70575	-2.13677
H	5.40483	-3.23758	-2.77834
H	4.40757	-4.65239	-2.31560

22_QChem_Model_B3LYP_Os1h_diff.xyz /// -2207.17995773226

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C	1.56303	-0.70222	0.42200
C	2.89495	-0.26764	0.65686
C	3.86605	-1.21527	0.99263
H	4.87771	-0.85917	1.15804
C	3.57398	-2.57980	1.12624
S	4.79737	-3.80765	1.55379
C	2.25439	-3.02786	0.91945
C	1.28819	-2.07763	0.57398
H	0.27331	-2.43220	0.42024
C	3.30302	1.18936	0.59234
H	2.86927	1.75800	1.42159
H	2.97045	1.67108	-0.33241
H	4.39074	1.29153	0.64812
C	1.87779	-4.48291	1.05746
H	2.07987	-4.85752	2.06843
H	2.44836	-5.11454	0.36532
H	0.81496	-4.62939	0.84930
C	0.31440	1.41905	-1.86787
C	-0.63355	2.29424	-2.47439
C	-0.33123	2.82461	-3.73118
H	-1.04919	3.49361	-4.20089

C	0.85024	2.51395	-4.40961
C	1.77962	1.64056	-3.84503
C	1.48943	1.10613	-2.57997
H	2.20254	0.41318	-2.14242
C	-1.95699	2.64751	-1.83078
H	-2.53185	1.75046	-1.58155
H	-2.56267	3.25853	-2.50639
H	-1.82921	3.21247	-0.90096
C	3.06815	1.28927	-4.55223
H	3.91393	1.86048	-4.14916
H	3.00699	1.50681	-5.62264
H	3.31253	0.22823	-4.43575
C	-1.68233	-0.50271	-0.23844
C	-1.90243	-1.49452	-1.22968
C	-3.13117	-2.16053	-1.26011
H	-3.27230	-2.92241	-2.01938
C	-4.16657	-1.86703	-0.36260
S	-5.74387	-2.70341	-0.37643
C	-3.98043	-0.86078	0.60786
C	-2.74496	-0.20743	0.64113
H	-2.60848	0.57101	1.38513
C	-0.87761	-1.82075	-2.29556
H	0.14732	-1.74244	-1.92363
H	-0.96143	-1.12748	-3.14032
H	-1.01853	-2.83522	-2.68194
C	-5.06809	-0.49580	1.58779
H	-5.34916	-1.35125	2.21444
H	-5.97942	-0.16769	1.07311
H	-4.74389	0.31247	2.24853
C	-0.05332	1.88814	1.43021
C	-0.21403	1.55571	2.80617
C	-0.25005	2.59948	3.73633
H	-0.38163	2.35521	4.78829
C	-0.11981	3.93866	3.36309
H	-0.15746	4.71474	4.12421
C	0.07137	4.28385	2.02386
C	0.10067	3.24621	1.08119
H	0.25622	3.50582	0.03837
C	-0.33654	0.13086	3.30435
H	-0.26745	0.09864	4.39564
H	0.45320	-0.50774	2.89853
H	-1.29226	-0.32483	3.02324
C	0.26713	5.72184	1.60179
H	1.31442	6.03111	1.71114
H	-0.33550	6.40214	2.21211
H	-0.00900	5.87252	0.55406

Os	0.04028	0.53339	-0.06777
C	-5.60512	-3.87524	-1.76335
H	-6.56710	-4.39066	-1.80333
H	-4.81656	-4.61216	-1.59375
H	-5.44092	-3.35886	-2.71198
C	6.32674	-2.84014	1.76472
H	1.03819	2.94801	-5.38878
H	7.09401	-3.56667	2.04029
H	6.22903	-2.10588	2.56763
H	6.62294	-2.34680	0.83613

23_QChem_Model_B3LYP_Si1h_sim.xyz /// -2091.13741268375
53

C	1.53416	0.37403	-0.04326
C	1.55948	1.56386	-0.80020
C	2.69894	2.35714	-0.88378
C	3.87110	1.99091	-0.20114
C	3.86668	0.81861	0.56477
C	2.71495	0.03179	0.63569
Si	-0.00000	-0.72817	0.00001
C	0.04950	-1.83340	1.53700
C	-1.53416	0.37403	0.04328
C	-0.04951	-1.83339	-1.53700
C	0.81116	-3.01854	1.55351
C	-0.63455	-1.48399	2.71595
C	-1.55948	1.56386	0.80022
C	-2.71495	0.03179	-0.63567
C	-0.81117	-3.01853	-1.55351
C	0.63454	-1.48398	-2.71594
C	0.89417	-3.81384	2.69818
C	-0.55699	-2.27663	3.86282
C	-2.69895	2.35714	0.88380
C	-3.86668	0.81861	-0.56475
C	-0.89418	-3.81383	-2.69818
C	0.55698	-2.27662	-3.86281
C	0.20959	-3.44311	3.85700
C	-3.87110	1.99091	0.20116
C	-0.20960	-3.44310	-3.85700
H	0.66762	1.88736	-1.33135
H	2.68183	3.26721	-1.47781
S	5.26821	3.08090	-0.37826
H	4.74925	0.50894	1.11329
H	2.74485	-0.86873	1.24353
H	1.33898	-3.33425	0.65681
H	-1.24215	-0.58328	2.73811

H	-0.66763	1.88736	1.33137
H	-2.74486	-0.86872	-1.24352
H	-1.33899	-3.33425	-0.65681
H	1.24214	-0.58327	-2.73809
H	1.48809	-4.72385	2.68332
H	-1.09814	-1.98547	4.75915
H	-2.68184	3.26720	1.47783
H	-4.74926	0.50895	-1.11328
H	-1.48810	-4.72384	-2.68332
H	1.09814	-1.98546	-4.75914
H	0.26933	-4.06190	4.74824
S	-5.26821	3.08090	0.37828
C	-6.57759	2.26396	-0.58957
H	-7.46035	2.89730	-0.47960
H	-6.80440	1.26968	-0.19786
H	-6.31758	2.20215	-1.64887
C	6.57761	2.26391	0.58951
H	-0.26934	-4.06188	-4.74824
H	7.46035	2.89727	0.47959
H	6.80443	1.26966	0.19772
H	6.31762	2.20200	1.64881

24_QChem_Model_B3LYP_Si1h_diff.xyz /// -2091.13746426853

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C	-0.11304	1.96593	1.55831
C	0.19303	1.42744	2.82389
C	0.07789	2.19242	3.98604
C	-0.34013	3.52244	3.90834
C	-0.63992	4.08062	2.66475
C	-0.52685	3.30972	1.50610
Si	-0.00911	0.89818	-0.00193
C	0.06999	2.00309	-1.53733
C	1.54499	-0.17172	0.10851
C	-1.53990	-0.20451	-0.13326
C	-1.09728	2.58513	-2.07000
C	1.29201	2.30062	-2.16821
C	2.73842	0.32217	0.67439
C	1.57768	-1.48225	-0.39525
C	-1.95252	-0.73814	-1.37178
C	-2.29347	-0.56733	0.99495
C	-1.04605	3.43241	-3.17834
C	1.34898	3.14637	-3.27772
C	3.89718	-0.44555	0.72861
C	2.73208	-2.26622	-0.34815

C	-3.04439	-1.59367	-1.47504
C	-3.39397	-1.42275	0.90810
C	0.17948	3.71513	-3.78464
C	3.90695	-1.75343	0.21555
C	-3.77845	-1.94911	-0.33121
H	0.53998	0.39988	2.90370
H	0.32033	1.75314	4.95010
H	-0.42649	4.12077	4.81129
H	-0.95805	5.11746	2.59558
H	-0.75704	3.76427	0.54635
H	-2.06299	2.36615	-1.62081
H	2.21209	1.86113	-1.79219
H	2.76256	1.32382	1.09646
H	0.68043	-1.91408	-0.83140
H	-1.41733	-0.47354	-2.28047
H	-2.02616	-0.17173	1.97144
H	-1.96153	3.86696	-3.57090
H	2.30549	3.35812	-3.74813
H	4.79829	-0.03465	1.17643
H	2.70071	-3.27281	-0.74972
H	-3.33400	-1.98672	-2.44615
H	-3.94358	-1.66739	1.81016
H	0.22192	4.37151	-4.64960
S	5.44286	-2.64887	0.33800
S	-5.15361	-3.05328	-0.58065
C	5.03904	-4.28941	-0.34262
C	-5.81509	-3.30645	1.09789
H	5.95674	-4.87532	-0.25789
H	4.75411	-4.23054	-1.39567
H	4.25166	-4.77928	0.23499
H	-6.64654	-4.00473	0.98186
H	-6.19256	-2.37567	1.52765
H	-5.06808	-3.75194	1.75895

25_QChem_Model_B3LYP_C1h_sim.xyz /// -1839.70375063244

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C	1.22143	0.00043	-0.14374
C	1.47927	0.93190	0.87531
C	2.52271	1.85052	0.79337
C	3.34417	1.88698	-0.34195
C	3.08281	0.98226	-1.37826
C	2.04289	0.05815	-1.27698
C	0.00001	-0.95122	0.00004
H	0.84110	0.95058	1.75341

H	2.67767	2.53939	1.61565
S	4.70729	3.01345	-0.57247
H	3.69213	0.99906	-2.27793
H	1.87287	-0.61602	-2.10743
C	-0.13937	-1.90460	-1.22230
C	-1.22139	0.00048	0.14375
C	0.13936	-1.90450	1.22245
C	0.89173	-2.82857	-1.47554
C	-1.27170	-1.95537	-2.04331
C	-1.47921	0.93187	-0.87537
C	-2.04285	0.05830	1.27697
C	-0.89176	-2.82843	1.47577
C	1.27168	-1.95522	2.04347
C	0.81000	-3.73783	-2.52639
H	1.76420	-2.84145	-0.82976
C	-1.36175	-2.87566	-3.09385
H	-2.10127	-1.28230	-1.86507
C	-2.52262	1.85054	-0.79350
H	-0.84103	0.95048	-1.75348
C	-3.08275	0.98244	1.37818
H	-1.87285	-0.61582	2.10748
C	-0.81005	-3.73758	2.52671
H	-1.76422	-2.84134	0.82999
C	1.36170	-2.87541	3.09411
H	2.10127	-1.28219	1.86517
C	-0.32140	-3.76529	-3.34666
H	1.62656	-4.43373	-2.69815
H	-2.25620	-2.89168	-3.71063
C	-3.34408	1.88710	0.34181
H	-2.67755	2.53937	-1.61582
H	-3.69210	0.99929	2.27783
C	0.32133	-3.76499	3.34699
H	-1.62663	-4.43345	2.69853
H	2.25615	-2.89139	3.71089
H	-0.39119	-4.47757	-4.16379
S	-4.70713	3.01367	0.57229
H	0.39110	-4.47719	4.16419
C	4.64198	4.07260	0.90810
C	-4.64204	4.07245	-0.90855
H	5.44874	4.79814	0.78446
H	4.81946	3.50097	1.82220
H	3.69212	4.60811	0.97615
H	-5.44884	4.79796	-0.78501
H	-4.81956	3.50057	-1.82248
H	-3.69222	4.60801	-0.97683

26_QChem_Model_B3LYP_C1h_diff.xyz /// -1839.70392246166

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C	-0.13245	-1.49197	1.38318
C	-1.27322	-2.28818	1.60032
C	-1.46619	-2.97404	2.79661
C	-0.52668	-2.87088	3.82582
C	0.59804	-2.07329	3.63552
C	0.79348	-1.39247	2.42829
C	0.01405	-0.75172	0.02070
H	-2.02455	-2.36417	0.82044
H	-2.35679	-3.58271	2.92766
H	1.33393	-1.96916	4.42827
H	1.67626	-0.77417	2.31944
C	1.21035	0.24173	0.04601
C	-1.33118	-0.00532	-0.21336
C	0.30725	-1.75496	-1.13516
C	2.51934	-0.26782	0.04154
C	1.07262	1.63579	0.04458
C	-1.85948	0.78806	0.81870
C	-2.08404	-0.09258	-1.39166
C	0.64780	-1.24539	-2.40268
C	0.28426	-3.14610	-0.98249
C	3.63835	0.56192	0.06024
H	2.67022	-1.34254	0.01619
C	2.18401	2.47822	0.05041
H	0.08758	2.08461	0.02144
C	-3.05994	1.48247	0.68213
H	-1.32642	0.85888	1.76181
C	-3.29143	0.58945	-1.53831
H	-1.74186	-0.70781	-2.21460
C	0.92266	-2.08888	-3.47608
H	0.70606	-0.17072	-2.54462
C	0.56913	-3.99660	-2.05686
H	0.05278	-3.58390	-0.01936
C	3.48282	1.95482	0.06438
H	4.62432	0.11120	0.06334
H	2.03543	3.55455	0.03419
C	-3.79543	1.39185	-0.50696
H	-3.41375	2.08113	1.51380
H	-3.84768	0.49005	-2.46672
C	0.88339	-3.47565	-3.30895
H	1.17627	-1.66144	-4.44234
H	0.54638	-5.07201	-1.90288
S	4.82863	3.12474	0.09209

S	-5.34582	2.21808	-0.80879
H	1.10318	-4.13662	-4.14248
C	-5.66622	3.10923	0.74796
H	-6.62013	3.62012	0.60139
H	-4.89463	3.85559	0.95162
H	-5.75945	2.42254	1.59256
C	6.30654	2.08202	-0.12959
H	-0.67674	-3.39906	4.76313
H	7.14816	2.77570	-0.18511
H	6.25551	1.51137	-1.05984
H	6.46191	1.40945	0.71729

27_QChem_Model_B3LYP_Os1h-Au1_sim.xyz /// -2478.06722984796

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C	0.26142	-2.20372	1.70082
C	-0.65011	-3.21215	2.12007
C	-0.35715	-3.91374	3.29262
H	-1.04748	-4.68590	3.62521
C	0.79766	-3.66510	4.03817
H	0.98510	-4.24019	4.94195
C	1.71697	-2.69675	3.62814
C	1.42983	-1.98241	2.45589
H	2.14134	-1.23853	2.11095
C	-1.87633	-3.59168	1.31852
H	-1.59878	-4.16433	0.42696
H	-2.43766	-2.71864	0.97294
H	-2.55548	-4.20918	1.91344
C	2.96733	-2.40596	4.42500
H	3.31727	-3.29577	4.95683
H	2.78708	-1.62696	5.17642
H	3.77969	-2.05467	3.78168
C	-1.59066	0.05547	0.06447
C	-1.92354	0.99078	-0.95812
C	-3.05214	1.79196	-0.79222
H	-3.30066	2.48277	-1.59015
C	-3.84724	1.74115	0.36420
S	-5.27798	2.75878	0.60560
C	-3.52957	0.83248	1.39713
C	-2.40920	0.01968	1.21675
H	-2.16113	-0.66991	2.01767
C	-1.08257	1.17889	-2.20280
H	-0.12932	1.66312	-1.96531
H	-1.60333	1.80504	-2.93295
H	-0.84251	0.22843	-2.68810

C	-4.37288	0.71825	2.64244
H	-5.41096	0.45635	2.39835
H	-4.40338	1.66304	3.19866
H	-3.97730	-0.05211	3.30890
C	1.57442	0.11298	-0.24411
C	1.89530	1.18908	0.63430
C	3.04031	1.94322	0.37881
H	3.28690	2.73774	1.07557
C	3.86146	1.70736	-0.73527
S	5.36453	2.59567	-1.04277
C	3.53484	0.68052	-1.64620
C	2.39772	-0.08171	-1.37529
H	2.14485	-0.87171	-2.07571
C	1.04083	1.56130	1.82756
H	0.91097	0.72511	2.52216
H	0.04000	1.87615	1.51594
H	1.49303	2.38641	2.38485
C	4.39284	0.37795	-2.84943
H	5.40696	0.08308	-2.54975
H	4.49317	1.25006	-3.50659
H	3.96289	-0.43880	-3.43406
C	-0.09489	-2.46810	-1.51810
C	0.91780	-3.43586	-1.76879
C	0.74592	-4.30098	-2.85406
H	1.52265	-5.03254	-3.06597
C	-0.38718	-4.25765	-3.66770
H	-0.47513	-4.94717	-4.50376
C	-1.41009	-3.34042	-3.41462
C	-1.24233	-2.45650	-2.33947
H	-2.03176	-1.73679	-2.14358
C	2.13774	-3.60182	-0.88754
H	2.93637	-4.12217	-1.42442
H	1.89965	-4.19085	0.00534
H	2.53971	-2.64713	-0.53782
C	-2.66592	-3.31246	-4.25408
H	-3.41309	-4.01979	-3.87292
H	-2.45869	-3.58885	-5.29262
H	-3.12869	-2.32109	-4.25271
Os	0.01926	-1.13955	0.00074
C	5.38078	3.90673	0.22422
C	-5.30159	3.85204	-0.85170
H	6.29576	4.47187	0.03973
H	5.42093	3.48371	1.22824
H	4.51280	4.55831	0.10446
H	-6.16892	4.49892	-0.71102
H	-5.42918	3.28247	-1.77280

H	-4.39277	4.45622	-0.88340
Au	7.39590	1.06159	-0.03516
Au	-7.55828	1.30520	0.06762

28_QChem_Model_B3LYP_Os1h-Au1_diff.xyz /// -2478.06795840824

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C	1.75464	0.59369	-0.49117
C	2.90037	1.42565	-0.66051
C	4.11317	0.83428	-1.00620
H	4.97666	1.47964	-1.12644
C	4.24941	-0.55223	-1.18569
S	5.78827	-1.32266	-1.59613
C	3.14025	-1.40221	-0.97363
C	1.92587	-0.80196	-0.64408
H	1.06792	-1.45213	-0.50164
C	2.86922	2.91853	-0.41546
H	2.86791	3.13825	0.65851
H	1.97780	3.38639	-0.84021
H	3.74575	3.40636	-0.85205
C	3.25055	-2.90222	-1.09152
H	3.96817	-3.30869	-0.36806
H	3.59322	-3.20604	-2.08766
H	2.28405	-3.37699	-0.90520
C	-0.78817	2.69405	-1.19303
C	-1.98843	3.41627	-0.95486
C	-2.41124	4.32969	-1.92692
H	-3.32594	4.89161	-1.75084
C	-1.70757	4.53148	-3.11435
C	-0.53730	3.81381	-3.37805
C	-0.09943	2.90516	-2.40597
H	0.81203	2.34546	-2.59705
C	-2.84960	3.20418	0.27149
H	-3.42123	2.27229	0.19529
H	-3.56754	4.02129	0.38741
H	-2.26003	3.14547	1.19051
C	0.24557	4.02954	-4.65243
H	0.78760	4.98308	-4.63100
H	-0.41283	4.05406	-5.52721
H	0.98196	3.23565	-4.80679
C	-1.47663	-0.11732	-0.00962
C	-1.79501	-0.89120	-1.16295
C	-2.84090	-1.80899	-1.08734
H	-3.06963	-2.39098	-1.97369
C	-3.60094	-1.98420	0.08039

S	-4.95115	-3.11877	0.20287
C	-3.33810	-1.18920	1.22024
C	-2.27901	-0.28716	1.14406
H	-2.06118	0.30823	2.02622
C	-1.09162	-0.70167	-2.48877
H	-0.01771	-0.54978	-2.36357
H	-1.48309	0.18004	-3.00879
H	-1.23829	-1.56653	-3.14242
C	-4.17806	-1.29507	2.46774
H	-4.15518	-2.30710	2.88946
H	-5.22894	-1.05949	2.25339
H	-3.82560	-0.60171	3.23513
C	0.33962	1.92985	1.93349
C	0.73539	1.07771	3.00108
C	0.99337	1.65946	4.24553
H	1.28382	1.01526	5.07238
C	0.89333	3.03604	4.45774
H	1.09843	3.44340	5.44477
C	0.53321	3.89224	3.41508
C	0.25730	3.31785	2.16553
H	-0.03511	3.97568	1.35093
C	0.93149	-0.41230	2.83084
H	0.96131	-0.91582	3.80164
H	1.87584	-0.62750	2.31814
H	0.13452	-0.86988	2.23842
C	0.45375	5.38816	3.61276
H	1.36884	5.88443	3.26593
H	0.32446	5.64408	4.66845
H	-0.38083	5.82407	3.05442
Os	-0.04706	1.28409	0.05859
C	-4.89610	-4.05819	-1.35924
H	-5.70954	-4.78177	-1.28664
H	-3.94150	-4.58063	-1.44820
H	-5.07240	-3.41052	-2.21844
C	6.83346	0.05321	-2.18135
H	-2.07726	5.25150	-3.84079
H	7.76021	-0.41467	-2.51759
H	7.06348	0.75181	-1.37685
H	6.34598	0.55992	-3.01667
Au	7.22245	-1.85794	0.68442
Au	-7.28750	-1.74671	-0.24549

29_QChem_Model_B3LYP_Si1h-Au1_sim.xyz /// -2362.01801287426

C	1.49798	-0.60254	0.51529
C	1.68890	0.60312	-0.18983
C	2.74463	1.46118	0.09837
C	3.65542	1.13364	1.11483
C	3.49201	-0.05781	1.83023
C	2.42145	-0.90252	1.53087
Si	0.08068	-1.78460	0.08539
C	-0.32311	-2.87399	1.57709
C	-1.42862	-0.73822	-0.38476
C	0.57167	-2.87926	-1.37731
C	0.41342	-4.04663	1.83436
C	-1.33744	-2.52482	2.48734
C	-1.71599	0.47383	0.27545
C	-2.31279	-1.13905	-1.40040
C	-0.09085	-4.09820	-1.62197
C	1.57476	-2.48641	-2.28210
C	0.15441	-4.83202	2.95929
C	-1.60193	-3.30794	3.61216
C	-2.82175	1.24734	-0.06161
C	-3.43356	-0.38291	-1.74642
C	0.22755	-4.88561	-2.73005
C	1.89852	-3.27148	-3.39015
C	-0.85446	-4.46259	3.85088
C	-3.68589	0.82346	-1.08329
C	1.22314	-4.47183	-3.61721
H	0.99498	0.88594	-0.97703
H	2.86883	2.38071	-0.46660
S	4.95239	2.31897	1.41678
H	4.17974	-0.33401	2.62151
H	2.30836	-1.81460	2.11096
H	1.18962	-4.35847	1.13975
H	-1.93451	-1.63330	2.31384
H	-1.05337	0.83578	1.05720
H	-2.12443	-2.06134	-1.94315
H	-0.85661	-4.44502	-0.93215
H	2.11511	-1.55816	-2.11677
H	0.73465	-5.73373	3.13607
H	-2.39311	-3.01933	4.29870
H	-3.01181	2.18183	0.45893
H	-4.08889	-0.73794	-2.53358
H	-0.29637	-5.82285	-2.89749
H	2.67942	-2.94787	-4.07287
H	-1.06062	-5.07465	4.72471
S	-5.05688	1.90281	-1.44847
C	-5.82990	1.14940	-2.91860
H	-6.66233	1.80526	-3.17840

H	-6.21557	0.15437	-2.69472
H	-5.11251	1.11878	-3.74113
C	6.05106	1.48240	2.60823
H	1.47533	-5.08489	-4.47815
H	6.90231	2.15291	2.73712
H	6.40151	0.52898	2.21080
H	5.54343	1.34716	3.56538
Au	-6.97152	1.45290	0.34179
Au	6.54409	2.26917	-0.80601

30_QChem_Model_B3LYP_Si1h-Au1_diff.xyz /// -2362.01893203589

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C	-0.12956	3.12585	1.30131
C	0.12610	2.98657	2.68031
C	-0.00364	4.06626	3.55519
C	-0.38746	5.31720	3.06720
C	-0.63964	5.48050	1.70439
C	-0.51124	4.39636	0.83362
Si	0.00021	1.64559	0.13262
C	0.05120	2.21983	-1.66558
C	1.58235	0.68725	0.54688
C	-1.49453	0.50769	0.37231
C	-1.13271	2.54198	-2.35800
C	1.27168	2.37380	-2.34868
C	2.73315	1.34731	1.02312
C	1.67047	-0.70507	0.37026
C	-1.85956	-0.43751	-0.60924
C	-2.27160	0.54468	1.54269
C	-1.09833	3.00608	-3.67416
C	1.31089	2.83570	-3.66541
C	3.90884	0.65832	1.30463
C	2.84302	-1.41154	0.63512
C	-2.93066	-1.30603	-0.42792
C	-3.35449	-0.31263	1.73967
C	0.12533	3.15407	-4.33008
C	3.96933	-0.73075	1.11343
C	-3.68569	-1.25033	0.75485
H	0.44009	2.02384	3.07770
H	0.19958	3.93326	4.61442
H	-0.48550	6.16029	3.74549
H	-0.93375	6.45256	1.31806
H	-0.70581	4.54218	-0.22543
H	-2.09601	2.42113	-1.86819
H	2.20440	2.12451	-1.84967

H	2.71004	2.42025	1.19279
H	0.80479	-1.26128	0.02142
H	-1.30710	-0.48845	-1.54410
H	-2.04098	1.26696	2.32087
H	-2.02527	3.24616	-4.18774
H	2.26563	2.94293	-4.17286
H	4.77777	1.19394	1.67678
H	2.86592	-2.48285	0.47175
H	-3.19309	-2.01589	-1.20779
H	-3.92918	-0.23619	2.65508
H	0.15430	3.51142	-5.35577
S	5.52697	-1.50967	1.48569
S	-5.04660	-2.39334	0.87291
C	5.12502	-3.28779	1.55463
C	-5.74036	-2.08917	2.53088
H	6.05260	-3.78435	1.84495
H	4.81186	-3.66492	0.58080
H	4.35646	-3.46416	2.30979
H	-6.58393	-2.77528	2.62186
H	-6.10338	-1.06485	2.62043
H	-4.99750	-2.31458	3.29874
Au	-7.05494	-1.31180	-0.62386
Au	7.05986	-1.51303	-0.75045

31_QChem_Model_B3LYP_C1h-Au1_sim.xyz /// -2110.58746744725

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C	-1.28459	-0.62797	0.25867
C	-1.69851	0.17788	-0.81921
C	-2.75800	1.06845	-0.70549
C	-3.42400	1.21068	0.52115
C	-3.00928	0.44012	1.61290
C	-1.95418	-0.46222	1.47882
C	-0.04471	-1.54471	0.08938
H	-1.18885	0.09805	-1.77368
H	-3.06568	1.64157	-1.57328
S	-4.84254	2.25978	0.74979
H	-3.50696	0.54587	2.57245
H	-1.65561	-1.04121	2.34435
C	0.13911	-2.53637	1.27172
C	1.11534	-0.52160	-0.02758
C	-0.14924	-2.47050	-1.15490
C	-0.93076	-3.37364	1.63492
C	1.36704	-2.73304	1.91669
C	1.50378	0.22679	1.09703

C	1.72876	-0.20519	-1.24988
C	0.98736	-3.18719	-1.56913
C	-1.35732	-2.72353	-1.81713
C	-0.79011	-4.33830	2.62963
H	-1.88441	-3.27707	1.12535
C	1.51291	-3.70591	2.91051
H	2.22737	-2.13220	1.64630
C	2.49928	1.19670	1.02976
H	1.02455	0.04418	2.05325
C	2.70966	0.77777	-1.33859
H	1.44859	-0.73639	-2.15162
C	0.92694	-4.09041	-2.62738
H	1.93084	-3.04258	-1.05216
C	-1.42223	-3.63640	-2.87457
H	-2.26387	-2.21278	-1.51369
C	0.43547	-4.50755	3.27855
H	-1.63808	-4.96521	2.89065
H	2.47857	-3.83280	3.39192
C	3.11667	1.48024	-0.19620
H	2.78069	1.72410	1.93388
H	3.17125	0.98680	-2.29957
C	-0.28150	-4.31834	-3.29043
H	1.82453	-4.62345	-2.92787
H	-2.37390	-3.81020	-3.36892
H	0.54847	-5.26099	4.05254
S	4.44845	2.63613	-0.41429
H	-0.33198	-5.02465	-4.11391
C	-4.48555	3.68975	-0.33317
C	4.57821	3.47199	1.20027
H	-5.27992	4.41295	-0.13968
H	-4.51436	3.40910	-1.38620
H	-3.51721	4.11675	-0.06557
H	5.38086	4.20219	1.08593
H	4.84982	2.76467	1.98434
H	3.64282	3.98422	1.43477
Au	6.70616	1.12058	-0.27534
Au	-6.81047	1.18375	-0.76841

32_QChem_Model_B3LYP_C1h-Au1_diff.xyz /// -2110.58604061701

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C	-0.14473	1.72743	1.72705
C	1.04740	2.11481	2.36788
C	1.10782	2.28219	3.74931
C	-0.02524	2.05578	4.53485

C	-1.20926	1.66078	3.91824
C	-1.26849	1.49794	2.52972
C	-0.14422	1.56359	0.17832
H	1.94160	2.27949	1.77488
H	2.04365	2.58278	4.21194
H	-2.09784	1.46845	4.51296
H	-2.20314	1.17780	2.08614
C	-1.44943	0.86364	-0.30135
C	1.10055	0.70521	-0.18871
C	-0.08970	2.94997	-0.53091
C	-2.65043	1.59754	-0.32083
C	-1.50797	-0.46874	-0.72805
C	1.37164	-0.45771	0.55624
C	1.98998	1.01897	-1.22535
C	-0.31995	3.01340	-1.91867
C	0.16585	4.15234	0.13886
C	-3.85610	1.02725	-0.71401
H	-2.64330	2.63757	-0.01188
C	-2.70638	-1.04934	-1.14514
H	-0.60972	-1.07181	-0.75963
C	2.46337	-1.27586	0.28133
H	0.72370	-0.72338	1.38540
C	3.08478	0.20655	-1.51722
H	1.84710	1.91171	-1.82091
C	-0.27303	4.22218	-2.60920
H	-0.54627	2.10157	-2.46285
C	0.20570	5.36907	-0.55093
H	0.32770	4.15458	1.20937
C	-3.89213	-0.30802	-1.13969
H	-4.75953	1.62615	-0.68172
H	-2.71243	-2.08082	-1.48523
C	3.32891	-0.95131	-0.77078
H	2.63400	-2.15092	0.89828
H	3.75252	0.48179	-2.32856
C	-0.00801	5.41152	-1.92603
H	-0.45117	4.23510	-3.68090
H	0.40180	6.28488	-0.00034
S	-5.38452	-1.15702	-1.61697
S	4.78607	-1.88419	-1.19788
H	0.02346	6.35682	-2.45996
C	4.53212	-3.49395	-0.37717
H	5.37134	-4.11659	-0.69163
H	3.59391	-3.93829	-0.71580
H	4.55038	-3.39700	0.70867
C	-6.43550	0.17664	-2.29064
H	0.02002	2.17896	5.61302

H	-7.31963	-0.32082	-2.69326
H	-5.90298	0.69623	-3.08953
H	-6.74629	0.87016	-1.50953
Au	6.78304	-0.90185	0.35532
Au	-6.79202	-1.60630	0.69674

33_FHI-aims_Molecule_Os1.xyz /// -566287.731908578 eV

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xyz file created automatically from geometry.in.

