

Electronic Supplementary Information 2

Relative stability of SCM-14 germanosilicate with different distribution of germanium ions in absence and presence of structure-directing agents

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Content:

Cartesian coordinates (in Å) and computed relative energies (in eV) of the optimized structures:

Structures without SDA

S14a
S14b
S14c
S14d
S14e
S14f
S14g
S14h
S14i

Structures with SDA

Series 1

S14a_1
S14b_1
S14c_1
S14d_1
S14e_1
S14f_1
S14g_1
S14h_1
S14i_1

Series 2

S14a_2
S14a_3
S14a_4
S14a_5
S14a_6
S14a_7
S14a_8

S14a_9
S14a_10
S14a_11
S14a_12
S14a_13
S14a_14
S14a_15
S14a_16
Series 3
S14b_4
S14b_6
S14b_17
S14e_4
S14e_6
S14e_17
S14i_4
S14i_6
S14i_17
S14c_4
S14c_6
S14c_17

Cartesian coordinates (in Å) and computed relative energies (in eV) of the optimized structures

S14a, Rel. E = 0.00

Ge	16.08643	10.73983	2.634519
Ge	16.18141	10.18622	5.780928
Ge	4.842512	10.20543	5.396276
Ge	4.799607	6.968589	4.897739
Ge	16.22336	7.006664	5.118647
Ge	16.07536	7.568968	1.968687
Ge	12.96423	7.044394	5.2665
Ge	8.072701	6.958812	4.888912
Ge	8.102724	10.21407	5.361345
Ge	12.82424	7.562326	2.115491
Ge	12.80573	10.74724	2.777077
Ge	12.93693	10.19916	5.932553
Si	5.639893	16.34661	5.346708
Si	15.33913	16.248	5.517679
Si	5.584155	1.337919	1.936061
Si	15.37278	1.447064	2.280847
Si	4.797979	7.540317	1.813844
Si	5.601892	15.98932	2.272412
Si	15.28819	1.651528	5.380435
Si	4.827038	10.52441	2.301886
Si	15.38942	16.0753	2.417089
Si	5.627105	1.697387	5.003111
Si	2.399917	1.359947	2.036775
Si	2.443201	1.707149	5.111248
Si	18.52636	16.09545	2.469544
Si	18.43133	16.287	5.562968
Si	7.977166	7.485051	1.789337
Si	2.459379	16.3555	5.467624
Si	18.50894	1.461662	2.318191
Si	8.004668	10.46983	2.261023
Si	18.38225	1.665912	5.404277
Si	2.415427	16.02655	2.393653
Si	3.910277	5.372698	7.324672
Si	17.03177	12.39989	0.258934
Si	17.01672	5.341635	7.477221
Si	3.967872	12.31615	7.559845
Si	14.43826	14.25386	0.104612
Si	6.451702	3.417446	7.338984
Si	6.47681	14.25976	7.473464
Si	14.3994	3.459289	0.094159
Si	1.469048	3.439206	7.469523

Si	19.5098	14.3656	0.148445
Si	19.47914	3.413082	0.125263
Si	1.491297	14.29205	0.080194
Si	11.86846	12.41242	0.424492
Si	8.970732	5.303012	7.310247
Si	8.986917	12.34401	7.565238
Si	11.8622	5.331941	0.018589
O	3.988099	1.614346	1.80277
O	16.8901	15.77349	5.712232
O	16.96215	15.66093	2.301785
O	4.040701	2.016783	5.191326
O	16.83339	2.164756	5.521409
O	4.000669	15.7116	2.196056
O	4.055854	16.07002	5.597011
O	16.94061	1.865277	2.125801
O	14.45985	11.42699	2.9002
O	6.431169	6.241111	4.87415
O	6.381652	7.163354	1.864051
O	14.56135	10.92911	5.862407
O	6.471708	10.91778	5.563924
O	14.45012	6.833073	1.989341
O	14.5736	6.334682	4.968985
O	6.423441	10.78091	2.483148
O	6.373237	2.216735	0.839478
O	14.41264	15.33157	6.474691
O	14.5313	15.01778	1.540608
O	6.462305	2.816936	5.825079
O	14.35346	2.666253	6.248195
O	6.383708	14.85384	1.407219
O	6.492309	15.47923	6.405525
O	14.50401	2.379304	1.298181
O	17.05025	12.00228	1.850858
O	3.757955	5.807611	5.747763
O	4.045456	6.697155	0.664383
O	17.18429	11.04565	6.943441
O	3.804665	11.06628	6.526636
O	17.01768	6.72616	0.751331
O	17.19217	5.732666	5.889143
O	4.158008	11.76028	1.494677
O	5.91911	17.46833	1.65861
O	15.16279	0.116828	5.931494
O	15.17773	17.58994	1.846289
O	5.962528	0.217914	5.598906
O	15.98445	9.304389	1.56312
O	4.862456	8.483996	5.846314
O	4.600598	9.127288	1.486394

O	16.17553	8.450032	6.177545
O	6.057149	1.757236	3.438168
O	14.90029	16.02881	3.965497
O	14.86243	1.67316	3.811762
O	6.067279	15.92556	3.829801
O	16.91797	10.37644	4.16256
O	4.128329	7.188641	3.272254
O	4.138201	10.42466	3.778732
O	16.93647	7.33505	3.52259
O	2.056416	17.49331	1.781101
O	18.50221	0.152372	5.975017
O	18.74244	17.60782	1.899296
O	2.13964	0.228854	5.742652
O	12.81756	9.298176	1.717987
O	8.153506	8.490047	5.823646
O	8.192874	9.067261	1.44847
O	13.0416	8.465344	6.356806
O	1.971774	1.762174	3.556422
O	18.94898	16.0578	4.038349
O	18.91435	1.694614	3.873015
O	1.987944	15.96525	3.959094
O	12.08356	10.4337	4.376785
O	8.68049	7.123944	3.228675
O	8.74084	10.36526	3.711841
O	12.11611	7.422499	3.750799
O	1.57834	2.242969	0.972669
O	19.39213	15.49016	6.574993
O	19.43729	15.05652	1.624982
O	1.64399	2.833687	5.962903
O	19.30016	2.640966	6.296758
O	1.59012	14.90194	1.584192
O	1.667406	15.46414	6.553856
O	19.4447	2.382364	1.380451
O	11.85197	12.0408	2.025822
O	9.05826	5.751773	5.732667
O	8.666287	6.623919	0.619191
O	12.02376	11.00831	7.192057
O	9.12739	11.19724	6.406071
O	11.81797	6.637157	1.006302
O	12.02087	5.782962	6.044064
O	8.672671	11.66803	1.42109
O	5.205785	4.429497	7.558818
O	15.67799	13.22182	7.487958
O	15.65439	4.493074	0.129421
O	5.218294	13.27559	7.170335
O	2.574173	4.581496	0.175038

O	18.33311	13.28944	7.539804
O	18.3158	4.507322	0.34758
O	2.590924	13.14031	7.451195
O	13.0408	13.45025	0.044678
O	7.837436	4.194988	0.000147
O	7.856587	13.44994	7.248649
O	13.02399	4.267763	0.380905
O	0.006567	4.132516	0.054812
O	0.014306	13.62471	7.547739
O	10.43328	13.09245	0.064457
O	10.39659	4.631329	0.138029

S14b, Rel. E = 0.44

Ge	16.1087	10.76912	2.533163
Ge	16.20639	10.18407	5.672351
Ge	4.779002	10.2113	5.3986
Ge	4.801076	7.01055	4.971472
Ge	16.27122	6.995366	5.078827
Ge	16.11466	7.578658	1.944379
Ge	12.97835	6.982065	5.160629
Ge	12.8647	7.521282	2.02443
Ge	18.60743	15.92121	2.670855
Ge	18.4531	16.41098	5.806108
Ge	12.82842	10.72313	2.66455
Ge	12.94257	10.14838	5.807137
Si	5.631871	16.28937	5.35872
Si	15.25601	16.33033	5.586045
Si	5.640062	1.399808	2.011864
Si	15.34629	1.318749	2.145982
Si	4.879882	7.487601	1.849991
Si	5.589302	16.01361	2.234321
Si	15.25566	1.742479	5.191268
Si	4.849	10.50918	2.25965
Si	15.30306	15.96673	2.548094
Si	5.664888	1.655009	5.121573
Si	2.49484	1.453264	2.074047
Si	2.498223	1.696818	5.188079
Si	8.032991	7.476898	2.024814
Si	8.015935	7.119862	5.068954
Si	7.980851	10.22577	5.4357
Si	2.475351	16.32961	5.419935
Si	18.53263	1.340735	2.190462
Si	8.005178	10.52057	2.381738
Si	18.35582	1.840986	5.241484
Si	2.45339	16.08095	2.298461
Si	3.92975	5.329999	7.352855
Si	16.97903	12.4534	0.137271

Si	16.99984	5.326452	-0.12639
Si	3.914158	12.33637	-0.03052
Si	14.38545	14.28446	0.137733
Si	6.49862	3.421101	7.430284
Si	6.484827	14.23323	-0.09517
Si	14.401	3.416523	-0.02255
Si	1.452084	3.464393	7.509082
Si	19.47805	14.30272	0.291018
Si	19.42859	3.423167	0.02225
Si	1.433253	14.32894	0.019607
Si	11.86503	12.37607	0.313502
Si	8.982474	5.432539	7.429212
Si	8.956241	12.23972	0.023647
Si	11.89794	5.272013	-0.08244
O	4.068192	1.762867	1.788525
O	16.79166	15.79286	5.779415
O	16.87674	15.54082	2.599301
O	4.090437	2.003037	5.369315
O	16.79083	2.297123	5.227689
O	4.008595	15.66584	2.029814
O	4.055221	16.0141	5.668985
O	16.93897	1.634089	2.029758
O	14.46813	11.43441	2.771408
O	6.500524	6.491919	5.076673
O	6.456083	7.087481	1.905538
O	14.56428	10.86875	5.70673
O	6.448287	10.78343	5.597253
O	14.50275	6.821554	1.994981
O	14.62127	6.333193	4.906152
O	6.422863	10.90626	2.367161
O	6.545769	2.282558	1.004416
O	14.35367	15.52942	6.670974
O	14.51132	14.85432	1.663248
O	6.551885	2.731135	5.951836
O	14.33888	2.776325	6.057176
O	6.44957	14.92521	1.386364
O	6.531895	15.3744	6.338175
O	14.57263	2.206576	1.044285
O	17.03372	12.05122	1.728058
O	3.844052	5.750096	5.767909
O	4.138511	6.644608	0.692823
O	17.14924	11.09406	6.84064
O	3.7346	11.18759	6.416493
O	17.00673	6.731921	0.694802
O	17.20579	5.704353	5.870133
O	4.065553	11.66416	1.442856

O	5.901135	17.52339	1.696236
O	15.16956	0.239423	5.838689
O	15.10004	-0.26814	1.85503
O	5.982793	0.148351	5.654284
O	16.027	9.305	1.498303
O	4.596722	8.518023	5.907152
O	4.707895	9.071072	1.500141
O	16.2565	8.460963	6.109721
O	6.048502	1.746435	3.547619
O	14.72836	15.9971	4.074592
O	14.78084	1.687669	3.635182
O	5.972338	15.91927	3.810075
O	16.94835	10.4214	4.062945
O	4.205971	7.147624	3.307246
O	4.184783	10.40409	3.741448
O	16.99401	7.339667	3.487194
O	2.184368	17.59219	1.76479
O	18.46632	0.446149	6.077393
O	18.89783	-0.21825	1.875572
O	2.159353	0.1958	5.736447
O	12.8624	9.257821	1.627916
O	8.035443	8.619528	5.729354
O	8.236567	9.059154	1.690729
O	13.00752	8.417603	6.237503
O	2.109827	1.799816	3.615226
O	19.3005	15.96131	4.307786
O	18.94465	1.704204	3.731591
O	2.097245	15.99178	3.876701
O	12.08913	10.39202	4.253892
O	8.563492	7.18752	3.539223
O	8.527739	10.50242	3.922638
O	12.1165	7.312796	3.636858
O	1.596168	2.33882	1.078342
O	19.36017	15.76486	7.161199
O	19.43853	14.55909	1.906245
O	1.646829	2.786103	6.035106
O	19.21621	2.92664	6.072628
O	1.507482	15.06623	1.470626
O	1.589481	15.40686	6.401662
O	19.36722	2.224988	1.123051
O	11.85059	11.99663	1.912377
O	8.949678	6.121675	5.946154
O	8.871384	6.597438	0.968974
O	12.07142	10.98435	7.076342
O	8.884859	11.03531	6.509225
O	11.92616	6.616132	0.846126

O	12.09301	5.670253	5.931319
O	8.812325	11.62909	1.528366
O	5.142933	4.289191	0.026635
O	15.61162	13.26483	7.381539
O	15.63039	4.478616	0.100582
O	5.186379	13.2909	7.254474
O	2.521271	4.651626	0.165021
O	18.26538	13.36538	-0.21141
O	18.27772	4.493108	0.405222
O	2.555487	13.1878	7.504025
O	12.98733	13.48544	-0.02839
O	7.788868	4.366392	0.020243
O	7.823658	13.35166	7.335486
O	13.00536	4.165087	0.341615
O	-0.03081	4.114749	0.059739
O	-0.02805	13.61622	7.49485
O	10.40406	12.97843	-0.07145
O	10.39805	4.647829	0.043132

S14c, Rel. E = 1.12

Ge	5.686074	1.363814	1.882831
Ge	16.20694	10.30398	5.475702
Ge	4.7674	7.42625	2.045885
Ge	15.96664	7.492415	1.980697
Ge	16.30194	7.084919	5.124373
Ge	5.596183	1.790866	5.016229
Ge	2.435429	1.290119	1.78458
Ge	12.72423	7.374212	2.423907
Ge	18.63629	15.9803	2.679086
Ge	18.42844	16.41156	5.872164
Ge	18.35301	1.864896	5.292568
Ge	2.180277	1.695122	4.910808
Si	5.595152	16.39231	5.476868
Si	15.24145	16.30549	5.58159
Si	15.89624	10.60345	2.349223
Si	15.35708	1.327605	2.185987
Si	4.888842	10.15605	5.478805
Si	4.919183	7.132504	5.171353
Si	15.16668	1.715838	5.207572
Si	4.763306	10.57346	2.418554
Si	15.39175	15.95398	2.532381
Si	5.665916	15.91371	2.416703
Si	2.405118	16.30131	5.384894
Si	2.599169	15.85369	2.333547
Si	7.978956	7.46586	1.888667
Si	8.124272	7.214382	4.956218

Si	8.083365	10.23239	5.322167
Si	18.51183	1.382285	2.188789
Si	12.79076	10.55812	2.636378
Si	13.0579	10.3165	5.678494
Si	13.10471	7.229077	5.467602
Si	7.898598	10.54904	2.283587
Si	3.975285	5.302897	7.512431
Si	16.9568	12.42366	0.047526
Si	16.95708	5.316003	-0.14173
Si	3.993897	12.27006	0.062154
Si	14.40751	14.28768	0.118004
Si	6.518591	3.532928	7.403104
Si	6.526323	14.27865	0.051258
Si	14.3689	3.364736	-0.0085
Si	1.387216	3.420599	7.251967
Si	19.55282	14.26238	0.394288
Si	19.44174	3.535356	0.086597
Si	1.52409	14.18393	7.56643
Si	11.92485	12.26335	0.281002
Si	9.020404	5.483785	7.290529
Si	8.969713	12.30801	7.529461
Si	11.92808	5.351065	0.197708
O	4.044217	2.057922	1.788084
O	16.77391	15.77128	5.816612
O	16.94371	15.43851	2.592268
O	3.881112	2.221478	4.820417
O	16.65925	2.388013	5.250956
O	4.141679	15.32949	2.429869
O	4.006548	16.04617	5.537113
O	16.92627	1.765957	2.167409
O	14.34698	11.05485	2.567097
O	6.526394	6.910701	5.059617
O	6.443632	6.912623	1.75968
O	14.56273	10.95682	5.683206
O	6.484573	10.47034	5.507027
O	14.36081	6.733547	2.107953
O	14.58072	6.623929	5.122961
O	6.335275	10.99561	2.344308
O	6.684903	2.141481	0.656628
O	14.27635	15.49517	6.609707
O	14.56706	14.8897	1.626619
O	6.342299	3.18056	5.816135
O	14.21151	2.712568	6.080362
O	6.596041	14.86161	1.584654
O	6.384989	15.47875	6.550727
O	14.55536	2.158025	1.061725

O	16.68259	11.71336	1.482593
O	4.260065	5.939966	6.043412
O	3.701156	6.488691	1.007702
O	17.24764	11.34402	6.443823
O	4.142879	11.05519	6.586853
O	16.77189	6.733065	0.62603
O	17.17958	5.721581	5.863669
O	3.912135	11.69453	1.594964
O	5.699605	17.32303	1.587886
O	15.15506	0.210974	5.854277
O	15.2666	-0.26701	1.854779
O	5.826362	0.258903	5.897851
O	15.88799	9.197783	1.514387
O	4.626442	8.589128	5.854489
O	4.537652	9.139598	1.660694
O	16.49299	8.628407	6.013797
O	6.44674	1.705441	3.456838
O	14.78415	15.9981	4.044737
O	14.69302	1.62981	3.65055
O	6.160005	16.11345	3.959914
O	16.6776	10.42041	3.76818
O	4.22999	7.090387	3.696383
O	4.308041	10.48866	3.982414
O	16.93112	7.223095	3.460396
O	2.562919	17.2546	1.490016
O	18.4506	0.421331	6.332896
O	18.76426	-0.18319	1.794854
O	2.013352	0.141577	5.770493
O	12.59055	9.083181	1.933046
O	8.453401	8.671827	5.62394
O	8.028628	9.07058	1.604321
O	13.19976	8.741261	6.058408
O	1.494568	1.578251	3.270148
O	19.27698	16.15358	4.328618
O	19.08859	1.657073	3.698362
O	1.980101	16.01734	3.830832
O	12.35726	10.49319	4.209156
O	8.561555	7.186341	3.387987
O	8.517078	10.55689	3.785644
O	12.19628	7.235545	4.110599
O	1.547258	1.993891	0.444149
O	19.36522	15.63882	7.132819
O	19.63308	14.69473	1.976572
O	1.269728	3.020225	5.662673
O	19.27142	3.118817	6.105716
O	1.748329	14.78006	1.478384

O	1.621275	15.32371	6.406714
O	19.31441	2.284365	1.114617
O	11.9124	11.6426	1.799009
O	8.936566	6.073029	5.771513
O	8.871307	6.705929	0.773374
O	12.17346	11.05434	6.806034
O	8.881522	11.20551	6.334655
O	11.68845	6.252411	1.544037
O	12.40542	6.300711	6.568867
O	8.705857	11.61451	1.385291
O	5.247235	4.387637	0.368668
O	15.69104	13.37951	7.289883
O	15.66179	4.352586	0.055206
O	5.260175	13.27341	7.493701
O	2.637283	4.405076	7.488498
O	18.32578	13.26142	0.139937
O	18.29786	4.624159	0.457393
O	2.612833	13.02447	7.27664
O	13.05698	13.40169	0.100772
O	7.869667	4.391001	7.569318
O	7.905532	13.50473	7.28905
O	13.00868	4.156222	0.389331
O	0.021192	4.160827	0.173946
O	0.022311	13.54656	7.550657
O	10.47339	12.93069	-0.02657
O	10.45932	4.736748	7.450642

S14d, Rel. E = 1.23

Ge	16.21739	10.60884	2.655944
Ge	16.19965	10.20051	5.801833
Ge	4.822063	10.21072	5.337233
Ge	4.745388	6.956937	4.893459
Ge	5.651555	16.36904	5.348497
Ge	15.27739	1.552087	2.438697
Ge	2.356517	1.299831	1.858296
Ge	8.0177	6.929864	4.863723
Ge	8.077251	10.17658	5.358674
Ge	2.373913	1.782528	4.994443
Ge	12.84239	10.65382	2.68908
Ge	12.97154	10.26217	5.834119
Si	16.02228	7.059341	5.27458
Si	15.43614	16.13626	5.471394
Si	5.571912	1.327501	1.831986
Si	16.05262	7.494171	2.193291
Si	4.743091	7.542209	1.822044
Si	5.599545	15.96498	2.274798

Si	15.34089	1.505638	5.60735
Si	4.82845	10.52581	2.242046
Si	15.38575	16.11745	2.352923
Si	5.603986	1.800331	4.862787
Si	12.97163	7.134362	5.28468
Si	12.90225	7.534748	2.209997
Si	18.50652	16.25184	2.31647
Si	18.51463	16.22102	5.410682
Si	7.934332	7.470327	1.782112
Si	2.450616	16.33863	5.532528
Si	18.47933	1.629653	2.392727
Si	8.024013	10.42563	2.256081
Si	18.43085	1.59063	5.503392
Si	2.462892	15.91558	2.475225
Si	3.941593	5.32207	7.335192
Si	17.07612	12.34865	0.330965
Si	16.94094	5.396142	0.036415
Si	3.994612	12.35009	-0.10238
Si	14.4691	14.19642	0.097367
Si	6.500438	3.385879	7.256873
Si	6.512952	14.2503	-0.11794
Si	14.3572	3.472767	0.226673
Si	1.424127	3.493287	7.355378
Si	19.52482	14.37759	0.045535
Si	19.4831	3.493711	0.167958
Si	1.499102	14.27702	0.130655
Si	11.89832	12.37927	0.382158
Si	8.963375	5.300634	7.28011
Si	9.003844	12.28212	7.575686
Si	11.89338	5.497695	0.008241
O	4.030274	1.868651	1.755288
O	16.99171	15.65427	5.550653
O	16.9644	15.73142	2.198112
O	4.055459	2.328785	4.823665
O	16.87473	2.061666	5.644405
O	4.046975	15.5323	2.501825
O	3.99429	15.79851	5.622919
O	16.93614	2.156675	2.217389
O	14.54001	11.21949	2.727522
O	6.373363	6.220191	4.856363
O	6.33378	7.216277	1.917631
O	14.59862	10.99245	5.808947
O	6.456084	10.90728	5.529616
O	14.47161	7.118214	2.064512
O	14.48161	6.509603	5.247407
O	6.433642	10.71771	2.438866

O	6.409262	2.131712	0.705071
O	14.53173	15.15519	6.376749
O	14.52525	15.0525	1.485098
O	6.475882	2.889811	5.699142
O	14.4311	2.412568	6.584247
O	6.35144	14.81568	1.407173
O	6.700778	15.5224	6.470901
O	14.18488	2.670963	1.635546
O	17.16797	11.90309	1.903435
O	3.734639	5.7865	5.771858
O	4.041667	6.647124	0.679718
O	17.19718	10.98641	7.020573
O	3.802788	11.10218	6.458181
O	16.89123	6.569801	1.164893
O	16.92546	5.987988	6.097928
O	4.230418	11.78213	1.410766
O	5.663157	17.42429	1.531808
O	15.30703	-0.05542	6.067297
O	15.11912	-0.08208	1.758702
O	5.713604	0.396732	5.694286
O	16.29101	9.060974	1.773323
O	4.795918	8.493466	5.809969
O	4.528958	9.120666	1.458748
O	16.09922	8.462123	6.119226
O	6.154021	1.634215	3.334807
O	14.94499	16.07271	3.919686
O	14.72126	1.602021	4.108833
O	6.322677	16.0602	3.734128
O	17.01111	10.43228	4.23564
O	4.058005	7.193758	3.274911
O	4.132506	10.4721	3.719722
O	16.54112	7.242306	3.738861
O	2.252977	17.26589	1.579927
O	18.58335	0.042383	5.98031
O	18.61369	0.102275	1.831784
O	2.326384	0.234715	5.886214
O	12.6882	9.109243	1.808159
O	8.069221	8.452758	5.812108
O	8.223794	9.035007	1.426876
O	13.03252	8.526265	6.138606
O	1.56706	1.641928	3.417386
O	19.00087	16.16953	3.861694
O	18.9141	1.696633	3.956386
O	1.912955	16.08325	4.002345
O	12.10453	10.52618	4.304265
O	8.648189	7.088957	3.210949

O	8.736135	10.30973	3.717065
O	12.42796	7.326421	3.76211
O	1.436415	2.083097	0.589878
O	19.48732	15.29064	6.291925
O	19.43251	15.31183	1.381266
O	1.504988	3.114867	5.766308
O	19.33451	2.541244	6.442018
O	1.659893	14.75826	1.683214
O	1.607257	15.50633	6.642271
O	19.44126	2.603402	1.532199
O	11.92399	11.98823	1.972277
O	9.019905	5.732799	5.698028
O	8.54353	6.587465	0.587423
O	12.07586	10.97321	7.160802
O	9.113532	11.12675	6.421809
O	12.04067	6.605303	1.199381
O	11.97691	6.16229	6.108354
O	8.728345	11.62632	1.448984
O	5.283916	4.429622	-0.05487
O	15.6818	13.12148	0.038434
O	15.68268	4.400698	0.244938
O	5.225714	13.33454	7.074541
O	2.638978	4.471069	0.207511
O	18.32625	13.30466	0.002822
O	18.33569	4.617564	0.229232
O	2.607117	13.15907	7.393265
O	13.04374	13.44741	0.010607
O	7.92272	4.094573	7.538493
O	7.856105	13.37537	7.291979
O	13.03193	4.369281	0.106367
O	0.004809	4.234936	0.064546
O	0.02327	13.60105	0.024291
O	10.44954	13.03239	0.03352
O	10.43811	4.786617	0.136185

S14e, Rel. E = 1.35

Ge	4.755785	7.566909	2.069921
Ge	16.20544	10.235	5.456169
Ge	15.21167	1.34422	5.449256
Ge	16.02463	7.359353	1.868918
Ge	16.2557	7.059236	5.044838
Ge	15.1961	15.81309	4.947459
Ge	8.007619	7.57971	1.964284
Ge	12.77737	7.308981	2.27592
Ge	2.430042	16.41385	5.680786
Ge	18.45038	15.7384	5.023854

Ge	18.44177	1.239172	5.609798
Ge	2.412033	16.08813	2.498277
Si	5.615858	16.41598	5.622347
Si	5.53233	1.824778	5.261733
Si	15.40009	16.23923	1.831456
Si	5.736941	16.1006	2.57102
Si	4.839379	10.27502	5.547229
Si	4.838799	7.311706	5.132462
Si	5.683878	1.431321	2.219527
Si	4.844244	10.74622	2.501785
Si	15.93856	10.46352	2.302803
Si	15.41422	1.554663	2.313687
Si	18.51677	16.23769	1.917625
Si	2.435795	1.835185	5.148106
Si	13.05503	7.179766	5.357462
Si	8.063152	7.329003	5.033583
Si	8.052394	10.28282	5.510827
Si	18.52383	1.537665	2.475622
Si	12.83914	10.46142	2.563532
Si	7.945653	10.73515	2.461269
Si	2.482594	1.453214	2.055336
Si	13.04883	10.2483	5.626024
Si	3.929296	5.478472	7.482047
Si	17.02914	12.30658	0.045121
Si	16.93625	5.19638	-0.3187
Si	4.060389	12.42597	0.124672
Si	14.41923	14.14806	-0.29394
Si	6.407692	3.533312	0.075785
Si	6.596468	14.41011	0.191163
Si	14.29681	3.405185	0.052714
Si	1.435547	3.545054	7.417868
Si	19.55453	14.16325	-0.15856
Si	19.46819	3.287442	0.228795
Si	1.504785	14.23878	0.227499
Si	11.958	12.19227	0.254804
Si	8.881229	5.489694	7.339837
Si	9.007184	12.40663	0.117162
Si	11.80974	5.331683	0.054703
O	4.090702	1.690766	2.015332
O	16.80912	15.03994	4.952152
O	16.95797	15.745	1.860389
O	3.986526	2.347161	5.21869
O	16.84071	2.027632	5.752856
O	4.15065	15.72666	2.506573
O	4.096449	15.81252	5.747139
O	16.96386	2.017359	2.537904

O	14.39701	10.94497	2.506475
O	6.443523	7.256159	4.860269
O	6.379412	6.866094	1.817872
O	14.55979	10.88371	5.677889
O	6.445908	10.49807	5.628061
O	14.39961	6.623165	1.945435
O	14.54154	6.571067	5.05425
O	6.39688	11.24322	2.508085
O	6.518919	2.363379	1.196973
O	14.10748	14.6716	5.76802
O	14.59235	15.429	0.694434
O	6.379158	2.871661	6.169705
O	14.10626	2.339095	6.405453
O	6.563294	14.97627	1.727047
O	6.512595	15.66035	6.737654
O	14.63401	2.66184	1.448929
O	16.7419	11.57449	1.461113
O	4.359437	6.043131	6.014355
O	3.718203	6.720273	0.931058
O	17.28861	11.25222	6.405997
O	4.112733	11.2136	6.636287
O	16.9759	6.490655	0.675172
O	17.19828	5.731069	5.743754
O	3.978405	11.83481	1.650532
O	6.018723	17.56913	1.910394
O	15.17015	-0.37758	5.911437
O	15.3588	0.135767	1.51018
O	5.612685	0.321804	5.904817
O	15.95331	9.074628	1.431556
O	4.48097	8.71578	5.890026
O	4.731936	9.304926	1.729523
O	16.42249	8.553469	6.015419
O	6.125397	1.792116	3.7478
O	14.65495	15.98245	3.270293
O	14.67144	1.438106	3.761217
O	6.212191	16.11036	4.132411
O	16.67676	10.28473	3.745712
O	4.085544	7.251254	3.683696
O	4.312808	10.63606	4.038056
O	16.91395	7.211476	3.404571
O	2.115404	17.6133	1.619349
O	18.37933	17.21482	6.037639
O	18.60566	0.138338	1.640886
O	2.331353	0.443194	5.998597
O	12.66893	9.018718	1.800586
O	8.436408	8.719093	5.820074

O	8.02512	9.320391	1.640598
O	13.14135	8.668608	6.01566
O	1.97018	1.692558	3.592407
O	19.13907	15.93185	3.40439
O	19.12403	1.348141	3.976587
O	1.662638	16.13152	4.104932
O	12.39902	10.3931	4.131759
O	8.75165	7.308792	3.552415
O	8.521955	10.61663	3.979441
O	12.22491	7.23136	3.956092
O	1.777122	2.46262	1.006149
O	19.47983	14.56054	5.843705
O	19.39936	15.47896	0.795292
O	1.483036	2.890501	5.92286
O	19.52435	2.085041	6.707785
O	1.629064	14.67566	1.793865
O	1.471117	15.59584	6.903402
O	19.41902	2.661151	1.731681
O	11.92977	11.53131	1.750255
O	8.593061	6.02398	5.828812
O	8.975445	6.790694	0.732021
O	12.14229	11.03482	6.707841
O	8.781733	11.25431	6.574423
O	11.6785	6.260272	1.392382
O	12.26031	6.220908	6.368396
O	8.809306	11.81386	1.62167
O	5.059458	4.404538	0.36772
O	15.7937	13.29362	7.296724
O	15.48712	4.468428	-0.24988
O	5.368699	13.37219	7.536522
O	2.479906	4.77263	7.435583
O	18.40739	13.11153	0.252329
O	18.16201	4.216069	0.044763
O	2.716879	13.26422	7.381735
O	13.16298	13.26469	0.192368
O	7.724381	4.46067	0.208205
O	7.999561	13.65489	7.48328
O	12.86262	4.122752	0.252901
O	-0.07043	4.125289	0.079648
O	0.081578	13.46651	0.06636
O	10.53984	12.94539	-0.00084
O	10.32094	4.725045	7.374295

S14f, Rel. E = 1.36

Ge	5.712802	1.483677	2.055636
Ge	16.31761	10.41863	5.281578

Ge	4.828194	10.19896	5.429254
Ge	4.908488	7.003583	4.953348
Ge	16.31348	7.133124	5.176654
Ge	5.662948	15.93917	2.300237
Ge	2.232924	16.27343	5.186899
Ge	12.76668	7.289973	2.452583
Ge	18.72257	16.00753	2.758304
Ge	18.4274	16.33694	5.91704
Ge	12.69426	10.53085	2.578945
Ge	13.11928	10.32924	5.729307
Si	5.478121	16.28705	5.451441
Si	15.26822	16.2577	5.571595
Si	15.85695	10.43438	2.207857
Si	15.43043	1.361108	2.232793
Si	4.821806	7.523841	1.829183
Si	15.8944	7.333335	2.090426
Si	15.26601	1.65584	5.285636
Si	4.752383	10.53934	2.289534
Si	15.43664	16.01208	2.525622
Si	5.486598	1.624345	5.209182
Si	2.578239	1.530973	1.983629
Si	2.324965	1.707872	5.053126
Si	7.985281	7.538176	1.828401
Si	8.100943	7.177235	4.873677
Si	8.01256	10.2846	5.279505
Si	18.59633	1.418256	2.381795
Si	13.19175	7.187457	5.558554
Si	7.909461	10.58609	2.229242
Si	18.34419	1.761089	5.456795
Si	2.518255	16.12846	2.086347
Si	3.974614	5.358142	7.382761
Si	16.96599	12.34255	7.518699
Si	16.98871	5.360717	7.522774
Si	3.901124	12.30437	0.015595
Si	14.42666	14.28541	0.141293
Si	6.53864	3.522046	7.4703
Si	6.510682	14.17146	7.534731
Si	14.41656	3.375929	0.007362
Si	1.448831	3.455873	7.40508
Si	19.5008	14.20088	0.5132
Si	19.45027	3.489954	0.194171
Si	1.382269	14.27744	7.41196
Si	11.8818	12.35819	0.334469
Si	9.034759	5.515509	7.202728
Si	8.970438	12.2854	7.442462
Si	11.92096	5.315081	0.221003

O	4.079185	2.183718	1.90111
O	16.78792	15.67487	5.783751
O	17.00512	15.56129	2.606208
O	3.917716	2.049949	5.140753
O	16.78753	2.24047	5.380674
O	3.970216	15.37575	2.199286
O	3.9242	15.77933	5.428051
O	17.011	1.749465	2.186296
O	14.38283	11.10375	2.446279
O	6.610459	6.49571	4.936535
O	6.405378	7.131425	1.767861
O	14.69047	11.13445	5.52543
O	6.48599	10.82986	5.529022
O	14.41685	6.642675	2.2302
O	14.65111	6.493581	5.30742
O	6.325264	10.96097	2.29914
O	6.824263	2.494639	1.12539
O	14.29623	15.43591	6.578041
O	14.63636	14.9357	1.618409
O	6.281971	2.707376	6.094523
O	14.29052	2.638843	6.139068
O	6.656425	14.69972	1.500459
O	6.28639	15.44223	6.559547
O	14.62429	2.268415	1.174584
O	16.64825	11.22379	1.055186
O	4.004636	5.727503	5.784108
O	3.987386	6.694698	0.718795
O	17.35978	11.58314	6.11829
O	3.782363	11.09412	6.518342
O	16.70469	6.651559	0.875854
O	17.30913	5.913654	6.004426
O	3.895057	11.68954	1.527422
O	5.864042	17.50803	1.45871
O	15.2085	0.147706	5.913504
O	15.27067	17.48808	1.845646
O	5.580807	0.147912	5.886599
O	15.66102	8.896703	1.735171
O	4.747122	8.492745	5.927315
O	4.609674	9.108768	1.516165
O	16.53401	8.755351	5.919375
O	6.20591	1.576238	3.750503
O	14.80234	16.02322	4.02738
O	14.81799	1.619754	3.72345
O	6.18195	16.04304	3.991573
O	16.76265	10.48621	3.566867
O	4.236827	7.167002	3.322326

O	4.162655	10.40045	3.800648
O	16.77416	7.163195	3.462505
O	2.727637	17.66291	1.596758
O	18.4176	0.358984	6.290398
O	18.96965	17.58256	1.96102
O	1.984554	0.247665	5.736544
O	12.48354	8.931304	1.785763
O	8.084426	8.674134	5.536972
O	8.132867	9.132902	1.51432
O	13.44988	8.661264	6.200645
O	1.920211	1.701743	3.471226
O	19.3461	16.06556	4.423797
O	18.97294	1.637234	3.959735
O	1.719529	16.13578	3.502912
O	12.11818	10.43617	4.264602
O	8.586089	7.255449	3.320934
O	8.49455	10.57836	3.747672
O	12.33028	7.288132	4.172734
O	1.636017	2.247411	0.890226
O	19.2501	15.57727	7.262491
O	19.65469	14.66782	2.074542
O	1.507649	2.844491	5.884656
O	19.18101	2.836453	6.316782
O	1.607421	15.35457	1.01368
O	1.220777	15.08616	6.003058
O	19.44124	2.404545	1.411751
O	11.71656	11.83997	1.885609
O	9.095343	6.213758	5.724932
O	8.802768	6.681625	0.73099
O	12.23415	11.01034	7.076402
O	8.957455	11.09215	6.325277
O	11.72798	6.120774	1.634769
O	12.35635	6.328113	6.624448
O	8.671634	11.69895	1.343264
O	5.254843	4.455379	0.221974
O	15.67691	13.31467	7.369882
O	15.68827	4.387802	7.573336
O	5.26768	13.14293	7.370289
O	2.593253	4.567766	0.055633
O	18.28287	13.16621	0.35223
O	18.31673	4.613668	0.490185
O	2.602018	13.23007	7.382962
O	13.02485	13.4799	0.154667
O	7.855533	4.423047	7.277486
O	7.884604	13.43695	7.088843
O	13.0191	4.130499	0.329711

O	0.006567	4.156602	0.103577
O	20.89766	13.49247	0.062266
O	10.45102	12.97007	7.447407
O	10.44079	4.733298	7.461825

S14g, Rel. E = 1.43

Ge	5.692452	1.430116	1.993962
Ge	15.252947	16.080452	5.415105
Ge	15.993693	10.484468	2.398291
Ge	4.918588	7.052633	4.996650
Ge	16.214985	7.193136	5.309412
Ge	5.706811	15.899362	2.383101
Ge	8.016626	10.285174	5.352717
Ge	18.686625	1.594459	2.634534
Ge	18.698523	16.055500	2.597691
Ge	2.214513	1.680647	4.845017
Ge	7.965796	7.612711	1.798042
Ge	12.987246	10.379876	5.504285
Si	5.458574	16.378340	5.486831
Si	15.498688	1.559610	2.379939
Si	4.719026	7.482749	1.901059
Si	16.206007	10.314485	5.516127
Si	4.812763	10.209337	5.451653
Si	15.982412	7.369595	2.169801
Si	15.260160	1.558449	5.453961
Si	4.666836	10.520522	2.409559
Si	15.505366	16.175856	2.287686
Si	5.515960	1.687927	5.119629
Si	2.524272	1.386410	1.752395
Si	18.375059	16.167131	5.732636
Si	12.813060	10.401550	2.390574
Si	8.141410	7.150263	4.928000
Si	2.261528	16.300797	5.186202
Si	12.902303	7.326806	2.379909
Si	13.010706	7.248728	5.460281
Si	7.828005	10.683511	2.238221
Si	18.299606	1.547754	5.748570
Si	2.548187	15.995493	2.160913
Si	3.961613	5.350314	7.424325
Si	16.989487	12.339969	0.094737
Si	17.023561	5.337345	0.001256
Si	3.927622	12.219979	0.048817
Si	14.376048	14.225045	0.067400
Si	6.519007	3.533065	7.428105
Si	6.468976	14.199946	7.585671
Si	14.429996	3.408319	0.099264

Si	1.455185	3.408367	7.240025
Si	19.541134	14.250098	0.273418
Si	19.531891	3.458768	0.384394
Si	1.477225	14.237485	7.410713
Si	11.858742	12.351522	0.214423
Si	9.067845	5.465036	7.208694
Si	8.922460	12.444426	7.530806
Si	11.939561	5.403053	0.149173
O	4.026973	2.037967	1.793683
O	16.907057	15.435353	5.639139
O	17.008308	15.540603	2.381646
O	3.943011	2.065475	4.948583
O	16.786802	2.139768	5.607612
O	4.028379	15.308808	2.272476
O	3.867894	16.083191	5.337943
O	17.016279	2.177418	2.389442
O	14.312833	11.074982	2.371562
O	6.617408	6.539466	4.922546
O	6.288094	7.048046	1.750771
O	14.678836	10.898383	5.534821
O	6.332166	10.816360	5.527649
O	14.451656	6.815995	2.282398
O	14.532689	6.647916	5.463046
O	6.236482	10.944101	2.431872
O	6.766665	2.391639	0.981387
O	14.130394	14.974823	6.219462
O	14.666710	15.343419	1.199335
O	6.238104	2.852629	5.979544
O	14.283444	2.528199	6.317276
O	6.701740	14.686904	1.553734
O	6.070625	15.477262	6.673489
O	14.569291	2.445988	1.402764
O	17.037766	11.610603	1.550639
O	4.021215	5.800504	5.854294
O	3.857481	6.654148	0.806696
O	17.100080	11.275629	6.459269
O	3.936096	11.001169	6.557422
O	16.789722	6.503028	1.090058
O	17.249542	5.996110	6.102197
O	3.811397	11.626559	1.572769
O	5.877984	17.435448	1.489822
O	15.124299	0.035823	6.050421
O	15.568967	0.030857	1.82714
O	5.682852	0.244632	5.87106
O	15.998936	8.902042	1.609487
O	4.803529	8.617681	5.836808