Os	8.90975420	8.86077436	8.56934924
C	7.03086100	7.92364283	10.74702191
C	8.84597024	7.27613581	7.34479036
C	7.73200946	6.41123824	7.44427556
H	6.94039109	6.64745851	8.15905904
C	7.56889268	5.26577797	6.64929289
C	8.59195718	4.96055776	5.72656461
C	9.68632705	5.83546884	5.58868727
H	10.44998431	5.58957003	4.84644459
C	10.99292307	7.92402418	6.06857961
H	11.51356934	8.23719371	6.98476558
H	10.64502267	8.84350657	5.57425630
H	11.72603600	7.44058887	5.40877777
C	9.83254242	6.99808749	6.35046828
C	6.32583922	4.42676134	6.79587272
H	5.48990386	5.03389022	7.16786258
H	6.47353224	3.60252909	7.51209753
H	6.04423943	3.97919630	5.83205134
C	4.30799758	11.29189489	10.23261743
H	4.68607069	11.97772574	9.46385355
H	3.29937341	10.96369085	9.93375559
H	4.19281883	11.85707671	11.17134895
H	14.49367579	6.73925900	9.97419776
H	13.59999466	5.80648322	11.18268935
C	10.73039685	9.72684757	10.82040988
C	10.49293073	8.76895148	9.79087523
C	11.40271103	7.69420023	9.66049981
H	11.21451846	6.92691550	8.90599786
C	12.54564391	7.55302924	10.45514006
C	12.79019603	8.53670408	11.44146742
C	11.87724833	9.59202463	11.60965013
H	12.04905783	10.34004919	12.38501430

C	9.76981475	10.85461615	11.12101342
H	9.45158919	11.38572868	10.21256322
C	13.48623689	6.39322533	10.25687006
H	8.85642872	10.47236053	11.60052367
H	10.22727058	11.58903810	11.79800203
C	5.23581457	10.11873671	10.41045649
C	9.04976295	10.47060017	7.38646824
C	10.15867583	11.33311156	7.55595234
H	10.90566734	11.09620867	8.31646612
C	10.36198311	12.48402474	6.78755666
C	9.40503022	12.79186368	5.79272911
C	8.31119113	11.93182686	5.59172553
H	7.58210238	12.15412685	4.81105947
C	6.95772563	9.86527656	6.01211244
H	6.38422736	9.56866817	6.90215293
H	7.31421260	8.93666538	5.54171744
H	6.26619029	10.35578432	5.31359131
C	8.11731173	10.77312322	6.35144896
C	11.56247057	13.36341070	7.02136394
H	12.20313641	12.94819184	7.80979642
H	11.26259049	14.38020192	7.32259402
H	12.16699346	13.46835825	6.10624193
C	4.96720937	9.10878167	11.36355696
C	5.86863868	8.04141586	11.51619951
H	5.67549284	7.26934533	12.26249317
C	7.97779045	6.77994694	11.03109794
H	8.31011051	6.27571290	10.11241229
H	8.88410657	7.14019784	11.54028006
H	7.50187659	6.02799660	11.67538907
H	13.12134115	5.72300124	9.46814927
C	7.29655472	8.91263650	9.75488622
C	6.39373731	9.99459449	9.63447078
H	6.60248389	10.78390395	8.90848225
S	8.52126616	3.55887217	4.62351283
S	14.26171956	8.34890231	12.40941443
S	3.48347615	9.28245218	12.31539656
S	9.67936661	14.26891810	4.85521460
C	3.50238572	7.83925704	13.41052625
H	2.59066860	7.92773760	14.01428441
H	3.46426452	6.89995192	12.84411407
H	4.37334770	7.84969527	14.07843780
C	8.29255461	14.30604609	3.68950326
H	8.44413428	15.21587382	3.09566811
H	8.30514220	13.43735539	3.01901864
H	7.32834953	14.37662091	4.20874261
C	8.65058437	2.14339324	5.77013566

H	8.72618557	1.25246851	5.13308576
H	9.55612224	2.22741251	6.38279215
H	7.76553818	2.04776803	6.41051383
C	14.22837685	9.77537816	13.52623487
H	15.14732032	9.69317429	14.12016366
H	14.24766989	10.72238795	12.97178012
H	13.36363947	9.74309793	14.20131251

34_FHI-aims_Molecule_Os2.xyz /// -591429.938924243 eV

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xyz file created automatically from geometry.in.

Os	8.90149632	8.84413334	8.70333636
C	6.93360248	8.00455442	10.86099975
C	8.91109137	7.26431644	7.47424884
C	7.84863715	6.33797132	7.52866391
H	7.01254614	6.53304118	8.20482321
C	7.79284658	5.17946019	6.73620211
C	8.85908566	4.93090215	5.84111502
C	9.89503346	5.88507657	5.75006652
H	10.71292501	5.69096123	5.05036955
C	11.07153191	8.03428169	6.28808547
H	11.53797442	8.37058559	7.22510411
H	10.69965090	8.93604320	5.77880287
H	11.85687249	7.58998125	5.66162342
C	9.94960723	7.04783492	6.51884687
C	6.58098750	4.28266412	6.84642150
H	5.70084350	4.86829804	7.14504790
H	6.71785221	3.49708382	7.60647776
H	6.35809870	3.78041066	5.89612834
C	4.39156490	11.48511789	10.12273968
H	4.51463049	11.77807732	9.07141573
H	3.32860356	11.28001476	10.30607999
H	4.66361343	12.35934658	10.73509551
H	14.34051948	6.37023175	10.63330595
H	12.98861192	5.27971315	10.97351038
C	10.68496539	9.61490333	11.04356779
C	10.44249281	8.70076302	9.97514925
C	11.30697640	7.59308387	9.83451098
H	11.12685066	6.87935354	9.02817284
C	12.40519740	7.35656856	10.67527923
C	12.65286275	8.27327868	11.72234299
C	11.78708594	9.37809415	11.86786620
H	11.97034337	10.06925480	12.69559057
C	9.76989640	10.77745994	11.34852780
H	9.50843986	11.35252162	10.44877905

C	13.28982026	6.16417560	10.39015693
H	8.82219951	10.42543938	11.78345850
H	10.23791186	11.46400185	12.06702152
C	5.25470974	10.28425919	10.43713508
C	9.00098259	10.46231670	7.52840560
C	10.02748746	11.40861898	7.72939701
H	10.78153213	11.21496638	8.49614016
C	10.15005551	12.58739819	6.97498798
C	9.20333836	12.82569946	5.95268626
C	8.20159315	11.85856678	5.72497696
H	7.47271610	12.05085789	4.93255020
C	6.98901333	9.69626304	6.10256382
H	6.42259731	9.34945487	6.97899771
H	7.41774460	8.80097506	5.62838750
H	6.27587727	10.14572013	5.39811405
C	8.07249700	10.68491921	6.46780077
C	11.30425736	13.52012506	7.26227748
C	4.94076423	9.35002519	11.45007519
C	5.78352649	8.23125323	11.61985566
H	5.54212193	7.52200070	12.41682018
C	7.81273374	6.82016861	11.18795134
H	8.11470683	6.26371984	10.28900747
H	8.73939945	7.14462320	11.68485700
H	7.29335171	6.12399114	11.86028200
H	13.22492596	5.88686596	9.32942433
C	7.25536379	8.94769374	9.83970042
C	6.40360485	10.06006758	9.66279950
H	6.63848337	10.78949014	8.88492554
C	8.94009312	3.72442759	4.98003456
C	9.25769877	3.83811938	3.61458913
C	9.39199054	2.71709109	2.79299065
C	9.21690734	1.42945185	3.32314672
C	8.90073408	1.29877950	4.69003341
C	8.76333792	2.42385571	5.49599321
H	8.77535574	0.30368172	5.12213671
H	8.54727706	2.29028035	6.55676398
H	9.62703548	2.85881704	1.73868740
H	9.38512916	4.83086579	3.17824396
S	9.35565419	-0.07176727	2.39742800
C	9.90417628	0.48352716	0.76226448
H	10.03532195	-0.43481375	0.17686960
H	10.86524440	1.01029306	0.82000457
H	9.14970982	1.11149550	0.27151134
C	3.76730105	9.49783535	12.34854653
C	2.86315970	8.43247949	12.53903625
C	1.77907927	8.54646756	13.40399296

C	1.56140969	9.73751596	14.12472605
C	3.53772427	10.67883622	13.07514928
C	2.45830050	10.80353964	13.95215922
H	2.32975239	11.73481875	14.50285564
H	3.00637354	7.50464949	11.98159347
H	4.23345892	11.51350276	12.97663962
H	1.08824983	7.70917284	13.52188368
S	0.15429395	9.76823650	15.19684385
C	0.22991100	11.41426423	15.95066927
H	-0.63151581	11.45989889	16.62830303
H	0.13208075	12.20761193	15.19848899
H	1.14938427	11.54931140	16.53459999
C	13.78682245	8.12874630	12.67022781
C	14.02728820	6.93205272	13.36717644
C	14.64870481	9.21478229	12.92975988
C	15.70415437	9.10583209	13.82949639
C	15.93491312	7.89817892	14.51769102
C	15.07895692	6.81145677	14.27816012
H	15.21866939	5.86639235	14.80217009
H	13.36232201	6.08045685	13.21746163
H	14.49698290	10.15504921	12.39610804
H	16.36400143	9.95913781	13.99913617
S	17.30599497	7.87610449	15.63555735
C	17.27431988	6.19817768	16.31844855
H	18.11934206	6.15590585	17.01667462
H	17.42175576	5.44216176	15.53637069
H	16.34606440	6.00428038	16.87100122
C	9.21642761	14.03061132	5.08474879
C	9.12725253	13.89933614	3.68736731
C	9.07724102	15.01209985	2.84536388
C	9.10702003	16.30729675	3.38562290
C	9.19839335	16.45536720	4.78402302
C	9.25574015	15.33808142	5.61146044
H	9.11091696	12.90038249	3.24648213
H	9.01779787	14.85847734	1.76863224
H	9.21034221	17.45558251	5.22201850
H	9.29712333	15.48209481	6.69205243
S	9.02990542	17.79643342	2.43320388
C	8.90380599	17.20121349	0.72682678
H	8.84147472	18.10636184	0.11033618
H	7.99686477	16.60283413	0.57338668
H	9.79510312	16.63246105	0.43288923
H	11.65822814	14.02207176	6.35204883
H	12.14337833	12.96520709	7.70303658
H	11.02506893	14.30778599	7.97997102

35_FHI-aims_Molecule_Os3.xyz /// -616572.512776929 eV

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xyz file created automatically from geometry.in.

Os	8.91682219	8.74315871	8.55649843
C	7.05132307	7.92221336	10.80676794
C	8.91304582	7.13697996	7.36337473
C	7.92344858	6.14922006	7.54801160
H	7.13172449	6.32392680	8.28011760
C	7.88848081	4.94738751	6.82191067
C	8.88488231	4.73177060	5.84307135
C	9.83580363	5.74882984	5.61361633
H	10.59584067	5.57826753	4.84568736
C	10.91741907	7.98546120	5.97916504
H	11.46360766	8.35093362	6.86123410
H	10.45021676	8.86514146	5.51216663
H	11.65350259	7.57667050	5.27380533
C	9.88011312	6.94428182	6.33157925
C	6.77071681	3.96655256	7.09324447
H	5.88414905	4.49433941	7.46979560
H	7.05398628	3.22461085	7.85648594
H	6.48793189	3.41069606	6.18982814
C	4.36168928	11.27893690	10.01634400
H	4.41018468	11.50610159	8.94282226
H	3.31784447	11.06550563	10.28037298
H	4.65238912	12.19581620	10.55283437
H	14.58603480	6.59644352	10.24112663
H	13.31908773	5.40501878	10.57167146
C	10.71674158	9.55488405	10.85743178
C	10.50404350	8.65158500	9.77300560
C	11.44315423	7.61742833	9.56941535
H	11.28404373	6.91028280	8.75278094
C	12.58864602	7.44473458	10.36243212
C	12.80661480	8.35262810	11.42370110
C	11.86475368	9.38262576	11.63202765
H	12.02701328	10.06474636	12.47123873
C	9.73330491	10.63976410	11.23043876
H	9.39093991	11.21601672	10.35912218
C	13.54605432	6.32760605	10.01451299
H	8.83396581	10.21141645	11.69746231
H	10.18404300	11.34154400	11.94541248
C	5.27363011	10.11949280	10.34740963
C	8.97126532	10.38335373	7.41055836
C	9.96131545	11.35682944	7.65836614
H	10.72273052	11.15689520	8.41556844
C	10.03198578	12.57615183	6.96526873

C	9.07585757	12.82463785	5.95501893
C	8.12376793	11.82518266	5.66446841
H	7.39570540	12.02272982	4.87231320
C	7.00612565	9.59238015	5.94251971
H	6.42253396	9.22016840	6.79773163
H	7.47847117	8.71412594	5.47812137
H	6.30179804	10.02255353	5.21766015
C	8.04234064	10.61296235	6.35193977
C	11.14362004	13.54284474	7.30311070
C	5.03524953	9.22384230	11.41438442
C	5.92266778	8.14270827	11.59867238
H	5.73897701	7.46392772	12.43639504
C	7.98863884	6.79035221	11.15885959
H	8.29944068	6.21175810	10.27742259
H	8.90926416	7.17335757	11.62435026
H	7.51355931	6.09915621	11.86820537
H	13.47417879	6.08350758	8.94607051
C	7.29890134	8.82904686	9.73287745
C	6.39796885	9.89804159	9.53749006
H	6.57751040	10.60123872	8.72180770
C	8.97348762	3.48868750	5.03455911
C	9.09100249	3.54811980	3.63218897
C	9.21159461	2.38921345	2.86673719
C	9.22934904	1.11550356	3.46834604
C	9.12429632	1.05788123	4.87209218
C	8.99429249	2.21582755	5.63582813
H	9.18205871	0.09093227	5.37526378
H	8.94936656	2.13610201	6.72306744
H	9.25752120	2.47086087	1.77916794
H	9.05650742	4.51974209	3.13519613
C	3.90041707	9.38022135	12.35959650
C	3.05070337	8.29756545	12.65720124
C	2.00141197	8.43014959	13.56561007
C	3.65948651	10.59876369	13.02208320
C	2.61453064	10.73041337	13.93340118
H	2.44340836	11.69575340	14.41338420
H	3.21294112	7.34022546	12.15772695
H	4.31197201	11.45182462	12.83100836
H	1.37230583	7.56547006	13.78562806
C	13.98198598	8.28451882	12.32899105
C	14.36088380	7.09428277	12.97903613
C	14.73552893	9.44285818	12.60246922
C	15.81744354	9.41250457	13.47962891
C	16.19660477	8.22181283	14.12957772
C	15.44148348	7.06380193	13.85894732
H	15.71673069	6.11936584	14.33181159

H	13.78798296	6.18206225	12.80770857
H	14.46788409	10.38002077	12.11028741
H	16.36418586	10.33459503	13.68527390
C	9.04098157	14.08873791	5.17473134
C	9.04457150	14.06819157	3.76704025
C	8.99672190	15.24863872	3.02645287
C	8.93244526	16.50487234	3.66052920
C	8.90934264	16.52274626	5.06918214
C	8.96731565	15.34342119	5.80834437
H	9.12034126	13.10989844	3.24926015
H	9.04762460	15.19764052	1.93732380
H	8.81082514	17.47565841	5.59222344
H	8.91941826	15.39141393	6.89744548
H	11.46929301	14.11265300	6.42317889
H	12.00916160	13.00213843	7.70920235
H	10.83133488	14.27415600	8.06532040
C	17.34087465	8.19425980	15.06765165
C	17.32294570	7.38473008	16.22270132
C	18.38912831	7.36943274	17.11441355
C	19.52837141	8.16599437	16.88313733
C	19.56454592	8.97092883	15.73340236
C	18.48567617	8.98074620	14.84803260
H	16.44107073	6.78031022	16.44312646
H	18.33850452	6.74535246	18.00910319
H	20.43498187	9.58786656	15.51305329
H	18.54998843	9.59646403	13.94897610
C	0.64546045	9.80126828	15.18848509
C	-0.59502836	9.16154056	14.98443508
C	-1.64738566	9.32087249	15.87912291
C	-1.49832334	10.12720962	17.02544117
C	-0.26568754	10.76197801	17.24703313
C	0.78135805	10.59835227	16.33896079
C	1.75834141	9.65070870	14.22481004
H	-0.74817528	8.55682649	14.08874031
H	-2.60345500	8.83109346	15.68422277
H	-0.10779741	11.37939583	18.13060572
H	1.73728408	11.08226758	16.54680056
C	8.89769706	17.76318053	2.88204721
C	8.22610189	17.84861804	1.64442898
C	8.19477465	19.03359694	0.91742085
C	8.84077404	20.18906565	1.40127461
C	9.51520583	20.11886363	2.63066918
C	9.53784123	18.92416092	3.35140017
H	7.69312674	16.97767923	1.25876535
H	7.65557439	19.07404972	-0.03129621
H	10.03673670	20.98779719	3.03046534

H	10.09372961	18.88852548	4.29005849
C	9.35148354	-0.11782845	2.65962539
C	8.68447496	-1.29977002	3.02735670
C	8.78953814	-2.46895366	2.27244525
C	9.57966372	-2.49218588	1.11219398
C	10.25570332	-1.31549569	0.73231090
C	10.14022028	-0.15644659	1.49091395
H	8.04141425	-1.30120969	3.90929975
H	8.24198403	-3.35526120	2.59127256
H	10.88919597	-1.31957531	-0.15713549
H	10.69877260	0.73082224	1.18769394
S	9.79842198	-3.90053891	0.06616025
C	8.85790817	-5.20538025	0.89982608
H	8.99698783	-6.09935755	0.27955801
H	7.78750495	-4.96769938	0.94435982
H	9.25051079	-5.40502787	1.90498172
S	20.81944943	8.06534596	18.08708018
C	22.04884461	9.25868287	17.49838466
H	22.84918388	9.23890084	18.24828380
H	21.63290436	10.27305000	17.44837111
H	22.46551095	8.96495318	16.52669679
S	8.74044500	21.63510680	0.38877667
C	9.59585307	22.89897116	1.36542506
H	9.52704684	23.81740720	0.76955944
H	10.65466605	22.65056204	1.51362932
H	9.09997318	23.06306612	2.33052253
S	-2.90431886	10.25552994	18.09010081
C	-2.37570406	11.44166327	19.35365298
H	-3.24651287	11.57097649	20.00793091
H	-2.11635432	12.41114262	18.90968305
H	-1.53915570	11.05476438	19.94923253

36_FHI-aims_Molecule_Si1.xyz /// -80899.498231165 eV

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Si	9.10870003	8.88775035	8.53925315
C	7.48899895	8.11611843	10.78069387
C	8.99803911	7.34838133	7.44386935
C	8.09190603	6.31116458	7.72846754
H	7.42905183	6.39436984	8.59280256
C	7.99284525	5.17135965	6.92572013
C	8.81219627	5.03606309	5.79443806
C	9.72762267	6.06408932	5.48914041
H	10.36441757	5.97524067	4.60603071
C	9.81159397	7.19402741	6.29887550

C	10.64587040	9.56841279	10.86377741
C	10.62885967	8.83144447	9.66433320
C	11.78625146	8.08824412	9.35234646
H	11.81741186	7.48620686	8.44084023
C	12.89914903	8.08315592	10.18955383
C	12.89590476	8.82855592	11.38556031
C	11.75360038	9.57478895	11.71548297
H	11.71384488	10.15719733	12.63568077
C	5.35720344	9.81193619	10.20961591
C	9.17932139	10.40870992	7.41849572
C	9.95519849	11.54189114	7.74090243
H	10.57442351	11.53680818	8.64133404
C	9.96719428	12.67433761	6.93108414
C	9.19473768	12.71648412	5.75346768
C	8.41957593	11.59696902	5.41089830
H	7.81680262	11.59287984	4.50297342
C	8.42055247	10.46767588	6.23434775
C	5.27566078	8.94945095	11.32071286
C	6.35853980	8.10040734	11.60172065
H	6.33238977	7.42719008	12.45825041
C	7.58521619	8.96128042	9.65849417
C	6.49069038	9.81143563	9.39921183
H	6.52650865	10.49554568	8.54773438
S	8.77684072	3.65503757	4.69103437
S	14.35796541	8.74441893	12.37670657
S	3.79021258	9.02628121	12.27733035
S	9.28621263	14.20433083	4.80310576
C	4.04518099	7.77378440	13.56100804
H	3.12822770	7.78884660	14.16296370
H	4.16945672	6.77310062	13.12770325
H	4.89766752	8.02206700	14.20589139
C	8.21077869	13.87237919	3.38324022
H	8.25456441	14.78246325	2.77220858
H	8.57860215	13.02669453	2.78856459
H	7.17211167	13.70262228	3.69371075
C	7.48738923	2.58766611	5.38601393
H	7.44042211	1.72066871	4.71559714
H	7.74931252	2.24338161	6.39454116
H	6.51031958	3.08721364	5.39126641
C	13.95203852	9.75803100	13.82275109
H	14.84655353	9.72257023	14.45700993
H	13.75654566	10.80101722	13.54315470
H	13.10317491	9.34216583	14.38052491
H	8.32062136	7.45290146	11.03437303
H	4.52623945	10.48388125	9.98359635
H	13.77820707	7.49168865	9.92386574

H	10.51557250	7.98247121	6.01908860
H	7.26935663	4.39931887	7.18616295
H	7.81762742	9.60716518	5.93214323
H	10.58278536	13.53413066	7.20503160
H	9.76538816	10.14579865	11.15792907

37_FHI-aims_Molecule_Si2.xyz /// -106041.994090932 eV

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Si	8.91100222	8.81544315	8.74028177
C	7.12014286	8.03943904	10.85642269
C	8.86817166	7.30870601	7.59531167
C	7.94051178	6.25729671	7.71457056
H	7.16439447	6.30300653	8.48259234
C	7.97241460	5.15893234	6.85164598
C	8.94011425	5.06212980	5.83300037
C	9.86937158	6.11404607	5.70897265
H	10.64783531	6.05700328	4.94566162
C	9.82774505	7.21210943	6.56576099
C	10.51193414	9.55448719	11.01338678
C	10.38192612	8.66757766	9.92417018
C	11.35353587	7.65730812	9.79390532
H	11.29096445	6.94826921	8.96534494
C	12.39946375	7.53298697	10.70976065
C	12.52186514	8.41798251	11.79719131
C	11.56082180	9.43998765	11.92573720
H	11.61325198	10.12255894	12.77648831
C	5.31659068	10.12609636	10.48275619
C	9.05557615	10.34181415	7.62967023
C	9.98282864	11.37808164	7.84556781
H	10.68980100	11.30899378	8.67593754
C	10.03900049	12.49031699	7.00230164
C	9.16305731	12.61723621	5.90702477
C	8.23320596	11.58155461	5.68687222
H	7.52160045	11.66268782	4.86279001
C	8.18743930	10.46899704	6.52508510
C	5.09547967	9.21800480	11.53500048
C	6.01400420	8.16211245	11.69750430
H	5.88394948	7.45899600	12.52276751
C	7.35201549	8.95262440	9.80640112
C	6.41984225	9.99410712	9.63824561
H	6.56120850	10.72367444	8.83755463
C	8.98836900	3.90149866	4.91520532
C	9.35090046	4.05780566	3.56539071
C	9.42135266	2.97053154	2.69366134