O	4.506664	9.078334	1.661019
O	16.342207	8.787760	6.087591
O	6.251644	1.614664	3.664166
O	14.743223	16.058971	3.723598
O	14.856288	1.584430	3.878304
O	6.222683	16.015858	4.07792
O	16.761904	10.365591	3.985114
O	4.172109	7.102067	3.395251
O	4.169137	10.429656	3.959618
O	16.732143	7.257916	3.617689
O	2.661638	17.485912	1.511524
O	18.152367	17.701868	6.182718
O	18.974422	17.684465	1.90423
O	1.839999	0.121037	5.62611
O	12.818115	8.866318	1.839337
O	8.191335	8.566313	5.761171
O	8.065973	9.323965	1.349816
O	12.923898	8.731440	6.155883
O	1.708842	1.676403	3.145693
O	19.166916	16.068214	4.306401
O	19.131886	1.646609	4.347653
O	1.849784	16.077404	3.626837
O	12.229555	10.409321	3.910487
O	8.682712	7.374159	3.404769
O	8.571742	10.556481	3.686617
O	12.428169	7.282496	3.939264
O	1.696670	2.045754	0.523364
O	19.302351	15.518964	6.879189
O	19.666267	14.798002	1.815214
O	1.367333	3.002562	5.654832
O	19.124720	2.319876	6.891022
O	1.644069	15.076434	1.200406
O	1.491544	15.234732	6.123697
O	19.739344	2.775014	1.85494
O	11.839892	11.298331	1.459062
O	9.088320	6.058352	5.681311
O	8.927626	6.728951	0.638789
O	12.069774	11.570560	6.394112
O	9.030370	11.224004	6.446569
O	11.970644	6.361776	1.472513
O	12.130424	6.262428	6.374307
O	8.449677	11.920694	1.410253
O	5.273807	4.489666	0.258352
O	15.622101	13.194630	7.539105
O	15.745901	4.345803	7.581424
O	5.295618	13.082453	7.499138

O	2.628022	4.459575	7.584894
O	18.318121	13.238447	0.053411
O	18.390144	4.593577	0.417494
O	2.638910	13.127748	7.286132
O	13.012954	13.455535	0.464015
O	7.874191	4.397974	7.356711
O	7.868574	13.580609	7.031928
O	13.080750	4.271813	0.292323
O	0.037388	4.121057	0.009061
O	0.015426	13.516052	7.47632
O	10.410398	13.088990	0.108526
O	10.469220	4.718122	7.582966

S14h, Rel. E = 1.49

Ge	5.653161	1.351618	1.944085
Ge	16.18145	10.29867	5.443599
Ge	4.745763	7.436179	2.08761
Ge	15.97831	7.511482	1.928234
Ge	16.24344	7.085844	5.0748
Ge	5.604312	1.791474	5.082509
Ge	2.412607	1.278168	1.969105
Ge	12.73213	7.404943	2.349236
Ge	18.59931	16.01359	2.562075
Ge	18.4188	16.43088	5.758114
Ge	18.35046	1.882072	5.173353
Ge	2.562541	15.77498	2.514357
Si	5.681086	16.40667	5.549765
Si	15.23589	16.31719	5.510716
Si	15.93412	10.61399	2.31143
Si	15.33017	1.344394	2.106746
Si	4.910697	10.16415	5.508512
Si	4.887772	7.149026	5.215322
Si	15.16437	1.723247	5.133557
Si	4.788839	10.58502	2.447246
Si	15.37273	15.96759	2.462289
Si	5.72034	15.89118	2.511958
Si	2.493004	16.33138	5.598378
Si	2.306488	1.620506	5.066048
Si	7.964176	7.449419	1.922096
Si	8.098431	7.192167	4.992114
Si	8.110452	10.19995	5.347853
Si	18.47161	1.413498	2.060766
Si	12.82008	10.56815	2.563546
Si	13.03371	10.32363	5.613114
Si	13.05137	7.241406	5.399671
Si	7.928057	10.52976	2.306062

Si	3.963973	5.312724	7.564693
Si	16.95811	12.43072	0.011938
Si	16.94207	5.316648	-0.20709
Si	4.014753	12.29603	0.102206
Si	14.39711	14.30104	0.056059
Si	6.497171	3.529428	7.469478
Si	6.555118	14.29397	0.120499
Si	14.35548	3.370304	-0.08229
Si	1.408686	3.372841	7.360229
Si	19.55025	14.28839	0.280739
Si	19.43937	3.552221	-0.04389
Si	1.534625	14.14311	0.094428
Si	11.92327	12.28012	0.215393
Si	8.993202	5.452333	7.332205
Si	8.97902	12.28065	7.554358
Si	11.9063	5.3671	0.129813
O	4.016074	2.050558	1.839417
O	16.76784	15.77698	5.744612
O	16.91872	15.43308	2.51593
O	3.863994	2.099925	4.921403
O	16.6535	2.400207	5.161483
O	4.241223	15.19058	2.580051
O	4.095429	16.03985	5.588385
O	16.89003	1.818552	2.056813
O	14.3796	11.05202	2.518515
O	6.494256	6.936952	5.096756
O	6.420454	6.920871	1.789824
O	14.54	10.96257	5.63649
O	6.51256	10.43183	5.525508
O	14.37172	6.758221	2.074498
O	14.52541	6.610888	5.087306
O	6.366422	10.9907	2.349473
O	6.633593	2.120503	0.697712
O	14.27825	15.50205	6.540729
O	14.52677	14.91765	1.560925
O	6.306675	3.205702	5.875627
O	14.20799	2.717157	6.007104
O	6.679915	14.88454	1.649575
O	6.474028	15.5075	6.630006
O	14.49615	2.160874	0.993473
O	16.7294	11.73879	1.466781
O	4.236677	5.954396	6.092784
O	3.669954	6.499919	1.055871
O	17.22095	11.32298	6.427847
O	4.21804	11.09825	6.61955
O	16.77292	6.719691	0.588872

O	17.13006	5.726287	5.797751
O	3.939649	11.70756	1.628475
O	5.633941	17.30324	1.683199
O	15.1608	0.222268	5.788637
O	15.27117	-0.25302	1.786411
O	5.899197	0.274008	5.966961
O	15.94989	9.217768	1.456236
O	4.59628	8.608767	5.894047
O	4.532432	9.15041	1.70102
O	16.40843	8.6167	5.987411
O	6.423836	1.724956	3.506356
O	14.76844	16.01834	3.975185
O	14.67939	1.628849	3.580232
O	6.259765	16.1322	4.036301
O	16.68562	10.42031	3.744636
O	4.203001	7.100435	3.737821
O	4.339706	10.51006	4.013152
O	16.90671	7.253664	3.430161
O	2.479858	17.26084	1.521442
O	18.43892	0.439963	6.217278
O	18.69509	-0.15688	1.663372
O	2.216707	0.209975	5.891261
O	12.61877	9.106334	1.835052
O	8.478907	8.639796	5.655244
O	8.045574	9.050565	1.626968
O	13.15694	8.748385	6.006988
O	1.668341	1.432614	3.573341
O	19.24962	16.21001	4.201437
O	19.06411	1.68275	3.566588
O	1.865168	15.94153	4.132865
O	12.36223	10.49167	4.128365
O	8.533905	7.157167	3.423482
O	8.541092	10.52775	3.810865
O	12.17257	7.288328	4.025054
O	1.395652	2.120405	0.817236
O	19.39238	15.64141	6.978201
O	19.61637	14.75307	1.853154
O	1.453887	2.764686	5.842674
O	19.28248	3.137411	5.971259
O	1.647875	14.52507	1.67977
O	1.773551	15.4493	6.742355
O	19.2802	2.299809	0.979698
O	11.95225	11.66199	1.731729
O	8.866123	6.022809	5.809372
O	8.850003	6.678587	0.809632
O	12.1401	11.07974	6.723261

O	8.902255	11.17371	6.363603
O	11.70359	6.285796	1.466088
O	12.29659	6.309358	6.462901
O	8.763206	11.58344	1.41674
O	5.249974	4.419203	0.430117
O	15.68358	13.3804	7.268215
O	15.66717	4.331722	0.00703
O	5.226514	13.37121	7.568184
O	2.648896	4.382401	7.546285
O	18.32137	13.28377	0.043613
O	18.30887	4.645962	0.344175
O	2.605681	12.99191	7.300824
O	13.04521	13.42112	0.010133
O	7.871128	4.342323	0.069367
O	7.878325	13.44351	7.335008
O	13.01306	4.19677	0.293635
O	0.014588	4.179265	0.048836
O	0.025051	13.56002	7.469583
O	10.46317	12.94717	-0.04266
O	10.43881	4.715457	7.46364

S14i, Rel. E = 1.50

Ge	4.755866	7.469809	2.057159
Ge	16.16074	10.26376	5.390875
Ge	5.756791	1.420877	2.193328
Ge	15.96227	7.44285	1.904826
Ge	16.25632	7.040676	5.064875
Ge	15.17724	16.27358	5.474921
Ge	8.014305	7.56607	1.835504
Ge	12.71716	7.266101	2.356537
Ge	18.61695	15.96205	2.616749
Ge	18.42515	16.37321	5.787382
Ge	18.35999	1.838824	5.169354
Ge	2.529057	15.98795	2.408352
Si	5.574789	16.37961	5.574426
Si	5.534755	1.743324	5.30563
Si	15.37657	15.9593	2.39177
Si	5.770882	15.96658	2.521458
Si	4.869464	10.18281	5.538252
Si	4.944237	7.18952	5.129419
Si	15.19389	1.752604	5.073648
Si	4.770186	10.65669	2.501578
Si	15.86515	10.55454	2.253913
Si	15.37926	1.313394	2.026924
Si	2.423795	16.33061	5.509188
Si	2.385942	1.666651	5.109551

Si	13.08038	7.173797	5.417978
Si	8.162642	7.289066	4.920497
Si	8.073436	10.24629	5.404718
Si	18.51544	1.346262	2.055386
Si	12.7612	10.44197	2.53568
Si	7.872614	10.70694	2.361158
Si	2.523585	1.42207	2.020472
Si	13.0228	10.26029	5.586417
Si	3.993068	5.38503	7.506984
Si	16.94376	12.3705	-0.05168
Si	16.95655	5.277045	-0.21787
Si	3.997376	12.30242	0.133831
Si	14.3921	14.18815	0.017969
Si	6.480241	3.553349	0.068688
Si	6.542965	14.30429	0.15656
Si	14.35173	3.358787	-0.14063
Si	1.465731	3.442461	7.388391
Si	19.53054	14.22343	0.317889
Si	19.46517	3.476162	-0.03768
Si	1.507792	14.20031	0.046031
Si	11.8983	12.17189	0.216353
Si	8.98563	5.50037	7.219204
Si	8.962448	12.36737	0.006153
Si	11.87436	5.287789	0.118397
O	4.076713	1.91697	1.939967
O	16.81461	15.60954	5.750609
O	16.91188	15.46194	2.64705
O	3.953063	2.119981	5.196123
O	16.68697	2.42857	5.105235
O	4.221572	15.45436	2.415387
O	4.005323	15.95031	5.561821
O	16.94225	1.779475	1.999049
O	14.30459	10.9739	2.45227
O	6.543869	7.11696	4.834825
O	6.393054	6.830877	1.719958
O	14.51861	10.92714	5.600874
O	6.470319	10.45487	5.573943
O	14.36759	6.657701	2.036051
O	14.54946	6.528996	5.112306
O	6.31555	11.17916	2.46272
O	6.808625	2.401071	1.177536
O	14.0703	15.36475	6.510541
O	14.64353	14.84958	1.478386
O	6.267381	2.873791	6.195772
O	14.2331	2.770112	5.918097
O	6.662006	14.87526	1.692071

O	6.346385	15.53373	6.705019
O	14.54955	2.141665	0.919195
O	16.63405	11.68495	1.39179
O	4.47909	5.94598	6.055432
O	3.684043	6.623053	0.941554
O	17.23013	11.26829	6.364814
O	4.147115	11.07932	6.666165
O	16.83385	6.677579	0.594727
O	17.17832	5.705381	5.795442
O	3.863746	11.72165	1.660926
O	5.970534	17.41549	1.78182
O	15.16786	0.306157	5.846062
O	15.31505	-0.27967	1.66668
O	5.703434	0.25658	5.962368
O	15.89117	9.145475	1.424758
O	4.587404	8.606075	5.864662
O	4.656606	9.20944	1.743735
O	16.4035	8.588077	5.950856
O	6.266722	1.746055	3.851587
O	14.58893	16.03989	3.819985
O	14.74132	1.582297	3.513913
O	6.207239	16.07606	4.092155
O	16.63157	10.38866	3.683429
O	4.170138	7.095901	3.693569
O	4.283847	10.54976	4.052893
O	16.89144	7.211074	3.410659
O	2.377794	17.55285	1.572971
O	18.3644	0.392972	6.21678
O	18.7251	-0.23088	1.681521
O	2.208959	0.209534	5.821801
O	12.57714	8.964632	1.835009
O	8.488886	8.691931	5.699795
O	7.957406	9.305981	1.516533
O	13.19448	8.693113	5.985733
O	1.951027	1.603212	3.540254
O	19.29767	16.16978	4.24511
O	19.084	1.613474	3.570913
O	1.82057	16.01793	4.025117
O	12.33636	10.38958	4.107777
O	8.786539	7.321836	3.41313
O	8.494188	10.5897	3.861365
O	12.19698	7.165104	4.046392
O	1.704008	2.337981	0.97401
O	19.3677	15.60064	7.048564
O	19.56029	14.64615	1.903513
O	1.457439	2.720877	5.920028

O	19.33643	3.055302	5.97668
O	1.626418	14.7291	1.583184
O	1.62967	15.44921	6.600888
O	19.36463	2.212142	0.984184
O	11.84134	11.49079	1.703697
O	8.824189	6.023808	5.685048
O	9.018113	6.81489	0.60417
O	12.1015	11.01097	6.678755
O	8.828128	11.2074	6.459527
O	11.67994	6.112279	1.51903
O	12.33041	6.300761	6.53245
O	8.698667	11.80367	1.510622
O	5.148201	4.389576	0.495989
O	15.69043	13.32673	7.140137
O	15.62271	4.369175	-0.01797
O	5.293221	13.2752	0.028301
O	2.600737	4.584999	7.364859
O	18.32085	13.20112	0.043279
O	18.28062	4.520586	0.332015
O	2.642854	13.09254	7.315262
O	13.09211	13.24581	0.120617
O	7.769195	4.51876	0.016331
O	7.923956	13.5774	7.308541
O	12.95859	4.091139	0.246728
O	0.019331	4.142712	0.090416
O	0.024923	13.52634	7.510286
O	10.48746	12.93349	-0.0525
O	10.39715	4.692107	7.352355

S14a_1, Rel. E = 1.84

Ge	16.33703	10.78823	2.616764
Ge	16.15573	10.16374	5.620618
Ge	4.783098	10.15681	5.449386
Ge	4.705881	6.904243	4.999576
Ge	16.30002	7.04617	5.189432
Ge	16.14372	7.606541	2.076098
Ge	13.07744	7.064784	5.215294
Ge	7.996059	6.927636	4.935601
Ge	8.037629	10.18579	5.364525
Ge	12.89662	7.72052	2.029038
Ge	13.17855	10.81498	2.619287
Ge	13.02231	10.21871	5.761089
Ge	16.33703	10.78823	10.20446
Ge	16.15573	10.16374	13.20832
Ge	4.783098	10.15681	13.03709
Ge	4.705881	6.904243	12.58728

Ge	16.30002	7.04617	12.77713
Ge	16.14372	7.606541	9.663798
Ge	13.07744	7.064784	12.80299
Ge	7.996059	6.927636	12.5233
Ge	8.037629	10.18579	12.95223
Ge	12.89662	7.72052	9.616738
Ge	13.17855	10.81498	10.20699
Ge	13.02231	10.21871	13.34879
Si	5.555694	16.26603	5.363501
Si	15.36589	16.32273	5.595985
Si	5.523449	1.29211	2.048486
Si	15.30057	1.388366	2.20162
Si	4.672737	7.425845	1.925273
Si	5.559654	15.95158	2.334586
Si	15.32618	1.742622	5.27346
Si	4.725579	10.47167	2.34512
Si	15.28191	16.00204	2.52138
Si	5.555873	1.597102	5.091437
Si	2.441463	1.260815	2.10798
Si	2.468762	1.608099	5.146341
Si	18.46038	15.96662	2.532249
Si	18.50971	16.36312	5.562852
Si	7.799542	7.387425	1.818316
Si	2.493495	16.25754	5.473761
Si	18.47689	1.364606	2.153107
Si	7.864965	10.40192	2.231163
Si	18.47062	1.781452	5.185008
Si	2.493708	15.93408	2.455199
Si	3.912804	5.235334	7.43479
Si	17.03493	12.40672	0.149594
Si	17.0749	5.344419	15.15287
Si	3.893025	12.29509	0.040873
Si	14.40888	14.2739	0.160966
Si	6.485671	3.317673	7.431546
Si	6.450519	14.24138	15.124
Si	14.43904	3.479761	0.054436
Si	1.476259	3.248468	7.534684
Si	19.44242	14.37713	0.110106
Si	19.48691	3.369447	-0.00367
Si	1.443222	14.29764	0.111766
Si	11.90441	12.38865	0.270756
Si	8.964991	5.25186	7.345798
Si	8.962399	12.28599	7.567644
Si	11.93192	5.405913	-0.0535
Si	5.555694	16.26603	12.9512
Si	15.36589	16.32273	13.18368

Si	5.523449	1.29211	9.636185
Si	15.30057	1.388366	9.78932
Si	4.672737	7.425845	9.512973
Si	5.559654	15.95158	9.922285
Si	15.32618	1.742622	12.86116
Si	4.725579	10.47167	9.932819
Si	15.28191	16.00204	10.10908
Si	5.555873	1.597102	12.67914
Si	2.441463	1.260815	9.69568
Si	2.468762	1.608099	12.73404
Si	18.46038	15.96662	10.11995
Si	18.50971	16.36312	13.15055
Si	7.799542	7.387425	9.406015
Si	2.493495	16.25754	13.06146
Si	18.47689	1.364606	9.740807
Si	7.864965	10.40192	9.818862
Si	18.47062	1.781452	12.77271
Si	2.493708	15.93408	10.0429
Si	3.912804	5.235334	15.02249
Si	17.03493	12.40672	7.737294
Si	17.0749	5.344419	7.565168
Si	3.893025	12.29509	7.628572
Si	14.40888	14.2739	7.748665
Si	6.485671	3.317673	15.01925
Si	6.450519	14.24138	7.536301
Si	14.43904	3.479761	7.642136
Si	1.476259	3.248468	15.12238
Si	19.44242	14.37713	7.697806
Si	19.48691	3.369447	7.584029
Si	1.443222	14.29764	7.699466
Si	11.90441	12.38865	7.858456
Si	8.964991	5.25186	14.9335
Si	8.962399	12.28599	15.15535
Si	11.93192	5.405913	7.534195
O	3.974826	1.55514	1.627565
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O	16.88155	1.662617	1.965253
O	14.7483	11.64425	2.707484
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O	6.237095	6.973094	1.981342
O	14.59817	11.00226	5.982756

O	6.403736	10.87222	5.605038
O	14.51721	6.901489	1.953716
O	14.67689	6.284794	5.211783
O	6.307285	10.84294	2.458196
O	6.40846	2.179886	0.99332
O	14.46188	15.51213	6.665842
O	14.4064	14.93986	1.661271
O	6.464609	2.666999	5.94497
O	14.40678	2.756681	6.155209
O	6.459672	14.88409	1.446961
O	6.476813	15.39704	6.409728
O	14.44432	2.268443	1.153598
O	17.29106	12.02272	1.727013
O	3.707541	5.737494	5.875721
O	3.904675	6.578286	0.788829
O	17.11188	11.06188	6.86143
O	3.750165	11.04686	6.567761
O	17.09434	6.680891	0.887412
O	17.25878	5.762882	5.99314
O	3.947335	11.64259	1.537901
O	6.006762	17.44376	1.81975
O	15.07865	0.218555	5.846751
O	14.96621	17.50881	1.966039
O	6.024709	0.111093	5.58725
O	16.44585	9.308603	1.610482
O	4.713562	8.442682	5.926176
O	4.53811	9.026171	1.597799
O	16.45157	8.496752	6.222513
O	5.922386	1.870388	3.524736
O	14.85418	15.91738	4.097501
O	14.84048	1.800103	3.718945
O	5.961205	15.66766	3.891965
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O	3.98498	7.126521	3.389642
O	4.0645	10.40353	3.842054
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O	2.001818	17.40143	1.959968
O	18.71718	0.26032	5.704381
O	18.75329	17.47327	2.002409
O	2.043955	0.109118	5.636747
O	13.34238	9.392316	1.549715
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O	18.93566	15.82743	4.083754

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O	1.583392	2.669775	6.020403
O	19.31795	2.838932	6.051248
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O	1.599445	15.43161	6.565847
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O	12.07329	11.98485	1.842745
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O	12.04934	5.817229	5.963609
O	8.645424	11.51387	1.376819
O	5.316116	4.446014	0.043549
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O	3.974826	1.55514	9.215264
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F	4.056286	17.55668	11.33123
F	14.92285	9.119253	11.68682
C	9.664765	16.23354	0.960476
C	9.442758	16.66932	7.103067
C	8.824319	0.360369	7.2514
C	9.575537	0.970074	0.84986
C	11.13069	16.42258	3.486891
C	11.89403	16.55682	4.612217
C	11.81369	1.224637	4.459459
C	11.05476	1.157705	3.324026
C	10.69586	17.5867	2.772354
C	20.48241	7.821178	1.644255
C	20.32459	7.683934	0.128499
C	19.4763	8.906377	7.348749
C	20.01338	10.01	0.669264
C	0.572141	9.180218	4.060996
C	1.092238	9.860826	5.128411
C	0.648635	11.95033	4.104426
C	0.123798	11.33276	3.001273
C	0.072964	9.901978	2.929186
C	9.664765	16.23354	8.548176
C	9.442758	16.66932	14.69077
C	8.824319	0.360369	14.8391
C	9.575537	0.970074	8.43756
C	11.13069	16.42258	11.07459
C	11.89403	16.55682	12.19992
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C	10.69586	17.5867	10.36005
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C	20.32459	7.683934	7.716198
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C	20.01338	10.01	8.256964
C	0.572141	9.180218	11.6487
C	1.092238	9.860826	12.71611
C	0.648635	11.95033	11.69213
C	0.123798	11.33276	10.58897
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H	8.746474	15.81408	1.403821
H	10.47458	15.49919	1.064167
H	10.41513	16.72738	6.596916
H	8.801859	15.97289	6.55199
H	8.913665	0.978797	6.348971
H	7.757812	0.269717	7.489704
H	10.46475	1.547101	0.539488
H	8.937437	1.62941	1.457244
H	10.876	15.42237	3.144135
H	12.27835	15.70804	5.175815
H	12.14684	2.163377	4.900471
H	10.75119	2.082152	2.838033
H	12.85993	0.15934	5.881255
H	19.61173	7.397051	2.174271
H	0.471619	7.350217	2.0279
H	0.39033	7.725489	7.237802
H	19.85552	6.731242	7.443081
H	19.5373	9.185833	6.289243
H	18.42166	8.719799	7.583642
H	20.83698	10.58578	0.209864
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H	8.746474	15.81408	8.991521
H	10.47458	15.49919	8.651867
H	10.41513	16.72738	14.18462
H	8.801859	15.97289	14.13969
H	8.913665	0.978797	13.93667
H	7.757812	0.269717	15.0774
H	10.46475	1.547101	8.127188
H	8.937437	1.62941	9.044944
H	10.876	15.42237	10.73183
H	12.27835	15.70804	12.76352
H	12.14684	2.163377	12.48817
H	10.75119	2.082152	10.42573
H	12.85993	0.15934	13.46896
H	19.61173	7.397051	9.761971
H	0.471619	7.350217	9.6156
H	0.39033	7.725489	14.8255

H	19.85552	6.731242	15.03078
H	19.5373	9.185833	13.87694
H	18.42166	8.719799	15.17134
H	20.83698	10.58578	7.797564
H	19.234	10.72077	8.564015
H	0.551884	8.092409	11.6727
H	1.505308	9.359254	13.59037
H	0.723825	13.03419	11.78234
H	20.6835	11.95024	9.772736
H	1.560662	11.69975	13.52755

S14b_1, Rel. E = 2.63

Ge	16.27145	10.74398	2.521279
Ge	16.20353	10.16057	5.569444
Ge	4.732728	10.18066	5.433071
Ge	4.686564	6.978837	5.045202
Ge	16.33364	7.031837	5.106339
Ge	16.23192	7.590947	2.040889
Ge	13.11583	6.98178	5.070877
Ge	13.06499	7.549615	1.909709
Ge	18.56286	15.84799	2.640566
Ge	18.50142	16.37039	5.776139
Ge	13.0942	10.65998	2.505126
Ge	13.02793	10.13278	5.662301
Ge	16.27145	10.74398	10.10898
Ge	16.20353	10.16057	13.15715
Ge	4.732728	10.18066	13.02077
Ge	4.686564	6.978837	12.6329
Ge	16.33364	7.031837	12.69404
Ge	16.23192	7.590947	9.628589
Ge	13.11583	6.98178	12.65858
Ge	13.06499	7.549615	9.49741
Ge	18.56286	15.84799	10.22827
Ge	18.50142	16.37039	13.36384
Ge	13.0942	10.65998	10.09283
Ge	13.02793	10.13278	13.25
Si	5.55468	16.26494	5.36488
Si	15.29896	16.31108	5.561948
Si	5.578689	1.375638	2.100292
Si	15.34596	1.352009	2.152039
Si	4.764963	7.415742	1.93135
Si	5.56556	16.02064	2.325975
Si	15.31753	1.750217	5.190627
Si	4.749051	10.50193	2.307213
Si	15.26259	15.97595	2.495564
Si	5.588387	1.611408	5.156815

Si	2.501395	1.365154	2.133252
Si	2.497957	1.652297	5.179973
Si	7.851019	7.403245	2.038909
Si	7.929388	7.120451	5.097249
Si	7.933641	10.23453	5.392785
Si	2.492299	16.29397	5.416072
Si	18.54629	1.310496	2.171475
Si	7.835525	10.47908	2.324745
Si	18.42955	1.838769	5.202221
Si	2.502629	16.02028	2.390124
Si	3.913909	5.272297	7.442564
Si	17.00709	12.43895	0.088059
Si	17.08127	5.354835	15.0988
Si	3.89214	12.3314	0.036478
Si	14.36397	14.27627	0.105733
Si	6.50946	3.375933	7.484376
Si	6.468587	14.25472	15.14987
Si	14.44893	3.46937	15.1522
Si	1.471399	3.321631	7.55342
Si	19.48636	14.27616	0.238197
Si	19.47236	3.380111	0.01283
Si	1.448351	14.35516	0.047209
Si	11.88873	12.3016	0.181946
Si	8.96193	5.415964	7.443626
Si	8.930182	12.22616	-0.00337
Si	11.94632	5.356444	15.00256
Si	5.55468	16.26494	12.95258
Si	15.29896	16.31108	13.14965
Si	5.578689	1.375638	9.687992
Si	15.34596	1.352009	9.739738
Si	4.764963	7.415742	9.519051
Si	5.56556	16.02064	9.913675
Si	15.31753	1.750217	12.77833
Si	4.749051	10.50193	9.894914
Si	15.26259	15.97595	10.08326
Si	5.588387	1.611408	12.74451
Si	2.501395	1.365154	9.720952
Si	2.497957	1.652297	12.76767
Si	7.851019	7.403245	9.62661
Si	7.929388	7.120451	12.68495
Si	7.933641	10.23453	12.98048
Si	2.492299	16.29397	13.00377
Si	18.54629	1.310496	9.759175
Si	7.835525	10.47908	9.912445
Si	18.42955	1.838769	12.78992
Si	2.502629	16.02028	9.977824

Si	3.913909	5.272297	15.03026
Si	17.00709	12.43895	7.675759
Si	17.08127	5.354835	7.511098
Si	3.89214	12.3314	7.624177
Si	14.36397	14.27627	7.693433
Si	6.50946	3.375933	15.07208
Si	6.468587	14.25472	7.562165
Si	14.44893	3.46937	7.564499
Si	1.471399	3.321631	15.14112
Si	19.48636	14.27616	7.825896
Si	19.47236	3.380111	7.60053
Si	1.448351	14.35516	7.634909
Si	11.88873	12.3016	7.769646
Si	8.96193	5.415964	15.03133
Si	8.930182	12.22616	7.584334
Si	11.94632	5.356444	7.41486
O	4.038438	1.697091	1.67899
O	16.81758	15.79679	5.803916
O	16.82415	15.51999	2.452752
O	4.052736	2.000132	5.548665
O	16.85042	2.268213	5.228594
O	4.027111	15.60449	1.958349
O	4.027637	15.9395	5.848308
O	16.94315	1.599149	2.033345
O	14.65493	11.52	2.595989
O	6.400543	6.539874	5.171556
O	6.301106	6.882608	1.972442
O	14.60522	10.92894	5.822627
O	6.393377	10.74974	5.618834
O	14.6603	6.757403	1.866218
O	14.72922	6.228736	5.068685
O	6.288744	11.02454	2.359512
O	6.51016	2.266573	1.083449
O	14.33489	15.53588	6.620734
O	14.38347	14.92778	1.613409
O	6.511302	2.658386	6.025434
O	14.37911	2.739661	6.081614
O	6.480052	14.97138	1.435924
O	6.473535	15.35624	6.379342
O	14.56427	2.255746	1.066574
O	17.19528	12.0216	1.661808
O	3.745846	5.733366	5.866838
O	3.956402	6.621042	0.781411
O	17.12228	11.11008	6.770305
O	3.725406	11.15991	6.489329
O	17.16846	6.697013	0.821902

O	17.30536	5.778092	5.945168
O	3.866766	11.58903	1.487643
O	6.010906	17.51905	1.831309
O	15.16647	0.227289	5.804669
O	15.02743	17.47402	1.876368
O	6.019452	0.10643	5.638497
O	16.44552	9.281875	1.500476
O	4.425025	8.506845	5.946558
O	4.671544	9.020432	1.617684
O	16.42866	8.485968	6.14894
O	5.978159	1.894348	3.597154
O	14.76277	15.96272	4.055419
O	14.79237	1.742899	3.646581
O	5.968811	15.7166	3.878113
O	17.11018	10.62256	4.089468
O	4.063253	7.110463	3.388648
O	4.09124	10.4357	3.801277
O	17.14988	7.182942	3.528843
O	2.076082	17.51122	1.911304
O	18.54578	0.410397	5.976171
O	18.88048	17.43576	1.927032
O	2.064609	0.145462	5.640316
O	13.27178	9.250662	1.418768
O	8.023719	8.635923	5.712257
O	7.786938	8.988023	1.680787
O	12.95615	8.416266	6.130216
O	2.140625	1.938548	3.618094
O	19.24489	15.76343	4.282339
O	18.9891	1.758085	3.679551
O	2.113827	15.69734	3.94114
O	12.25825	10.41397	4.067215
O	8.430561	7.130134	3.545549
O	8.404768	10.49977	3.85483
O	12.30384	7.180598	3.495635
O	1.548198	2.173746	1.093371
O	19.4153	15.75838	7.138671
O	19.40075	14.50789	1.857342
O	1.603062	2.705991	6.056394
O	19.27832	2.912934	6.047695
O	1.554366	14.98848	1.528357
O	1.552037	15.44035	6.450567
O	19.35824	2.123376	1.04391
O	12.00805	11.84981	1.744765
O	8.862235	6.122117	5.968592
O	8.74465	6.572026	0.985223
O	11.98557	11.01968	6.782611

O	8.85326	11.11095	6.390832
O	12.04379	6.683959	0.756332
O	12.11422	5.717084	5.831964
O	8.730293	11.48297	1.433
O	5.263369	4.410754	0.074271
O	15.6492	13.32561	7.444752
O	15.70195	4.482616	0.098476
O	5.213434	13.22029	7.414222
O	2.58742	4.46303	0.260866
O	18.29001	13.35994	14.85018
O	18.33063	4.443334	0.416378
O	2.525994	13.15937	7.414293
O	12.97061	13.48459	15.02966
O	7.893236	4.220731	0.034351
O	7.838415	13.39694	7.388627
O	13.02663	4.201767	0.252291
O	0.014643	4.057875	0.113384
O	-0.00293	13.58222	7.509832
O	10.3959	12.94702	15.15022
O	10.4406	4.739888	0.018316
O	10.4786	8.92985	2.478504
O	4.038438	1.697091	9.266689
O	16.81758	15.79679	13.39162
O	16.82415	15.51999	10.04045
O	4.052736	2.000132	13.13637
O	16.85042	2.268213	12.81629
O	4.027111	15.60449	9.546048
O	4.027637	15.9395	13.43601
O	16.94315	1.599149	9.621045
O	14.65493	11.52	10.18369
O	6.400543	6.539874	12.75926
O	6.301106	6.882608	9.560142
O	14.60522	10.92894	13.41033
O	6.393377	10.74974	13.20653
O	14.6603	6.757403	9.453918
O	14.72922	6.228736	12.65639
O	6.288744	11.02454	9.947212
O	6.51016	2.266573	8.671149
O	14.33489	15.53588	14.20843
O	14.38347	14.92778	9.201109
O	6.511302	2.658386	13.61313
O	14.37911	2.739661	13.66931
O	6.480052	14.97138	9.023624
O	6.473535	15.35624	13.96704
O	14.56427	2.255746	8.654274
O	17.19528	12.0216	9.249508

O	3.745846	5.733366	13.45454
O	3.956402	6.621042	8.369111
O	17.12228	11.11008	14.35801
O	3.725406	11.15991	14.07703
O	17.16846	6.697013	8.409602
O	17.30536	5.778092	13.53287
O	3.866766	11.58903	9.075343
O	6.010906	17.51905	9.419009
O	15.16647	0.227289	13.39237
O	15.02743	17.47402	9.464067
O	6.019452	0.10643	13.2262
O	16.44552	9.281875	9.088177
O	4.425025	8.506845	13.53426
O	4.671544	9.020432	9.205384
O	16.42866	8.485968	13.73664
O	5.978159	1.894348	11.18485
O	14.76277	15.96272	11.64312
O	14.79237	1.742899	11.23428
O	5.968811	15.7166	11.46581
O	17.11018	10.62256	11.67717
O	4.063253	7.110463	10.97635
O	4.09124	10.4357	11.38898
O	17.14988	7.182942	11.11654
O	2.076082	17.51122	9.499004
O	18.54578	0.410397	13.56387
O	18.88048	17.43576	9.514732
O	2.064609	0.145462	13.22802
O	13.27178	9.250662	9.006468
O	8.023719	8.635923	13.29996
O	7.786938	8.988023	9.268487
O	12.95615	8.416266	13.71792
O	2.140625	1.938548	11.20579
O	19.24489	15.76343	11.87004
O	18.9891	1.758085	11.26725
O	2.113827	15.69734	11.52884
O	12.25825	10.41397	11.65491
O	8.430561	7.130134	11.13325
O	8.404768	10.49977	11.44253
O	12.30384	7.180598	11.08334
O	1.548198	2.173746	8.68107
O	19.4153	15.75838	14.72637
O	19.40075	14.50789	9.445042
O	1.603062	2.705991	13.64409
O	19.27832	2.912934	13.6354
O	1.554366	14.98848	9.116057
O	1.552037	15.44035	14.03827

O	19.35824	2.123376	8.63161
O	12.00805	11.84981	9.332465
O	8.862235	6.122117	13.55629
O	8.74465	6.572026	8.572923
O	11.98557	11.01968	14.37031
O	8.85326	11.11095	13.97853
O	12.04379	6.683959	8.344031
O	12.11422	5.717084	13.41966
O	8.730293	11.48297	9.0207
O	5.263369	4.410754	7.661971
O	15.6492	13.32561	15.03245
O	15.70195	4.482616	7.686175
O	5.213434	13.22029	15.00192
O	2.58742	4.46303	7.848566
O	18.29001	13.35994	7.262475
O	18.33063	4.443334	8.004079
O	2.525994	13.15937	15.00199
O	12.97061	13.48459	7.441964
O	7.893236	4.220731	7.622051
O	7.838415	13.39694	14.97633
O	13.02663	4.201767	7.839991
O	0.014643	4.057875	7.701084
O	-0.00293	13.58222	15.09753
O	10.3959	12.94702	7.562522
O	10.4406	4.739888	7.606017
O	10.4786	8.92985	10.0662
F	4.068943	17.61205	3.754768
F	14.90178	8.882595	3.874081
F	4.068943	17.61205	11.34247
F	14.90178	8.882595	11.46178
C	9.661726	16.19491	0.975364
C	9.440991	16.61544	7.113792
C	8.841943	0.316615	7.242857
C	9.604741	0.932133	0.830354
C	11.09869	16.39599	3.510378
C	11.8483	16.52908	4.643732
C	11.7941	1.197318	4.474891
C	11.05162	1.13012	3.328873
C	10.68735	17.55881	2.780555
C	20.4575	7.822603	1.606751
C	20.29469	7.720453	0.089118
C	19.45695	8.956604	7.331976
C	19.98183	10.03617	0.68926
C	0.585643	9.116059	4.036344
C	1.139618	9.768717	5.104195
C	0.630265	11.88449	4.168098

C	0.078044	11.29593	3.063281
C	0.050396	9.868396	2.942231
C	9.661726	16.19491	8.563064
C	9.440991	16.61544	14.70149
C	8.841943	0.316615	14.83056
C	9.604741	0.932133	8.418055
C	11.09869	16.39599	11.09808
C	11.8483	16.52908	12.23143
C	11.7941	1.197318	12.06259
C	11.05162	1.13012	10.91657
C	10.68735	17.55881	10.36826
C	20.4575	7.822603	9.19445
C	20.29469	7.720453	7.676818
C	19.45695	8.956604	14.91968
C	19.98183	10.03617	8.27696
C	0.585643	9.116059	11.62404
C	1.139618	9.768717	12.6919
C	0.630265	11.88449	11.7558
C	0.078044	11.29593	10.65098
C	0.050396	9.868396	10.52993
N	12.18471	0.060261	5.116038
N	10.01609	17.46582	1.634523
N	1.151843	11.12618	5.168913
N	20.49476	9.278266	1.845044
N	12.18471	0.060261	12.70374
N	10.01609	17.46582	9.222223
N	1.151843	11.12618	12.75661
N	20.49476	9.278266	9.432744
H	10.59926	8.115411	3.008149
H	10.60688	9.628638	3.151557
H	8.742819	15.78714	1.426777
H	10.46863	15.45743	1.084677
H	10.41354	16.65382	6.607599
H	8.79351	15.91951	6.570443
H	8.937617	0.920036	6.330858
H	7.77459	0.246728	7.485424
H	10.50516	1.486618	0.510148
H	8.977776	1.61208	1.426239
H	10.83431	15.39663	3.172779
H	12.21304	15.68053	5.219705
H	12.12596	2.136111	4.916721
H	10.76165	2.054244	2.834011
H	12.78986	0.130332	5.933181
H	19.5935	7.380579	2.132889
H	0.451772	7.346823	1.971497
H	0.358821	7.760162	7.197182

H	19.81261	6.780158	7.384851
H	19.53796	9.262311	6.28096
H	18.39946	8.764532	7.545997
H	20.80319	10.63152	0.251776
H	19.19462	10.73184	1.012289
H	0.579454	8.028268	4.026398
H	1.602651	9.244534	5.939507
H	0.691463	12.96553	4.294412
H	20.60002	11.93708	2.284697
H	1.64673	11.58004	5.938795
H	10.59926	8.115411	10.59585
H	10.60688	9.628638	10.73926
H	8.742819	15.78714	9.014478
H	10.46863	15.45743	8.672377
H	10.41354	16.65382	14.1953
H	8.79351	15.91951	14.15814
H	8.937617	0.920036	13.91856
H	7.77459	0.246728	15.07312
H	10.50516	1.486618	8.097847
H	8.977776	1.61208	9.013939
H	10.83431	15.39663	10.76048
H	12.21304	15.68053	12.80741
H	12.12596	2.136111	12.50442
H	10.76165	2.054244	10.42171
H	12.78986	0.130332	13.52088
H	19.5935	7.380579	9.720588
H	0.451772	7.346823	9.559197
H	0.358821	7.760162	14.78488
H	19.81261	6.780158	14.97255
H	19.53796	9.262311	13.86866
H	18.39946	8.764532	15.1337
H	20.80319	10.63152	7.839476
H	19.19462	10.73184	8.599989
H	0.579454	8.028268	11.6141
H	1.602651	9.244534	13.52721
H	0.691463	12.96553	11.88211
H	20.60002	11.93708	9.872396
H	1.64673	11.58004	13.52649