C	9.13050997	1.67606226	3.15338018
C	8.75974884	1.50489859	4.50239414
C	8.68887142	2.59710321	5.36014689
H	8.54064286	0.50397809	4.87961217
H	8.42833090	2.43135851	6.40698436
H	9.69609843	3.14377378	1.65381359
H	9.55868038	5.05642719	3.17690439
S	9.19085778	0.21680148	2.15639909
C	9.78121319	0.82021226	0.55339088
H	9.86055763	-0.07294164	-0.07843109
H	10.77187941	1.28449688	0.63986285
H	9.06796084	1.51690434	0.09483507
C	3.95279481	9.38866623	12.46061895
C	3.22034458	8.28445869	12.94213032
C	2.15632279	8.45131800	13.82185273
C	1.78686725	9.73769297	14.26354705
C	3.56988710	10.66640178	12.90459980
C	2.50872967	10.84619641	13.79294043
H	2.25912688	11.85433422	14.12198926
H	3.47496461	7.27927654	12.60114445
H	4.13464454	11.53986319	12.57344181
H	1.59954052	7.57961738	14.17146889
S	0.42452220	9.82576572	15.38732646
C	0.30794487	11.59037312	15.78018540
H	-0.52473495	11.67191918	16.48966175
H	0.07536979	12.18955833	14.89047187
H	1.22367623	11.95611315	16.26203490
C	13.61033010	8.26186493	12.78838356
C	14.00764391	6.98793305	13.23038928
C	14.27770349	9.37884918	13.33167901
C	15.29484981	9.22816938	14.26783279
C	15.67976393	7.94523013	14.70636549
C	15.02152501	6.82423438	14.17548219
H	15.28470036	5.81819698	14.50028790
H	13.49164076	6.10419537	12.85062052
H	14.01073624	10.38190598	12.99376532
H	15.80347244	10.10952094	14.66377524
S	16.97985336	7.87727165	15.90295107
C	17.13939247	6.10879435	16.26100379
H	17.93737931	6.03857781	17.01046002
H	17.43779325	5.54031136	15.37099649
H	16.21401675	5.70003294	16.68658886
C	9.21145989	13.79312066	5.00919186
C	8.97451886	13.66355910	3.62927700
C	8.99672756	14.76577268	2.77421261
C	9.25544990	16.04889443	3.28188645

C	9.50320909	16.19291188	4.66174906
C	9.48349800	15.08577052	5.50281700
H	8.79367133	12.67395545	3.20587545
H	8.81926484	14.61295974	1.71031962
H	9.69728205	17.18457750	5.07523992
H	9.64886865	15.23012881	6.57192811
S	9.29649425	17.52427018	2.30876877
C	8.83302084	16.95171261	0.65338679
H	8.81341571	17.85543797	0.03194010
H	7.83501345	16.49549546	0.65135911
H	9.57580466	16.25604066	0.24252595
H	10.79491033	13.25865226	7.17733111
H	7.45802856	9.68234787	6.31365047
H	10.56003598	8.01259437	6.42936242
H	7.21565812	4.37802931	6.95002446
H	4.60554646	10.93794761	10.31641978
H	7.83479802	7.23376220	11.04495344
H	9.76186799	10.33384012	11.17275873
H	13.14551303	6.74779603	10.57144180

38_FHI-aims_Molecule_Si3.xyz /// -131184.575636874 eV

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Si	8.93387805	8.79884423	8.61242825
C	7.29597147	8.11440206	10.89012046
C	8.87080938	7.27620812	7.48951868
C	8.11125344	6.13660598	7.81676995
H	7.46332779	6.15077063	8.69667514
C	8.15309518	4.98493088	7.02986962
C	8.95627011	4.92379908	5.87514072
C	9.70059798	6.06784376	5.53026387
H	10.34625938	6.04373687	4.64985705
C	9.65814287	7.21605405	6.32143018
C	10.54265950	9.40751876	10.93433000
C	10.45867676	8.67614410	9.73144657
C	11.55102469	7.85143421	9.39980261
H	11.52699513	7.26299284	8.47966547
C	12.67033551	7.75840478	10.22704369
C	12.74642860	8.48563292	11.42990477
C	11.66071030	9.31777278	11.76472482
H	11.67656342	9.86955939	12.70689139
C	5.24264067	9.89646869	10.28988526
C	9.01405332	10.34719301	7.52542340
C	9.74830828	11.48595550	7.90927559
H	10.35439097	11.45928960	8.81820850

C	9.73486057	12.65158562	7.14246459
C	8.99175679	12.72523199	5.94911011
C	8.26803126	11.58522462	5.55123815
H	7.66791730	11.62107413	4.63948419
C	8.27772868	10.42427110	6.32540427
C	5.14576581	9.11850176	11.45937043
C	6.19148637	8.21608083	11.73636962
H	6.15915323	7.61936491	12.65030473
C	7.40569830	8.90397730	9.72654693
C	6.34853942	9.79109948	9.44582383
H	6.39287222	10.42184470	8.55482268
C	9.03026094	3.69249393	5.05570346
C	9.10589183	3.75070898	3.65097114
C	9.20193884	2.59035967	2.88611251
C	9.23333920	1.31756133	3.48999361
C	9.15157209	1.26121532	4.89533599
C	9.04814311	2.42077771	5.65972372
H	9.21360926	0.29463137	5.39834287
H	9.02871394	2.34468640	6.74830223
H	9.21957822	2.66916349	1.79767982
H	9.05388823	4.71931192	3.15036037
C	4.00012930	9.26763139	12.38650696
C	3.46648213	8.16500703	13.08086653
C	2.40696633	8.31726528	13.97276678
C	3.41878256	10.52885680	12.61968352
C	2.36094558	10.68124547	13.51211259
H	1.92385699	11.67081139	13.65775686
H	3.88080373	7.16989944	12.90897900
H	3.81833485	11.40737057	12.11000352
H	2.03215641	7.44461967	14.51065753
C	13.92206806	8.36288584	12.32257174
C	14.56713903	7.12467192	12.50567908
C	14.42982564	9.47410483	13.02224879
C	15.53222587	9.35375042	13.86519313
C	16.17673502	8.11513294	14.05050486
C	15.66695606	7.00352434	13.35157934
H	16.15413239	6.03252014	13.45834854
H	14.18702489	6.23980599	11.99192380
H	13.96151337	10.45125470	12.89007613
H	15.88914730	10.23098415	14.40775704
C	8.97043365	13.96403796	5.13781609
C	9.02818134	13.91746810	3.73219870
C	9.00681892	15.08415768	2.97133798
C	8.91354843	16.35200165	3.57917051
C	8.85157123	16.39529292	4.98625203
C	8.88616218	15.22997668	5.74792831

H	9.13152042	12.95279020	3.23187823
H	9.09956347	15.01328933	1.88627383
H	8.73506954	17.35652793	5.48975050
H	8.80284805	15.29644478	6.83427671
C	17.34665901	7.98462468	14.94698081
C	17.53086545	6.83645385	15.74562407
C	18.62986411	6.70851179	16.58717067
C	19.59809148	7.72998002	16.66050420
C	19.42831945	8.87875756	15.87118037
C	18.31828744	8.99742181	15.03308109
H	16.78299331	6.04175197	15.72656474
H	18.74073389	5.81358253	17.20283862
H	20.16199418	9.68383974	15.89410864
H	18.22325492	9.88784124	14.40879757
C	0.72075447	9.75077767	15.17598622
C	-0.28909073	8.77562939	15.31347040
C	-1.33405424	8.93619627	16.21594351
C	-1.40978383	10.08590351	17.02747466
C	-0.40982567	11.06357764	16.90421897
C	0.63223975	10.89298927	15.99148143
C	1.83237501	9.58059341	14.21430120
H	-0.27034880	7.88825628	14.67833536
H	-2.10893471	8.17048432	16.29024316
H	-0.42783221	11.95976463	17.52367036
H	1.41161144	11.65517673	15.93557225
C	8.87605707	17.59188822	2.77283062
C	8.26241016	17.62355496	1.50259222
C	8.21621545	18.78971259	0.74736216
C	8.78748255	19.98208283	1.23571264
C	9.40564026	19.96549868	2.49652440
C	9.44523286	18.78849037	3.24494960
H	7.78304357	16.72376150	1.11298435
H	7.71988127	18.78685751	-0.22528400
H	9.87037291	20.86443194	2.90050380
H	9.95718420	18.79761227	4.20894061
C	9.36083440	0.08517103	2.68149009
C	8.71688879	-1.10738855	3.05697873
C	8.84171884	-2.27754049	2.30675951
C	9.62816000	-2.29051557	1.14368061
C	10.27754942	-1.10198164	0.75385368
C	10.14271658	0.05786953	1.50762440
H	8.07868377	-1.11733724	3.94243437
H	8.31339550	-3.17342707	2.63133835
H	10.90371389	-1.09668312	-0.14070971
H	10.68147773	0.95523630	1.19863302
S	9.87497267	-3.69979009	0.10560995

C	8.97240456	-5.02244417	0.95295202
H	9.13391428	-5.91727258	0.33924191
H	7.89605470	-4.81337062	0.99919377
H	9.37299413	-5.20306271	1.95839357
S	20.95273018	7.45328549	17.76237919
C	21.98456378	8.92736074	17.55013507
H	22.84263594	8.77560072	18.21653425
H	21.45610944	9.83965348	17.85438131
H	22.34715091	9.01841472	16.51847883
S	8.67082068	21.40178027	0.18919448
C	9.37805292	22.73170674	1.19656635
H	9.28944725	23.63578161	0.58169031
H	10.43886274	22.55458548	1.41394452
H	8.81265526	22.87366688	2.12656106
S	-2.78366407	10.17887355	18.13620607
C	-2.53651477	11.75471986	18.99489661
H	-3.38159661	11.83847040	19.68927875
H	-2.56304991	12.60273429	18.29881300
H	-1.60214112	11.75757758	19.57057559
H	8.10367602	7.42983286	11.16229521
H	4.43434038	10.58356375	10.03207256
H	7.69755702	9.56173096	5.98736041
H	10.33397623	13.50981043	7.45426913
H	7.53356645	4.12661905	7.29809050
H	10.25639353	8.08118512	6.02382126
H	13.50786033	7.12500280	9.92839477
H	9.70692297	10.03920671	11.24643195

39_FHI-aims_Molecule_C1.xyz /// -74034.593620248 eV

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C	9.10499136	8.87354668	8.54725309
C	7.75215050	8.05453570	10.54865038
C	9.01276072	7.62115361	7.63264042
C	8.03973417	6.62666012	7.78014537
H	7.28807391	6.70960277	8.56399413
C	7.98451862	5.51522777	6.93011943
C	8.91365525	5.36646012	5.89399967
C	9.89019858	6.36876656	5.72086693
H	10.61776893	6.28456616	4.91088223
C	9.92762837	7.47035929	6.56837773
C	10.45291494	9.70546841	10.54888595
C	10.34588243	8.79775049	9.47923873
C	11.37079226	7.84826507	9.34320503
H	11.32566639	7.10305443	8.54974629

C	12.45321077	7.81301294	10.22389653
C	12.55195944	8.73340510	11.28147551
C	11.53210695	9.68727275	11.43307386
H	11.56244264	10.41432552	12.24393321
C	5.70601534	9.88397054	10.15018895
C	9.18658137	10.10980117	7.60915242
C	10.11997056	11.14680957	7.76676781
H	10.85467762	11.10400368	8.56993912
C	10.14910315	12.23959521	6.89963007
C	9.23831551	12.33789041	5.83368049
C	8.30839009	11.30080168	5.65317581
H	7.59434471	11.32735714	4.83047041
C	8.29602658	10.21041288	6.52454499
C	5.59817899	8.95951336	11.20333072
C	6.64484843	8.04289616	11.39683210
H	6.61040232	7.31769448	12.20913131
C	7.86040014	8.95520865	9.47339535
C	6.81626465	9.87716033	9.30365298
H	6.86473780	10.61678442	8.50503656
S	8.95026354	4.00774459	4.76146894
S	13.96363417	8.59026375	12.33927713
S	4.13837189	9.04235615	12.20128274
S	9.36385201	13.77474339	4.80758506
C	4.40247386	7.75041833	13.44399210
H	3.51318088	7.78286350	14.08537191
H	4.47342393	6.75534881	12.98605641
H	5.29001252	7.95578428	14.05622588
C	8.09707306	13.51063185	3.53947521
H	8.16583218	14.38575961	2.88158006
H	8.29866864	12.60681503	2.95042368
H	7.08971592	13.47119320	3.97324798
C	7.58061122	2.96142937	5.32154738
H	7.58306746	2.09657205	4.64694606
H	7.73678573	2.61174468	6.35010301
H	6.61587327	3.47755040	5.23390665
C	13.69054144	9.86939700	13.59268009
H	14.54753259	9.79037058	14.27296337
H	13.67911575	10.87446308	13.15210872
H	12.76866021	9.68746566	14.15991794
H	8.55778745	7.34174258	10.73461038
H	4.91521389	10.62036301	9.99175952
H	13.22606032	7.05231715	10.09311745
H	10.67922258	8.24227707	6.39202485
H	7.19999626	4.77591283	7.08737287
H	7.57784616	9.40839771	6.34330392
H	10.89558499	13.02278815	7.04865928

H 9.66149457 10.43998305 10.71034782

40_FHI-aims_Molecule_C2.xyz /// -99177.166157066 eV

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C	8.93721315	8.80092377	8.73299032
C	7.46099835	7.95841434	10.64353560
C	8.87541938	7.57604900	7.78113447
C	7.88648560	6.58476116	7.83358503
H	7.07894721	6.65777891	8.56156912
C	7.89614611	5.50337467	6.94533025
C	8.89672944	5.36610666	5.96840266
C	9.88083509	6.37335302	5.90646194
H	10.68717033	6.29569767	5.17491029
C	9.86235790	7.45293040	6.78323088
C	10.26129199	9.60360105	10.76797763
C	10.13456912	8.67370261	9.71656972
C	11.07900985	7.63951090	9.65765624
H	11.01699367	6.88604978	8.87365618
C	12.10910840	7.54298803	10.59753472
C	12.24009425	8.47346024	11.64133746
C	11.29090966	9.51388413	11.70147859
H	11.33364556	10.23688444	12.51832016
C	5.64567333	10.03999181	10.39036292
C	9.07228112	10.04678257	7.81644783
C	10.05901191	11.03062087	7.96305287
H	10.81082132	10.93663352	8.74617870
C	10.11867671	12.13180337	7.10180653
C	9.19275483	12.29751539	6.05828675
C	8.21115646	11.29809105	5.90212192
H	7.46071951	11.39738991	5.11571195
C	8.16143621	10.19846104	6.75237237
C	5.43920932	9.09284663	11.40630962
C	6.37077885	8.03990039	11.50633293
H	6.26635256	7.30179834	12.30391524
C	7.66841182	8.90962317	9.62470467
C	6.73610925	9.95116021	9.52069592
H	6.85738800	10.71941219	8.75830682
C	8.92685093	4.21752907	5.03537573
C	9.36342849	4.37047396	3.70730901
C	9.42123699	3.29143085	2.82428551
C	9.04151732	2.00861013	3.25061603
C	8.59426361	1.84149221	4.57670574
C	8.53789933	2.92541930	5.44605916
H	8.30573903	0.84866586	4.92820444

H	8.21790811	2.76158890	6.47665829
H	9.75647945	3.46250070	1.80189114
H	9.64294316	5.36112257	3.34432976
S	9.07939528	0.55921405	2.23816482
C	9.79120487	1.14802458	0.68015206
H	9.86798759	0.25744291	0.04422729
H	10.79554851	1.56466065	0.83103969
H	9.14048955	1.88134479	0.18688227
C	4.30972019	9.21855031	12.35479495
C	3.61446385	8.08844041	12.83219298
C	2.56318972	8.21346070	13.73418232
C	2.16692106	9.48274830	14.20138917
C	3.90041892	10.47852349	12.82579082
C	2.84977738	10.61690318	13.73385533
H	2.57889658	11.61338998	14.08126661
H	3.88775187	7.09528394	12.47085549
H	4.43549273	11.37237554	12.49974574
H	2.03625956	7.32203568	14.08063001
S	0.82585968	9.51806706	15.35337587
C	0.64179714	11.27793230	15.74181826
H	-0.18502443	11.32841430	16.46089981
H	0.37413018	11.86235425	14.85227703
H	1.54686551	11.68405588	16.21094133
C	13.31667705	8.34904186	12.64968617
C	13.73483204	7.08872160	13.11208273
C	13.95885174	9.48416687	13.18643665
C	14.97020240	9.36407310	14.13338700
C	15.37895353	8.09412580	14.58766515
C	14.74628589	6.95512389	14.06435991
H	15.02720159	5.95776199	14.40096642
H	13.23946997	6.18957140	12.74115549
H	13.67827424	10.47862638	12.83445263
H	15.45813444	10.25997253	14.52292175
S	16.67077931	8.06397897	15.79497390
C	16.90686956	6.29820774	16.12503970
H	17.70901499	6.25083738	16.87177940
H	17.22718025	5.75837776	15.22478608
H	16.00187784	5.84214897	16.54621044
C	9.23877193	13.46642848	5.15165416
C	8.90585701	13.34504376	3.79083034
C	8.92477937	14.44330483	2.93013108
C	9.27897377	15.71351801	3.41260986
C	9.62176125	15.84922059	4.77288140
C	9.60253638	14.74636539	5.61975290
H	8.64998340	12.36440695	3.38545811
H	8.67008754	14.29697845	1.88107347

H	9.88933224	16.83170232	5.16724648
H	9.84230412	14.88524975	6.67547124
S	9.33212459	17.18292359	2.43024442
C	8.73462052	16.63161258	0.81179802
H	8.71347279	17.53527518	0.19013481
H	7.71875688	16.22126145	0.87808651
H	9.41545905	15.90256907	0.35407316
H	10.92346856	12.85855928	7.22855857
H	7.39337810	9.43941082	6.59236524
H	10.63559893	8.21862835	6.69726016
H	7.08902436	4.77006215	6.99694555
H	4.93448780	10.85854182	10.26421211
H	8.18882030	7.15744549	10.78613655
H	9.51834729	10.39616641	10.87529594
H	12.83545058	6.73352193	10.50334158

41_FHI-aims_Molecule_C3.xyz /// -124319.725560289 eV

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C	8.96993192	8.78735914	8.58935790
C	7.59493255	8.04614865	10.62170189
C	8.87134927	7.54134251	7.66777710
C	7.98685665	6.47910037	7.90219266
H	7.26758136	6.53773127	8.71811926
C	7.99583632	5.33671055	7.09740151
C	8.88637045	5.20846545	6.01839030
C	9.74710386	6.29218671	5.75646660
H	10.46021514	6.22708192	4.93236401
C	9.73619494	7.43000264	6.56085777
C	10.32648138	9.51000999	10.63987902
C	10.21177711	8.66250524	9.51943260
C	11.24086328	7.73367014	9.31105653
H	11.19445057	7.04537358	8.46843468
C	12.33926475	7.66021352	10.17204812
C	12.45842731	8.51181399	11.28267298
C	11.42220061	9.44176200	11.49697464
H	11.45676107	10.09667904	12.36960308
C	5.59471845	9.91112678	10.16098923
C	9.08065030	10.05034262	7.69105224
C	9.95811190	11.11067796	7.95869485
H	10.66555657	11.03925563	8.78370998
C	9.95781348	12.26834754	7.17635465
C	9.08391765	12.41457128	6.08620119
C	8.23160424	11.33310574	5.78969037
H	7.53175767	11.41159785	4.95541655

C	8.23349664	10.18010751	6.57246312
C	5.47617880	9.06570171	11.27646920
C	6.50247977	8.12281323	11.48252782
H	6.46693490	7.46802326	12.35515325
C	7.71759943	8.89978458	9.50696943
C	6.69072601	9.83103804	9.29787463
H	6.73979471	10.51997145	8.45600140
C	8.93209204	3.97368810	5.20215834
C	9.12445493	4.01636687	3.80817633
C	9.18622518	2.84658762	3.05355577
C	9.06773924	1.57896702	3.65760699
C	8.87442928	1.53871798	5.05260062
C	8.80435317	2.70784966	5.80579456
H	8.82112900	0.57402189	5.56009181
H	8.69363150	2.64098812	6.88963416
H	9.29591180	2.91721924	1.96994642
H	9.19118487	4.98265074	3.30468400
C	4.33516372	9.18059960	12.21349932
C	3.77805774	8.04774195	12.83759196
C	2.71472249	8.16542755	13.73037245
C	3.77517719	10.43573456	12.52067562
C	2.71212734	10.55331522	13.41211226
H	2.29101107	11.53995117	13.61328705
H	4.17623877	7.05752588	12.60893549
H	4.19388100	11.33599242	12.06753565
H	2.32117841	7.26881100	14.21281756
C	13.62216449	8.42893490	12.19451511
C	14.21476531	7.19075121	12.50823848
C	14.18004502	9.58489484	12.77396669
C	15.28323252	9.50636241	13.62081459
C	15.88078901	8.26851950	13.92915513
C	15.31762388	7.11224380	13.35486311
H	15.76579274	6.13818704	13.55877388
H	13.79411958	6.27353653	12.09217169
H	13.75336274	10.56220678	12.54126437
H	15.68034382	10.42040349	14.06621977
C	9.05038393	13.66420025	5.29253136
C	8.88840678	13.64677951	3.89421332
C	8.84756124	14.82991174	3.15933270
C	8.95686087	16.08655110	3.78790481
C	9.11497206	16.10134453	5.18792105
C	9.16521835	14.91885119	5.92157519
H	8.83125702	12.68970448	3.37228981
H	8.76414479	14.77799092	2.07237162
H	9.15838620	17.05639590	5.71422969
H	9.25125207	14.96603414	7.00871610

C	17.06210113	8.18332981	14.81603916
C	17.23211880	7.10363655	15.70803732
C	18.34707287	7.01394070	16.53306125
C	19.34682333	8.00651337	16.49606478
C	19.18994950	9.08887477	15.61561200
C	18.06395701	9.16948701	14.79473226
H	16.46112010	6.33417854	15.77535913
H	18.44627526	6.17305374	17.22252609
H	19.94727893	9.86943148	15.55239570
H	17.98117784	10.00519677	14.09750337
C	1.04024347	9.55286232	15.00221816
C	0.01737101	8.58443638	15.07707278
C	-1.03267640	8.70768410	15.97984590
C	-1.10037516	9.81152380	16.85326286
C	-0.08887081	10.78348349	16.79069874
C	0.95880783	10.64987053	15.87844941
C	2.15863169	9.42156924	14.04219514
H	0.03055129	7.73299634	14.39438649
H	-1.81672579	7.94826519	16.00788417
H	-0.10171497	11.64433037	17.45836636
H	1.74799294	11.40383642	15.87047663
C	8.90247122	17.34528279	3.01177423
C	8.09893254	17.46230943	1.85796998
C	8.03573883	18.64767436	1.13487700
C	8.78132415	19.77381869	1.53731335
C	9.58932838	19.67191890	2.68092930
C	9.64313963	18.47643517	3.39921267
H	7.48498016	16.61790019	1.54028571
H	7.39057290	18.71295871	0.25641119
H	10.19151116	20.51644109	3.01445899
H	10.30134427	18.41713469	4.26773854
C	9.15321794	0.33357198	2.86313826
C	8.40205328	-0.80510826	3.20494117
C	8.49347795	-1.99119597	2.47529765
C	9.35145167	-2.07607548	1.36711985
C	10.10446214	-0.94059534	1.00769433
C	10.00319717	0.23562709	1.74159689
H	7.70781473	-0.75965716	4.04595439
H	7.88277609	-2.84320258	2.77239318
H	10.78547679	-0.99165050	0.15573605
H	10.62431158	1.08770742	1.46001529
S	9.56733104	-3.51618557	0.36495534
C	8.54697901	-4.76701659	1.18785799
H	8.69263697	-5.68527674	0.60566748
H	7.48284779	-4.49967335	1.16695772
H	8.88072612	-4.94154765	2.21864012

S	20.72545447	7.77776830	17.57880738
C	21.75288152	9.23963542	17.27778131
H	22.61858806	9.12278848	17.94124213
H	21.22465110	10.16491437	17.54111672
H	22.10471035	9.27948302	16.23886515
S	8.62349975	21.22255383	0.53648248
C	9.59413591	22.46679617	1.42624463
H	9.47645107	23.39115382	0.84745216
H	10.65943756	22.20499626	1.46234188
H	9.20361846	22.62890227	2.43913203
S	-2.47917539	9.85864255	17.95892452
C	-2.20453257	11.36916045	18.92105892
H	-3.04553362	11.41950147	19.62350189
H	-2.22038059	12.26250686	18.28362286
H	-1.26755889	11.31920965	19.49027078
H	8.38805140	7.32877660	10.83919856
H	4.80968072	10.63963764	9.95055556
H	7.55163796	9.36657075	6.31834573
H	10.66893359	13.06434317	7.40546863
H	7.27880964	4.53874812	7.29981128
H	10.42451858	8.24589857	6.33323188
H	13.12916160	6.93751151	9.95975432
H	9.52783574	10.22018178	10.86038152

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Au	4.38560132	10.91066622	14.99358719
Au	3.61040906	11.23845871	17.64636229
Au	6.34770246	11.12055387	16.91641837
Au	4.64944026	13.42261796	16.06789118
Au	2.83942000	11.69465700	20.24769400
Au	5.63042300	11.51628000	19.54460300
Au	8.42142700	11.33790300	18.84151200
Au	4.08044300	13.80565100	18.72472900
Au	6.87144600	13.62727400	18.02163800
Au	5.32146500	15.91664600	17.20176400
Au	8.11246900	15.73826900	16.49867300
Au	2.069482	12.154876	22.988360
Au	4.860486	11.976499	22.285269
Au	7.651489	11.798122	21.582179
Au	10.442493	11.619745	20.879088
Au	3.310505	14.265871	21.465396
Au	6.101509	14.087494	20.762305
Au	8.892513	13.909116	20.059214