S14c_1, Rel. E = 2.60

Ge	5.654307	1.377632	2.212536
Ge	16.202583	10.236287	5.247922
Ge	4.806616	10.176227	5.477568
Ge	4.786730	6.962034	5.011203
Ge	16.323477	7.136057	5.093198
Ge	5.602126	16.009796	2.435547

Ge	2.375293	16.229685	5.237044
Ge	12.849936	7.542197	2.225256
Ge	18.650927	15.929163	2.680950
Ge	18.523287	16.391254	5.837338
Ge	13.070798	10.683320	2.480039
Ge	13.112131	10.170852	5.670914
Ge	5.654307	1.377632	9.800236
Ge	16.202583	10.236287	12.835622
Ge	4.806616	10.176227	13.065269
Ge	4.786730	6.962034	12.598903
Ge	16.323477	7.136057	12.680898
Ge	5.602126	16.009796	10.023248
Ge	2.375293	16.229685	12.824743
Ge	12.849936	7.542197	9.812957
Ge	18.650927	15.929163	10.268650
Ge	18.523287	16.391254	13.425038
Ge	13.070798	10.683320	10.067739
Ge	13.112131	10.170852	13.258614
Si	5.551533	16.198908	5.529007
Si	15.327096	16.286161	5.568891
Si	16.165771	10.588037	2.241808
Si	15.347380	1.305330	2.161951
Si	4.753333	7.467502	1.895249
Si	16.014669	7.480428	1.991198
Si	15.269592	1.728252	5.177344
Si	4.748831	10.535876	2.354846
Si	15.330171	15.934731	2.521591
Si	5.523168	1.593695	5.308009
Si	2.515855	1.437413	2.005069
Si	2.381491	1.663211	5.125074
Si	7.870358	7.443589	1.930873
Si	7.984602	7.099380	4.999993
Si	7.977188	10.232452	5.383169
Si	18.556587	1.351409	2.236935
Si	13.148149	7.072099	5.388306
Si	7.874333	10.525790	2.332269
Si	18.373930	1.838074	5.276335
Si	2.516535	16.058437	2.081561
Si	3.896813	5.330290	7.440173
Si	16.963734	12.362751	15.012469
Si	16.979933	5.394821	15.055830
Si	3.879664	12.292527	0.075957
Si	14.387853	14.270571	0.099316
Si	6.495361	3.476487	7.613772
Si	6.478560	14.165711	0.096951
Si	14.413322	3.403265	-0.029749

Si	1.408757	3.401299	7.468694
Si	19.464933	14.261162	0.321911
Si	19.399113	3.480757	0.06283
Si	1.359775	14.233716	7.444886
Si	11.901480	12.346565	0.175473
Si	9.000089	5.462467	7.339097
Si	8.952208	12.211964	7.560804
Si	11.948902	5.333702	0.060248
Si	5.551533	16.198908	13.116707
Si	15.327096	16.286161	13.156591
Si	16.165771	10.588037	9.829508
Si	15.347380	1.305330	9.749651
Si	4.753333	7.467502	9.482948
Si	16.014669	7.480428	9.578897
Si	15.269592	1.728252	12.765043
Si	4.748831	10.535876	9.942546
Si	15.330171	15.934731	10.10929
Si	5.523168	1.593695	12.895708
Si	2.515855	1.437413	9.592768
Si	2.381491	1.663211	12.712774
Si	7.870358	7.443589	9.518574
Si	7.984602	7.099380	12.587693
Si	7.977188	10.232452	12.970869
Si	18.556587	1.351409	9.824635
Si	13.148149	7.072099	12.976006
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Si	3.896813	5.330290	15.027874
Si	16.963734	12.362751	7.42477
Si	16.979933	5.394821	7.46813
Si	3.879664	12.292527	7.663656
Si	14.387853	14.270571	7.687016
Si	6.495361	3.476487	0.026072
Si	6.478560	14.165711	7.684651
Si	14.413322	3.403265	7.557951
Si	1.408757	3.401299	15.056395
Si	19.464933	14.261162	7.909611
Si	19.399113	3.480757	7.650529
Si	1.359775	14.233716	15.032586
Si	11.901480	12.346565	7.763173
Si	9.000089	5.462467	14.926797
Si	8.952208	12.211964	15.148503
Si	11.948902	5.333702	7.647947
O	4.038439	1.965067	1.712193
O	16.852346	15.782968	5.81253

O	16.916632	15.569081	2.516266
O	3.948002	2.005816	5.390119
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O	14.297729	2.689376	6.067336
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O	17.028229	11.528263	1.232092
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O	19.319365	2.278222	8.747912
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O	8.98841	6.156043	13.437795
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O	5.221449	4.480677	7.79383
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C	9.644452	16.195713	0.936614
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C	19.458042	8.981342	7.392388
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C	0.629516	9.139638	4.064887
C	1.170001	9.791561	5.139891
C	0.663635	11.908443	4.203571
C	0.130808	11.320877	3.088566
C	0.104286	9.893245	2.966624
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C	9.43974	16.612364	14.659285
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H	19.791225	6.797974	15.028614
H	19.481672	9.270288	13.922734
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H	20.887314	10.604515	7.824202
H	19.302015	10.795877	8.617199
H	0.625265	8.051787	11.639738
H	1.623032	9.268658	13.568783
H	0.710779	12.989117	11.928708
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S14d_1, Rel. E = 3.48

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Ge	2.428464	1.258484	1.876008
Ge	7.949498	6.989779	4.853323
Ge	7.985486	10.25723	5.345249
Ge	2.401377	1.706604	5.026005
Ge	12.95554	10.40028	2.325706
Ge	13.07097	10.34893	5.509942
Ge	16.06768	10.38052	10.11538
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Si	15.43117	16.05717	5.504014
Si	5.623226	1.38615	1.935405
Si	16.22037	7.275198	2.31893
Si	4.659581	7.513284	1.869964
Si	5.663637	15.98625	2.231472
Si	15.42595	1.482147	5.633639
Si	4.638981	10.56183	2.347606
Si	15.40627	16.08527	2.38995
Si	5.613567	1.799831	5.009776
Si	13.07357	7.236945	5.306927
Si	13.19154	7.32118	2.225872
Si	18.55142	16.18593	2.417973
Si	18.4799	16.10718	5.490387
Si	7.79504	7.546431	1.7618
Si	2.371129	16.26466	5.488253
Si	18.54797	1.586977	2.474744
Si	7.772827	10.56303	2.226406
Si	18.47048	1.515557	5.584632
Si	2.550136	15.85145	2.408726
Si	3.904268	5.313514	14.98917
Si	17.02634	12.28428	0.214265
Si	16.98348	5.30114	0.085406
Si	3.897952	12.31085	0.002351
Si	14.42291	14.16814	0.139294
Si	6.516086	3.462774	14.95155
Si	6.443022	14.29605	-0.18289
Si	14.34494	3.423503	0.205089
Si	1.439204	3.413275	14.96022
Si	19.49763	14.32627	0.164425
Si	19.53806	3.364831	0.218574
Si	1.447171	14.22769	0.073156
Si	11.83262	12.32834	0.125602
Si	8.957413	5.440506	14.87676
Si	8.911096	12.34823	15.11213
Si	11.95916	5.464575	-0.01195
Si	16.17081	7.159035	12.95976
Si	15.43117	16.05717	13.09171
Si	5.623226	1.38615	9.523105
Si	16.22037	7.275198	9.90663
Si	4.659581	7.513284	9.457664
Si	5.663637	15.98625	9.819172
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Si	4.638981	10.56183	9.935306
Si	15.40627	16.08527	9.977651
Si	5.613567	1.799831	12.59748

Si	13.07357	7.236945	12.89463
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Si	18.55142	16.18593	10.00567
Si	18.4799	16.10718	13.07809
Si	7.79504	7.546431	9.349501
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Si	6.516086	3.462774	7.363848
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Si	5.643206	16.31461	13.1213
Si	15.5883	1.370914	9.797812
Si	4.995399	7.45156	9.436624
Si	16.28541	10.18902	13.24407
Si	4.804802	10.14563	13.02197
Si	16.31883	7.435673	9.604161
Si	15.47438	1.588939	12.8833
Si	4.79262	10.54982	10.0179
Si	15.52138	15.98693	9.945493
Si	5.773806	1.709928	12.84843
Si	2.658804	1.347629	9.369234
Si	18.53953	16.09427	13.33756
Si	13.02873	10.41082	9.957906
Si	8.102262	6.96258	12.66037
Si	2.495444	16.28252	12.87278
Si	13.23901	7.368988	9.633456
Si	13.17221	6.980527	12.69731
Si	7.881874	10.72012	9.893731
Si	18.52269	1.477192	13.17375
Si	2.665271	15.98118	9.791742
Si	4.051988	5.331167	15.02686
Si	17.08647	12.20648	7.832686
Si	17.16621	5.340369	7.471908
Si	4.042714	12.22089	7.626235
Si	14.50909	14.08539	7.684234
Si	6.669025	3.476155	0.034589
Si	6.590841	14.18459	7.661511
Si	14.59273	3.38567	7.584925

Si	1.592938	3.409867	14.91958
Si	19.63103	14.09843	7.85638
Si	19.65756	3.394975	7.833589
Si	1.595045	14.24721	15.0721
Si	11.96856	12.11776	7.713379
Si	9.185368	5.421048	14.95767
Si	9.029695	12.35918	15.1652
Si	12.1333	5.334432	7.471776
O	4.19016	1.827745	1.484294
O	17.04762	15.41064	5.688824
O	17.06625	15.46941	2.431324
O	4.209197	2.183116	5.398962
O	17.01597	2.092317	5.418478
O	4.173357	15.37763	2.019797
O	4.051939	15.97533	5.616871
O	17.14214	1.85788	2.164779
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O	6.565279	6.493305	5.373715
O	6.534598	7.051759	1.574515
O	14.74663	10.73457	5.894293
O	6.361607	10.60411	5.559178
O	14.78427	6.876342	1.952784
O	14.70436	6.415332	5.153599
O	6.318169	11.11953	2.515993
O	6.811083	2.387902	1.213536
O	14.28119	15.15485	6.441524
O	14.63814	14.98394	1.453249
O	6.649411	2.730476	6.172931
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O	6.763795	14.62913	1.632089
O	6.335303	15.48966	6.749075
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O	17.07825	11.69663	1.776559
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O	17.15599	10.97794	6.780461
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O	17.1419	6.610307	0.884811
O	17.33452	5.866084	5.937231
O	3.898951	11.58801	1.540972
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O	15.26114	0.105444	5.983801
O	15.4542	17.50856	1.761653
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O	16.51529	9.010229	1.634849
O	4.568342	8.566323	5.746997

O	4.742842	9.074528	1.747906
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O	14.82602	15.97973	3.836685
O	15.00377	1.556314	3.733873
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O	16.91161	10.65715	4.215129
O	4.448576	6.956769	3.322233
O	4.20013	10.51292	3.953419
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O	2.431938	17.44908	1.555411
O	18.36043	17.65815	6.126442
O	19.14811	17.44563	1.826393
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O	19.30641	1.474416	4.161679
O	2.130196	15.89934	3.74227
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O	8.640242	10.53045	3.757068
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O	19.36668	2.320136	6.651888
O	1.734967	14.9481	1.342128
O	1.611693	15.28986	6.241456
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O	11.96151	11.33523	1.551397
O	9.085809	5.90401	5.809163
O	9.189855	6.758507	0.704585
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O	9.011236	11.09393	6.549123
O	12.36045	6.499076	0.991076
O	12.29989	5.878012	5.940098
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O	17.01597	2.092317	13.00618
O	4.173357	15.37763	9.607497
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O	6.368697	1.910335	11.34797
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O	15.00377	1.556314	11.32157
O	6.313869	15.72849	11.74253
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O	18.36043	17.65815	13.71414
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O	19.30641	1.474416	11.74938
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O	19.69269	14.57616	9.428519
O	1.598077	2.975563	13.34446
O	19.36668	2.320136	14.23959
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O	1.611693	15.28986	13.82916
O	19.81757	2.603184	9.2558
O	11.96151	11.33523	9.139096
O	9.085809	5.90401	13.39686
O	9.189855	6.758507	8.292285
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O	15.83278	4.416468	7.646278
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O	2.705315	4.500926	7.768432
O	18.48854	13.01055	7.597682
O	18.47262	4.48012	7.885803
O	2.709032	13.07696	14.8446
O	13.14856	13.23282	7.71153
O	8.025236	4.372375	0.133909
O	7.989907	13.51972	14.71729
O	13.16839	4.113973	7.77521
O	0.144372	4.142859	7.58131
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O	10.55352	12.94319	7.583821
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O	10.26741	8.499482	10.08636
F	4.542186	0.012243	3.377461
F	14.93903	9.019988	3.77721
F	4.542186	0.012243	10.96516
F	14.93903	9.019988	11.36491
C	9.738732	16.249	0.916681
C	9.523149	16.66851	7.053023
C	8.978125	0.393698	7.166593
C	9.725211	0.988384	0.775484
C	11.1634	16.42028	3.458083
C	11.93432	16.53743	4.578727
C	11.89523	1.206699	4.432477
C	11.13538	1.156148	3.297112
C	10.76554	17.59165	2.733735
C	20.5862	7.772342	1.668524
C	20.41521	7.668451	0.151827
C	19.54535	8.885233	7.402529
C	20.05519	9.974843	0.759208
C	0.716857	9.088348	4.089907
C	1.269778	9.750987	5.152566
C	0.729797	11.85456	4.208971
C	0.175625	11.2566	3.110898
C	0.164268	9.827605	2.994707
C	9.738732	16.249	8.504381
C	9.523149	16.66851	14.64072
C	8.978125	0.393698	14.75429
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C	11.93432	16.53743	12.16643

C	11.89523	1.206699	12.02018
C	11.13538	1.156148	10.88481
C	10.76554	17.59165	10.32144
C	20.5862	7.772342	9.256225
C	20.41521	7.668451	7.739527
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C	20.05519	9.974843	8.346908
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H	8.845803	15.98715	6.525528
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H	7.905368	0.364866	7.38557
H	10.63868	1.536931	0.483496
H	9.086071	1.665559	1.361045
H	10.8766	15.42695	3.121272
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H	12.23119	2.13835	4.885411
H	10.83047	2.086136	2.822475
H	12.92048	0.120497	5.856392
H	19.72921	7.322366	2.200271
H	0.587786	7.307807	2.028602
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H	1.745486	9.235065	5.985591
H	0.775667	12.93638	4.331965

H	20.68309	11.88779	2.332211
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H	0.587786	7.307807	9.616302
H	0.476037	7.736576	14.84455
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S14f_1, Rel. E = 1.91

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Ge	16.15965	7.433017	1.798525
Ge	16.12018	6.974762	4.827203
Ge	15.33668	16.11937	5.270936
Ge	8.133287	7.432666	2.282143
Ge	13.01561	7.322552	1.993265
Ge	2.437495	16.36055	5.724136
Ge	18.60261	16.13422	5.267958
Ge	18.59403	1.671902	5.04247
Ge	2.49089	15.94109	2.717713
Ge	4.942784	7.466134	9.736109
Ge	16.19234	10.0528	12.93706

Ge	15.31394	1.692657	12.63631
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Ge	16.12018	6.974762	12.4149
Ge	15.33668	16.11937	12.85864
Ge	8.133287	7.432666	9.869843
Ge	13.01561	7.322552	9.580965
Ge	2.437495	16.36055	13.31184
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Ge	18.59403	1.671902	12.63017
Ge	2.49089	15.94109	10.30541
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Si	5.598003	15.93248	2.519399
Si	4.700139	10.22436	5.552721
Si	4.69194	7.203156	5.408909
Si	5.446464	1.302875	2.155313
Si	4.782243	10.70364	2.571219
Si	16.09642	10.54732	2.277287
Si	15.35923	1.336907	1.924286
Si	18.47814	16.01275	2.113207
Si	2.365033	1.713156	5.20764
Si	13.00502	6.933372	5.135976
Si	7.764212	7.164872	5.506486
Si	7.942037	10.17823	5.555294
Si	18.45144	1.3487	1.908595
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Si	7.907737	10.64181	2.524353
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Si	17.01491	5.306318	-0.38149
Si	4.05827	12.39537	0.165171
Si	14.42386	14.06822	-0.16353
Si	6.39743	3.388703	15.17134
Si	6.613507	14.34297	0.157639
Si	14.40023	3.448647	-0.17506
Si	1.471595	3.374606	15.17013
Si	19.61047	14.13888	-0.11314
Si	19.52329	3.411253	-0.19437
Si	1.533688	14.25032	0.330206
Si	11.96522	12.02456	0.10779
Si	8.936657	5.246916	0.09448
Si	8.966919	12.28594	0.159664
Si	11.85503	5.303826	-0.14873

Si	5.599029	16.30985	13.17796
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Si	5.446464	1.302875	9.743013
Si	4.782243	10.70364	10.15892
Si	16.09642	10.54732	9.864986
Si	15.35923	1.336907	9.511986
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Si	2.365033	1.713156	12.79534
Si	13.00502	6.933372	12.72368
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Si	18.45144	1.3487	9.496295
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Si	2.301373	1.256312	9.736946
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Si	17.01491	5.306318	7.206207
Si	4.05827	12.39537	7.752871
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Si	11.96522	12.02456	7.69549
Si	8.936657	5.246916	7.68218
Si	8.966919	12.28594	7.747365
Si	11.85503	5.303826	7.438971
O	3.88347	1.385313	1.749462
O	16.96038	15.4385	5.48702
O	16.93874	15.45159	2.178774
O	3.950968	1.874318	5.56812
O	16.94318	2.372967	5.164449
O	4.10503	15.48485	2.034825
O	4.123951	16.06719	6.240152
O	16.89792	1.858811	1.987571
O	14.53329	11.00944	2.41741
O	6.212351	7.120261	5.996505

O	6.519752	6.99751	1.524834
O	14.52866	10.59899	5.698272
O	6.322486	10.25552	5.623018
O	14.57465	6.612197	1.568924
O	14.49115	6.272848	5.199068
O	6.35507	11.13266	2.541245
O	6.278358	2.15946	1.051932
O	14.1847	15.14846	6.203207
O	14.51981	14.91469	1.230307
O	6.370353	2.78078	6.062957
O	14.20795	2.790074	5.901544
O	6.615987	14.95512	1.670168
O	6.589403	15.52627	6.632662
O	14.49839	2.184272	0.857332
O	16.88161	11.70611	1.435132
O	3.793362	6.07024	6.156725
O	3.763168	6.612112	1.151743
O	17.19315	11.03463	6.43482
O	4.050392	11.14106	6.710505
O	17.09506	6.66501	0.505634
O	17.08309	5.670907	5.629946
O	3.960879	11.78688	1.675171
O	5.996798	17.46819	2.104187
O	15.14663	0.096182	5.873332
O	15.29221	-0.23957	1.492201
O	6.032272	0.182973	5.595688
O	16.26762	9.170591	1.404011
O	4.129436	8.709286	5.754405
O	4.557563	9.205235	1.971005
O	16.56064	8.394418	5.84514
O	5.776561	1.958894	3.615849
O	14.72957	15.98383	3.609426
O	14.66698	1.533853	3.401848
O	5.877551	15.66193	4.110234
O	16.81811	10.50337	3.740512
O	4.6083	6.933042	3.813102
O	4.223684	10.8052	4.102433
O	17.00257	6.867164	3.263223
O	1.740049	17.4239	2.0234
O	18.60586	0.097932	5.896904
O	18.44502	17.49276	1.459678
O	1.774134	0.306916	5.798207
O	12.87362	9.044759	1.638288
O	8.420807	8.641037	5.804868
O	8.026941	9.178664	1.834266
O	12.88919	8.420185	5.814778

O	2.044279	1.924776	3.624113
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O	19.15734	1.534347	3.372499
O	1.914181	15.36804	4.332603
O	12.45325	10.33039	4.001244
O	7.78405	6.827232	3.92555
O	8.47581	10.61456	4.06567
O	12.3485	6.938915	3.618687
O	1.497519	2.134811	1.039271
O	19.68464	15.05704	6.125911
O	19.38319	15.04828	1.208451
O	1.621031	2.899779	6.034939
O	19.61749	2.842588	5.853024
O	1.584651	14.57411	1.907125
O	1.527047	15.61601	7.063912
O	19.27888	2.154732	0.803198
O	12.06485	11.49421	1.645483
O	8.632042	6.071119	6.31412
O	9.082262	6.236558	1.378858
O	12.09361	10.82636	6.59804
O	8.603209	11.13361	6.665578
O	11.85847	6.508741	0.936892
O	12.01972	5.912738	5.938521
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O	5.236312	4.504065	0.209567
O	15.76769	13.21511	14.73499
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O	5.399877	13.27457	15.11382
O	2.603096	4.465775	0.353313
O	18.43258	13.0499	-0.20277
O	18.34192	4.467929	0.021805
O	2.696102	13.20534	14.98774
O	13.09679	13.16039	-0.13985
O	7.855094	4.054147	0.280354
O	8.040074	13.59034	15.10734
O	13.01269	4.204686	0.163822
O	0.01831	4.118905	0.136792
O	0.134115	13.40583	0.021757
O	10.51323	12.74905	-0.05784
O	10.41105	4.535702	-0.06851
O	10.03053	8.087749	3.037393
O	3.88347	1.385313	9.337162
O	16.96038	15.4385	13.07472
O	16.93874	15.45159	9.766474
O	3.950968	1.874318	13.15582
O	16.94318	2.372967	12.75215

O	4.10503	15.48485	9.622524
O	4.123951	16.06719	13.82785
O	16.89792	1.858811	9.575271
O	14.53329	11.00944	10.00511
O	6.212351	7.120261	13.58421
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O	14.49115	6.272848	12.78677
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O	6.278358	2.15946	8.639632
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O	14.20795	2.790074	13.48924
O	6.615987	14.95512	9.257868
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O	14.49839	2.184272	8.445031
O	16.88161	11.70611	9.022832
O	3.793362	6.07024	13.74443
O	3.763168	6.612112	8.739443
O	17.19315	11.03463	14.02252
O	4.050392	11.14106	14.2982
O	17.09506	6.66501	8.093333
O	17.08309	5.670907	13.21765
O	3.960879	11.78688	9.262871
O	5.996798	17.46819	9.691887
O	15.14663	0.096182	13.46103
O	15.29221	-0.23957	9.079901
O	6.032272	0.182973	13.18339
O	16.26762	9.170591	8.991711
O	4.129436	8.709286	13.34211
O	4.557563	9.205235	9.558704
O	16.56064	8.394418	13.43284
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O	14.66698	1.533853	10.98955
O	5.877551	15.66193	11.69793
O	16.81811	10.50337	11.32821
O	4.6083	6.933042	11.4008
O	4.223684	10.8052	11.69013
O	17.00257	6.867164	10.85092
O	1.740049	17.4239	9.6111
O	18.60586	0.097932	13.4846
O	18.44502	17.49276	9.047378

O	1.774134	0.306916	13.38591
O	12.87362	9.044759	9.225987
O	8.420807	8.641037	13.39257
O	8.026941	9.178664	9.421966
O	12.88919	8.420185	13.40248
O	2.044279	1.924776	11.21181
O	19.14786	16.07215	11.18072
O	19.15734	1.534347	10.9602
O	1.914181	15.36804	11.9203
O	12.45325	10.33039	11.58894
O	7.78405	6.827232	11.51325
O	8.47581	10.61456	11.65337
O	12.3485	6.938915	11.20639
O	1.497519	2.134811	8.62697
O	19.68464	15.05704	13.71361
O	19.38319	15.04828	8.796151
O	1.621031	2.899779	13.62264
O	19.61749	2.842588	13.44072
O	1.584651	14.57411	9.494825
O	1.527047	15.61601	14.65161
O	19.27888	2.154732	8.390898
O	12.06485	11.49421	9.233183
O	8.632042	6.071119	13.90182
O	9.082262	6.236558	8.966558
O	12.09361	10.82636	14.18574
O	8.603209	11.13361	14.25328
O	11.85847	6.508741	8.524591
O	12.01972	5.912738	13.52622
O	8.782041	11.71433	9.262588
O	5.236312	4.504065	7.797266
O	15.76769	13.21511	7.14729
O	15.70872	4.372134	7.554958
O	5.399877	13.27457	7.52612
O	2.603096	4.465775	7.941013
O	18.43258	13.0499	7.384927
O	18.34192	4.467929	7.609505
O	2.696102	13.20534	7.400043
O	13.09679	13.16039	7.447848
O	7.855094	4.054147	7.868054
O	8.040074	13.59034	7.519642
O	13.01269	4.204686	7.751522
O	0.01831	4.118905	7.724492
O	0.134115	13.40583	7.609457
O	10.51323	12.74905	7.529865
O	10.41105	4.535702	7.519187
O	10.03053	8.087749	10.62509

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F	14.88789	8.387243	3.702627
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F	14.88789	8.387243	11.29033
C	9.772214	16.37392	0.865859
C	9.47841	16.83067	7.027763
C	8.734861	0.44997	7.236017
C	9.475655	1.097815	0.817637
C	11.15938	16.60794	3.416418
C	11.91501	16.76329	4.542533
C	11.69734	1.425135	4.4373
C	10.93553	1.335494	3.305858
C	10.6635	0.054958	2.722989
C	20.58369	7.985565	1.851025
C	20.41208	7.745863	0.348898
C	19.58378	8.955644	7.484857
C	20.1455	10.10888	0.730371
C	0.66269	9.482047	4.183763
C	1.189724	10.21983	5.210711
C	0.874794	12.24133	4.016054
C	0.337633	11.56077	2.954853
C	0.215349	10.13623	2.991697
C	9.772214	16.37392	8.45356
C	9.47841	16.83067	14.61546
C	8.734861	0.44997	14.82372
C	9.475655	1.097815	8.405337
C	11.15938	16.60794	11.00412
C	11.91501	16.76329	12.13023
C	11.69734	1.425135	12.025
C	10.93553	1.335494	10.89356
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C	20.58369	7.985565	9.438725
C	20.41208	7.745863	7.936597
C	19.58378	8.955644	15.07256
C	20.1455	10.10888	8.31807
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C	1.189724	10.21983	12.79841
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C	0.337633	11.56077	10.54255
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N	12.18217	0.302185	5.036934
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H	8.914679	15.84571	1.313876
H	10.65957	15.72782	0.935825
H	10.42834	17.00632	6.508754
H	8.90073	16.08896	6.467076
H	8.723929	1.094577	6.34837
H	7.694316	0.251713	7.519139
H	10.31539	1.734313	0.486539
H	8.814751	1.70874	1.448666
H	10.95495	15.60215	3.057257
H	12.33384	15.92394	5.094572
H	11.9813	2.370463	4.896025
H	10.57255	2.248386	2.839185
H	12.80611	0.391135	5.839764
H	19.7166	7.605619	2.420614
H	0.573547	7.532966	2.254999
H	0.475198	7.739654	7.452655
H	19.92272	6.786132	7.73286
H	19.65865	9.159081	6.409034
H	18.5219	8.798078	7.714463
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H	1.566143	9.764799	6.125103
H	1.019476	13.32286	4.012845
H	0.039469	12.12754	2.075985
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H	9.969643	8.832557	11.25711
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H	10.65957	15.72782	8.523525
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H	8.90073	16.08896	14.05478
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H	7.694316	0.251713	15.10684
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H	8.814751	1.70874	9.036366
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H	12.80611	0.391135	13.42746
H	19.7166	7.605619	10.00831

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H	0.475198	7.739654	15.04036
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H	19.39032	10.8637	8.580146
H	0.59374	8.401403	11.87807
H	1.566143	9.764799	13.7128
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S14g_1, Rel. E = 2.33

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Ge	4.690814	7.306523	2.054388
Ge	15.992622	7.637922	2.044458
Ge	16.310331	7.097962	5.045557
Ge	5.605370	1.720034	5.169613
Ge	2.423413	1.187984	1.859941
Ge	12.857762	7.529164	2.203107
Ge	18.572105	16.016176	2.565710
Ge	18.513617	16.498644	5.764502
Ge	18.395773	1.986850	5.166782
Ge	2.344836	1.687488	5.036167
Ge	5.546008	1.186942	9.685889
Ge	16.314413	10.273301	12.920919
Ge	4.690814	7.306523	9.642088
Ge	15.992622	7.637922	9.632158
Ge	16.310331	7.097962	12.633257
Ge	5.605370	1.720034	12.757313
Ge	2.423413	1.187984	9.447641
Ge	12.857762	7.529164	9.790808
Ge	18.572105	16.016176	10.153410
Ge	18.513617	16.498644	13.352201
Ge	18.395773	1.986850	12.754481
Ge	2.344836	1.687488	12.623866
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Si	15.321530	16.362728	5.556243
Si	16.208532	10.723145	2.292935
Si	15.264938	1.385067	2.151932
Si	4.768554	10.019024	5.534759
Si	4.702699	6.988686	5.150585
Si	15.205938	1.807714	5.159802
Si	4.740138	10.511803	2.467305

Si	15.294763	16.000380	2.491164
Si	5.702296	15.820710	2.459203
Si	2.463373	16.209944	5.462850
Si	2.538189	15.771252	2.421901
Si	7.867829	7.339209	1.984209
Si	7.934006	7.031059	5.033979
Si	7.960785	10.058455	5.461097
Si	18.465172	1.410763	2.074311
Si	13.134190	10.639051	2.424958
Si	13.145226	10.303530	5.494720
Si	13.145259	7.210187	5.346682
Si	7.828146	10.459105	2.407862
Si	3.917718	5.163263	15.103301
Si	16.970478	12.493933	-0.064851
Si	16.973278	5.458302	-0.115035
Si	3.910668	12.150934	0.099194
Si	14.353361	14.335217	0.082878
Si	6.540378	3.377641	0.017906
Si	6.467696	14.112400	0.100477
Si	14.388731	3.490441	-0.035316
Si	1.333276	3.293206	14.978995
Si	19.522564	14.354284	0.221401
Si	19.396944	3.604820	0.012505
Si	1.503935	14.123425	0.066594
Si	11.971138	12.279787	0.101432
Si	8.936649	5.386827	15.020557
Si	8.937751	12.115073	0.054853
Si	11.904016	5.463907	0.04841
Si	5.629664	16.252754	13.111679
Si	15.321530	16.362728	13.143943
Si	16.208532	10.723145	9.880634
Si	15.264938	1.385067	9.739632
Si	4.768554	10.019024	13.122458
Si	4.702699	6.988686	12.738285
Si	15.205938	1.807714	12.747501
Si	4.740138	10.511803	10.055004
Si	15.294763	16.000380	10.078865
Si	5.702296	15.820710	10.046903
Si	2.463373	16.209944	13.05055
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Si	7.867829	7.339209	9.571909
Si	7.934006	7.031059	12.62168
Si	7.960785	10.058455	13.048797
Si	18.465172	1.410763	9.662011
Si	13.134190	10.639051	10.012658
Si	13.145226	10.303530	13.082419

Si	13.145259	7.210187	12.934382
Si	7.828146	10.459105	9.995563
Si	3.917718	5.163263	7.515601
Si	16.970478	12.493933	7.522849
Si	16.973278	5.458302	7.472664
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Si	14.353361	14.335217	7.670578
Si	6.540378	3.377641	7.605606
Si	6.467696	14.112400	7.688177
Si	14.388731	3.490441	7.552383
Si	1.333276	3.293206	7.391295
Si	19.522564	14.354284	7.809101
Si	19.396944	3.604820	7.600205
Si	1.503935	14.123425	7.654294
Si	11.971138	12.279787	7.689132
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Si	8.937751	12.115073	7.642553
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O	3.947522	2.203602	5.634553
O	16.685884	2.464192	5.154034
O	4.125302	15.529581	2.161884
O	4.041894	16.064295	5.805376
O	16.857235	1.692747	2.125203
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O	6.36136	10.262324	5.711618
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O	6.417261	15.341513	6.630749
O	14.483809	2.253002	1.039873
O	17.002111	11.870043	1.434623
O	4.04254	5.786716	6.002681
O	3.66974	6.468246	0.903902
O	17.234034	11.348035	6.415754

O	3.976955	10.907063	6.635096
O	16.869656	6.8418	0.688175
O	17.231405	5.809473	5.894532
O	3.827208	11.586794	1.634061
O	6.222257	17.23884	1.847338
O	15.180241	0.278188	5.777936
O	15.037168	-0.213415	1.86554
O	6.099471	0.092043	5.744162
O	16.360641	9.314081	1.483717
O	4.366098	8.460974	5.804238
O	4.530989	9.055179	1.757436
O	16.744764	8.640309	5.870659
O	6.17088	2.081204	3.524675
O	14.797151	15.981092	4.052024
O	14.642371	1.739834	3.628447
O	6.046617	15.671535	4.049191
O	16.966215	10.728554	3.741797
O	4.040178	6.923912	3.65964
O	4.281492	10.477046	4.036986
O	16.972475	6.938225	3.394062
O	1.972755	17.168001	1.821102
O	18.495253	0.513496	6.170437
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O	1.908351	0.031049	5.572721
O	13.028546	9.217182	1.641618
O	8.337245	8.486883	5.661578
O	7.797377	8.954003	1.800849
O	13.048452	8.741905	5.919842
O	1.915077	2.024847	3.34824
O	19.259966	16.098434	4.200642
O	19.084911	1.763379	3.552353
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O	12.557874	10.537321	3.967207
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O	12.449359	7.131183	3.882008
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O	1.770504	14.583483	1.594349
O	1.673935	15.296433	6.560646
O	19.175817	2.281055	0.931073
O	12.191333	11.698939	1.606533
O	8.661597	5.879158	5.894974

O	8.798221	6.680634	0.841524
O	12.235538	11.181678	6.524899
O	8.7981	10.956635	6.507191
O	11.743026	6.493504	1.293077
O	12.199839	6.261097	6.263724
O	8.753021	11.451268	1.529348
O	5.253669	4.34686	0.330552
O	15.589432	13.350255	14.90124
O	15.705894	4.415834	0.057486
O	5.157454	13.154703	15.061822
O	2.60186	4.257334	0.092314
O	18.242573	13.494731	-0.21438
O	18.3125	4.707868	0.458105
O	2.486068	12.856072	14.882343
O	12.918256	13.598739	-0.110139
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O	-0.010133	4.158943	0.191534
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O	10.433583	4.745754	15.094748
O	10.552588	8.766814	2.789307
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O	16.848625	15.852116	13.390756
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O	4.125302	15.529581	9.749583
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O	6.353594	6.741321	9.416847
O	14.661119	10.876533	13.19622
O	6.36136	10.262324	13.299317
O	14.430677	6.803723	9.346512
O	14.640334	6.569723	13.026147
O	6.285311	11.011272	9.947009
O	6.633872	2.06905	8.539735
O	14.343439	15.614607	14.213636
O	14.440108	14.928135	9.198434
O	6.592092	2.928855	13.624574
O	14.233521	2.745284	13.662429
O	6.531037	14.657208	9.22589
O	6.417261	15.341513	14.218449

O	14.483809	2.253002	8.627573
O	17.002111	11.870043	9.022324
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O	3.66974	6.468246	8.491602
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O	6.222257	17.23884	9.435037
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O	6.099471	0.092043	13.331861
O	16.360641	9.314081	9.071418
O	4.366098	8.460974	13.391938
O	4.530989	9.055179	9.345137
O	16.744764	8.640309	13.45836
O	6.17088	2.081204	11.112375
O	14.797151	15.981092	11.639724
O	14.642371	1.739834	11.216146
O	6.046617	15.671535	11.636891
O	16.966215	10.728554	11.329497
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O	16.972475	6.938225	10.981762
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O	18.495253	0.513496	13.758137
O	18.758863	-0.155709	9.28472
O	1.908351	0.031049	13.16042
O	13.028546	9.217182	9.229318
O	8.337245	8.486883	13.249278
O	7.797377	8.954003	9.388549
O	13.048452	8.741905	13.507542
O	1.915077	2.024847	10.93594
O	19.259966	16.098434	11.788342
O	19.084911	1.763379	11.140053
O	2.156137	15.556771	11.580534
O	12.557874	10.537321	11.554908
O	8.444685	6.959924	11.06695
O	8.347341	10.514813	11.535612
O	12.449359	7.131183	11.469707
O	1.332737	1.917162	8.256742
O	19.554214	15.747343	14.551878
O	19.513025	14.719872	9.407551
O	1.253935	2.861382	13.40513
O	19.25692	3.252642	13.591821

O	1.770504	14.583483	9.182049
O	1.673935	15.296433	14.148346
O	19.175817	2.281055	8.518773
O	12.191333	11.698939	9.194233
O	8.661597	5.879158	13.482675
O	8.798221	6.680634	8.429223
O	12.235538	11.181678	14.112598
O	8.7981	10.956635	14.094892
O	11.743026	6.493504	8.880777
O	12.199839	6.261097	13.851424
O	8.753021	11.451268	9.117048
O	5.253669	4.34686	7.918252
O	15.589432	13.350255	7.31354
O	15.705894	4.415834	7.645186
O	5.157454	13.154703	7.474122
O	2.60186	4.257334	7.680014
O	18.242573	13.494731	7.37332
O	18.3125	4.707868	8.045804
O	2.486068	12.856072	7.294643
O	12.918256	13.598739	7.477561
O	7.89086	4.251851	7.885022
O	7.82884	13.273919	7.388856
O	13.004332	4.274866	7.857831
O	-0.010133	4.158943	7.779235
O	-0.020108	13.522453	7.54071
O	10.419173	12.789211	7.561538
O	10.433583	4.745754	7.507049
O	10.552588	8.766814	10.377007
F	4.209965	0.324946	3.521771
F	15.018969	8.655009	3.686744
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F	15.018969	8.655009	11.274445
C	9.698653	16.199139	0.937158
C	9.473744	16.600992	7.070471
C	8.886657	0.307749	7.182702
C	9.638908	0.935779	0.767991
C	11.129475	16.433619	3.476262
C	11.866112	16.587873	4.615514
C	11.716862	1.252934	4.464719
C	10.992285	1.165213	3.309274
C	10.688054	17.58493	2.746051
C	20.485302	7.828635	1.678948
C	20.313147	7.704389	0.164583
C	19.462366	8.930195	7.403853
C	20.006908	10.027347	0.728605
C	0.639396	9.167233	4.078835

C	1.183006	9.837772	5.141047
C	0.74476	11.935082	4.131699
C	0.192442	11.328891	3.036568
C	0.123475	9.898601	2.960642
C	9.698653	16.199139	8.524858
C	9.473744	16.600992	14.658171
C	8.886657	0.307749	14.770402
C	9.638908	0.935779	8.355691
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C	11.866112	16.587873	12.203215
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C	10.992285	1.165213	10.896974
C	10.688054	17.58493	10.333752
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H	10.441566	16.616899	6.555643
H	8.814218	15.901039	6.545554
H	8.983049	0.901986	6.264526
H	7.822047	0.249255	7.430557
H	10.542444	1.490845	0.457258
H	8.995781	1.614689	1.346689
H	10.906658	15.42771	3.128902
H	12.258922	15.749651	5.187764
H	12.002148	2.198658	4.922348
H	10.664814	2.080249	2.821167
H	12.744153	0.215548	5.92284
H	19.615627	7.409065	2.214827

H	0.474854	7.348465	2.049224
H	0.374255	7.746322	7.265338
H	19.834444	6.758063	7.477099
H	19.515656	9.21485	6.345761
H	18.410433	8.733335	7.643587
H	20.819653	10.612014	0.261515
H	19.228994	10.732322	1.057439
H	0.610622	8.079976	4.098435
H	1.609236	9.326043	6.002736
H	0.835059	13.017745	4.221341
H	20.747505	11.953985	2.228582
H	1.669973	11.677961	5.959385
H	10.200656	8.03373	10.919413
H	10.912148	9.402221	11.02874
H	8.781376	15.793098	8.982479
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H	10.441566	16.616899	14.143343
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H	8.983049	0.901986	13.852225
H	7.822047	0.249255	15.018257
H	10.542444	1.490845	8.044958
H	8.995781	1.614689	8.934388
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H	12.002148	2.198658	12.510048
H	10.664814	2.080249	10.408867
H	12.744153	0.215548	13.51054
H	19.615627	7.409065	9.802527
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H	19.834444	6.758063	15.064799
H	19.515656	9.21485	13.933461
H	18.410433	8.733335	0.055887
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H	19.228994	10.732322	8.645139
H	0.610622	8.079976	11.686135
H	1.609236	9.326043	13.590435
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S14h_1, Rel. E = 2.38