Au	4.551528	16.376865	19.942431
Au	7.342531	16.198488	19.239340
Au	5.792550	18.487859	18.419466
Au	1.760524	16.555242	20.645521
Au	1.299545	12.615096	25.729027
Au	4.090548	12.436719	25.025936
Au	6.881552	12.258341	24.322845
Au	9.672556	12.079964	23.619754
Au	12.463559	11.901587	22.916664
Au	2.540568	14.726090	24.206062
Au	5.331572	14.547713	23.502971
Au	8.122575	14.369336	22.799880
Au	10.913579	14.190959	22.096789
Au	3.781590	16.837084	22.683097
Au	6.572594	16.658707	21.980006
Au	9.363598	16.480330	21.276915
Au	5.022613	18.948079	21.160132
Au	7.813616	18.769701	20.457042
Au	6.263636	21.059073	19.637167
S	3.62909054	9.43763515	13.20325897
Os	8.34680016	8.88032844	8.60980860
C	6.63912776	7.84005761	10.89959773
C	8.43414775	7.32658927	7.33759331
C	7.32210891	6.45655934	7.24382618
H	6.47204068	6.60633818	7.91463047
C	7.23936424	5.39469573	6.33191938
C	8.34397261	5.19547396	5.47609701
C	9.44622840	6.06054371	5.52496111
H	10.28365442	5.92084544	4.84046704
C	10.71206219	8.04702899	6.35507345
H	11.05930148	8.35652836	7.34937892
H	10.45750910	8.96360659	5.80215204
H	11.55094415	7.56287199	5.83702023
C	9.51691658	7.12651229	6.42805697
C	6.01862083	4.51406311	6.28015043
H	5.29466173	4.80622908	7.05081553
H	6.27713400	3.45528089	6.43650785
H	5.51632471	4.58115744	5.30160720
C	4.25669104	11.49863487	11.05930977
H	4.50711645	12.15184745	10.21433715
H	3.17537113	11.29445173	11.02541743
H	4.44878696	12.06149604	11.98780310
H	13.70363041	6.63484985	10.65866528
H	12.61689384	5.91750875	11.85403489
C	10.14807034	9.97706226	10.78371554
C	9.90198432	8.91207662	9.87037915

C	10.73831694	7.77152928	9.93304471
H	10.55770609	6.93993871	9.24725027
C	11.79542905	7.64383968	10.83931674
C	12.04115592	8.72216480	11.72442835
C	11.21944285	9.86012000	11.67563742
H	11.40056456	10.69115828	12.35844672
C	9.27016650	11.20326260	10.87778610
H	8.91243632	11.54081613	9.89611968
C	12.64670473	6.40188209	10.86493587
H	8.38181676	10.99390067	11.49307276
H	9.80972367	12.03751381	11.34637089
C	5.06288137	10.22775803	11.01019110
C	8.33337859	10.40616176	7.31800267
C	9.46469067	11.25461033	7.26387607
H	10.27142995	11.11694541	7.98770452
C	9.61811560	12.26097152	6.30630483
C	8.58440988	12.42897214	5.35151642
C	7.44553311	11.60762099	5.40794928
H	6.64385797	11.73917028	4.68011166
C	6.07266663	9.71384950	6.30482424
H	5.72202060	9.42292245	7.30524858
H	6.28946491	8.78661901	5.75303232
H	5.24434105	10.22109765	5.79141557
C	7.29663797	10.59783130	6.36313085
C	10.84846884	13.12916248	6.28993343
H	11.54051841	12.84375238	7.09223475
H	10.59164228	14.19234878	6.42081309
H	11.38151995	13.04744910	5.32924665
C	4.89684842	9.19763386	11.96049715
C	5.67170310	8.03126074	11.89220471
H	5.54112215	7.24017165	12.63141723
C	7.47733946	6.58445694	10.93667599
H	7.69084243	6.20250054	9.92934146
H	8.44735920	6.78153454	11.41761313
H	6.97466173	5.78924607	11.50397221
H	12.30442777	5.67554368	10.11689595
C	6.83473005	8.86637656	9.93022842
C	6.02879437	10.02695641	10.01498481
H	6.16556782	10.82503066	9.28108962
S	13.39568148	8.54500296	12.84579565
S	8.81833957	13.68608967	4.13288318
C	3.50828788	7.82077429	14.02386073
H	2.70815128	7.93739672	14.76389715
H	3.22397235	7.06145239	13.28520748
H	4.43825217	7.55321906	14.53583081
C	7.38073723	13.50382386	3.04449369

H	7.52808839	14.24989175	2.25401045
H	7.34533229	12.50593094	2.58980319
H	6.44299909	13.72481117	3.56935843
C	10.03052447	3.56872275	3.87571920
H	10.04770530	2.64083802	3.29220768
H	10.36873694	4.39646795	3.24430223
H	10.65891933	3.46206063	4.76806578
C	13.35746838	10.07408741	13.81765595
H	14.18254655	9.97502213	14.53369280
H	13.53493676	10.95701945	13.19110705
H	12.41614600	10.17613792	14.37183651
S	8.29748728	3.77075300	4.38989975
Au	7.14973068	4.17684832	2.28714270
Au	6.18653790	3.02969077	-0.03498745
Au	4.79777102	5.14555489	1.23653592
Au	7.57004065	5.54866222	-0.06106827
Au	5.26452400	1.98748800	-2.43106400
Au	3.82913000	4.11982000	-1.12390600
Au	2.39373500	6.25215100	0.18325300
Au	6.39348000	4.63934500	-2.33636500
Au	4.95808600	6.77167600	-1.02920700
Au	7.52243600	7.29120200	-2.24166600
Au	6.08704200	9.42353400	-0.93450700
Au	4.299379	0.919676	-4.929890
Au	2.863985	3.052007	-3.622732
Au	1.428591	5.184339	-2.315574
Au	-0.006803	7.316670	-1.008415
Au	5.428336	3.571533	-4.835191
Au	3.992941	5.703864	-3.528033
Au	2.557547	7.836196	-2.220874
Au	6.557292	6.223390	-4.740491
Au	5.121898	8.355721	-3.433334
Au	7.686248	8.875247	-4.645792
Au	3.686504	10.488053	-2.126175
Au	3.334235	-0.148136	-7.428716
Au	1.898841	1.984195	-6.121558
Au	0.463447	4.116526	-4.814399
Au	-0.971947	6.248858	-3.507241
Au	-2.407341	8.381189	-2.200083
Au	4.463191	2.503720	-7.334017
Au	3.027797	4.636052	-6.026858
Au	1.592403	6.768383	-4.719700
Au	0.157009	8.900715	-3.412542
Au	5.592147	5.155577	-7.239318
Au	4.156753	7.287909	-5.932159
Au	2.721359	9.420241	-4.625001

Au	6.721103	7.807435	-7.144618
Au	5.285710	9.939766	-5.837460
Au	7.850060	10.459292	-7.049919

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Au	16.17283968	9.34945319	18.22301543
Au	14.19755985	9.22073787	20.08340923
Au	16.90145480	9.43783579	20.89737462
Au	15.49244891	11.72883558	19.44133993
Au	12.19519300	9.19779400	21.92583300
Au	14.93335000	9.36688400	22.81451900
Au	17.67150700	9.53597500	23.70320500
Au	13.71070900	11.60961400	21.47617400
Au	16.44886500	11.77870400	22.36485900
Au	15.22622300	14.02143400	21.02651400
Au	17.96438100	14.19052400	21.91520000
Au	10.051694	9.180363	23.854813
Au	12.789851	9.349454	24.743499
Au	15.528007	9.518545	25.632184
Au	18.266164	9.687635	26.520870
Au	11.567208	11.592184	23.405153
Au	14.305366	11.761274	24.293839
Au	17.043523	11.930365	25.182525
Au	13.082724	14.004004	22.955494
Au	15.820880	14.173094	23.844180
Au	14.598239	16.415824	22.505835
Au	10.344567	13.834913	22.066809
Au	7.908194	9.162933	25.783793
Au	10.646351	9.332024	26.672479
Au	13.384508	9.501115	27.561164
Au	16.122665	9.670205	28.449850
Au	18.860821	9.839296	29.338536
Au	9.423709	11.574754	25.334134
Au	12.161866	11.743844	26.222819
Au	14.900022	11.912935	27.111505
Au	17.638180	12.082025	28.000191
Au	10.939224	13.986574	24.884474
Au	13.677381	14.155664	25.773160
Au	16.415538	14.324755	26.661846
Au	12.454740	16.398394	24.434815
Au	15.192896	16.567484	25.323500
Au	13.970255	18.810214	23.985155
Os	8.84909803	8.88345587	8.86200499

C	6.83050242	8.06597411	10.97780697
C	8.90309190	7.26006103	7.69324173
C	7.81646479	6.35985942	7.71307285
H	6.97907128	6.55643790	8.38688508
C	7.73130691	5.23448105	6.87697227
C	8.79008674	4.99742458	5.96876877
C	9.86955533	5.90566396	5.94254376
H	10.68857948	5.70977103	5.24487981
C	11.12962154	7.97194741	6.59473285
H	11.53721169	8.31565082	7.55587294
H	10.82938358	8.87203457	6.03735325
H	11.94248262	7.48598224	6.03816248
C	9.95983380	7.03004607	6.76338649
C	6.49669046	4.36577147	6.95094316
H	5.64388151	4.94591809	7.32830270
H	6.63580909	3.51321367	7.63422051
H	6.22997191	3.95356160	5.96889910
C	4.21600438	11.44078742	10.02468992
H	4.36977369	11.69283509	8.96709571
H	3.15170794	11.21697918	10.17358969
H	4.44543609	12.34759485	10.60630117
H	14.20559468	6.60626851	11.23781834
H	12.83461918	5.55581609	11.63043668
C	10.51861999	9.85601908	11.20629980
C	10.33115804	8.85142142	10.21024898
C	11.21036343	7.74671106	10.20323321
H	11.07214584	6.96525221	9.45289572
C	12.27037527	7.59261155	11.11035637
C	12.47175882	8.60764647	12.07388336
C	11.59227756	9.71122778	12.08668881
H	11.73681492	10.47692768	12.85422250
C	9.57621973	11.02432008	11.37256977
H	9.36694187	11.53264515	10.42059518
C	13.16321833	6.37979459	10.97750135
H	8.60748521	10.68815051	11.77177987
H	9.99063439	11.76527104	12.06918384
C	5.09985306	10.27888593	10.41815890
C	8.98288313	10.43611923	7.60452654
C	10.03111620	11.36630386	7.76710763
H	10.75700030	11.21104951	8.56887478
C	10.21318219	12.47849683	6.92908865
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C	8.27690337	11.71485890	5.68074491
H	7.57628180	11.86746596	4.85509969
C	6.99367623	9.61867949	6.17387239
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H	7.41176749	8.70599040	5.72365515
H	6.28339775	10.05421451	5.45812485
C	8.08992693	10.60457881	6.50518532
C	11.39026989	13.39245499	7.17858950
C	4.77137232	9.35925088	11.44112649
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H	5.39094508	7.57772846	12.48453470
C	7.72875727	6.91626393	11.36986640
H	8.09254509	6.35540238	10.49696206
H	8.61749591	7.27951457	11.90732401
H	7.19914124	6.21355243	12.02707813
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C	7.16662207	8.99126503	9.94472070
C	6.28899158	10.07052926	9.70203923
H	6.53446822	10.78501664	8.91356399
C	8.81057293	3.86534462	5.00872872
C	9.12137700	4.09538674	3.65612719
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H	8.69172095	1.73104759	0.09795804
C	3.55178509	9.48084005	12.27916215
C	2.72533316	8.36138024	12.51020689
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H	-0.94707247	11.20088612	16.57695793
H	-0.15920946	12.08855928	15.24120221
H	0.84425616	11.22115582	16.47497295
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C	14.84250339	7.43372034	14.82192539
H	14.97534670	6.55457977	15.45177801
H	13.15804226	6.58172147	13.80162595
H	14.26498796	10.57441420	12.60877072
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H	18.41866256	6.90402515	16.94645647
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C	9.41649466	15.92378698	3.01800298
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Au	-6.14498200	14.76708200	13.05263700
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Au	-7.876932	8.391023	9.237246
Au	-9.227687	9.287093	11.622277

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Au	-9.127045	12.068290	12.377707
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Au	-7.675648	13.953415	10.748105
Au	-6.224251	15.838542	9.118504
Au	-9.026403	14.849486	13.133137
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Au	-9.407598	7.577356	6.932714
Au	-10.758353	8.473426	9.317746
Au	-12.109108	9.369497	11.702778
Au	-13.459863	10.265567	14.087808
Au	-7.956201	9.462482	5.303113
Au	-9.306956	10.358552	7.688144
Au	-10.657711	11.254623	10.073175
Au	-12.008466	12.150693	12.458207
Au	-7.855558	12.243678	6.058542
Au	-9.206314	13.139749	8.443574
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Au	-7.754917	15.024875	6.813972
Au	-9.105671	15.920945	9.199003
Au	-7.654274	17.806071	7.569402

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Au	23.81199075	4.17788316	15.99625102
Au	23.92361569	3.75989318	19.03010816
Au	21.56112100	0.01743600	17.06450200
Au	23.58172300	1.47687000	15.61430400
Au	25.60232600	2.93630400	14.16410500
Au	23.83532900	1.10741500	18.46299500
Au	25.85593100	2.56684800	17.01279700
Au	26.10953700	2.19739200	19.86148800
Au	28.13013900	3.65682600	18.41129000
Au	21.313599	-2.834509	16.716660
Au	23.334202	-1.375075	15.266461
Au	25.354804	0.084358	13.816263
Au	27.375407	1.543792	12.366065
Au	23.587807	-1.744532	18.115153
Au	25.608410	-0.285098	16.664954
Au	27.629012	1.174336	15.214756

Au	25.862016	-0.654554	19.513645
Au	27.882618	0.804880	18.063448
Au	28.136223	0.435424	20.912139
Au	23.841413	-2.113988	20.963844
Au	21.066078	-5.686455	16.368817
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Au	25.107283	-2.767588	13.468420
Au	27.127886	-1.308154	12.018222
Au	29.148488	0.151280	10.568024
Au	23.340286	-4.596478	17.767310
Au	25.360889	-3.137044	16.317112
Au	27.381491	-1.677610	14.866914
Au	29.402093	-0.218176	13.416715
Au	25.614494	-3.506500	19.165803
Au	27.635096	-2.047066	17.715605
Au	29.655699	-0.587632	16.265406
Au	27.888702	-2.416522	20.564296
Au	29.909304	-0.957089	19.114098
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S	21.14692587	7.62927365	18.04159863
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C	8.98306345	4.90826971	6.01126968
C	9.96578238	5.88443826	5.74008186
H	10.70733293	5.66701251	4.96603063
C	11.12402567	8.09646844	6.03086399
H	11.71543706	8.44244017	6.89180084
H	10.67377979	8.99218052	5.57752770
H	11.81903638	7.65902315	5.30147075
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H	3.62554139	11.34939452	10.30262543
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H	12.45906517	10.24617449	12.45381166
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C	13.72087181	6.36350526	10.08257156
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C	5.58441621	10.41586370	10.41558974
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C	10.20521397	11.59677569	7.65605119
H	11.00756974	11.40536014	8.37235632
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H	9.12516164	15.62902378	7.01702711
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H	12.21775215	13.28592907	7.62311313
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C	18.60241396	7.24486682	17.17461243
C	19.84623005	7.79501961	16.82421115
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H	8.95549607	24.06180983	0.73993240
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Au	2.59947100	25.78806700	2.57228900
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Au	1.921948	29.093482	4.862903
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Au	-2.480991	24.630297	6.370679
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Au	-3.951816	24.484227	-1.114395
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Au	-1.468205	29.663294	-0.592504
Au	-0.563995	30.575161	1.989502
Au	-0.226399	32.252827	-0.331558

45_FHI-aims_Junction_Si1.xyz /// -39719139.529123940 eV

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Au	7.56038627	4.41691485	2.25686022
Au	6.44327098	3.34124035	-0.04066251
Au	5.17959784	5.46272001	1.33748815
Au	7.82083338	5.89818379	-0.02265301

Au	5.44310200	2.37092900	-2.40556300
Au	4.09360200	4.49358700	-0.99523300
Au	2.74410200	6.61624600	0.41509600
Au	6.60662800	5.00787100	-2.31283300
Au	5.25712900	7.13052900	-0.90250400
Au	7.77015500	7.64481300	-2.22010400
Au	6.42065500	9.76747200	-0.80977500
Au	4.353563	1.361805	-4.877491
Au	3.004064	3.484464	-3.467162
Au	1.654565	5.607122	-2.056833
Au	0.305065	7.729781	-0.646504
Au	5.517090	3.998747	-4.784762
Au	4.167591	6.121406	-3.374433
Au	2.818091	8.244064	-1.964104
Au	6.680616	6.635689	-4.692033
Au	5.331117	8.758347	-3.281704
Au	7.844143	9.272631	-4.599304
Au	8.030116	4.513030	-6.102362
Au	3.264025	0.352681	-7.349420
Au	1.914526	2.475339	-5.939092
Au	0.565026	4.597998	-4.528762
Au	-0.784473	6.720657	-3.118433
Au	-2.133972	8.843315	-1.708104
Au	4.427552	2.989623	-7.256691
Au	3.078052	5.112282	-5.846362
Au	1.728553	7.234940	-4.436033
Au	0.379054	9.357599	-3.025704
Au	5.591079	5.626565	-7.163962
Au	4.241579	7.749224	-5.753633
Au	2.892079	9.871882	-4.343304
Au	6.754605	8.263507	-7.071233
Au	5.405106	10.386165	-5.660904
Au	7.918132	10.900449	-6.978503
S	8.55958070	3.46645591	4.25635340
Si	9.13219097	8.35130246	8.52677023
C	7.58448183	7.48167344	10.77960483
C	9.01709882	6.84693656	7.36824965
C	8.03457520	5.85778780	7.54720727
H	7.36556914	5.90801601	8.40907456
C	7.85751292	4.81703523	6.62866576
C	8.68212538	4.74782581	5.50090167
C	9.68767614	5.70943807	5.30433412
H	10.33084701	5.65763800	4.42355177
C	9.83983056	6.74456683	6.22525170
C	10.67835251	9.09832465	10.80321533
C	10.67014989	8.29724569	9.64471533

C	11.81207058	7.51074531	9.39559824
H	11.84891783	6.86147749	8.51775717
C	12.91244472	7.52582149	10.25470876
C	12.89039245	8.33788106	11.40043828
C	11.76802804	9.12702287	11.67711150
H	11.72235018	9.75593619	12.56536653
C	5.45314672	9.22365656	10.36180834
C	9.17165530	9.87465674	7.41710972
C	9.97730667	11.00266235	7.68069100
H	10.63947703	11.00907706	8.54991710
C	9.96509709	12.11793820	6.84738528
C	9.13707289	12.14903843	5.70628377
C	8.32804609	11.03501361	5.42648263
H	7.68221987	11.02023768	4.54916377
C	8.35389410	9.92350620	6.27076914
C	5.41057068	8.32625368	11.44837219
C	6.49219122	7.45149424	11.64938806
H	6.49508353	6.74996336	12.48311476
C	7.64219316	8.36675621	9.68467356
C	6.54792893	9.23814365	9.50094535
H	6.55535058	9.95187514	8.67362103
S	3.97594430	8.39640224	12.47540682
S	9.20660374	13.60707666	4.71507527
C	4.29273583	7.14188796	13.74353118
H	3.41554256	7.17252674	14.40132635
H	4.37505984	6.13816316	13.30795800
H	5.18673313	7.38133762	14.33306475
C	8.01641684	13.28245573	3.38814448
H	8.03780376	14.18132729	2.75980874
H	8.31174791	12.41841985	2.77983509
H	7.00133347	13.14898815	3.78227619
C	7.29190748	2.33903521	4.90740028
H	7.20022478	1.54945452	4.15275312
H	7.63920615	1.90714162	5.85374070
H	6.32686357	2.84258334	5.02493202
C	14.06358424	9.65068327	13.63121166
H	14.96315158	9.67020944	14.25734863
H	13.96024626	10.60548893	13.10143801
H	13.19148065	9.44181357	14.25944422
H	8.41654279	6.79943154	10.97567826
H	4.62338983	9.91528776	10.20058705
H	13.78371274	6.90412076	10.03976324
H	10.60012528	7.50445909	6.02841068
H	7.06896104	4.08513835	6.79886488
H	7.72293784	9.06895988	6.01260183
H	10.60457297	12.97421417	7.07257644

H	9.80437288	9.70644078	11.04949336
S	14.35750587	8.31961760	12.42783814
Au	14.29738164	6.27883225	13.73523560
Au	12.98629307	3.91463776	14.12703764
Au	15.82068092	4.00819656	14.10690381
Au	14.23752329	5.32157912	16.32638232
Au	11.64941800	1.59007200	14.62444100
Au	14.53197400	1.63097400	14.55332800
Au	17.41453000	1.67187500	14.48221600
Au	13.12611800	2.86654000	16.74713800
Au	16.00867300	2.90744200	16.67602500
Au	14.60281800	4.14300800	18.86983500
Au	17.48537400	4.18391000	18.79872200
Au	10.254396	-0.883872	15.123811
Au	13.136952	-0.842971	15.052698
Au	16.019507	-0.802069	14.981586
Au	18.902063	-0.761167	14.910473
Au	11.731096	0.392596	17.246508
Au	14.613652	0.433497	17.175396
Au	17.496207	0.474399	17.104283
Au	13.207796	1.669064	19.369205
Au	16.090351	1.709966	19.298093
Au	14.684496	2.945532	21.491902
Au	18.972907	1.750867	19.226980
Au	8.859375	-3.357817	15.623181
Au	11.741930	-3.316915	15.552069
Au	14.624486	-3.276013	15.480956
Au	17.507041	-3.235112	15.409843
Au	20.389596	-3.194210	15.338731
Au	10.336074	-2.081349	17.745878
Au	13.218630	-2.040447	17.674766
Au	16.101185	-1.999545	17.603653
Au	18.983741	-1.958644	17.532541
Au	11.812774	-0.804881	19.868576
Au	14.695329	-0.763979	19.797463
Au	17.577885	-0.723077	19.726350
Au	13.289474	0.471588	21.991273
Au	16.172029	0.512489	21.920160
Au	14.766173	1.748056	24.113970

46_FHI-aims_Junction_Si2.xyz /// -39744281.998911940 eV

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Au	6.56827730	18.74501675	2.50442517
Au	3.92298203	18.55915546	1.91861850

Au	4.78139831	19.65830219	4.40089417
Au	5.31291929	21.07416410	1.70633732
Au	1.25907900	18.46363900	1.29556700
Au	2.10462300	19.55080100	3.82914000
Au	2.95016700	20.63796200	6.36271300
Au	2.62336100	21.00239700	1.39200400
Au	3.46890400	22.08955800	3.92557600
Au	3.98764200	23.54115500	1.48843900
Au	4.83318600	24.62831700	4.02201300
Au	-1.546183	18.358416	0.635802
Au	-0.700639	19.445578	3.169375
Au	0.144904	20.532739	5.702948
Au	0.990448	21.619901	8.236521
Au	-0.181901	20.897174	0.732238
Au	0.663642	21.984336	3.265811
Au	1.509186	23.071498	5.799384
Au	1.182380	23.435932	0.828675
Au	2.027924	24.523093	3.362247
Au	2.546662	25.974690	0.925111
Au	0.336837	22.348770	-1.704898
Au	-4.351445	18.253193	-0.023962
Au	-3.505902	19.340355	2.509610
Au	-2.660358	20.427517	5.043183
Au	-1.814814	21.514678	7.576756
Au	-0.969271	22.601840	10.110329
Au	-2.987164	20.791951	0.072473
Au	-2.141620	21.879113	2.606047
Au	-1.296077	22.966274	5.139619
Au	-0.450533	24.053436	7.673192
Au	-1.622882	23.330709	0.168909
Au	-0.777339	24.417871	2.702483
Au	0.068205	25.505033	5.236056
Au	-0.258600	25.869467	0.265346
Au	0.586943	26.956628	2.798918
Au	1.105681	28.408225	0.361782
S	8.83976200	17.92705607	2.47522081
Si	9.11054337	9.15170047	8.82354382
C	7.37063182	8.49485913	11.02224936
C	9.09424726	7.63918328	7.68919080
C	8.16447747	6.59064158	7.82024841
H	7.39925063	6.63903452	8.59887766
C	8.17828454	5.49603923	6.95281199
C	9.12693186	5.40096464	5.91625415
C	10.06454316	6.44497329	5.78641514
H	10.83035048	6.38658194	5.01043102
C	10.04288414	7.53871471	6.64976970

C	10.62620553	9.85736927	11.17426425
C	10.56530226	9.02617328	10.03641052
C	11.56792326	8.04763600	9.89739013
H	11.55800659	7.38009272	9.03287303
C	12.56878132	7.89001550	10.85728617
C	12.61086966	8.70909920	12.00063201
C	11.62876956	9.70935295	12.13305107
H	11.61762164	10.34053277	13.02391017
C	5.40365167	10.35943028	10.38412737
C	9.21653613	10.67471243	7.69736145
C	9.93252621	11.84226258	8.01964987
H	10.54141375	11.87436548	8.92638600
C	9.89660110	12.96818873	7.19388236
C	9.13917023	12.97162942	6.00723425
C	8.43014687	11.80247638	5.67361980
H	7.81371780	11.78267092	4.77279239
C	8.47223853	10.68089967	6.49993059
C	5.24814706	9.57942210	11.54630893
C	6.25022017	8.63312285	11.84112781
H	6.17179412	8.03265675	12.74954009
C	7.54067356	9.28906752	9.86886778
C	6.52550219	10.21760260	9.56698949
H	6.61499375	10.85171938	8.68201510
C	9.13955744	4.25321990	4.98193821
C	9.45530779	4.42849198	3.62296529
C	9.47831302	3.35538567	2.73169927
C	9.18727667	2.05693124	3.18071533
C	8.86694420	1.86704153	4.54023824
C	8.84138948	2.94533186	5.41730499
H	8.64828119	0.86275142	4.90862559
H	8.61635194	2.76655189	6.47023303
H	9.71480098	3.54252034	1.68489481
H	9.66028291	5.43118330	3.24340010
S	9.18779770	0.61522263	2.15903781
C	9.68397445	1.24604990	0.53515285
H	9.70585321	0.36658705	-0.12011677
H	10.68560997	1.69325983	0.56517597
H	8.95282712	1.96311728	0.14027373
C	4.08857417	9.76925645	12.44563726
C	3.49360473	8.68316060	13.12059602
C	2.41687983	8.86786604	13.98004657
C	1.89255515	10.15693097	14.20498822
C	3.55127913	11.04837552	12.67386893
C	2.47421932	11.24731758	13.53825646
H	2.10293680	12.25918590	13.69620151
H	3.86569874	7.67171941	12.94792169

H	4.00497058	11.91612264	12.19166599
H	1.96851772	8.00731025	14.48062681
S	0.53390343	10.27175438	15.32809497
C	0.14622620	12.04108538	15.35257110
H	-0.69993913	12.13879150	16.04372131
H	-0.16049677	12.40033644	14.36213352
H	0.98726133	12.63315876	15.73495515
C	13.62898255	8.49606304	13.05607645
C	14.01917451	7.19711110	13.42629236
C	14.21649881	9.57835136	13.74221467
C	15.15038535	9.37358984	14.75323954
C	15.52024600	8.06632274	15.10927367
C	14.95229488	6.97557849	14.44082637
H	15.21276255	5.95208633	14.70610381
H	13.56027869	6.33717680	12.93622917
H	13.95055749	10.59973907	13.46643891
H	15.58888852	10.22857639	15.27076350
C	16.90826860	6.11386314	16.63545036
H	17.61985040	5.99734582	17.46066680
H	17.31524810	5.64724252	15.73014956
H	15.94631920	5.67295302	16.91742116
C	9.07761340	14.16341227	5.12940176
C	9.03521816	14.02817573	3.72989779
C	8.95084549	15.13954769	2.89042332
C	8.91621930	16.42499439	3.44448106
C	8.96504561	16.58580130	4.83911550
C	9.04149805	15.46736318	5.66408217
H	9.08982296	13.03428931	3.28338724
H	8.92144948	14.98825660	1.81239973
H	8.93047917	17.58449891	5.27784345
H	9.04791144	15.60690962	6.74588566
C	9.10249886	17.35171257	0.77083898
H	9.10000509	18.26140015	0.15945658
H	8.29699178	16.68917088	0.43767354
H	10.08027274	16.85960088	0.70130148
H	10.48564458	13.84814542	7.45986003
H	7.90848503	9.79167672	6.20740249
H	10.77930898	8.33430458	6.50571483
H	7.41844814	4.71898488	7.05760344
H	4.62861060	11.07829174	10.11149710
H	8.14398078	7.77737669	11.30909280
H	9.85026837	10.60874074	11.34219192
H	13.33487066	7.12531981	10.71346835
S	16.76455706	7.90907675	16.38682783
Au	15.80513679	8.74622654	18.43690952
Au	13.76456405	8.33270421	20.19909095