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Ge	16.28882	10.27378	5.292557
Ge	4.68385	7.336925	2.091513
Ge	15.9859	7.644008	1.996114

Ge	16.27061	7.119139	5.001042
Ge	5.553697	1.695124	5.206177
Ge	2.367728	1.224241	2.154086
Ge	12.83721	7.54817	2.179379
Ge	18.54179	16.02331	2.4654
Ge	18.54403	16.50946	5.659416
Ge	18.42175	2.002139	5.052258
Ge	2.493543	15.76811	2.547841
Ge	5.472961	1.172855	9.686704
Ge	16.28882	10.27378	12.88026
Ge	4.68385	7.336925	9.679214
Ge	15.9859	7.644008	9.583814
Ge	16.27061	7.119139	12.58874
Ge	5.553697	1.695124	12.79388
Ge	2.367728	1.224241	9.741786
Ge	12.83721	7.54817	9.767078
Ge	18.54179	16.02331	10.0531
Ge	18.54403	16.50946	13.24712
Ge	18.42175	2.002139	12.63996
Ge	2.493543	15.76811	10.13554
Si	5.676449	16.21316	5.506709
Si	15.34609	16.38328	5.504347
Si	16.21607	10.74442	2.256736
Si	15.24525	1.39617	2.086924
Si	4.825166	10.05158	5.555624
Si	4.719916	7.025411	5.17459
Si	15.22191	1.822469	5.096755
Si	4.786657	10.53484	2.487981
Si	15.28179	16.00243	2.446027
Si	5.716424	15.80634	2.440721
Si	2.540795	16.17302	5.644437
Si	2.367595	1.572969	5.305956
Si	7.861103	7.324824	1.994488
Si	7.945609	7.019741	5.027259
Si	8.014414	10.05216	5.44983
Si	18.4271	1.424327	1.95087
Si	13.14229	10.66108	2.368215
Si	13.11523	10.32856	5.436625
Si	13.1122	7.227418	5.328454
Si	7.869874	10.4476	2.402512
Si	3.908848	5.205718	7.546185
Si	16.96601	12.49851	-0.1069
Si	16.94707	5.45802	15.00314
Si	3.939432	12.17897	0.126763
Si	14.35524	14.35773	0.034659
Si	6.496349	3.381557	7.618303

Si	6.509161	14.11616	0.087618
Si	14.37148	3.490937	15.08858
Si	1.332988	3.289085	7.591447
Si	19.51864	14.35167	0.124655
Si	19.38517	3.611814	15.07383
Si	1.491782	14.07355	0.176267
Si	11.97554	12.31618	0.038052
Si	8.915864	5.358433	7.430677
Si	8.969576	12.09585	7.62907
Si	11.88349	5.473161	0.024634
Si	5.676449	16.21316	13.09441
Si	15.34609	16.38328	13.09205
Si	16.21607	10.74442	9.844436
Si	15.24525	1.39617	9.674623
Si	4.825166	10.05158	13.14332
Si	4.719916	7.025411	12.76229
Si	15.22191	1.822469	12.68446
Si	4.786657	10.53484	10.07568
Si	15.28179	16.00243	10.03373
Si	5.716424	15.80634	10.02842
Si	2.540795	16.17302	13.23214
Si	2.367595	1.572969	12.89366
Si	7.861103	7.324824	9.582188
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Si	13.14229	10.66108	9.955914
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Si	7.869874	10.4476	9.990212
Si	3.908848	5.205718	15.13388
Si	16.96601	12.49851	7.480803
Si	16.94707	5.45802	7.415443
Si	3.939432	12.17897	7.714463
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Si	6.509161	14.11616	7.675318
Si	14.37148	3.490937	7.500879
Si	1.332988	3.289085	0.003748
Si	19.51864	14.35167	7.712355
Si	19.38517	3.611814	7.486133
Si	1.491782	14.07355	7.763967
Si	11.97554	12.31618	7.625751
Si	8.915864	5.358433	15.01838
Si	8.969576	12.09585	0.04137
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O	16.87545	15.87563	5.731391
O	16.837	15.51792	2.401358
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O	4.177819	15.27159	2.261146
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O	16.82685	1.74985	2.016737
O	14.6591	11.24613	2.364479
O	6.330082	6.857697	5.040786
O	6.338577	6.737824	1.885484
O	14.63629	10.88022	5.575853
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O	14.41422	6.825812	1.731333
O	14.61106	6.604832	5.456513
O	6.335839	11.02436	2.371226
O	6.55228	2.063589	0.953568
O	14.37932	15.64185	6.58718
O	14.40928	14.9418	1.568177
O	6.507364	2.940445	6.044015
O	14.24965	2.761234	6.012052
O	6.612712	14.69066	1.614652
O	6.521928	15.3157	6.579538
O	14.42755	2.243279	0.982777
O	17.01807	11.88734	1.399437
O	4.062163	5.833607	6.039115
O	3.654376	6.496392	0.949076
O	17.204	11.33503	6.391486
O	4.040627	10.94235	6.655812
O	16.85519	6.836095	0.645883
O	17.17958	5.810624	5.834974
O	3.881113	11.61286	1.660255
O	6.049927	17.221	1.696661
O	15.20448	0.296952	5.726152
O	15.0475	17.49354	1.815806
O	5.957724	0.076028	5.857288
O	16.3612	9.32663	1.462297
O	4.424477	8.49609	5.847493
O	4.561973	9.082279	1.772915
O	16.74768	8.647548	5.827219
O	6.183475	1.92346	3.565517
O	14.79389	15.99693	4.010486
O	14.64025	1.751851	3.570543
O	6.189909	15.79741	4.006224
O	16.95367	10.75417	3.713569
O	4.0214	6.979621	3.698607

O	4.327721	10.49365	4.057054
O	16.9468	6.943324	3.35559
O	1.92047	17.23637	1.730602
O	18.56231	0.527678	6.050428
O	18.66828	17.54951	1.579227
O	2.264109	0.043644	5.87504
O	13.03564	9.231261	1.600008
O	8.359211	8.473289	5.652246
O	7.813268	8.938695	1.800985
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O	1.830045	1.688088	3.778794
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O	12.54667	10.56794	3.903202
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O	8.41486	10.49499	3.935065
O	12.45487	7.097687	3.8523
O	1.234164	2.216734	1.21124
O	19.57817	15.73368	6.848001
O	19.48364	14.7322	1.717439
O	1.355931	2.510762	6.162198
O	19.28628	3.280185	5.877789
O	1.621013	14.41844	1.756253
O	1.789579	15.35305	6.828825
O	19.13964	2.265613	0.784315
O	12.22319	11.72701	1.533638
O	8.642102	5.85378	5.894325
O	8.759392	6.64952	0.837514
O	12.20125	11.22082	6.450862
O	8.871879	10.93266	6.493312
O	11.73126	6.492875	1.276489
O	12.15298	6.291732	6.246305
O	8.808266	11.41867	1.513665
O	5.238288	4.378274	0.365815
O	15.58632	13.3611	7.29185
O	15.68964	4.409359	0.038845
O	5.157242	13.2145	7.490539
O	2.581359	4.316109	7.667641
O	18.23753	13.49187	-0.30693
O	18.29843	4.704145	0.360679
O	2.485026	12.83177	7.345811
O	12.91896	13.63359	-0.19582
O	7.881504	4.205832	0.28742
O	7.824567	13.21263	7.377378
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O	-0.03617	4.187294	0.112254
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O	10.42189	12.82832	15.12692
O	10.41821	4.736154	7.501324
O	10.60241	8.717312	2.759142
O	3.914266	1.775326	9.026835
O	16.87545	15.87563	13.31909
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O	16.70556	2.469285	12.66544
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O	4.1194	15.80639	13.30713
O	16.82685	1.74985	9.604436
O	14.6591	11.24613	9.952178
O	6.330082	6.857697	12.62849
O	6.338577	6.737824	9.473185
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O	6.421475	10.29831	13.29023
O	14.41422	6.825812	9.319033
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O	6.507364	2.940445	13.63172
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O	6.612712	14.69066	9.202352
O	6.521928	15.3157	14.16724
O	14.42755	2.243279	8.570477
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O	4.062163	5.833607	13.62682
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O	17.204	11.33503	13.97919
O	4.040627	10.94235	14.24351
O	16.85519	6.836095	8.233582
O	17.17958	5.810624	13.42267
O	3.881113	11.61286	9.247955
O	6.049927	17.221	9.284361
O	15.20448	0.296952	13.31385
O	15.0475	17.49354	9.403506
O	5.957724	0.076028	13.44499
O	16.3612	9.32663	9.049997
O	4.424477	8.49609	13.43519
O	4.561973	9.082279	9.360616
O	16.74768	8.647548	13.41492
O	6.183475	1.92346	11.15322

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O	14.64025	1.751851	11.15824
O	6.189909	15.79741	11.59392
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O	4.0214	6.979621	11.28631
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O	16.9468	6.943324	10.94329
O	1.92047	17.23637	9.318302
O	18.56231	0.527678	13.63813
O	18.66828	17.54951	9.166927
O	2.264109	0.043644	13.46274
O	13.03564	9.231261	9.187709
O	8.359211	8.473289	13.23995
O	7.813268	8.938695	9.388684
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O	1.830045	1.688088	11.36649
O	19.26626	16.13344	11.66779
O	19.06945	1.775312	11.00776
O	1.929736	15.6158	11.81566
O	12.54667	10.56794	11.4909
O	8.472657	6.943728	11.0643
O	8.41486	10.49499	11.52277
O	12.45487	7.097687	11.44
O	1.234164	2.216734	8.798941
O	19.57817	15.73368	14.4357
O	19.48364	14.7322	9.305139
O	1.355931	2.510762	13.7499
O	19.28628	3.280185	13.46549
O	1.621013	14.41844	9.343952
O	1.789579	15.35305	14.41653
O	19.13964	2.265613	8.372015
O	12.22319	11.72701	9.121338
O	8.642102	5.85378	13.48202
O	8.759392	6.64952	8.425215
O	12.20125	11.22082	14.03856
O	8.871879	10.93266	14.08101
O	11.73126	6.492875	8.864189
O	12.15298	6.291732	13.834
O	8.808266	11.41867	9.101364
O	5.238288	4.378274	7.953515
O	15.58632	13.3611	14.87955
O	15.68964	4.409359	7.626544
O	5.157242	13.2145	15.07824
O	2.581359	4.316109	0.079941
O	18.23753	13.49187	7.28077
O	18.29843	4.704145	7.948379

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O	12.91896	13.63359	7.391883
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O	7.824567	13.21263	14.96508
O	12.99017	4.285558	7.791144
O	-0.03617	4.187294	7.699954
O	-0.02367	13.50867	15.05854
O	10.42189	12.82832	7.539215
O	10.41821	4.736154	15.08902
O	10.60241	8.717312	10.34684
F	4.127371	0.147676	3.454649
F	15.00869	8.676403	3.68582
F	4.127371	0.147676	11.04235
F	15.00869	8.676403	11.27352
C	9.728433	16.18329	0.952374
C	9.507356	16.5944	7.088006
C	8.889969	0.289055	7.203931
C	9.619462	0.920613	0.803089
C	11.14219	16.4203	3.494935
C	11.89081	16.57502	4.626453
C	11.73358	1.239493	4.48033
C	10.99216	1.151667	3.335281
C	10.6902	17.57175	2.771136
C	20.46164	7.853468	1.676577
C	20.27821	7.747802	0.161562
C	19.4414	8.987652	7.417062
C	19.99961	10.06705	0.754297
C	0.650884	9.159929	4.084024
C	1.208354	9.817688	5.147992
C	0.763098	11.92741	4.168182
C	0.197392	11.33417	3.072573
C	0.12335	9.905315	2.979914
C	9.728433	16.18329	8.540074
C	9.507356	16.5944	14.67571
C	8.889969	0.289055	14.79163
C	9.619462	0.920613	8.390789
C	11.14219	16.4203	11.08264
C	11.89081	16.57502	12.21415
C	11.73358	1.239493	12.06803
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C	10.6902	17.57175	10.35884
C	20.46164	7.853468	9.264277
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C	19.4414	8.987652	15.00476
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C	1.208354	9.817688	12.73569
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H	10.47988	16.63752	6.584062
H	8.869843	15.88496	6.549492
H	8.996805	0.891821	6.291979
H	7.821227	0.212647	7.434011
H	10.51662	1.491688	0.502912
H	8.961856	1.585717	1.382163
H	10.91564	15.41376	3.151135
H	12.29099	15.73721	5.194058
H	12.02431	2.185625	4.933567
H	10.65463	2.066411	2.853345
H	12.78559	0.203021	5.922172
H	19.59326	7.432984	2.2135
H	0.45035	7.362594	2.034628
H	0.336456	7.783121	7.256628
H	19.78636	6.810092	7.467505
H	19.49663	9.285045	6.362588
H	18.3871	8.799992	7.652767
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H	19.23103	10.77761	1.092488
H	0.620373	8.072378	4.092533
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H	0.853947	13.00902	4.266951
H	20.74397	11.97122	2.278358
H	1.700533	11.64924	5.985299
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H	7.821227	0.212647	15.02171
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H	0.45035	7.362594	9.622328
H	0.336456	7.783121	14.84433
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H	19.49663	9.285045	13.95029
H	18.3871	8.799992	0.065067
H	20.81803	10.64772	7.879754
H	19.23103	10.77761	8.680188
H	0.620373	8.072378	11.68023
H	1.644664	9.294893	13.5858
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S14i_1, Rel. E = 2.62

Ge	4.858265	7.431499	2.0339
Ge	16.22041	10.21182	5.279483
Ge	5.462471	1.20276	2.319097
Ge	16.11905	7.568908	1.936326
Ge	16.22826	7.042259	4.938901
Ge	15.31793	16.31219	5.448768
Ge	8.110826	7.486218	2.061442
Ge	13.0176	7.366686	2.079282
Ge	18.57712	15.95588	2.47666
Ge	18.55465	16.40974	5.655948
Ge	18.46917	1.899292	4.987658
Ge	2.574533	15.93928	2.508016
Ge	4.858265	7.431499	9.6216
Ge	16.22041	10.21182	12.86718
Ge	5.462471	1.20276	9.906797
Ge	16.11905	7.568908	9.524026
Ge	16.22826	7.042259	12.5266
Ge	15.31793	16.31219	13.03647
Ge	8.110826	7.486218	9.649141
Ge	13.0176	7.366686	9.666983
Ge	18.57712	15.95588	10.06436
Ge	18.55465	16.40974	13.24365

Ge	18.46917	1.899292	12.57536
Ge	2.574533	15.93928	10.09572
Si	5.631251	16.2763	5.56874
Si	5.589127	1.676044	5.371182
Si	15.29761	15.94803	2.358796
Si	5.73351	15.86572	2.494002
Si	4.735373	10.08843	5.569581
Si	4.70738	7.080141	5.237036
Si	15.29246	1.818881	4.985568
Si	4.742939	10.66014	2.573581
Si	16.1258	10.66175	2.207872
Si	15.32698	1.320025	1.962511
Si	2.508186	16.23158	5.608957
Si	2.46598	1.60558	5.261683
Si	13.06366	7.104452	5.218134
Si	7.891745	7.013399	5.20198
Si	7.973181	10.05869	5.510293
Si	18.50163	1.325482	1.888237
Si	13.02443	10.48656	2.353171
Si	7.812714	10.6795	2.509765
Si	2.392479	1.343215	2.154014
Si	13.058	10.19094	5.420957
Si	3.913575	5.31581	7.566337
Si	16.96421	12.42059	15.02317
Si	17.007	5.384219	14.94766
Si	3.968951	12.25525	0.163915
Si	14.35214	14.22687	-0.02098
Si	6.473806	3.394484	0.169569
Si	6.531783	14.20581	0.140227
Si	14.43473	3.437899	14.98682
Si	1.42971	3.322365	7.587386
Si	19.53329	14.25791	0.141254
Si	19.46353	3.493325	15.00621
Si	1.507877	14.17556	0.150268
Si	11.93129	12.15567	0.034148
Si	8.964393	5.308296	7.502192
Si	8.918314	12.18111	0.093764
Si	11.90081	5.338415	-0.07796
Si	5.631251	16.2763	13.15644
Si	5.589127	1.676044	12.95888
Si	15.29761	15.94803	9.946496
Si	5.73351	15.86572	10.0817
Si	4.735373	10.08843	13.15728
Si	4.70738	7.080141	12.82474
Si	15.29246	1.818881	12.57327
Si	4.742939	10.66014	10.16128

Si	16.1258	10.66175	9.795572
Si	15.32698	1.320025	9.550211
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Si	2.46598	1.60558	12.84938
Si	13.06366	7.104452	12.80584
Si	7.891745	7.013399	12.78968
Si	7.973181	10.05869	13.09799
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Si	13.02443	10.48656	9.940871
Si	7.812714	10.6795	10.09747
Si	2.392479	1.343215	9.741714
Si	13.058	10.19094	13.00866
Si	3.913575	5.31581	15.15404
Si	16.96421	12.42059	7.435469
Si	17.007	5.384219	7.359961
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Si	14.35214	14.22687	7.566716
Si	6.473806	3.394484	7.757268
Si	6.531783	14.20581	7.727926
Si	14.43473	3.437899	7.39912
Si	1.42971	3.322365	15.17509
Si	19.53329	14.25791	7.728954
Si	19.46353	3.493325	7.418511
Si	1.507877	14.17556	7.737967
Si	11.93129	12.15567	7.621848
Si	8.964393	5.308296	15.08989
Si	8.918314	12.18111	7.681465
Si	11.90081	5.338415	7.509744
O	3.894946	1.655297	1.577986
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O	16.85631	15.50815	2.529968
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O	16.78257	2.462493	4.944225
O	4.213499	15.43014	2.031735
O	4.076524	16.00147	5.948591
O	16.90814	1.684715	1.92114
O	14.54471	11.07626	2.282346
O	6.301277	6.980121	5.509511
O	6.45952	6.896722	1.534844
O	14.56266	10.798	5.560967
O	6.35624	10.18637	5.634074
O	14.58195	6.674985	1.641769
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O	6.278663	11.22548	2.562072
O	6.520176	2.210139	1.254935
O	14.18605	15.52775	6.562953

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O	14.33918	2.805049	5.870718
O	6.653491	14.75682	1.673509
O	6.48719	15.43284	6.67301
O	14.51552	2.165247	0.848616
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O	3.947441	5.886559	6.026638
O	3.717141	6.630266	0.948251
O	17.18667	11.23469	6.36172
O	4.056202	10.98526	6.733135
O	17.02925	6.751649	0.626373
O	17.15834	5.761555	5.780332
O	3.844134	11.70988	1.699477
O	6.228085	17.32024	1.925899
O	15.24116	0.360409	5.75658
O	15.13304	17.42067	1.660672
O	6.020372	0.140163	5.765046
O	16.37091	9.262012	1.393493
O	4.221489	8.557609	5.786071
O	4.607523	9.19658	1.876683
O	16.58795	8.564005	5.825542
O	5.991933	1.993426	3.829183
O	14.61783	15.97175	3.850832
O	14.72586	1.655999	3.45811
O	6.035555	15.67665	4.094704
O	16.84228	10.6751	3.677685
O	4.327885	6.945677	3.663758
O	4.211764	10.64398	4.119032
O	17.04134	6.950213	3.347829
O	1.913247	17.48045	1.923861
O	18.45688	0.435062	6.014391
O	18.71094	17.44427	1.526604
O	2.065906	0.081943	5.692782
O	12.88097	9.061504	1.572107
O	8.444666	8.50471	5.63493
O	7.790889	9.226554	1.791103
O	13.00638	8.617167	5.835176
O	2.144817	1.856362	3.686845
O	19.32519	16.10465	4.080419
O	19.13843	1.645316	3.368307
O	2.119233	15.54178	4.178815
O	12.48223	10.40601	3.897229
O	8.192196	6.690678	3.648442
O	8.442534	10.59995	4.025793
O	12.36124	7.109547	3.728315