Au	16.43925904	8.50939294	21.13290154
Au	15.04680902	10.91058142	19.92905694
Au	11.68903200	8.04265000	21.93560900
Au	14.39182600	8.16719400	22.93323100
Au	17.09462100	8.29173700	23.93085300
Au	13.14828700	10.52805500	21.83970400
Au	15.85108100	10.65259800	22.83732500
Au	14.60754200	13.01345900	21.74379800
Au	17.31033600	13.13800200	22.74142000
Au	9.487128	7.733372	23.771861
Au	12.189922	7.857915	24.769483
Au	14.892716	7.982458	25.767104
Au	17.595510	8.107002	26.764726
Au	10.946382	10.218776	23.675955
Au	13.649177	10.343319	24.673577
Au	16.351971	10.467862	25.671199
Au	12.405637	12.704180	23.580050
Au	15.108431	12.828723	24.577672
Au	13.864892	15.189584	23.484145
Au	17.811225	12.953267	25.575294
Au	7.285224	7.424093	25.608113
Au	9.988017	7.548636	26.605734
Au	12.690811	7.673180	27.603356
Au	15.393606	7.797723	28.600978
Au	18.096399	7.922266	29.598600
Au	8.744478	9.909497	25.512207
Au	11.447272	10.034041	26.509829
Au	14.150066	10.158584	27.507451
Au	16.852860	10.283127	28.505073
Au	10.203732	12.394901	25.416302
Au	12.906527	12.519445	26.413924
Au	15.609321	12.643988	27.411546
Au	11.662988	14.880306	25.320397
Au	14.365781	15.004849	26.318019
Au	13.122242	17.365710	25.224492

47_FHI-aims_Junction_Si3.xyz /// -39769424.579884693 eV

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Au	5.79484207	22.48517401	0.52781031
Au	3.17110188	22.16463610	-0.16701899
Au	3.89986675	23.12615401	2.40833655
Au	4.39178718	24.77732302	-0.13353820
Au	0.53446300	21.93539000	-0.87993800
Au	1.25788400	22.87857100	1.74740500

Au	1.98130500	23.82175300	4.37474700
Au	1.71299300	24.54773700	-0.55967500
Au	2.43641400	25.49091800	2.06766700
Au	2.89152200	27.16008400	-0.23941300
Au	3.61494300	28.10326600	2.38793000
Au	-2.244736	21.686809	-1.608027
Au	-1.521315	22.629990	1.019316
Au	-0.797895	23.573171	3.646657
Au	-0.074473	24.516353	6.274000
Au	-1.066207	24.299156	-1.287765
Au	-0.342786	25.242337	1.339578
Au	0.380635	26.185519	3.966920
Au	0.112322	26.911503	-0.967502
Au	0.835743	27.854684	1.659840
Au	1.290851	29.523850	-0.647240
Au	-0.611099	25.968322	-3.594845
Au	-5.023936	21.438228	-2.336116
Au	-4.300515	22.381409	0.291226
Au	-3.577094	23.324590	2.918568
Au	-2.853673	24.267772	5.545911
Au	-2.130252	25.210952	8.173253
Au	-3.845407	24.050575	-2.015854
Au	-3.121986	24.993756	0.611489
Au	-2.398565	25.936937	3.238831
Au	-1.675144	26.880118	5.866173
Au	-2.666878	26.662922	-1.695592
Au	-1.943457	27.606103	0.931751
Au	-1.220036	28.549284	3.559094
Au	-1.488348	29.275269	-1.375329
Au	-0.764927	30.218450	1.252013
Au	-0.309819	31.887616	-1.055067
S	8.07207698	21.66811580	0.42582503
Si	9.16173241	8.89991472	8.54194082
C	7.51448005	8.23299359	10.82191676
C	9.11983987	7.34926389	7.45780394
C	8.33061739	6.23577747	7.80593327
H	7.67498200	6.28761770	8.67838538
C	8.34808293	5.06563815	7.04656980
C	9.15636144	4.95631551	5.89878371
C	9.93660540	6.07165169	5.53636951
H	10.58714660	6.01099818	4.66146263
C	9.91702215	7.24025401	6.29965276
C	10.68853395	9.55191126	10.90471758
C	10.67295260	8.83512601	9.69026045
C	11.80259805	8.04806263	9.39371452
H	11.83394715	7.47029805	8.46688947

C	12.88771420	7.97273908	10.26787988
C	12.89017955	8.67738005	11.48732478
C	11.76936542	9.47698593	11.78400443
H	11.72308134	10.01144842	12.73478445
C	5.44921833	9.98358543	10.17573734
C	9.19550702	10.44053019	7.43629216
C	9.85563281	11.62008620	7.83151218
H	10.46707007	11.62163784	8.73730911
C	9.75285714	12.79647147	7.08769139
C	8.98491308	12.84323146	5.90810854
C	8.34628318	11.65972772	5.49121875
H	7.73093815	11.66916819	4.58911177
C	8.44924855	10.48633434	6.24075803
C	5.35624816	9.23398805	11.36388662
C	6.40600693	8.34315852	11.66219086
H	6.37501303	7.76576813	12.58832920
C	7.62430896	9.00111087	9.64388693
C	6.55899924	9.87005495	9.33858196
H	6.59932135	10.48099889	8.43388726
C	9.18337622	3.70730711	5.10269025
C	9.27381830	3.73347652	3.69766806
C	9.29739672	2.55495729	2.95471520
C	9.23875503	1.29392573	3.58112923
C	9.15289237	1.26980085	4.98741336
C	9.12170974	2.44766297	5.72967825
H	9.14908064	0.31110915	5.50886958
H	9.09087473	2.39192142	6.81930172
H	9.32356362	2.61271207	1.86513846
H	9.28486388	4.69308773	3.17754375
C	4.21293613	9.40999424	12.28829628
C	3.67454395	8.33095248	13.01503575
C	2.61647690	8.51521946	13.90304641
C	3.63954450	10.68099447	12.48489806
C	2.58401466	10.86524764	13.37316751
H	2.15226900	11.86078728	13.48955314
H	4.08307315	7.32884723	12.87189401
H	4.04340762	11.54168750	11.94917084
H	2.23696986	7.66059693	14.46601793
C	14.02103877	8.56226564	12.43874758
C	14.72736926	7.35249946	12.58633860
C	14.42155755	9.65011957	13.23884277
C	15.47548380	9.53340708	14.14168834
C	16.18151914	8.32343015	14.28775720
C	15.78220803	7.23515745	13.48804830
H	16.31696641	6.28645207	13.55874223
H	14.43174979	6.48226894	11.99827842

H	13.90715809	10.60756284	13.14261812
H	15.74027916	10.39146089	14.76188847
C	8.84227440	14.10334179	5.13967469
C	8.83000462	14.10869115	3.73141684
C	8.69277993	15.29668094	3.01570494
C	8.55836797	16.53388043	3.67579930
C	8.56255809	16.52752709	5.08434938
C	8.70304219	15.34021103	5.79907228
H	8.96800743	13.17125073	3.18988636
H	8.73027540	15.26822296	1.92526303
H	8.41387013	17.46170712	5.62867369
H	8.66548938	15.36471301	6.88945279
C	17.30460283	8.19987563	15.24521803
C	17.55216754	6.99107612	15.92929410
C	18.61798341	6.86478369	16.81441219
C	19.46579400	7.95943650	17.05180257
C	19.23319847	9.17415540	16.39629000
C	18.16743854	9.28180105	15.50113905
H	16.88548682	6.14051958	15.78209710
H	18.78593436	5.91855479	17.33193311
H	19.87674399	10.03697452	16.56183131
H	18.02222629	10.22430590	14.97144886
C	0.94002303	9.99976444	15.06283360
C	-0.07801588	9.03911185	15.23498381
C	-1.12860308	9.24807705	16.12109395
C	-1.20157028	10.43338396	16.88022252
C	-0.18939398	11.39413233	16.72666585
C	0.85741101	11.17494392	15.83081590
C	2.05015677	9.78885800	14.10820378
H	-0.06362342	8.12541196	14.63806154
H	-1.91254684	8.49445314	16.21965059
H	-0.20280961	12.31498732	17.30857680
H	1.64478976	11.92645695	15.74979059
C	8.42756670	17.80002858	2.91752515
C	7.71856140	17.85817149	1.69933793
C	7.61295953	19.04389852	0.97867911
C	8.21278514	20.21755546	1.46555977
C	8.91112799	20.18833066	2.67839759
C	9.01511921	18.98939662	3.38621438
H	7.22198544	16.96410136	1.31985425
H	7.05330438	19.06237461	0.04169908
H	9.38958336	21.08213633	3.07620020
H	9.59197578	18.97604106	4.31212517
C	9.26828553	0.04031446	2.79560613
C	8.53972206	-1.09320798	3.19857204
C	8.56831490	-2.28253094	2.46880115

C	9.33980699	-2.37605596	1.29929608
C	10.07354011	-1.24730427	0.88212409
C	10.03386352	-0.06738785	1.61561758
H	7.91021524	-1.03947894	4.08865850
H	7.97589087	-3.12918846	2.81404686
H	10.68940294	-1.30624110	-0.01757907
H	10.63645950	0.78031257	1.28482843
S	9.46600305	-3.81727344	0.28417479
C	8.49215975	-5.05793986	1.17550303
H	8.58512184	-5.97578998	0.58205127
H	7.43251100	-4.77841735	1.23248442
H	8.89742051	-5.24029437	2.17894791
C	21.81601204	9.19280506	18.07442937
H	22.66928236	9.02372836	18.74141119
H	21.25044233	10.06352731	18.42205524
H	22.17166803	9.32580373	17.04562244
C	9.03860982	22.93449391	1.29923107
H	8.95234862	23.83540687	0.68106972
H	10.08806211	22.62055680	1.35085793
H	8.63091290	23.13606394	2.29531601
S	-2.58402338	10.59275832	17.96961011
C	-2.37026755	12.23939665	18.69456210
H	-3.23082773	12.37261604	19.36153950
H	-2.38998518	13.02246296	17.92604019
H	-1.44910899	12.30384480	19.28759798
H	8.32537260	7.55926423	11.11116337
H	4.63571377	10.65726497	9.90002686
H	7.92609338	9.59207822	5.89238945
H	10.29237062	13.68832288	7.41285399
H	7.70197290	4.23204720	7.32873628
H	10.53834831	8.08305719	5.98451335
H	13.75339608	7.36655047	9.99408248
H	9.82321316	10.15529689	11.19024314
S	20.82821268	7.67129745	18.17521441
Au	19.89336649	7.70290830	20.41360625
Au	17.95126896	7.01190459	22.19345131
Au	20.65671466	7.12200251	23.00731782
Au	19.10872459	9.67261391	22.18051224
Au	15.97455600	6.45048100	23.99670800
Au	18.72734200	6.49919200	24.85441300
Au	21.48012700	6.54790200	25.71211800
Au	17.39313400	8.95652000	24.14923100
Au	20.14591800	9.00523100	25.00693600
Au	18.81171100	11.46255900	24.30175400
Au	21.56449600	11.51127000	25.15945900
Au	13.883789	5.859424	25.892810

Au	16.636574	5.908135	26.750515
Au	19.389359	5.956845	27.608220
Au	22.142144	6.005556	28.465925
Au	15.302366	8.365463	26.045332
Au	18.055151	8.414174	26.903038
Au	20.807937	8.462884	27.760743
Au	16.720944	10.871502	26.197855
Au	19.473728	10.920213	27.055560
Au	18.139521	13.377541	26.350378
Au	22.226514	10.968923	27.913265
Au	11.793022	5.268367	27.788911
Au	14.545806	5.317078	28.646616
Au	17.298592	5.365788	29.504321
Au	20.051377	5.414499	30.362027
Au	22.804162	5.463210	31.219731
Au	13.211599	7.774406	27.941434
Au	15.964384	7.823117	28.799139
Au	18.717169	7.871827	29.656844
Au	21.469954	7.920538	30.514549
Au	14.630176	10.280445	28.093957
Au	17.382961	10.329156	28.951662
Au	20.135747	10.377866	29.809367
Au	16.048753	12.786484	28.246480
Au	18.801538	12.835195	29.104184
Au	17.467330	15.292523	28.399002

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Au	4.65114188	11.18745011	14.20952193
Au	3.69222859	12.21494298	16.60050075
Au	6.47454060	12.04448548	16.08644834
Au	4.69293788	13.91029999	14.49512264
Au	2.74466900	13.36028900	18.92048600
Au	5.57926100	13.15388300	18.43228100
Au	8.41385300	12.94747700	17.94407500
Au	3.98321300	15.00350200	16.90015900
Au	6.81780400	14.79709600	16.41195400
Au	5.22175600	16.64671500	14.87983300
Au	8.05634700	16.44030900	14.39162800
Au	1.785576	14.555993	21.363084
Au	4.620168	14.349587	20.874879
Au	7.454758	14.143182	20.386674
Au	10.289350	13.936776	19.898469
Au	3.024118	16.199206	19.342758

Au	5.858710	15.992800	18.854553
Au	8.693302	15.786394	18.366348
Au	4.262662	17.842419	17.322432
Au	7.097253	17.636013	16.834227
Au	5.501205	19.485632	15.302106
Au	1.428070	18.048825	17.810637
Au	0.826482	15.751697	23.805683
Au	3.661073	15.545292	23.317478
Au	6.495665	15.338886	22.829273
Au	9.330257	15.132480	22.341068
Au	12.164848	14.926074	21.852863
Au	2.065025	17.394911	21.785357
Au	4.899617	17.188505	21.297152
Au	7.734208	16.982099	20.808947
Au	10.568800	16.775693	20.320742
Au	3.303568	19.038124	19.765031
Au	6.138160	18.831718	19.276826
Au	8.972751	18.625312	18.788620
Au	4.542112	20.681337	17.744704
Au	7.376702	20.474931	17.256499
Au	5.780654	22.324550	15.724378
S	4.30396440	9.23840227	12.79755369
C	9.02528978	8.78470436	8.84522812
C	7.69427120	7.96461770	10.86859606
C	9.05013626	7.47080806	8.01578603
C	8.10592366	6.44460808	8.12990605
H	7.30884170	6.51296050	8.86984558
C	8.13498339	5.32100098	7.28951072
C	9.11882855	5.21295982	6.30432327
C	10.08657632	6.22555138	6.18031047
H	10.85714510	6.15947702	5.41007177
C	10.04313599	7.33036472	7.02173234
C	10.34848302	9.96983752	10.67529143
C	10.26119536	8.88752881	9.78001916
C	11.27586416	7.91856163	9.84258534
H	11.24619942	7.04410980	9.19287975
C	12.33667632	8.03277157	10.74153161
C	12.42038815	9.12703521	11.62087652
C	11.40632221	10.09997186	11.57467933
H	11.42479715	10.95892968	12.24482718
C	5.78604831	9.97321725	10.63701980
C	8.99247013	9.92000725	7.78498052
C	9.94866718	10.94461873	7.70583121
H	10.76494015	10.98792559	8.42651462
C	9.88873266	11.91661948	6.70582579
C	8.86353511	11.89846693	5.74311521

C	7.90784135	10.86902770	5.80350602
H	7.10474044	10.80877678	5.06961498
C	7.98485110	9.90003396	6.80336143
C	5.69626235	9.05160178	11.68779307
C	6.65954695	8.03969368	11.80213073
H	6.63017749	7.31831196	12.61747711
C	7.79652951	8.86814439	9.79447998
C	6.82471144	9.87800818	9.70791850
H	6.88082108	10.62226375	8.91479446
S	13.80443233	9.16165716	12.71783956
S	8.88546369	13.18153297	4.52797059
C	4.45225381	7.82176815	13.92643773
H	3.61312372	7.92442006	14.62408909
H	4.34703570	6.88976376	13.35754879
H	5.39406619	7.84836150	14.48465535
C	7.42936057	12.82982458	3.50771380
H	7.41265396	13.62303672	2.75021315
H	7.51273386	11.85902006	3.00265433
H	6.50418078	12.88144188	4.09573194
C	7.64889205	2.97993814	5.34962371
H	7.64012958	2.20606680	4.57343341
H	7.62687036	2.50579462	6.33632559
H	6.79512448	3.65417352	5.21010746
C	13.51859255	10.64095826	13.72522839
H	14.35945318	10.67338834	14.42900985
H	13.53111204	11.55423400	13.11682913
H	12.58256805	10.56824977	14.29314758
H	8.46088681	7.19924922	11.00234070
H	5.05499296	10.77908737	10.54737908
H	13.10451977	7.25671951	10.76524848
H	10.77994280	8.12309455	6.88403457
H	7.37220651	4.55304249	7.41317645
H	7.24173648	9.09957572	6.81016190
H	10.65059503	12.69805638	6.67014980
H	9.56425332	10.72934561	10.68469281
S	9.18898513	3.90578865	5.08143316
Au	10.91411746	2.26412290	5.57241082
Au	11.36750753	-0.31084732	6.39387727
Au	13.01711122	0.83826673	4.43795990
Au	13.02050795	1.91652793	7.29640249
Au	11.88064500	-2.80906800	7.37111300
Au	13.57266600	-1.72181500	5.30452000
Au	15.26468600	-0.63456100	3.23792800
Au	13.66824500	-0.62712600	7.97067400
Au	15.36026500	0.46012700	5.90408200
Au	15.45584400	1.55481500	8.57023600

Au	17.14786400	2.64206900	6.50364400
Au	12.408138	-5.438274	8.431720
Au	14.100158	-4.351020	6.365127
Au	15.792178	-3.263767	4.298535
Au	17.484198	-2.176513	2.231943
Au	14.195737	-3.256332	9.031282
Au	15.887757	-2.169078	6.964689
Au	17.579778	-1.081825	4.898097
Au	15.983337	-1.074390	9.630843
Au	17.675357	0.012863	7.564252
Au	17.770936	1.107551	10.230406
Au	19.367377	1.100117	5.497659
Au	12.935631	-8.067479	9.492327
Au	14.627650	-6.980226	7.425735
Au	16.319671	-5.892972	5.359142
Au	18.011691	-4.805718	3.292550
Au	19.703711	-3.718465	1.225958
Au	14.723230	-5.885538	10.091889
Au	16.415250	-4.798284	8.025297
Au	18.107270	-3.711030	5.958705
Au	19.799290	-2.623776	3.892112
Au	16.510829	-3.703596	10.691451
Au	18.202849	-2.616342	8.624859
Au	19.894870	-1.529088	6.558266
Au	18.298429	-1.521654	11.291013
Au	19.990449	-0.434400	9.224421
Au	20.086028	0.660288	11.890575

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Au	14.99521874	8.89929927	18.41315919
Au	12.79737444	8.40848445	19.94225718
Au	15.35162948	8.60791017	21.15460993
Au	14.03360286	11.02224602	19.87030277
Au	10.56808900	8.02814800	21.45465700
Au	13.14641000	8.17110100	22.73827700
Au	15.72473100	8.31405500	24.02189700
Au	11.98105100	10.53905200	21.57612300
Au	14.55937100	10.68200600	22.85974300
Au	13.39401200	13.04995700	21.69759000
Au	15.97233400	13.19291000	22.98121000
Au	8.189589	7.634113	23.036850
Au	10.767911	7.777067	24.320470
Au	13.346231	7.920020	25.604090

Au	15.924553	8.062973	26.887711
Au	9.602551	10.145018	23.158316
Au	12.180872	10.287971	24.441937
Au	14.759194	10.430924	25.725557
Au	11.015513	12.655922	23.279783
Au	13.593834	12.798875	24.563403
Au	12.428475	15.166827	23.401250
Au	8.437192	12.512969	21.996163
Au	5.811090	7.240079	24.619043
Au	8.389411	7.383032	25.902663
Au	10.967732	7.525986	27.186284
Au	13.546054	7.668939	28.469904
Au	16.124374	7.811892	29.753524
Au	7.224052	9.750983	24.740510
Au	9.802373	9.893937	26.024130
Au	12.380694	10.036890	27.307750
Au	14.959015	10.179843	28.591371
Au	8.637013	12.261888	24.861976
Au	11.215335	12.404841	26.145597
Au	13.793656	12.547794	27.429217
Au	10.049976	14.772792	24.983443
Au	12.628296	14.915745	26.267063
Au	11.462937	17.283696	25.104909
S	16.19413116	8.36703026	16.38620709
C	8.96746730	8.67413902	8.78698733
C	7.49379145	7.81314710	10.68365294
C	8.89423447	7.42848385	7.86112686
C	7.80183050	6.55009857	7.82856404
H	6.97328717	6.68505830	8.52307892
C	7.72589281	5.52082060	6.88424608
C	8.73720461	5.33114882	5.92901240
C	9.84402198	6.20308052	5.97115547
H	10.66230932	6.07271349	5.26043426
C	9.91547605	7.22725149	6.91088418
C	10.29154929	9.63749553	10.73730853
C	10.15819200	8.60965029	9.78195227
C	11.05464086	7.53507991	9.86333787
H	10.98491076	6.71181442	9.15253875
C	12.03662144	7.48338492	10.85951616
C	12.16425318	8.50599400	11.81406907
C	11.27263429	9.59409774	11.72246965
H	11.31266947	10.39027273	12.46787925
C	5.76863550	9.98308002	10.56516199
C	9.08307835	9.87488796	7.80887040
C	10.14074596	10.79420902	7.81388548
H	10.94075858	10.70398925	8.54849112

C	10.21055423	11.82373716	6.86842555
C	9.22604292	11.97692634	5.87790048
C	8.16761255	11.04567985	5.87034428
H	7.37074161	11.14258662	5.13088838
C	8.10479361	10.01789331	6.80506765
C	5.54327698	9.00119616	11.54413206
C	6.43171395	7.90701189	11.57778485
H	6.31421698	7.14212267	12.34754033
C	7.71471698	8.79528762	9.69801507
C	6.83204489	9.88308959	9.66254144
H	6.96929217	10.67475525	8.92664068
C	8.62943093	4.28055623	4.88900344
C	9.03941320	4.53358321	3.56644885
C	8.94505443	3.55844399	2.57310395
C	8.45008505	2.28791682	2.89319218
C	8.02623577	2.01429807	4.20403960
C	8.10916092	3.00329679	5.18127113
H	7.65039615	1.02262483	4.46177107
H	7.79998188	2.76848997	6.20090526
H	9.25333616	3.80312903	1.55748835
H	9.41159432	5.52380524	3.29941644
C	9.45460367	1.46850651	0.37109214
H	9.49241484	0.61666136	-0.31785083
H	10.45511377	1.66881181	0.77248024
H	9.05136032	2.33985270	-0.15466631
C	4.43693216	9.11865640	12.52003177
C	3.72224708	7.98443681	12.95802891
C	2.69431616	8.09176282	13.88755085
C	2.34043852	9.34650250	14.42347687
C	4.06972911	10.36454075	13.05796009
C	3.04195968	10.48493093	13.99460726
H	2.80225621	11.46996713	14.39355233
H	3.96167875	7.00327912	12.54403001
H	4.61959115	11.26030475	12.76319802
H	2.15255227	7.19779832	14.20296491
S	1.02419969	9.35536332	15.60262555
C	0.91487872	11.09040850	16.11188987
H	0.12197714	11.11683609	16.86937246
H	0.62928132	11.74173530	15.27619963
H	1.85246248	11.43451691	16.56657804
C	13.16382527	8.43800996	12.90659022
C	13.48148316	7.21624847	13.52917241
C	13.80766177	9.60006113	13.38045025
C	14.72245990	9.54699497	14.42802737
C	15.01239620	8.31797970	15.04234456
C	14.38829416	7.14936059	14.58818485

H	14.58469916	6.18696412	15.05919932
H	12.98112780	6.30180533	13.20706190
H	13.60859983	10.55955967	12.90122225
H	15.21784330	10.45826758	14.76732996
C	16.70035031	6.63122045	16.58330342
H	17.47316671	6.64686735	17.36037243
H	17.12605682	6.27172950	15.63896254
H	15.86991491	5.99993472	16.91439786
C	9.28900565	13.06130809	4.87237876
C	8.87074423	12.84613071	3.54710583
C	8.90211626	13.86406589	2.59336190
C	9.35390893	15.14667685	2.94338326
C	9.78441480	15.37460739	4.26609443
C	9.75362207	14.35037167	5.20622146
H	8.53522323	11.85280480	3.24339052
H	8.57846238	13.64613907	1.57626145
H	10.12822988	16.36891343	4.55830509
H	10.06280078	14.56303938	6.23124371
S	9.42703238	16.52324245	1.83721800
C	8.70037271	15.87989559	0.30682788
H	8.70140349	16.72764717	-0.38921029
H	7.66604501	15.54849663	0.46312070
H	9.30493890	15.07009237	-0.12062895
H	11.06782567	12.49954223	6.88495441
H	7.27678392	9.30852753	6.75538379
H	10.76999747	7.90613520	6.88963000
H	6.83597809	4.88879945	6.86156905
H	5.09111433	10.83572623	10.49140654
H	8.18737429	6.97478428	10.77325543
H	9.58412335	10.46825209	10.73303510
H	12.72166189	6.63348228	10.88044979
S	8.36771071	0.93321685	1.72806730
Au	6.19729295	0.77953423	0.64633176
Au	4.93579623	-0.15985614	-1.61931115
Au	3.67572064	-0.30765264	0.91042894
Au	4.26512303	2.39272366	-0.44378990
Au	3.61068900	-0.96404000	-3.89862800
Au	2.32250600	-1.16949500	-1.32681400
Au	1.03432300	-1.37495000	1.24500100
Au	2.78866800	1.42184700	-2.50303400
Au	1.50048600	1.21639200	0.06878000
Au	1.96664800	3.80773400	-1.10744100
Au	0.67846500	3.60227900	1.46437400
Au	2.214212	-1.794264	-6.281156
Au	0.926030	-1.999719	-3.709341
Au	-0.362153	-2.205174	-1.137527

Au	-1.650336	-2.410629	1.434288
Au	1.392192	0.591623	-4.885563
Au	0.104009	0.386168	-2.313748
Au	-1.184174	0.180713	0.258067
Au	0.570171	2.977510	-3.489968
Au	-0.718012	2.772055	-0.918154
Au	-0.251850	5.363397	-2.094375
Au	-2.006195	2.566600	1.653660
Au	0.817736	-2.624488	-8.663683
Au	-0.470447	-2.829943	-6.091869
Au	-1.758630	-3.035398	-3.520055
Au	-3.046813	-3.240853	-0.948240
Au	-4.334995	-3.446308	1.623574
Au	-0.004285	-0.238601	-7.268090
Au	-1.292468	-0.444056	-4.696275
Au	-2.580651	-0.649511	-2.124461
Au	-3.868834	-0.854966	0.447353
Au	-0.826306	2.147286	-5.872497
Au	-2.114489	1.941831	-3.300682
Au	-3.402672	1.736376	-0.728867
Au	-1.648327	4.533173	-4.476902
Au	-2.936509	4.327718	-1.905089
Au	-2.470347	6.919060	-3.081309

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Au	17.67809286	8.12829604	22.07969069
Au	20.38831953	8.28627689	22.87558777
Au	18.85759214	10.75339515	21.67590069
Au	15.69280700	7.86783400	23.94929100
Au	18.44947800	7.97698200	24.78876200
Au	21.20614900	8.08613100	25.62823200
Au	17.16566800	10.33858000	23.74447000
Au	19.92233800	10.44772800	24.58394000
Au	18.63852900	12.80932600	23.53964800
Au	21.39519900	12.91847400	24.37911900
Au	13.597539	7.596707	25.911993
Au	16.354210	7.705855	26.751463
Au	19.110879	7.815004	27.590934
Au	21.867550	7.924152	28.430404
Au	15.070399	10.067453	25.707171
Au	17.827070	10.176601	26.546642
Au	20.583741	10.285750	27.386112

Au	16.543260	12.538199	25.502350
Au	19.299930	12.647347	26.341820
Au	18.016121	15.008945	25.297528
Au	13.786589	12.429050	24.662880
Au	11.502270	7.325580	27.874695
Au	14.258940	7.434728	28.714165
Au	17.015611	7.543877	29.553635
Au	19.772282	7.653025	30.393106
Au	22.528952	7.762174	31.232576
Au	12.975131	9.796326	27.669873
Au	15.731802	9.905474	28.509344
Au	18.488472	10.014623	29.348814
Au	21.245142	10.123771	30.188284
Au	14.447991	12.267072	27.465051
Au	17.204662	12.376220	28.304522
Au	19.961333	12.485369	29.143993
Au	15.920852	14.737818	27.260230
Au	18.677522	14.846966	28.099700
Au	17.393713	17.208564	27.055409
S	20.60741826	8.30137766	18.02179278
C	9.13200717	9.12495728	8.65078035
C	7.75036352	8.36458615	10.66211580
C	9.01783265	7.86859900	7.74330244
C	8.08180631	6.84705991	7.95613385
H	7.33954830	6.94143150	8.74731296
C	8.06687110	5.69973891	7.15978932
C	8.98376106	5.52300878	6.11044367
C	9.89498707	6.56894784	5.86558218
H	10.62703680	6.46925368	5.06174047
C	9.90679132	7.71394172	6.66068089
C	10.49650296	9.89983879	10.67062428
C	10.37063236	9.00852873	9.58608571
C	11.37329983	8.04135386	9.43106617
H	11.31506315	7.31843132	8.61853771
C	12.45871176	7.97363046	10.30993933
C	12.58938654	8.86927391	11.38380676
C	11.57861208	9.83786479	11.54429797
H	11.61883576	10.52727595	12.38950906
C	5.79900193	10.29826093	10.28458507
C	9.25147079	10.36479823	7.72349463
C	10.20536533	11.37627795	7.90173361
H	10.95187493	11.29004236	8.69023190
C	10.23411499	12.50088458	7.07269656
C	9.31078757	12.66419640	6.02686312
C	8.37506351	11.63066063	5.82336494
H	7.63338102	11.72140657	5.02755655

C	8.35256556	10.50775985	6.64759627
C	5.65252491	9.40007107	11.35402606
C	6.65853435	8.42804601	11.52331538
H	6.60346188	7.73648312	12.36596458
C	7.88923295	9.25503616	9.57827157
C	6.89287927	10.22740655	9.41605644
H	6.96045470	10.95165232	8.60541228
C	8.99111806	4.27645617	5.31103691
C	9.21799130	4.28458633	3.92173836
C	9.21436503	3.10168232	3.18402953
C	8.99166453	1.85530663	3.80250638
C	8.77615501	1.84907133	5.19478669
C	8.77230334	3.03068304	5.93036965
H	8.64717231	0.89758871	5.71348442
H	8.63661556	2.98723067	7.01255617
H	9.34958438	3.14797772	2.10192412
H	9.35895676	5.23626867	3.40571857
C	4.50254811	9.47684099	12.28396778
C	3.91054113	8.31033122	12.80455718
C	2.84863965	8.37969512	13.70312831
C	3.97333427	10.71603234	12.69233776
C	2.91303060	10.78555893	13.59317858
H	2.51935825	11.76206481	13.88082083
H	4.28255429	7.33299945	12.49158054
H	4.41655990	11.63978727	12.31587135
H	2.42915065	7.45626675	14.10645671
C	13.73594771	8.79743790	12.31896406
C	14.30174072	7.56269102	12.69205415
C	14.29697297	9.96530995	12.87091274
C	15.37211722	9.90161175	13.75346768
C	15.93653083	8.66662777	14.12647210
C	15.37662239	7.49775048	13.57572445
H	15.80036085	6.52428247	13.82873429
H	13.87930143	6.63708857	12.29761589
H	13.89304463	10.93981025	12.59196894
H	15.76653248	10.82558062	14.17984300
C	9.31436829	13.88198119	5.18310568
C	9.01015948	13.83029714	3.80889726
C	8.99524310	14.98508801	3.02898048
C	9.28879657	16.24409186	3.58786752
C	9.59967638	16.29599515	4.96018103
C	9.60978955	15.14209377	5.73952839
H	8.81457616	12.86585594	3.33716309
H	8.79046240	14.90451499	1.95989294
H	9.79282698	17.26079281	5.43268703
H	9.81036041	15.22214924	6.80912312

C	17.07754022	8.60288999	15.06776850
C	17.18977214	7.56096871	16.01182149
C	18.25677311	7.50269076	16.90260628
C	19.24784182	8.49783904	16.87418346
C	19.15975886	9.54150061	15.94585595
C	18.08487095	9.58459193	15.05605137
H	16.41006055	6.80046331	16.07156588
H	18.30982565	6.69587578	17.63593493
H	19.91989777	10.31975620	15.89659525
H	18.04488432	10.38910816	14.32036809
C	1.22964006	9.69214439	15.11262181
C	0.17747634	8.75245783	15.11263613
C	-0.84521257	8.81132852	16.05250156
C	-0.85381818	9.81704122	17.04022671
C	0.18545962	10.76124139	17.05030840
C	1.20406087	10.69430609	16.09871229
C	2.33068597	9.61912033	14.12686362
H	0.14713660	7.97703438	14.34506937
H	-1.65290226	8.07717852	16.02203742
H	0.21762886	11.54620988	17.80500416
H	2.01724837	11.42081953	16.14712945
C	9.26503230	17.47561965	2.76652331
C	8.29398927	17.66460450	1.76202874
C	8.25091288	18.83367770	1.00855422
C	9.19663247	19.84718067	1.23241753
C	10.18106931	19.67599552	2.21344911
C	10.20264327	18.50488996	2.97171570
H	7.53496062	16.89902427	1.59515062
H	7.47421664	18.96760661	0.25365261
H	10.93982768	20.43781473	2.38827395
H	10.98716758	18.37592194	3.71897054
C	8.98330475	0.59355350	3.02976679
C	8.11786016	-0.46069333	3.37334515
C	8.10954293	-1.66424279	2.66767675
C	8.98086822	-1.85262310	1.58265357
C	9.84928405	-0.80233196	1.22228882
C	9.84589366	0.39360266	1.93157008
H	7.41267532	-0.33034955	4.19619488
H	7.41259015	-2.44695797	2.96506578
H	10.54113475	-0.93622390	0.38823926
H	10.55108008	1.17757708	1.64981358
S	9.07622345	-3.32668556	0.61210646
C	7.91161517	-4.45050925	1.42680360
H	7.97494469	-5.38851799	0.86170337
H	6.88160475	-4.07507685	1.37574672
H	8.20111273	-4.64177287	2.46803186

C	21.58908919	9.81444856	17.80342519
H	22.38828403	9.74846871	18.55054485
H	20.98533320	10.70880317	17.99103200
H	22.02791710	9.82561187	16.79863496
C	10.03940695	22.55957227	1.07674709
H	9.90757178	23.47912375	0.49488529
H	11.10153361	22.29536989	1.09254253
H	9.64222010	22.69634028	2.08981950
S	-2.19594348	9.78343520	18.18999008
C	-1.86105268	11.19124738	19.28040895
H	-2.68235063	11.19234686	20.00748129
H	-1.87282343	12.14029373	18.72947763
H	-0.91162605	11.06857986	19.81707208
H	8.52662066	7.62044919	10.84885719
H	5.03462029	11.05789825	10.11056134
H	7.61394619	9.72657649	6.45891141
H	11.00949912	13.25306412	7.22953543
H	7.30928105	4.93593143	7.34476569
H	10.63166271	8.50090058	6.44379608
H	13.22808241	7.21837144	10.13942100
H	9.71501090	10.64017215	10.85001991
S	9.04508265	21.30666848	0.20967727
Au	10.29032127	20.83246183	-1.80158368
Au	12.31254133	19.37633289	-2.90539660
Au	10.13871521	20.27944910	-4.48294388
Au	12.15307591	22.25904874	-3.26559087
Au	14.40265700	18.02284300	-4.02346100
Au	12.18590700	18.88227200	-5.65541000
Au	9.96915700	19.74170200	-7.28735900
Au	14.03857000	20.82452200	-4.60129300
Au	11.82182100	21.68395200	-6.23324100
Au	13.67448300	23.62620100	-5.17912500
Au	11.45773300	24.48563100	-6.81107400
Au	16.595417	16.577950	-5.215076
Au	14.378667	17.437380	-6.847025
Au	12.161918	18.296809	-8.478974
Au	9.945168	19.156239	-10.110923
Au	16.231330	19.379629	-5.792908
Au	14.014580	20.239059	-7.424857
Au	11.797830	21.098489	-9.056806
Au	15.867243	22.181309	-6.370740
Au	13.650493	23.040738	-8.002689
Au	15.503156	24.982988	-6.948572
Au	11.433743	23.900168	-9.634638
Au	18.788177	15.133057	-6.406692
Au	16.571427	15.992487	-8.038640

Au	14.354677	16.851917	-9.670589
Au	12.137927	17.711346	-11.302539
Au	9.921178	18.570776	-12.934487
Au	18.424090	17.934737	-6.984523
Au	16.207340	18.794166	-8.616473
Au	13.990590	19.653596	-10.248421
Au	11.773840	20.513026	-11.880370
Au	18.060003	20.736416	-7.562355
Au	15.843253	21.595846	-9.194304
Au	13.626503	22.455275	-10.826253
Au	17.695916	23.538095	-8.140187
Au	15.479166	24.397525	-9.772136
Au	17.331829	26.339774	-8.718019

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Au	-3.09056274	8.71671718	-6.66950561
Au	-5.66728912	8.39884528	-7.47927655
Au	-5.07602607	9.43931591	-4.89147071
Au	-4.44672744	11.00517677	-7.42858321
Au	-8.24814400	8.15358900	-8.31976500
Au	-7.68860000	9.16902200	-5.67937400
Au	-7.12905500	10.18445500	-3.03898300
Au	-7.08898100	10.77447700	-7.99860400
Au	-6.52943700	11.78991000	-5.35821400
Au	-5.92981900	13.39536500	-7.67744400
Au	-5.37027400	14.41079800	-5.03705300
Au	-10.976917	7.883381	-9.212315
Au	-10.417372	8.898814	-6.571924
Au	-9.857828	9.914247	-3.931534
Au	-9.298283	10.929680	-1.291143
Au	-9.817754	10.504269	-8.891155
Au	-9.258210	11.519702	-6.250764
Au	-8.698665	12.535135	-3.610373
Au	-8.658591	13.125157	-8.569994
Au	-8.099047	14.140590	-5.929604
Au	-7.499428	15.746045	-8.248833
Au	-9.218136	12.109724	-11.210384
Au	-13.705690	7.613174	-10.104864
Au	-13.146145	8.628606	-7.464474
Au	-12.586601	9.644039	-4.824084
Au	-12.027056	10.659472	-2.183693
Au	-11.467511	11.674905	0.456697
Au	-12.546527	10.234062	-9.783704

Au	-11.986982	11.249495	-7.143313
Au	-11.427438	12.264927	-4.502923
Au	-10.867893	13.280360	-1.862533
Au	-11.387364	12.854949	-9.462544
Au	-10.827819	13.870382	-6.822153
Au	-10.268275	14.885815	-4.181762
Au	-10.228201	15.475837	-9.141383
Au	-9.668656	16.491270	-6.500993
Au	-9.069038	18.096725	-8.820223
S	-0.83269973	7.86017620	-6.65943686
Si	-0.53923399	-0.98177114	-0.39339632
C	-2.26132259	-1.69367054	1.79935765
C	-0.54691266	-2.52259548	-1.49437649
C	-1.44093707	-3.58776585	-1.27394498
H	-2.18333247	-3.51500941	-0.47570837
C	-1.41709463	-4.73404647	-2.07064459
C	-0.49529143	-4.86423332	-3.12587279
C	0.39812006	-3.79978003	-3.35550051
H	1.13735420	-3.88276442	-4.15485009
C	0.36977793	-2.65499524	-2.55827718
C	0.95508587	-0.27375457	1.97779619
C	0.91307541	-1.08742642	0.82620846
C	1.92652474	-2.05451797	0.68363624
H	1.93580674	-2.70581795	-0.19317280
C	2.91114930	-2.22628677	1.65739431
C	2.92591595	-1.43488640	2.82106661
C	1.94177092	-0.43624598	2.95162265
H	1.91229326	0.17855461	3.85349685
C	-4.37184607	-0.03704063	1.05681668
C	-0.45508771	0.53850109	-1.52487003
C	0.24037319	1.71592157	-1.19102444
H	0.84052711	1.75358197	-0.27864153
C	0.19481156	2.84506375	-2.01132786
C	-0.55313248	2.84550793	-3.20464181
C	-1.23856375	1.66573149	-3.55150167
H	-1.84537539	1.63962528	-4.45873889
C	-1.18643152	0.53935515	-2.73073019
C	-4.50490983	-0.83103103	2.21109925
C	-3.42680699	-1.66465911	2.56561987
H	-3.49036349	-2.26829045	3.47321861
C	-2.12251787	-0.90011659	0.64152241
C	-3.20616704	-0.07275104	0.28974581
H	-3.14123150	0.55992791	-0.59857212
C	-0.46972448	-6.07981505	-3.97603990
C	-0.26310038	-5.98530355	-5.36565757
C	-0.24515666	-7.12848217	-6.16715267

C	-0.42936996	-8.39151827	-5.59546859
C	-0.63326237	-8.50096901	-4.21609807
C	-0.65512069	-7.35778595	-3.41470171
H	-0.76866708	-9.48325454	-3.76016026
H	-0.79170106	-7.45541210	-2.33619417
H	-0.09532498	-7.03191331	-7.24381971
H	-0.14503308	-5.00179023	-5.82411853
C	-5.73607407	-0.78098792	3.03694481
C	-6.27626086	-1.95142051	3.60332054
C	-7.43394864	-1.90050623	4.38217738
C	-8.07329092	-0.67847823	4.61527485
C	-6.39149533	0.44164339	3.27819592
C	-7.54653414	0.49251011	4.06059691
H	-8.03218819	1.45214408	4.24540964
H	-5.79786468	-2.91275876	3.40725411
H	-5.97260608	1.36375337	2.87130542
H	-7.84329596	-2.82045887	4.80300503
C	3.91091633	-1.68771044	3.89964905
C	4.27491976	-3.00414986	4.23567824
C	4.49241675	-0.63780364	4.63898986
C	5.40101503	-0.89090687	5.66327585
C	5.74396577	-2.21466175	5.98446591
C	5.17527628	-3.27362507	5.26704846
H	5.41074601	-4.30934923	5.50718592
H	3.81805800	-3.83999664	3.70393642
H	4.25055869	0.39640944	4.38959139
H	5.84875232	-0.06052040	6.21199477
C	7.35180197	-4.20098040	7.21640044
H	8.10678314	-4.35333202	7.99617340
H	7.78152354	-4.42659272	6.23291369
H	6.48261336	-4.83198836	7.42859522
C	-0.62530514	4.04771886	-4.06924000
C	-0.67216426	3.93538888	-5.47107325
C	-0.75290461	5.06078180	-6.29315182
C	-0.77841133	6.33802405	-5.71932066
C	-0.73233579	6.47545950	-4.32212494
C	-0.66077594	5.34397908	-3.51509362
H	-0.62242822	2.94897077	-5.93447260
H	-0.78483803	4.92685062	-7.37358851
H	-0.76287500	7.46755325	-3.86834989
H	-0.65493637	5.46780827	-2.43141537
C	-0.54530730	7.32358234	-8.37242792
H	-0.53789915	8.24754332	-8.96205832
H	-1.34660783	6.67092730	-8.73380233
H	0.43295754	6.83213348	-8.43889996
H	0.76831488	3.73196074	-1.73473067

H	-1.73254737	-0.35709362	-3.03482296
H	1.07709910	-1.84905183	-2.77270466
H	-2.14492446	-5.52825327	-1.89289234
H	-5.20117910	0.60151394	0.74634175
H	-1.43553640	-2.33173216	2.12483490
H	0.17418950	0.47226930	2.14655672
H	3.68350129	-2.98420904	1.51156498
H	-0.41391021	-9.28551185	-6.22072323
H	-8.97643016	-0.63815599	5.22599764
S	6.93486260	-2.43348667	7.30298531
Au	5.78633686	-2.18205795	9.41457555
Au	3.66826158	-3.02207609	10.90821077
Au	6.25103035	-2.92095648	12.06328970
Au	4.81663148	-0.38740886	11.24704140
Au	1.50300700	-3.73516000	12.39061000
Au	4.11576500	-3.70869200	13.61071500
Au	6.72852300	-3.68222300	14.83081900
Au	2.83230900	-1.22678800	12.89744800
Au	5.44506600	-1.20031900	14.11755200
Au	4.16161000	1.28158400	13.40428500
Au	6.77436800	1.30805300	14.62438900
Au	-0.807223	-4.482795	13.946160
Au	1.805535	-4.456327	15.166265
Au	4.418292	-4.429858	16.386368
Au	7.031050	-4.403390	17.606472
Au	0.522078	-1.974423	14.452997
Au	3.134836	-1.947954	15.673102
Au	5.747594	-1.921486	16.893206
Au	1.851380	0.533949	14.959835
Au	4.464137	0.560418	16.179939
Au	3.180680	3.042321	15.466672
Au	7.076894	0.586886	17.400043
Au	-3.117453	-5.230430	15.501710
Au	-0.504696	-5.203961	16.721814
Au	2.108062	-5.177493	17.941918
Au	4.720820	-5.151025	19.162022
Au	7.333577	-5.124556	20.382126
Au	-1.788152	-2.722058	16.008547
Au	0.824606	-2.695589	17.228652
Au	3.437363	-2.669121	18.448755
Au	6.050120	-2.642653	19.668859
Au	-0.458851	-0.213686	16.515384
Au	2.153906	-0.187217	17.735489
Au	4.766664	-0.160749	18.955593
Au	0.870450	2.294686	17.022222
Au	3.483207	2.321155	18.242326

Au 2.199751 4.803059 17.529059

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Au	-2.15554361	9.18399949	-5.90175502
Au	-4.85996497	9.45384705	-5.82613374
Au	-3.24239838	10.53485116	-3.74986409
Au	-3.17124004	11.65455117	-6.60573003
Au	-7.57028900	9.80503400	-5.80097500
Au	-5.95899900	10.87780700	-3.66350900
Au	-4.34770900	11.95058000	-1.52604300
Au	-5.83559500	12.05552800	-6.29288200
Au	-4.22430600	13.12830100	-4.15541700
Au	-4.10090200	14.30602100	-6.78478900
Au	-2.48961200	15.37879400	-4.64732300
Au	-10.430851	10.168664	-5.772355
Au	-8.819560	11.241438	-3.634889
Au	-7.208271	12.314210	-1.497424
Au	-5.596981	13.386984	0.640041
Au	-8.696157	12.419158	-6.264263
Au	-7.084867	13.491931	-4.126797
Au	-5.473577	14.564704	-1.989331
Au	-6.961463	14.669652	-6.756170
Au	-5.350174	15.742424	-4.618705
Au	-5.226770	16.920145	-7.248077
Au	-8.572753	13.596878	-8.893636
Au	-13.291412	10.532295	-5.743736
Au	-11.680122	11.605068	-3.606271
Au	-10.068832	12.677841	-1.468805
Au	-8.457542	13.750614	0.668661
Au	-6.846252	14.823387	2.806126
Au	-11.556718	12.782788	-6.235643
Au	-9.945428	13.855561	-4.098177
Au	-8.334139	14.928334	-1.960712
Au	-6.722849	16.001107	0.176753
Au	-9.822025	15.033282	-6.727551
Au	-8.210735	16.106055	-4.590085
Au	-6.599445	17.178828	-2.452619
Au	-8.087331	17.283775	-7.219458
Au	-6.476041	18.356548	-5.081993
Au	-6.352637	19.534269	-7.711365
S	-0.18665597	7.86833571	-6.34737142
Si	-0.58006942	-1.30785863	-0.57864036
C	-0.29802345	-2.70009729	-1.82673920

C	0.79120877	-0.42027129	1.80861388
C	0.76880560	-1.35810300	0.75543833
C	1.74849987	-2.36963146	0.77655592
H	1.78229321	-3.11202462	-0.02418946
C	2.69305825	-2.45275510	1.80138859
C	2.69955791	-1.51994037	2.85492634
C	1.73394033	-0.49424805	2.83491880
H	1.69922929	0.22984763	3.65139727
C	-0.52830699	0.35452687	-1.49566598
C	0.64387226	1.13043242	-1.58450274
H	1.54853320	0.80602836	-1.06411496
C	0.68464890	2.30913756	-2.33219322
C	-0.45081960	2.76248233	-3.03025615
C	-1.63038301	1.99930458	-2.93744329
H	-2.53776350	2.34549442	-3.43619408
C	-1.66421050	0.82522685	-2.18497575
C	-2.26987166	-1.52248380	0.24193509
C	3.68954586	-1.62409976	3.95351600
C	4.06654364	-2.87818041	4.46876867
C	4.28494388	-0.47681372	4.51613747
C	5.22844596	-0.57797974	5.53508128
C	5.59138437	-1.84090612	6.03092169
C	4.99995829	-2.99383085	5.49974387
H	5.24703823	-3.98220913	5.88503417
H	3.59768713	-3.78261048	4.07820641
H	4.03173988	0.50938271	4.12436258
H	5.69341547	0.32272081	5.93937305
C	7.40901024	-3.58378262	7.34370421
H	8.21824696	-3.60325592	8.08265503
H	7.80123642	-3.84075910	6.35229777
H	6.62111398	-4.27682192	7.65507617
C	-0.40770446	3.99824488	-3.84768729
C	-1.09293046	4.07633659	-5.07614050
C	-1.05773647	5.22973065	-5.85882743
C	-0.31209860	6.33577917	-5.43003881
C	0.37877126	6.28117631	-4.20952482
C	0.32258552	5.12820645	-3.42953220
H	-1.64782044	3.20952029	-5.43793553
H	-1.60587455	5.25347322	-6.80037041
H	0.95573110	7.14339933	-3.87138471
H	0.84404817	5.10974485	-2.47151504
C	-0.35468393	7.33934134	-8.08300914
H	-0.19204761	8.24616755	-8.67704580
H	-1.35238739	6.94430397	-8.29672154
H	0.42300771	6.59876757	-8.30420547
H	1.61966960	2.86876548	-2.40215950

H	-2.60513924	0.27154597	-2.13242619
H	0.05016411	0.38318589	1.83915812
H	3.45188107	-3.23732240	1.77195879
H	-1.07122709	-2.66140849	-2.60770092
H	-0.35380847	-3.69018509	-1.35105783
H	0.67729911	-2.60875343	-2.32545009
H	-3.08352201	-1.52326544	-0.49773386
H	-2.47175540	-0.71956023	0.96479727
H	-2.30915802	-2.47945759	0.78177935
S	6.82636971	-1.85994717	7.32708888
Au	5.67513483	-1.56499945	9.42692622
Au	3.55749854	-2.33876545	10.95242700
Au	6.15788304	-2.23173557	12.08376437
Au	4.72056970	0.29451069	11.20394642
Au	1.40321800	-2.99862900	12.47731100
Au	4.02982300	-2.95588400	13.66684100
Au	6.65642700	-2.91313900	14.85637000
Au	2.75353900	-0.48603400	12.90081500
Au	5.38014300	-0.44328800	14.09034400
Au	4.10385900	2.02656200	13.32431800
Au	6.73046400	2.06930700	14.51384800
Au	-0.893670	-3.688942	14.078445
Au	1.732934	-3.646197	15.267974
Au	4.359538	-3.603452	16.457504
Au	6.986142	-3.560707	17.647033
Au	0.456650	-1.176347	14.501948
Au	3.083255	-1.133602	15.691478
Au	5.709859	-1.090857	16.881008
Au	1.806971	1.336248	14.925452
Au	4.433575	1.378993	16.114981
Au	3.157291	3.848844	15.348955
Au	7.060179	1.421739	17.304511
Au	-3.190558	-4.379256	15.679578
Au	-0.563955	-4.336511	16.869108
Au	2.062650	-4.293766	18.058637
Au	4.689254	-4.251020	19.248167
Au	7.315857	-4.208275	20.437696
Au	-1.840238	-1.866661	16.103082
Au	0.786366	-1.823915	17.292611
Au	3.412970	-1.781170	18.482141
Au	6.039574	-1.738425	19.671671
Au	-0.489918	0.645935	16.526585
Au	2.136686	0.688680	17.716115
Au	4.763291	0.731425	18.905645
Au	0.860403	3.158530	16.950089
Au	3.487007	3.201275	18.139618

Au 2.210723 5.671126 17.373592

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Au	-3.32610042	8.47829706	-7.00544402
Au	-5.70885207	7.90222836	-8.17532319
Au	-5.60759548	8.79712708	-5.48044044
Au	-4.82588336	10.63419279	-7.85100773
Au	-8.11587900	7.43138100	-9.38903700
Au	-8.04344200	8.30062800	-6.64039700
Au	-7.97100500	9.16987500	-3.89175700
Au	-7.32687100	10.13062000	-8.75073100
Au	-7.25443400	10.99986700	-6.00209300
Au	-6.53786200	12.82985900	-8.11242700
Au	-6.46542500	13.69910500	-5.36378700
Au	-10.647283	6.935808	-10.678324
Au	-10.574846	7.805055	-7.929684
Au	-10.502409	8.674301	-5.181045
Au	-10.429971	9.543548	-2.432405
Au	-9.858274	9.635046	-10.040019
Au	-9.785837	10.504293	-7.291379
Au	-9.713400	11.373540	-4.542739
Au	-9.069266	12.334285	-9.401713
Au	-8.996829	13.203532	-6.653074
Au	-8.280258	15.033523	-8.763409
Au	-9.141703	11.465038	-12.150353
Au	-13.178686	6.440234	-11.967610
Au	-13.106249	7.309481	-9.218971
Au	-13.033812	8.178728	-6.470331
Au	-12.961375	9.047975	-3.721692
Au	-12.888938	9.917221	-0.973053
Au	-12.389678	9.139473	-11.329306
Au	-12.317241	10.008720	-8.580666
Au	-12.244804	10.877966	-5.832027
Au	-12.172367	11.747213	-3.083387
Au	-11.600670	11.838711	-10.691001
Au	-11.528232	12.707958	-7.942361
Au	-11.455795	13.577205	-5.193721
Au	-10.811661	14.537950	-10.052695
Au	-10.739224	15.407197	-7.304056
Au	-10.022653	17.237188	-9.414391
S	-0.95586348	8.11747532	-6.72415451
Si	-0.50058601	-0.69310557	-0.42973759
C	-2.36204993	-1.61701900	1.66176568

C	-0.36547566	-2.22240413	-1.55934768
C	-1.34717514	-3.22616149	-1.47418745
H	-2.14801157	-3.11583163	-0.73699052
C	-1.39641703	-4.34917715	-2.31352762
C	-0.40119270	-4.47143318	-3.31165361
C	0.57889731	-3.46790642	-3.41019946
H	1.34958610	-3.57666185	-4.17829616
C	0.62371241	-2.34949391	-2.56951817
C	1.02460123	0.21155911	1.92616584
C	0.94560662	-0.67692990	0.82164269
C	1.89464902	-1.71325999	0.74464106
H	1.84531295	-2.40969801	-0.09707911
C	2.89047070	-1.93730159	1.70525132
C	2.93969052	-1.06420962	2.81567205
C	2.02706331	0.00164937	2.88410375
H	2.07291656	0.66861524	3.74959240
C	-4.26294745	0.42716079	1.06636008
C	-0.50319589	0.83647049	-1.57676190
C	0.43647256	1.86207689	-1.37041772
H	1.17249403	1.74618874	-0.56888424
C	0.51210635	3.02688555	-2.14965381
C	-0.41430952	3.16914595	-3.20753705
C	-1.32810058	2.13002636	-3.45304645
H	-2.03843475	2.24979039	-4.27554284
C	-1.39453997	0.96750502	-2.67576854
C	-4.50380739	-0.47494957	2.12893678
C	-3.55207446	-1.47783762	2.38747344
H	-3.73945732	-2.16223110	3.21948034
C	-2.10821607	-0.71113501	0.59746947
C	-3.07114042	0.28230281	0.34302238
H	-2.89059357	0.99692326	-0.46428776
C	-0.36195526	-5.59026452	-4.29048291
C	-0.27695114	-5.31893897	-5.66690677
C	-0.20484668	-6.34150102	-6.61530055
C	-0.20443690	-7.68384875	-6.20504727
C	-0.28344527	-7.97021987	-4.82748732
C	-0.36517378	-6.94226791	-3.89350560
H	-0.27102013	-9.00878973	-4.49044393
H	-0.40326239	-7.19294697	-2.83236669
H	-0.15396070	-6.08131691	-7.67206342
H	-0.28686381	-4.28100276	-6.00595940
S	-0.11348057	-9.07267105	-7.29617085
C	0.05642446	-8.31910758	-8.93469753
H	0.13835813	-9.16256997	-9.63116098
H	0.96641828	-7.70964526	-9.00431336
H	-0.82687520	-7.72462039	-9.20089757

C	-5.71773295	-0.40232682	2.98269577
C	-6.50209247	-1.54813264	3.22616103
C	-7.62916004	-1.49473040	4.04059594
C	-8.01053041	-0.28492986	4.65432419
C	-6.10502035	0.79492346	3.60758434
C	-7.22879985	0.86026608	4.43292858
H	-7.48343137	1.80868384	4.90435599
H	-6.23288880	-2.49199732	2.74779699
H	-5.50263549	1.69370449	3.46833401
H	-8.22787936	-2.39392688	4.19949053
S	-9.46202637	-0.32861726	5.66291189
C	-9.64857191	1.38929334	6.20674017
H	-10.55540998	1.39846540	6.82384054
H	-9.79025294	2.06723565	5.35551847
H	-8.79913568	1.71378768	6.82117154
C	3.90538391	-1.25466671	3.93312482
C	3.92799254	-2.45445345	4.66670313
C	4.79258642	-0.23092000	4.31532874
C	5.68590697	-0.40588594	5.37187570
C	5.69181626	-1.61292080	6.08740820
C	4.80053547	-2.63598035	5.74043041
H	4.76927878	-3.57001086	6.30035433
H	3.22885010	-3.25213187	4.41185827
H	4.79969589	0.70686106	3.75728448
H	6.38344800	0.39039152	5.63696075
C	7.06528662	-3.53871626	7.65125952
H	7.86582545	-3.65252942	8.39140005
H	7.36812299	-3.99001961	6.69868838
H	6.15027688	-3.99841813	8.03756721
C	-0.47754855	4.37184522	-4.08065288
C	-0.45962773	4.23982919	-5.48091763
C	-0.59606872	5.34587024	-6.32220467
C	-0.74672089	6.62110225	-5.76504850
C	-0.75465639	6.77892302	-4.36987814
C	-0.62487702	5.66540165	-3.54407939
H	-0.33201139	3.24939063	-5.92125660
H	-0.58607256	5.19913172	-7.40165322
H	-0.87468202	7.77159084	-3.93221595
H	-0.66297319	5.79945689	-2.46254714
C	-0.37957902	7.65152575	-8.38576024
H	-0.43977122	8.57195637	-8.97779136
H	-1.01953714	6.88868826	-8.84043144
H	0.66182400	7.31388510	-8.32241619
C	1.58416625	4.04989807	-1.85326919
C	-2.38951402	-0.09924278	-3.07364707
C	1.69566963	-1.31090348	-2.81564807

C	-2.52217526	-5.34320603	-2.14952641
C	-5.24293408	1.50155905	0.65343016
C	-1.38360340	-2.68816703	2.09007616
C	0.03335850	1.32865174	2.16225617
C	3.86986320	-3.07185254	1.50843264
H	1.94715136	4.53914595	-2.76698173
H	2.43867718	3.57245352	-1.35513797
H	1.22211160	4.84383245	-1.18114382
H	-3.15822378	0.31619429	-3.73918867
H	-2.89564839	-0.54979287	-2.21028189
H	-1.88832973	-0.92056269	-3.60852259
H	2.53902839	-1.74715535	-3.36838092
H	2.08760004	-0.87824185	-1.88564820
H	1.30170551	-0.47340111	-3.41212352
H	-2.83906292	-5.76384749	-3.11304795
H	-3.38935269	-4.86381996	-1.67573366
H	-2.23005446	-6.18963015	-1.50792086
H	-5.12095280	1.73768574	-0.41230476
H	-5.08810980	2.43873606	1.21074299
H	-6.28232526	1.19209802	0.82426216
H	-0.89878757	-3.18224019	1.23771382
H	-1.88991428	-3.45902660	2.68709933
H	-0.57950334	-2.26056418	2.70901979
H	-0.29446112	1.80657939	1.23060006
H	0.46580254	2.10310166	2.81053272
H	-0.87271436	0.94615835	2.65733270
H	3.94156538	-3.33210035	0.44412070
H	3.55938349	-3.98310739	2.04327034
H	4.87429797	-2.81153339	1.86863245
S	6.87909801	-1.74208626	7.42250677
Au	5.79332991	-0.96046218	9.42926782
Au	3.59092847	-1.23233496	11.01041139
Au	6.16069463	-0.97217494	12.17908919
Au	4.90181618	1.32776760	10.66700708
Au	1.36160400	-1.39208500	12.56109200
Au	3.95421700	-1.18422700	13.80648900
Au	6.54683000	-0.97636900	15.05188500
Au	2.83792200	1.08069000	12.41369000
Au	5.43053300	1.28854800	13.65908600
Au	4.31423800	3.55346500	12.26628700
Au	6.90685000	3.76132400	13.51168400
Au	-1.011567	-1.559572	14.190773
Au	1.581045	-1.351714	15.436170
Au	4.173657	-1.143856	16.681566
Au	6.766270	-0.935998	17.926963
Au	0.464749	0.913204	14.043371

Au	3.057362	1.121062	15.288768
Au	5.649974	1.328920	16.534164
Au	1.941066	3.385979	13.895969
Au	4.533678	3.593837	15.141365
Au	3.417382	5.858754	13.748566
Au	7.126290	3.801695	16.386762
Au	-3.384739	-1.727058	15.820455
Au	-0.792127	-1.519200	17.065851
Au	1.800486	-1.311342	18.311248
Au	4.393098	-1.103484	19.556645
Au	6.985710	-0.895626	20.802041
Au	-1.908423	0.745717	15.673052
Au	0.684190	0.953575	16.918449
Au	3.276802	1.161433	18.163846
Au	5.869414	1.369291	19.409242
Au	-0.432106	3.218492	15.525650
Au	2.160506	3.426351	16.771047
Au	4.753119	3.634209	18.016444
Au	1.044211	5.691268	15.378248
Au	3.636822	5.899126	16.623644
Au	2.520527	8.164043	15.230845

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Au	-7.589680	0.833650	-0.326640
Au	-8.932933	0.079121	-2.764306
Au	-8.519170	-1.872886	-0.682403
Au	-10.416540	0.264503	-0.298459
Au	-10.276185	-0.675407	-5.201972
Au	-9.862422	-2.627415	-3.120068
Au	-9.448659	-4.579422	-1.038164
Au	-11.759792	-0.490026	-2.736125
Au	-11.346029	-2.442033	-0.654221
Au	-13.243398	-0.304644	-0.270278
Au	-12.829636	-2.256652	1.811626
Au	-11.619438	-1.429936	-7.639638
Au	-11.205675	-3.381944	-5.557734
Au	-10.791912	-5.333951	-3.475831
Au	-10.378150	-7.285959	-1.393927
Au	-13.103045	-1.244554	-5.173791
Au	-12.689282	-3.196562	-3.091887
Au	-12.275519	-5.148570	-1.009983
Au	-14.586651	-1.059173	-2.707944
Au	-14.172889	-3.011180	-0.626041

Au	-16.070258	-0.873791	-0.242097
Au	-15.000414	0.892835	-4.789848
Au	-12.962691	-2.184465	-10.077304
Au	-12.548928	-4.136472	-7.995401
Au	-12.135165	-6.088480	-5.913497
Au	-11.721402	-8.040488	-3.831593
Au	-11.307640	-9.992495	-1.749689
Au	-14.446297	-1.999083	-7.611457
Au	-14.032535	-3.951091	-5.529553
Au	-13.618772	-5.903098	-3.447650
Au	-13.205009	-7.855106	-1.365746
Au	-15.929904	-1.813701	-5.145611
Au	-15.516141	-3.765709	-3.063707
Au	-15.102379	-5.717717	-0.981803
Au	-17.413511	-1.628320	-2.679763
Au	-16.999748	-3.580327	-0.597860
Au	-18.897118	-1.442938	-0.213917
S	-5.67786	2.34456	0.71004
C	0.19568	-2.08819	1.74610
C	-0.68747	-3.16336	2.07482
C	-0.47995	-3.83334	3.29020
H	-1.16273	-4.64681	3.56255
C	0.57200	-3.49771	4.15649
H	0.69368	-4.04540	5.09726
C	1.47814	-2.47848	3.82370
C	1.27476	-1.78917	2.61121
H	1.98011	-1.00440	2.32162
C	-1.77750	-3.63389	1.13576
H	-1.36033	-4.29000	0.35169
H	-2.27823	-2.80317	0.61041
H	-2.54812	-4.20680	1.67590
C	2.65310	-2.14447	4.71305
H	2.49185	-2.50168	5.74240
H	2.83746	-1.05875	4.75301
H	3.58064	-2.61533	4.34177
C	-1.66423	0.13698	0.21933
C	-1.97451	1.21784	-0.67454
C	-3.19443	1.88616	-0.51701
H	-3.42700	2.68755	-1.22496
C	-4.10342	1.56889	0.51597
C	-3.79503	0.53333	1.43878
C	-2.58134	-0.14231	1.27054
H	-2.33743	-0.92729	1.99343
C	-1.04005	1.66998	-1.77682
H	-0.07086	2.00201	-1.36967
H	-1.47986	2.50856	-2.33880

H	-0.82220	0.86277	-2.49698
C	-4.75149	0.14644	2.53787
H	-5.72529	-0.16961	2.11840
H	-4.95434	0.99073	3.22068
H	-4.34664	-0.68518	3.13333
C	1.56249	0.15798	-0.10589
C	1.87325	1.25661	0.76578
C	3.09092	1.92383	0.58928
H	3.32641	2.73885	1.28055
C	3.99447	1.58939	-0.44362
C	3.68020	0.54130	-1.35039
C	2.46846	-0.13300	-1.16272
H	2.21036	-0.92375	-1.87432
C	0.93868	1.72606	1.86040
H	0.72691	0.93147	2.59607
H	-0.03364	2.04256	1.44788
H	1.37309	2.57902	2.40467
C	4.62785	0.14174	-2.45261
H	5.60564	-0.16755	-2.03713
H	4.82394	0.97760	-3.14758
H	4.21965	-0.69812	-3.03408
C	-0.24356	-2.16794	-1.55158
C	0.63662	-3.25683	-1.84471
C	0.40631	-3.97834	-3.02861
H	1.08116	-4.80809	-3.26995
C	-0.65105	-3.67824	-3.89948
H	-0.78561	-4.27080	-4.81092
C	-1.54652	-2.63797	-3.60423
C	-1.32723	-1.90116	-2.42427
H	-2.03345	-1.10555	-2.16756
C	1.76705	-3.68208	-0.93039
H	2.33239	-4.51402	-1.37856
H	1.38880	-4.02003	0.04916
H	2.48254	-2.86656	-0.72748
C	-2.72770	-2.33581	-4.49687
H	-3.55191	-3.05033	-4.32376
H	-2.45580	-2.40758	-5.56277
H	-3.12588	-1.32605	-4.31107
Os	-0.04065	-1.00253	0.07349
C	5.60875	3.64968	0.62805
C	-5.70062	3.62473	-0.58797
H	6.60950	4.09756	0.55033
H	5.49479	3.20623	1.62679
H	4.83584	4.40728	0.43122
H	-6.69850	4.08051	-0.51986
H	-5.58437	3.17202	-1.58224

H	-4.92329	4.37833	-0.39313
S	5.56940	2.35852	-0.65867
Au	7.486370	0.847760	0.370820
Au	8.044768	-1.561099	1.854548
Au	9.840958	-0.704017	-0.232308
Au	9.685118	0.779850	2.235426
Au	8.603164	-3.969957	3.338276
Au	10.399355	-3.112875	1.251420
Au	12.195545	-2.255793	-0.835436
Au	10.243515	-1.629008	3.719153
Au	12.039704	-0.771927	1.632298
Au	11.883864	0.711940	4.100031
Au	13.680055	1.569022	2.013175
Au	9.161562	-6.378816	4.822004
Au	10.957752	-5.521734	2.735148
Au	12.753942	-4.664652	0.648292
Au	14.550133	-3.807570	-1.438564
Au	10.801912	-4.037867	5.202882
Au	12.598102	-3.180785	3.116026
Au	14.394292	-2.323703	1.029170
Au	12.442262	-1.696919	5.583759
Au	14.238452	-0.839837	3.496904
Au	14.082612	0.644030	5.964637
Au	16.034642	0.017245	1.410048
Au	9.719960	-8.787675	6.305732
Au	11.516150	-7.930593	4.218876
Au	13.312340	-7.073511	2.132020
Au	15.108530	-6.216428	0.045164
Au	16.904720	-5.359347	-2.041692
Au	11.360310	-6.446726	6.686610
Au	13.156500	-5.589644	4.599754
Au	14.952690	-4.732562	2.512898
Au	16.748880	-3.875480	0.426042
Au	13.000659	-4.105778	7.067488
Au	14.796850	-3.248696	4.980632
Au	16.593040	-2.391613	2.893776
Au	14.641010	-1.764829	7.448365
Au	16.437199	-0.907747	5.361510
Au	16.281359	0.576120	7.829243

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Au	-7.066270	-1.940330	0.316590
Au	-9.784494	-2.089380	-0.634673

Au	-9.211943	-0.851899	1.906327
Au	-8.426528	0.452917	-0.542435
Au	-12.502717	-2.238431	-1.585936
Au	-11.930166	-1.000950	0.955064
Au	-11.357615	0.236532	3.496064
Au	-11.144751	0.303867	-1.493697
Au	-10.572200	1.541348	1.047302
Au	-9.786785	2.846164	-1.401459
Au	-9.214234	4.083646	1.139541
Au	-15.220940	-2.387481	-2.537199
Au	-14.648389	-1.150000	0.003801
Au	-14.075839	0.087481	2.544801
Au	-13.503287	1.324963	5.085801
Au	-13.862975	0.154816	-2.444961
Au	-13.290424	1.392297	0.096039
Au	-12.717873	2.629779	2.637040
Au	-12.505009	2.697114	-2.352722
Au	-11.932458	3.934595	0.188277
Au	-11.147043	5.239411	-2.260484
Au	-13.077560	1.459632	-4.893723
Au	-17.939164	-2.536532	-3.488462
Au	-17.366613	-1.299051	-0.947462
Au	-16.794062	-0.061569	1.593538
Au	-16.221511	1.175912	4.134538
Au	-15.648960	2.413394	6.675538
Au	-16.581198	0.005766	-3.396224
Au	-16.008647	1.243247	-0.855223
Au	-15.436096	2.480728	1.685776
Au	-14.863545	3.718210	4.226777
Au	-15.223233	2.548063	-3.303986
Au	-14.650682	3.785545	-0.762985
Au	-14.078131	5.023026	1.778015
Au	-13.865267	5.090361	-3.211747
Au	-13.292716	6.327842	-0.670747
Au	-12.507301	7.632659	-3.119509
S	-4.76485	-3.17259	0.39814
C	1.71656	0.60854	-0.51354
C	2.90909	1.39609	-0.63795
C	4.09894	0.76187	-1.01123
H	5.00024	1.37687	-1.09090
C	4.15916	-0.62087	-1.29174
C	2.99589	-1.42711	-1.14707
C	1.81255	-0.79063	-0.75810
H	0.91881	-1.41167	-0.63744
C	2.93722	2.87618	-0.32566
H	2.95134	3.05014	0.76445

H	2.04954	3.39652	-0.72158
H	3.83167	3.35639	-0.75378
C	3.03711	-2.91549	-1.38077
H	3.79544	-3.39647	-0.73462
H	3.30595	-3.15939	-2.42429
H	2.06081	-3.37431	-1.16413
C	-0.71155	2.78768	-1.24579
C	-1.93983	3.49136	-1.04998
C	-2.32063	4.43133	-2.02152
H	-3.25917	4.97944	-1.87907
C	-1.55087	4.67397	-3.16842
C	-0.35501	3.97149	-3.39167
C	0.04281	3.03362	-2.41929
H	0.96877	2.47003	-2.57701
C	-2.85238	3.21991	0.12467
H	-3.32905	2.22863	0.03108
H	-3.65360	3.97297	0.18587
H	-2.30855	3.22405	1.08426
C	0.49487	4.23050	-4.61415
H	1.21208	5.05186	-4.43590
H	-0.12275	4.52157	-5.47896
H	1.08066	3.34087	-4.89542
C	-1.45346	0.00364	0.02393
C	-1.84939	-0.72737	-1.14652
C	-2.84998	-1.69632	-1.02415
H	-3.14592	-2.24097	-1.92519
C	-3.47660	-1.98057	0.20966
C	-3.14305	-1.22780	1.37053
C	-2.14816	-0.25286	1.23984
H	-1.88738	0.33013	2.12919
C	-1.26840	-0.43233	-2.50992
H	-0.16678	-0.39659	-2.48845
H	-1.60901	0.55290	-2.87241
H	-1.57211	-1.19094	-3.24830
C	-3.84084	-1.45151	2.68823
H	-3.74629	-2.49790	3.02887
H	-4.92315	-1.23467	2.61076
H	-3.42033	-0.80130	3.46999
C	0.36221	2.07715	1.87529
C	0.81459	1.27451	2.97043
C	1.05066	1.91971	4.19567
H	1.38957	1.31630	5.04570
C	0.87253	3.30099	4.36643
H	1.06568	3.75448	5.34462
C	0.45773	4.10721	3.29533
C	0.21085	3.47470	2.06037

H	-0.10759	4.09298	1.21292
C	1.07280	-0.21057	2.85186
H	1.40265	-0.62753	3.81614
H	1.85726	-0.42038	2.10528
H	0.17385	-0.76656	2.53480
C	0.29887	5.60288	3.43995
H	1.17940	6.13932	3.04329
H	0.18527	5.89562	4.49562
H	-0.58000	5.97113	2.88612
Os	-0.03084	1.38587	0.03244
C	-4.85797	-3.99406	-1.22727
H	-5.66890	-4.72966	-1.12949
H	-3.90802	-4.50427	-1.44476
H	-5.12001	-3.27633	-2.01665
C	6.89731	-0.13915	-1.80103
H	-1.89193	5.41293	-3.90186
H	7.83451	-0.64720	-2.06802
H	7.00409	0.30197	-0.80029
H	6.65048	0.62222	-2.55567
S	5.63562	-1.45478	-1.78712
Au	6.721320	-2.912860	0.154690
Au	6.271692	-5.077874	2.005745
Au	8.877715	-4.704929	0.828712
Au	7.897684	-2.827783	2.786189
Au	5.822063	-7.242888	3.856800
Au	8.428087	-6.869943	2.679766
Au	11.034111	-6.496997	1.502732
Au	7.448056	-4.992797	4.637243
Au	10.054079	-4.619851	3.460210
Au	9.074048	-2.742705	5.417687
Au	11.680072	-2.369759	4.240654
Au	5.372435	-9.407903	5.707855
Au	7.978459	-9.034957	4.530821
Au	10.584483	-8.662011	3.353788
Au	13.190507	-8.289066	2.176754
Au	6.998427	-7.157811	6.488299
Au	9.604451	-6.784865	5.311265
Au	12.210476	-6.411920	4.134231
Au	8.624420	-4.907719	7.268742
Au	11.230443	-4.534774	6.091709
Au	10.250412	-2.657628	8.049186
Au	13.836468	-4.161828	4.914675
Au	4.922807	-11.572917	7.558909
Au	7.528831	-11.199971	6.381876
Au	10.134855	-10.827026	5.204843
Au	12.740879	-10.454080	4.027809

Au	15.346902	-10.081134	2.850776
Au	6.548799	-9.322825	8.339353
Au	9.154824	-8.949880	7.162320
Au	11.760847	-8.576934	5.985287
Au	14.366871	-8.203988	4.808253
Au	8.174792	-7.072734	9.119797
Au	10.780816	-6.699788	7.942764
Au	13.386840	-6.326842	6.765730
Au	9.800784	-4.822642	9.900241
Au	12.406808	-4.449697	8.723208
Au	11.426777	-2.572551	10.680685

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Au	-7.051630	1.375380	0.677270
Au	-9.551495	-0.058904	0.580512
Au	-7.649036	-0.617076	2.674539
Au	-9.083657	1.884420	2.659088
Au	-12.051360	-1.493187	0.483754
Au	-10.148900	-2.051359	2.577781
Au	-8.246441	-2.609532	4.671808
Au	-11.583521	0.450136	2.562330
Au	-9.681062	-0.108036	4.656356
Au	-11.115683	2.393459	4.640906
Au	-9.213223	1.835287	6.734933
Au	-14.551225	-2.927471	0.386996
Au	-12.648765	-3.485643	2.481023
Au	-10.746306	-4.043815	4.575049
Au	-8.843847	-4.601987	6.669076
Au	-14.083387	-0.984147	2.465572
Au	-12.180927	-1.542320	4.559599
Au	-10.278467	-2.100492	6.653626
Au	-13.615548	0.959176	4.544148
Au	-11.713089	0.401004	6.638175
Au	-13.147710	2.902499	6.622724
Au	-15.518008	1.517348	2.450121
Au	-17.051090	-4.361754	0.290239
Au	-15.148631	-4.919926	2.384265
Au	-13.246171	-5.478099	4.478292
Au	-11.343712	-6.036271	6.572319
Au	-9.441253	-6.594443	8.666345
Au	-16.583252	-2.418431	2.368814
Au	-14.680792	-2.976603	4.462841
Au	-12.778333	-3.534776	6.556868

Au	-10.875873	-4.092948	8.650895
Au	-16.115414	-0.475108	4.447390
Au	-14.212954	-1.033280	6.541417
Au	-12.310494	-1.591452	8.635444
Au	-15.647575	1.468215	6.525966
Au	-13.745116	0.910043	8.619993
Au	-15.179737	3.411539	8.604542
S	-5.13881	2.46345	-0.77053
C	1.44967	-0.49708	0.53351
C	1.70146	0.74482	-0.09786
C	2.86130	1.47754	0.16404
C	3.80861	0.98129	1.08373
C	3.57123	-0.23561	1.74721
C	2.39952	-0.95426	1.47121
Si	-0.05915	-1.53309	0.03427
C	-0.49372	-2.78237	1.39044
C	-1.51380	-0.35149	-0.25488
C	0.32179	-2.46916	-1.56819
C	0.25912	-3.97134	1.53984
C	-1.56123	-2.55834	2.28868
C	-1.82931	0.67375	0.67004
C	-2.34682	-0.48268	-1.38701
C	-0.42105	-3.62534	-1.90371
C	1.30748	-2.02685	-2.47830
C	-0.03552	-4.89304	2.55510
C	-1.86148	-3.48013	3.30170
C	-2.93123	1.51277	0.48667
C	-3.45564	0.34921	-1.59032
C	-0.19466	-4.30740	-3.10795
C	1.53866	-2.70820	-3.68197
C	-1.09723	-4.64768	3.43847
C	-3.75120	1.35316	-0.65100
C	0.78584	-3.84827	-3.99947
H	0.97600	1.14977	-0.81209
H	3.04601	2.42383	-0.35450
H	4.28838	-0.63444	2.46885
H	2.22854	-1.90053	1.99593
H	1.07407	-4.18859	0.83992
H	-2.17661	-1.65738	2.19133
H	-1.19600	0.82570	1.55118
H	-2.13079	-1.25551	-2.13245
H	-1.17752	-4.00530	-1.20778
H	1.90804	-1.14225	-2.23992
H	0.55835	-5.80768	2.65062
H	-2.69783	-3.28911	3.98156
H	-3.16062	2.28990	1.22298

H	-4.07820	0.20823	-2.47615
H	-0.77959	-5.20110	-3.34785
H	2.31098	-2.35085	-4.37044
H	-1.33288	-5.36956	4.22676
C	-5.84767	2.10786	-2.41165
H	-6.70335	2.79049	-2.51137
H	-6.21014	1.07228	-2.46433
H	-5.10613	2.31799	-3.19660
C	6.25812	1.05454	2.52080
H	0.96706	-4.38113	-4.93830
H	7.18685	1.63017	2.64039
H	6.50621	0.04509	2.16324
H	5.71345	1.02228	3.47621
S	5.28576	1.96178	1.27274
Au	6.691300	1.279810	-0.845040
Au	8.023243	-0.898503	-2.185465
Au	6.694353	1.145463	-3.725630
Au	9.128924	1.761989	-2.308375
Au	9.355186	-3.076816	-3.525888
Au	8.026296	-1.032850	-5.066054
Au	6.697405	1.011116	-6.606220
Au	10.460867	-0.416323	-3.648798
Au	9.131977	1.627642	-5.188964
Au	11.566548	2.244169	-3.771709
Au	10.237658	4.288135	-5.311874
Au	10.687129	-5.255129	-4.866313
Au	9.358239	-3.211162	-6.406478
Au	8.029349	-1.167197	-7.946644
Au	6.700458	0.876769	-9.486810
Au	11.792811	-2.594637	-4.989223
Au	10.463920	-0.550671	-6.529388
Au	9.135029	1.493296	-8.069554
Au	12.898491	0.065856	-5.112133
Au	11.569601	2.109821	-6.652298
Au	14.004173	2.726348	-5.235043
Au	10.240711	4.153787	-8.192464
Au	12.019072	-7.433441	-6.206737
Au	10.690182	-5.389476	-7.746902
Au	9.361292	-3.345510	-9.287068
Au	8.032401	-1.301544	-10.827234
Au	6.703511	0.742422	-12.367399
Au	13.124754	-4.772949	-6.329647
Au	11.795863	-2.728983	-7.869813
Au	10.466973	-0.685018	-9.409978
Au	9.138082	1.358948	-10.950144
Au	14.230435	-2.112457	-6.452557

Au	12.901544	-0.068491	-7.992723
Au	11.572654	1.975475	-9.532889
Au	15.336116	0.548035	-6.575468
Au	14.007226	2.592001	-8.115633
Au	16.441797	3.208527	-6.698378

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Au	7.143690	-1.473740	-0.623610
Au	9.928149	-1.180637	-1.314072
Au	8.107447	-2.433529	-3.166411
Au	7.932761	0.401325	-2.667468
Au	12.712607	-0.887533	-2.004532
Au	10.891905	-2.140425	-3.856871
Au	9.071203	-3.393318	-5.709211
Au	10.717219	0.694428	-3.357929
Au	8.896518	-0.558464	-5.210268
Au	8.721832	2.276390	-4.711325
Au	6.901130	1.023498	-6.563665
Au	15.497066	-0.594430	-2.694993
Au	13.676364	-1.847322	-4.547333
Au	11.855662	-3.100214	-6.399672
Au	10.034960	-4.353107	-8.252012
Au	13.501679	0.987532	-4.048389
Au	11.680977	-0.265360	-5.900729
Au	9.860274	-1.518253	-7.753069
Au	11.506291	2.569493	-5.401786
Au	9.685589	1.316601	-7.254125
Au	9.510904	4.151455	-6.755183
Au	13.326993	3.822386	-3.549447
Au	18.281525	-0.301326	-3.385455
Au	16.460823	-1.554218	-5.237794
Au	14.640121	-2.807111	-7.090133
Au	12.819419	-4.060003	-8.942473
Au	10.998717	-5.312895	-10.794812
Au	16.286137	1.280636	-4.738851
Au	14.465435	0.027743	-6.591191
Au	12.644734	-1.225149	-8.443530
Au	10.824031	-2.478041	-10.295869
Au	14.290750	2.862597	-6.092247
Au	12.470048	1.609705	-7.944587
Au	10.649346	0.356812	-9.796927
Au	12.295362	4.444559	-7.445644
Au	10.474661	3.191667	-9.297983

Au	10.299975	6.026520	-8.799040
S	5.47586	-1.91792	1.31617
C	-0.05073	2.93492	1.46675
C	0.17973	2.69183	2.84190
C	0.04630	3.71455	3.79216
C	-0.31768	5.00631	3.38383
C	-0.54612	5.26963	2.02561
C	-0.41269	4.24412	1.07833
Si	0.06561	1.53590	0.19535
C	0.15805	2.21812	-1.56662
C	1.61985	0.50115	0.54335
C	-1.46455	0.42495	0.35021
C	-1.00773	2.62742	-2.25590
C	1.40266	2.36859	-2.21878
C	2.72884	1.02784	1.24707
C	1.72472	-0.82450	0.06529
C	-1.86100	-0.44044	-0.69927
C	-2.23503	0.39961	1.53303
C	-0.93056	3.17424	-3.54504
C	1.48287	2.91282	-3.50834
C	3.88207	0.27014	1.46965
C	2.87646	-1.59458	0.26250
C	-2.95538	-1.29922	-0.56919
C	-3.34065	-0.44697	1.68084
C	0.31576	3.31790	-4.17242
C	3.95808	-1.05098	0.98181
C	-3.69822	-1.31256	0.63099
H	0.47655	1.69003	3.17383
H	0.23071	3.50496	4.85069
H	-0.41940	5.80672	4.12342
H	-0.82588	6.27730	1.70251
H	-0.58924	4.46352	0.01975
H	-1.98983	2.50754	-1.78440
H	2.32098	2.04885	-1.71391
H	2.68838	2.04902	1.64044
H	0.88462	-1.27523	-0.47450
H	-1.31670	-0.43004	-1.65024
H	-1.97827	1.06839	2.36171
H	-1.84442	3.48357	-4.06217
H	2.45676	3.01696	-3.99694
H	4.72452	0.69876	2.02194
H	2.92161	-2.60983	-0.13835
H	-3.25094	-1.94489	-1.40288
H	-3.91226	-0.42166	2.61094
H	0.37642	3.74087	-5.18013
C	5.08154	-3.65173	0.90384

C	-5.79710	-2.15999	2.33768
H	5.97452	-4.22900	1.18257
H	4.90283	-3.77206	-0.17388
H	4.21689	-3.98501	1.49658
H	-6.66817	-2.82800	2.39186
H	-6.13670	-1.11971	2.43510
H	-5.07336	-2.42561	3.12239
S	-5.07162	-2.44437	0.69046
Au	-6.984660	-1.348070	-0.750190
Au	-9.013156	-1.844348	-2.738850
Au	-9.487638	0.080128	-0.644306
Au	-7.583752	0.660168	-2.731081
Au	-11.041651	-2.340627	-4.727510
Au	-11.516133	-0.416151	-2.632966
Au	-11.990615	1.508326	-0.538421
Au	-9.612247	0.163890	-4.719740
Au	-10.086729	2.088365	-2.625196
Au	-8.182843	2.668405	-4.711971
Au	-8.657325	4.592881	-2.617426
Au	-13.070147	-2.836905	-6.716170
Au	-13.544629	-0.912428	-4.621626
Au	-14.019111	1.012047	-2.527082
Au	-14.493592	2.936523	-0.432537
Au	-11.640743	-0.332389	-6.708401
Au	-12.115225	1.592087	-4.613856
Au	-12.589707	3.516563	-2.519312
Au	-10.211339	2.172127	-6.700631
Au	-10.685821	4.096603	-4.606087
Au	-8.781935	4.676643	-6.692861
Au	-11.160302	6.021079	-2.511542
Au	-15.098643	-3.333182	-8.704830
Au	-15.573125	-1.408707	-6.610287
Au	-16.047607	0.515769	-4.515742
Au	-16.522088	2.440245	-2.421197
Au	-16.996570	4.364721	-0.326653
Au	-13.669239	-0.828667	-8.697061
Au	-14.143721	1.095809	-6.602516
Au	-14.618202	3.020285	-4.507973
Au	-15.092684	4.944761	-2.413428
Au	-12.239835	1.675849	-8.689292
Au	-12.714317	3.600325	-6.594747
Au	-13.188798	5.524801	-4.500202
Au	-10.810431	4.180365	-8.681521
Au	-11.284913	6.104840	-6.586978
Au	-9.381027	6.684881	-8.673752

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Au	6.640320	1.243150	0.648350
Au	7.279981	-0.663632	2.714959
Au	9.165491	-0.148431	0.594753
Au	8.668913	1.861063	2.602538
Au	7.919641	-2.570414	4.781568
Au	9.805151	-2.055212	2.661362
Au	11.690661	-1.540011	0.541155
Au	9.308574	-0.045719	4.669147
Au	11.194083	0.469483	2.548940
Au	10.697506	2.478976	4.556725
Au	12.583016	2.994178	2.436519
Au	8.559302	-4.477195	6.848178
Au	10.444812	-3.961994	4.727971
Au	12.330322	-3.446793	2.607765
Au	14.215832	-2.931592	0.487558
Au	9.948234	-1.952501	6.735756
Au	11.833744	-1.437299	4.615550
Au	13.719255	-0.922098	2.495343
Au	11.337167	0.572194	6.623335
Au	13.222676	1.087396	4.503128
Au	12.726099	3.096889	6.510913
Au	9.451657	0.056993	8.743541
Au	9.198963	-6.383977	8.914787
Au	11.084473	-5.868776	6.794581
Au	12.969983	-5.353575	4.674374
Au	14.855493	-4.838374	2.554167
Au	16.741003	-4.323173	0.433961
Au	10.587895	-3.859282	8.802366
Au	12.473406	-3.344081	6.682159
Au	14.358915	-2.828880	4.561953
Au	16.244425	-2.313679	2.441746
Au	11.976827	-1.334588	8.689944
Au	13.862338	-0.819386	6.569738
Au	15.747848	-0.304185	4.449531
Au	13.365760	1.190107	8.577523
Au	15.251270	1.705309	6.457316
Au	14.754692	3.714802	8.465101
S	4.71055	2.23915	-0.82578
C	-1.15861	-0.70795	0.19755
C	-1.55928	0.13637	-0.86356
C	-2.57601	1.08032	-0.71233
C	-3.20226	1.23978	0.54070

C	-2.79866	0.42721	1.61802
C	-1.79344	-0.52922	1.44314
C	0.02492	-1.68494	-0.01808
H	-1.06352	0.04942	-1.83510
H	-2.86894	1.69036	-1.56967
H	-3.27128	0.54305	2.59844
H	-1.50123	-1.14646	2.29591
C	0.24044	-2.63907	1.18855
C	1.22251	-0.72410	-0.23361
C	-0.20183	-2.64172	-1.21997
C	-0.82387	-3.47437	1.59505
C	1.48238	-2.79434	1.83105
C	1.61980	0.12559	0.82579
C	1.88039	-0.57218	-1.46971
C	0.85201	-3.49211	-1.62286
C	-1.44628	-2.78710	-1.85999
C	-0.66218	-4.40084	2.63075
H	-1.78828	-3.40514	1.08199
C	1.64888	-3.73140	2.86388
H	2.33701	-2.18563	1.52559
C	2.65805	1.04545	0.68182
H	1.10861	0.05539	1.79052
C	2.91321	0.35878	-1.63570
H	1.58720	-1.18953	-2.32203
C	0.67876	-4.42189	-2.65372
H	1.81705	-3.43277	-1.10983
C	-1.62465	-3.72756	-2.88774
H	-2.29404	-2.16862	-1.55504
C	0.57801	-4.53274	3.27471
H	-1.50668	-5.03042	2.92767
H	2.62746	-3.83049	3.34373
C	3.31381	1.17244	-0.56017
H	2.96059	1.65403	1.53754
H	3.40767	0.45456	-2.60731
C	-0.56335	-4.54279	-3.29604
H	1.51554	-5.06309	-2.94765
H	-2.60518	-3.81905	-3.36518
H	0.70784	-5.26050	4.08122
H	-0.70231	-5.27333	-4.09852
C	-4.40407	3.58584	-0.49027
C	4.34965	3.67717	0.24532
H	-5.17688	4.33908	-0.28055
H	-4.60757	3.13444	-1.47071
H	-3.40655	4.04833	-0.46143
H	5.15380	4.40089	0.04873
H	4.37504	3.40414	1.30932

H	3.37624	4.10549	-0.03508
S	-4.54490	2.35932	0.85336
Au	-6.736510	1.199550	0.067690
Au	-8.247509	0.330504	-2.229590
Au	-8.297116	-1.221774	0.200189
Au	-9.616625	1.340351	0.098840
Au	-9.758508	-0.538541	-4.526871
Au	-9.808115	-2.090819	-2.097091
Au	-9.857722	-3.643097	0.332689
Au	-11.127624	0.471305	-2.198440
Au	-11.177231	-1.080973	0.231339
Au	-12.496739	1.481152	0.129990
Au	-12.546346	-0.071127	2.559770
Au	-11.269507	-1.407587	-6.824151
Au	-11.319114	-2.959865	-4.394372
Au	-11.368721	-4.512143	-1.964593
Au	-11.418329	-6.064421	0.465187
Au	-12.638623	-0.397741	-4.495721
Au	-12.688230	-1.950019	-2.065941
Au	-12.737837	-3.502297	0.363838
Au	-14.007739	0.612106	-2.167290
Au	-14.057346	-0.940172	0.262489
Au	-15.376854	1.621952	0.161140
Au	-14.106953	-2.492450	2.692269
Au	-12.780507	-2.276633	-9.121432
Au	-12.830114	-3.828911	-6.691653
Au	-12.879721	-5.381189	-4.261873
Au	-12.929328	-6.933467	-1.832093
Au	-12.978935	-8.485745	0.597686
Au	-14.149622	-1.266787	-6.793001
Au	-14.199229	-2.819065	-4.363222
Au	-14.248836	-4.371342	-1.933443
Au	-14.298444	-5.923621	0.496337
Au	-15.518738	-0.256940	-4.464571
Au	-15.568345	-1.809218	-2.034791
Au	-15.617952	-3.361496	0.394988
Au	-16.887854	0.752906	-2.136140
Au	-16.937461	-0.799372	0.293639
Au	-18.256969	1.762753	0.192290

59_FHI-aims_Junction_C1h_diff.xyz /// -39688378.434473053 eV

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Au	-6.344060	-2.225760	0.122140
Au	-8.483648	-4.019814	0.842826

Au	-5.858261	-4.375846	1.981437
Au	-7.479288	-2.125392	2.771110
Au	-10.623237	-5.813868	1.563510
Au	-7.997849	-6.169900	2.702122
Au	-5.372461	-6.525933	3.840733
Au	-9.618876	-3.919446	3.491795
Au	-6.993488	-4.275478	4.630406
Au	-8.614515	-2.025024	5.420079
Au	-5.989127	-2.381057	6.558691
Au	-12.762826	-7.607922	2.284196
Au	-10.137437	-7.963954	3.422807
Au	-7.512050	-8.319987	4.561418
Au	-4.886662	-8.676019	5.700030
Au	-11.758465	-5.713500	4.212480
Au	-9.133077	-6.069533	5.351092
Au	-6.507688	-6.425565	6.489703
Au	-10.754103	-3.819078	6.140765
Au	-8.128716	-4.175111	7.279376
Au	-9.749743	-1.924657	8.069049
Au	-13.379492	-3.463046	5.002154
Au	-14.902414	-9.401976	3.004882
Au	-12.277027	-9.758009	4.143493
Au	-9.651638	-10.114041	5.282104
Au	-7.026250	-10.470073	6.420716
Au	-4.400863	-10.826105	7.559327
Au	-13.898053	-7.507554	4.933166
Au	-11.272665	-7.863587	6.071777
Au	-8.647278	-8.219619	7.210388
Au	-6.021889	-8.575651	8.349000
Au	-12.893693	-5.613133	6.861450
Au	-10.268304	-5.969165	8.000062
Au	-7.642916	-6.325197	9.138673
Au	-11.889331	-3.718711	8.789735
Au	-9.263944	-4.074743	9.928346
Au	-10.884970	-1.824289	10.718019
S	-5.30070	-0.78782	-1.83399
C	0.04504	1.74153	1.71905
C	1.26777	2.04486	2.36111
C	1.34226	2.18977	3.75122
C	0.19427	2.02329	4.54060
C	-1.02015	1.70850	3.92106
C	-1.09417	1.56891	2.52518
C	0.02570	1.61457	0.16883
H	2.17415	2.16069	1.75898
H	2.30320	2.42652	4.21842
H	-1.92273	1.56068	4.52203

H	-2.05317	1.30932	2.07108
C	-1.31092	0.98762	-0.32094
C	1.22239	0.71117	-0.23936
C	0.14032	3.01353	-0.50620
C	-2.48185	1.77836	-0.31139
C	-1.42634	-0.33169	-0.79954
C	1.45957	-0.47923	0.48572
C	2.09696	1.00231	-1.30419
C	-0.12048	3.12571	-1.89162
C	0.48785	4.18402	0.19150
C	-3.71606	1.27956	-0.73842
H	-2.42432	2.81328	0.03792
C	-2.64880	-0.84119	-1.25021
H	-0.54681	-0.97724	-0.84030
C	2.50402	-1.35028	0.16206
H	0.81946	-0.72336	1.33914
C	3.14304	0.13859	-1.64638
H	1.97672	1.92214	-1.88044
C	-0.01360	4.35316	-2.55587
H	-0.42153	2.23527	-2.45240
C	0.58769	5.41834	-0.47186
H	0.67379	4.14198	1.26668
C	-3.80426	-0.03712	-1.22866
H	-4.59619	1.92476	-0.69539
H	-2.70371	-1.86902	-1.62234
C	3.34817	-1.05136	-0.92370
H	2.65229	-2.25034	0.76353
H	3.80633	0.39523	-2.47837
C	0.34394	5.50988	-1.84661
H	-0.21799	4.40614	-3.62979
H	0.85449	6.31273	0.09965
H	0.42288	6.47226	-2.36115
C	4.45807	-3.63531	-0.55596
H	5.25685	-4.30387	-0.90738
H	3.47531	-4.04973	-0.82570
H	4.55585	-3.50694	0.53130
C	-6.51782	0.56742	-1.78384
H	0.25088	2.12917	5.62812
H	-7.45612	0.12563	-2.14783
H	-6.20450	1.38629	-2.44852
H	-6.66710	0.91713	-0.75303
S	4.72535	-2.05837	-1.43541
Au	6.822100	-1.264710	-0.111340
Au	8.031610	-1.093574	2.500873
Au	9.675677	-1.562808	0.178650
Au	8.447275	1.015368	0.578520

Au	9.241119	-0.922439	5.113086
Au	10.885186	-1.391672	2.790862
Au	12.529253	-1.860906	0.468639
Au	9.656785	1.186503	3.190732
Au	11.300851	0.717270	0.868510
Au	10.072450	3.295446	1.268379
Au	11.716517	2.826212	-1.053844
Au	10.450629	-0.751303	7.725298
Au	12.094696	-1.220536	5.403075
Au	13.738763	-1.689770	3.080852
Au	15.382830	-2.159003	0.758629
Au	10.866294	1.357639	5.802946
Au	12.510361	0.888406	3.480722
Au	14.154429	0.419172	1.158499
Au	11.281960	3.466581	3.880592
Au	12.926027	2.997348	1.558370
Au	11.697625	5.575524	1.958239
Au	14.570094	2.528115	-0.763854
Au	11.660139	-0.580167	10.337511
Au	13.304206	-1.049401	8.015288
Au	14.948273	-1.518634	5.693065
Au	16.592340	-1.987867	3.370842
Au	18.236407	-2.457101	1.048619
Au	12.075804	1.528775	8.415158
Au	13.719872	1.059542	6.092935
Au	15.363938	0.590308	3.770712
Au	17.008006	0.121075	1.448489
Au	12.491470	3.637717	6.492805
Au	14.135537	3.168484	4.170582
Au	15.779604	2.699250	1.848359
Au	12.907136	5.746659	4.570452
Au	14.551202	5.277426	2.248230
Au	13.322801	7.855602	2.648099

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Au	-3.06646376	8.55915687	-6.77780669
Au	-5.61143074	8.19891936	-7.66758186
Au	-5.12097700	9.23012732	-5.05577014
Au	-4.44174871	10.82392095	-7.57607631
Au	-8.17147800	7.91462400	-8.58527000
Au	-7.70201900	8.92429100	-5.92518800
Au	-7.23256000	9.93395900	-3.26510500
Au	-7.06235100	10.55115400	-8.21865600

Au	-6.59289200	11.56082100	-5.55857500
Au	-5.95322400	13.18768300	-7.85204400
Au	-5.48376500	14.19735100	-5.19196100
Au	-10.869621	7.607554	-9.555624
Au	-10.400163	8.617221	-6.895542
Au	-9.930704	9.626888	-4.235460
Au	-9.461245	10.636556	-1.575378
Au	-9.760494	10.244083	-9.189011
Au	-9.291036	11.253751	-6.528929
Au	-8.821577	12.263418	-3.868847
Au	-8.651368	12.880613	-8.822398
Au	-8.181909	13.890280	-6.162316
Au	-7.542241	15.517142	-8.455785
Au	-9.120826	11.870946	-11.482480
Au	-13.567765	7.300483	-10.525978
Au	-13.098306	8.310151	-7.865897
Au	-12.628847	9.319818	-5.205815
Au	-12.159389	10.329485	-2.545732
Au	-11.689930	11.339153	0.114349
Au	-12.458638	9.937013	-10.159366
Au	-11.989179	10.946680	-7.499283
Au	-11.519721	11.956348	-4.839202
Au	-11.050262	12.966015	-2.179119
Au	-11.349511	12.573542	-9.792753
Au	-10.880052	13.583210	-7.132670
Au	-10.410594	14.592877	-4.472588
Au	-10.240384	15.210072	-9.426139
Au	-9.770925	16.219739	-6.766057
Au	-9.131257	17.846602	-9.059526
S	-0.76764197	7.83822546	-6.59740267
Si	-0.39597374	-1.01083817	-0.33940609
C	-1.98376172	-1.75587555	1.94481024
C	-0.46807461	-2.53724944	-1.46167055
C	-1.27198511	-3.64798998	-1.13963036
H	-1.89975509	-3.62174099	-0.24558865
C	-1.29365516	-4.78504563	-1.95380337
C	-0.51072588	-4.83356965	-3.11135468
C	0.29174783	-3.73951795	-3.45246241
H	0.89921757	-3.76820647	-4.35942868
C	0.31038266	-2.60444679	-2.63617191
C	1.23373495	-0.37359676	1.96597500
C	1.13705157	-1.12344224	0.77520114
C	2.18693792	-2.01805581	0.48955382
H	2.15457305	-2.61796584	-0.42275230
C	3.26548298	-2.17921580	1.36016790
C	3.33882785	-1.45281111	2.56367045

C	2.31057866	-0.53048929	2.84025540
H	2.32563287	0.03013575	3.77706471
C	-4.19582301	-0.19648829	1.26245122
C	-0.37217153	0.52646908	-1.45082341
C	0.37597606	1.68090709	-1.15157323
H	1.03005208	1.69349136	-0.27620891
C	0.32030764	2.81525719	-1.96418132
C	-0.48862700	2.84250663	-3.11657354
C	-1.23492666	1.68923206	-3.42465474
H	-1.89206273	1.68717863	-4.29658821
C	-1.17479945	0.55899072	-2.60996998
C	-4.23671573	-0.99585292	2.40875363
C	-3.12682416	-1.77580804	2.74972419
H	-3.14959797	-2.39834835	3.64641062
C	-1.92448509	-0.96163446	0.78071779
C	-3.05145510	-0.18080445	0.45867286
H	-3.03489193	0.45669642	-0.42843629
C	4.42792361	-1.69486175	3.54005639
C	4.93143324	-2.99286398	3.74270551
C	4.96518677	-0.65399899	4.32528257
C	5.93522765	-0.90314729	5.29213614
C	6.40245334	-2.21274694	5.49421144
C	5.90912990	-3.25706650	4.70302119
H	6.25906115	-4.27985312	4.83413037
H	4.52568930	-3.82377718	3.16405178
H	4.62580397	0.37093046	4.16948236
H	6.33311526	-0.08144861	5.89017562
C	7.76127188	-4.25327044	6.92661965
H	8.45352800	-4.42032106	7.75988791
H	8.19773601	-4.65688297	6.00684813
H	6.79335605	-4.71769283	7.15173392
C	-0.55667947	4.04233505	-3.98444458
C	-0.66177672	3.92089369	-5.38319535
C	-0.73941125	5.04227310	-6.20967668
C	-0.69933219	6.32370448	-5.64534105
C	-0.58999916	6.47003251	-4.25299277
C	-0.52534391	5.34184177	-3.43942343
H	-0.66103760	2.93004203	-5.83949978
H	-0.82063975	4.90355805	-7.28709726
H	-0.56229152	7.46595402	-3.80752686
H	-0.46846875	5.47193416	-2.35786877
C	-0.31465532	7.30788949	-8.27817421
H	-0.27056444	8.23107266	-8.86745843
H	-1.06557965	6.63991845	-8.71196009
H	0.67375965	6.83367307	-8.24974988
H	0.93808858	3.68134335	-1.71848295

H	-1.76745301	-0.31703391	-2.88561513
H	0.93286181	-1.75359641	-2.92638050
H	-1.92820117	-5.63260773	-1.68726476
H	-5.05596190	0.42030752	0.99499376
H	-1.12156469	-2.36236129	2.23453938
H	0.43245123	0.31683913	2.24184077
H	4.06529813	-2.87492670	1.09920257
H	-5.12880771	-1.00734483	3.03756755
H	-0.52852565	-5.71938762	-3.74883207
S	7.56009029	-2.44905752	6.83774603
Au	9.74107910	-1.62807994	6.18808466
Au	12.38231343	-1.59925346	6.98685862
Au	11.65428337	-2.41166859	4.37049800
Au	11.25288736	0.48214952	5.34173683
Au	15.03673100	-1.43828400	7.72434200
Au	14.30225700	-2.29106300	5.06931400
Au	13.56778200	-3.14384200	2.41428600
Au	13.93096600	0.45863800	5.85489700
Au	13.19649200	-0.39414000	3.19987000
Au	12.82520100	2.35556100	3.98545200
Au	12.09072600	1.50278200	1.33042400
Au	17.817966	-1.275395	8.468693
Au	17.083491	-2.128174	5.813665
Au	16.349017	-2.980952	3.158638
Au	15.614543	-3.833731	0.503610
Au	16.712200	0.621528	6.599249
Au	15.977726	-0.231251	3.944221
Au	15.243252	-1.084030	1.289193
Au	15.606435	2.518450	4.729804
Au	14.871961	1.665672	2.074776
Au	14.500670	4.415373	2.860359
Au	14.137487	0.812893	-0.580252
Au	20.599200	-1.112506	9.213045
Au	19.864726	-1.965284	6.558018
Au	19.130252	-2.818063	3.902990
Au	18.395777	-3.670842	1.247961
Au	17.661303	-4.523621	-1.407066
Au	19.493435	0.784417	7.343600
Au	18.758961	-0.068362	4.688572
Au	18.024486	-0.921140	2.033545
Au	17.290012	-1.773919	-0.621483
Au	18.387670	2.681340	5.474156
Au	17.653195	1.828561	2.819128
Au	16.918721	0.975782	0.164100
Au	17.281904	4.578262	3.604711
Au	16.547430	3.725484	0.949683

Au	16.176139	6.475185	1.735266
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