O	1.414609	2.229212	1.198889
O	19.55845	15.65238	6.879745
O	19.44734	14.6126	1.739614
O	1.518515	2.605522	6.128428
O	19.41095	3.119531	5.818146
O	1.619728	14.6504	1.689418
O	1.654437	15.42154	6.72639
O	19.25475	2.157408	0.740787
O	12.08104	11.53754	1.532104
O	8.651329	5.840536	5.998329
O	9.077188	6.619847	0.875158
O	12.12792	11.04037	6.455384
O	8.694615	10.9305	6.661568
O	11.87635	6.36909	1.171772
O	12.11165	6.133779	6.106707
O	8.734861	11.69609	1.642263
O	5.235779	4.450807	0.33231
O	15.63325	13.32853	7.147355
O	15.71411	4.396168	0.011343
O	5.241686	13.22325	-0.0466
O	2.590554	4.422173	7.766046
O	18.29657	13.33743	-0.3054
O	18.3301	4.556695	0.235628
O	2.562019	12.97912	7.341159
O	12.96967	13.39885	-0.15391
O	7.88265	4.203318	0.362264
O	7.878419	13.37286	7.351981
O	13.02788	4.175863	0.097929
O	0.004561	4.127124	0.090153
O	0.028028	13.48045	7.505262
O	10.42405	12.77199	15.07927
O	10.44372	4.595375	7.479655
O	10.09216	8.343801	2.746855
O	3.894946	1.655297	9.165686
O	16.93421	15.6409	13.32343
O	16.85631	15.50815	10.11767
O	4.006258	1.934824	13.25954
O	16.78257	2.462493	12.53193
O	4.213499	15.43014	9.619435
O	4.076524	16.00147	13.53629
O	16.90814	1.684715	9.50884
O	14.54471	11.07626	9.870046
O	6.301277	6.980121	13.09721
O	6.45952	6.896722	9.122544
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O	6.35624	10.18637	13.22177

O	14.58195	6.674985	9.229468
O	14.55487	6.441645	12.82133
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O	6.520176	2.210139	8.842634
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O	6.653491	14.75682	9.261209
O	6.48719	15.43284	14.26071
O	14.51552	2.165247	8.436316
O	16.89642	11.8374	8.954097
O	3.947441	5.886559	13.61434
O	3.717141	6.630266	8.535952
O	17.18667	11.23469	13.94942
O	4.056202	10.98526	14.32084
O	17.02925	6.751649	8.214073
O	17.15834	5.761555	13.36803
O	3.844134	11.70988	9.287177
O	6.228085	17.32024	9.513599
O	15.24116	0.360409	13.34428
O	15.13304	17.42067	9.248372
O	6.020372	0.140163	13.35275
O	16.37091	9.262012	8.981194
O	4.221489	8.557609	13.37377
O	4.607523	9.19658	9.464382
O	16.58795	8.564005	13.41324
O	5.991933	1.993426	11.41688
O	14.61783	15.97175	11.43853
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O	6.035555	15.67665	11.6824
O	16.84228	10.6751	11.26539
O	4.327885	6.945677	11.25146
O	4.211764	10.64398	11.70673
O	17.04134	6.950213	10.93553
O	1.913247	17.48045	9.51156
O	18.45688	0.435062	13.60209
O	18.71094	17.44427	9.114305
O	2.065906	0.081943	13.28048
O	12.88097	9.061504	9.159806
O	8.444666	8.50471	13.22263
O	7.790889	9.226554	9.378803
O	13.00638	8.617167	13.42287
O	2.144817	1.856362	11.27455
O	19.32519	16.10465	11.66812
O	19.13843	1.645316	10.95601

O	2.119233	15.54178	11.76652
O	12.48223	10.40601	11.48493
O	8.192196	6.690678	11.23614
O	8.442534	10.59995	11.61349
O	12.36124	7.109547	11.31602
O	1.414609	2.229212	8.786589
O	19.55845	15.65238	14.46744
O	19.44734	14.6126	9.327314
O	1.518515	2.605522	13.71613
O	19.41095	3.119531	13.40585
O	1.619728	14.6504	9.277118
O	1.654437	15.42154	14.31409
O	19.25475	2.157408	8.328486
O	12.08104	11.53754	9.119804
O	8.651329	5.840536	13.58603
O	9.077188	6.619847	8.462858
O	12.12792	11.04037	14.04308
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O	12.11165	6.133779	13.69441
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O	15.71411	4.396168	7.599042
O	5.241686	13.22325	7.541101
O	2.590554	4.422173	0.178346
O	18.29657	13.33743	7.282303
O	18.3301	4.556695	7.823328
O	2.562019	12.97912	14.92886
O	12.96967	13.39885	7.433793
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O	10.42405	12.77199	7.491572
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F	14.94768	8.527516	3.549675
F	4.182392	-0.03764	11.12885
F	14.94768	8.527516	11.13738
C	9.702795	16.29214	0.961256
C	9.437154	16.71936	7.108887
C	8.791589	0.395713	7.269666
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C	11.09722	16.51471	3.512523
C	11.84523	16.65876	4.644677
C	11.737	1.325443	4.48721
C	10.99191	1.247741	3.345036
C	10.66663	17.67093	2.784663
C	20.4974	7.896808	1.713702
C	20.32682	7.748766	0.200565
C	19.4817	8.971666	7.409977
C	20.00558	10.08079	0.736983
C	0.641293	9.260689	4.098782
C	1.190646	9.938416	5.154055
C	0.778461	12.0268	4.116374
C	0.216035	11.41108	3.030362
C	0.131714	9.98125	2.970637
C	9.702795	16.29214	8.548956
C	9.437154	16.71936	14.69659
C	8.791589	0.395713	14.85737
C	9.566177	1.028544	8.424617
C	11.09722	16.51471	11.10022
C	11.84523	16.65876	12.23238
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C	20.32682	7.748766	7.788266
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H	10.39509	16.79957	6.581254
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H	10.44968	1.599852	0.500003
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H	10.84699	15.51212	3.173565
H	12.22357	15.81597	5.218839
H	12.04412	2.267741	4.93752
H	10.66858	2.16601	2.859818
H	12.76929	0.276661	5.934093
H	19.6338	7.475484	2.25829
H	0.492378	7.429521	2.087381
H	0.389741	7.778331	7.30479
H	19.84629	6.798006	7.529424
H	19.56644	9.247382	6.351067
H	18.42267	8.777228	7.618065
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H	19.21557	10.77647	1.058245
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H	1.614725	9.429238	6.01858
H	0.889618	13.10968	4.185029
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H	8.831267	1.009872	13.94916
H	7.740578	0.285595	15.14705
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H	8.932094	1.691655	9.031065
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H	0.389741	7.778331	14.89249
H	19.84629	6.798006	15.11712
H	19.56644	9.247382	13.93877
H	18.42267	8.777228	0.030365
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H	19.21557	10.77647	8.645945
H	0.603402	8.173326	11.72009

H	1.614725	9.429238	13.60628
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Ge	4.917614	10.09125	5.313342
Ge	4.834628	7.028541	5.02895
Ge	16.38195	7.076128	5.189423
Ge	16.04825	7.5948	2.083951
Ge	13.1117	7.064976	5.307505
Ge	8.054076	7.066887	4.979653
Ge	8.072498	10.23361	5.243953
Ge	12.77134	7.726218	2.128599
Ge	13.09173	10.84159	2.669843
Ge	13.03456	10.21171	5.850906
Ge	16.26735	10.80643	10.14258
Ge	16.18688	10.15832	13.14406
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Ge	4.834628	7.028541	12.61665
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Ge	16.04825	7.5948	9.671651
Ge	13.1117	7.064976	12.89521
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Ge	13.09173	10.84159	10.25754
Ge	13.03456	10.21171	13.43861
Si	5.603521	16.3043	5.417938
Si	15.34989	16.32434	5.593012
Si	5.610578	1.30687	2.000216
Si	15.29546	1.362306	2.176254
Si	4.733294	7.384383	1.945011
Si	5.644773	15.94613	2.378539
Si	15.26143	1.759239	5.231609
Si	4.762037	10.46585	2.239609
Si	15.32346	15.9709	2.525461
Si	5.579257	1.673946	5.065269
Si	2.414622	1.276843	2.008224
Si	2.389355	1.681154	5.051941
Si	18.49824	15.99864	2.572639
Si	18.4827	16.41196	5.601142
Si	7.791107	7.351875	1.832191
Si	2.405007	16.30757	5.447534

Si	18.47213	1.398802	2.190059
Si	7.826011	10.41468	2.104474
Si	18.39746	1.838111	5.206228
Si	2.432288	15.92216	2.437362
Si	3.924416	5.307475	7.407452
Si	17.02715	12.45602	0.075148
Si	17.03077	5.320821	15.12315
Si	3.877877	12.20837	15.07494
Si	14.40563	14.27975	0.137857
Si	6.484774	3.402446	7.418979
Si	6.425033	14.19172	-0.00929
Si	14.40194	3.431736	0.023015
Si	1.467481	3.325187	7.440067
Si	19.4602	14.45236	0.138727
Si	19.44942	3.407248	0.03707
Si	1.47613	14.25429	0.055428
Si	11.87132	12.4098	0.317695
Si	9.000132	5.305298	7.321476
Si	8.975693	12.29407	7.430792
Si	11.93205	5.364649	0.019281
Si	5.603521	16.3043	13.00564
Si	15.34989	16.32434	13.18071
Si	5.610578	1.30687	9.587916
Si	15.29546	1.362306	9.763954
Si	4.733294	7.384383	9.53271
Si	5.644773	15.94613	9.966239
Si	15.26143	1.759239	12.81931
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Si	15.32346	15.9709	10.11316
Si	5.579257	1.673946	12.65297
Si	2.414622	1.276843	9.595923
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Si	18.49824	15.99864	10.16034
Si	18.4827	16.41196	13.18884
Si	7.791107	7.351875	9.41989
Si	2.405007	16.30757	13.03523
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Si	7.826011	10.41468	9.692174
Si	18.39746	1.838111	12.79393
Si	2.432288	15.92216	10.02506
Si	3.924416	5.307475	14.99515
Si	17.02715	12.45602	7.662848
Si	17.03077	5.320821	7.535453
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Si	14.40563	14.27975	7.725557
Si	6.484774	3.402446	15.00668

Si	6.425033	14.19172	7.578409
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Si	1.467481	3.325187	15.02777
Si	19.4602	14.45236	7.726427
Si	19.44942	3.407248	7.62477
Si	1.47613	14.25429	7.643128
Si	11.87132	12.4098	7.905395
Si	9.000132	5.305298	14.90918
Si	8.975693	12.29407	15.01849
Si	11.93205	5.364649	7.606982
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O	4.040125	15.72482	2.268323
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O	14.47509	14.9016	1.653112
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O	6.385736	15.45727	6.542797
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O	17.19729	12.03199	1.64497
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O	17.20636	11.13777	6.738801
O	3.827683	11.10038	6.327158
O	16.89544	6.668034	0.820811
O	17.32409	5.758519	5.982154
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O	6.03723	17.43861	1.823396
O	15.06194	0.225001	5.792072
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O	5.963089	0.180958	5.604983

O	16.3307	9.298749	1.585904
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O	4.64361	8.970764	1.590417
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O	14.87815	15.8724	4.095085
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O	17.10422	10.758	4.119826
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O	17.02574	7.148323	3.527884
O	2.026169	17.4051	1.901664
O	18.63776	0.317982	5.726737
O	18.78016	17.51365	2.053473
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O	13.2567	9.391181	1.643885
O	8.520509	8.58868	5.807876
O	7.803426	8.927256	1.449453
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O	2.001792	1.84886	3.479617
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O	1.964059	15.74461	3.984762
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O	8.58157	7.080116	3.259614
O	8.590918	10.43747	3.549003
O	12.24613	7.301406	3.790904
O	1.597116	2.060331	0.86522
O	19.4039	15.75241	6.746998
O	19.35547	14.94678	1.6924
O	1.547712	2.773254	5.90388
O	19.23563	2.881855	6.098894
O	1.665202	14.79645	1.578026
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O	19.34218	2.147322	1.061386
O	11.99045	12.02516	1.906843
O	9.067413	5.817934	5.771179
O	8.625123	6.55204	0.702473
O	11.98895	11.08606	6.981143
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O	12.14654	5.772715	6.047938
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O	15.65521	13.30718	7.41452

O	15.74341	4.326125	0.119895
O	5.141369	13.24163	7.360081
O	2.615136	4.406691	0.155005
O	18.27987	13.44065	14.90998
O	18.36422	4.523772	0.463131
O	2.506194	13.07187	7.317316
O	12.97506	13.55707	-0.06931
O	7.926753	4.104066	-0.01339
O	7.831719	13.4493	7.308422
O	13.0518	4.230286	0.400963
O	0.021666	4.036176	0.103459
O	-0.04859	13.67992	7.527353
O	10.39931	13.08541	0.070408
O	10.45281	4.655824	0.127161
O	10.71119	8.660489	2.264542
O	4.013189	1.473427	9.348767
O	16.9173	16.00067	13.42843
O	16.91231	15.65879	9.98388
O	3.985943	1.937927	12.84251
O	16.81269	2.202922	12.95033
O	4.040125	15.72482	9.856024
O	4.008088	16.10158	13.19764
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C	10.72771	17.58361	2.71194
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C	19.41665	8.345717	0.670628
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H	12.78863	0.277623	5.874985
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Si	15.31374	1.415126	2.238333
Si	4.64815	7.436471	1.98054
Si	5.652273	15.95957	2.439002
Si	15.32624	1.75388	5.30968
Si	4.712134	10.53864	2.288432
Si	15.30641	16.01361	2.524712
Si	5.586635	1.69017	5.091086
Si	2.387656	1.251154	2.062122
Si	2.382918	1.696874	5.070459
Si	18.46871	15.98988	2.54693
Si	18.4951	16.35878	5.59551
Si	7.730964	7.38775	1.866804
Si	2.412629	16.32579	5.516574
Si	18.47772	1.389875	2.215193
Si	7.790284	10.44905	2.136143
Si	18.45172	1.780463	5.250705
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Si	3.902068	12.26861	15.11963
Si	14.41297	14.28936	0.16655
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C	11.16296	16.30707	3.550663
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C	20.20819	7.729891	0.005358
C	19.43191	9.013458	7.284312
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Ge	16.267475	7.064641	5.227664
Ge	16.170134	7.598570	2.099783
Ge	13.058539	7.050771	5.216780
Ge	7.971085	7.018848	5.036787
Ge	7.966125	10.206831	5.325771
Ge	12.928430	7.673028	2.039996
Ge	13.088086	10.776813	2.648268
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Si	15.334206	1.404595	2.218261
Si	4.730020	7.344188	1.908151
Si	5.636318	15.894363	2.426895

Si	15.345323	1.733027	5.304006
Si	4.713890	10.448419	2.167619
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Si	5.637891	1.648543	5.051953
Si	2.432960	1.229835	2.039768
Si	2.467485	1.697509	5.055312
Si	18.463522	15.959558	2.541700
Si	18.490948	16.328110	5.587162
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Si	2.427300	16.292082	5.504743
Si	18.496078	1.366388	2.191403
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Si	17.098343	5.352620	0.000737
Si	3.881947	12.234189	14.979790
Si	14.400530	14.259356	0.165271
Si	6.533522	3.326901	7.407299
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Si	1.518263	3.286541	7.468191
Si	19.457893	14.348753	0.140587
Si	19.509178	3.352952	0.030747
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O	1.622368	15.577994	14.295575
O	19.394678	2.120004	8.675165
O	11.996672	11.959183	9.460504
O	8.963656	5.764311	13.411549
O	8.621953	6.522447	8.355784
O	11.908344	11.062465	14.511316
O	9.035212	11.35097	13.751204
O	11.97906	6.702007	8.489001
O	12.054525	5.782864	13.54985
O	8.682647	11.39144	8.825931
O	5.288449	4.333992	7.617927
O	15.686358	13.310085	15.150879
O	15.76291	4.427037	7.817597
O	5.174583	13.217779	14.862274
O	2.658939	4.374915	7.804315
O	18.306213	13.301185	7.349785
O	18.404564	4.459526	7.977256
O	2.53964	13.145658	14.872284
O	12.987121	13.505249	7.514337
O	7.95581	4.042421	7.660368
O	7.843916	13.447262	14.951648
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O	0.07596	4.002152	7.71501
O	-0.012165	13.63735	15.151769
O	10.393983	13.054169	7.678023
O	10.470036	4.677841	7.729209
O	10.610932	8.794193	9.862934
F	6.010359	8.7464	4.132062
F	14.844834	9.10087	4.163031
F	6.010359	8.7464	11.719763
F	14.844834	9.10087	11.750731
C	9.735172	16.155642	0.958722
C	9.496724	16.543705	14.678521
C	8.870798	0.235193	14.785062
C	9.62833	0.887964	0.768847
C	11.175786	16.432905	3.482816
C	11.924334	16.604265	4.61349
C	11.81465	1.267043	4.403961
C	11.07245	1.162964	3.259049
C	10.734816	17.573954	2.737592
C	20.20562	10.703202	3.771753
C	20.072283	10.554295	5.287455
C	19.656111	9.092155	5.504725

C	20.266909	8.317395	4.336283
C	0.528149	10.089622	1.214846
C	1.329108	9.773147	0.151819
C	1.17257	7.467214	0.622617
C	0.405205	7.71386	1.72808
C	0.128235	9.061769	2.122984
C	9.735172	16.155642	8.546421
C	9.496724	16.543705	7.090821
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C	11.175786	16.432905	11.070516
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H	8.830944	15.724467	1.42057
H	10.558275	15.438937	1.074499
H	10.463653	16.591547	6.574391
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H	8.95014	0.825475	6.275073
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H	10.51755	1.449157	0.431148
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H	10.943926	15.421144	3.158144
H	12.316658	15.773308	5.197643
H	12.129693	2.220694	4.826376
H	10.76845	2.072258	2.745076

H	12.85619	0.247105	5.863294
H	19.278824	11.077178	3.309855
H	0.106792	11.372199	3.494438
H	0.115138	10.76113	5.755429
H	19.334139	11.249823	5.703924
H	19.977968	8.696485	6.476966
H	18.568071	9.002368	5.464598
H	0.31259	7.858634	4.589268
H	19.592661	7.528469	3.968418
H	0.260857	11.131076	1.375597
H	1.747883	10.518552	14.658224
H	1.421399	6.457636	0.310955
H	0.030085	6.872269	2.305659
H	2.424061	8.325356	6.772488
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H	10.599402	9.517329	10.524465
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H	10.558275	15.438937	8.662199
H	10.463653	16.591547	14.162091
H	8.862094	15.818383	14.159153
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S14a_5, Rel. E = 0.27

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Ge	16.2676	7.063352	5.226734
Ge	16.17292	7.59651	2.099649
Ge	13.0569	7.050088	5.214137
Ge	7.972456	7.017185	5.028594
Ge	7.96614	10.20452	5.324659
Ge	12.93397	7.670667	2.040393
Ge	13.08225	10.77423	2.64573
Ge	12.96246	10.19193	5.788184
Ge	16.24149	10.77324	10.24239
Ge	16.07742	10.16364	13.27561
Ge	4.773478	10.05909	12.80271
Ge	4.694798	7.011033	12.55018
Ge	16.2676	7.063352	12.81443
Ge	16.17292	7.59651	9.687349
Ge	13.0569	7.050088	12.80184
Ge	7.972456	7.017185	12.61629
Ge	7.96614	10.20452	12.91236
Ge	12.93397	7.670667	9.628093
Ge	13.08225	10.77423	10.23343
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Si	5.641314	1.227651	2.001748
Si	15.33599	1.406049	2.220527
Si	4.731634	7.349279	1.904846
Si	5.635852	15.89286	2.430027
Si	15.34476	1.731437	5.308516
Si	4.714018	10.45191	2.166318
Si	15.29945	16.01078	2.509049
Si	5.638069	1.646987	5.05355
Si	2.435444	1.235588	2.038346
Si	2.467429	1.701374	5.055411
Si	18.4658	15.96449	2.538992
Si	18.48709	16.32493	5.587598
Si	7.791809	7.343511	1.881115
Si	2.423056	16.29562	5.504739
Si	18.49698	1.366135	2.195479
Si	7.783967	10.40512	2.143009
Si	18.47743	1.741082	5.242049
Si	2.409841	15.89754	2.513373
Si	3.965165	5.239908	7.347091
Si	17.02604	12.38548	0.209755
Si	17.09876	5.35405	15.1733
Si	3.882379	12.23318	14.98063

Si	14.40152	14.258	0.163797
Si	6.534081	3.326162	7.409033
Si	6.430058	14.17443	0.013784
Si	14.4569	3.490536	0.073666
Si	1.518724	3.29175	7.467137
Si	19.45969	14.3467	0.143212
Si	19.51114	3.353848	0.034915
Si	1.479218	14.27983	0.096629
Si	11.87247	12.36355	0.292279
Si	8.98869	5.279894	7.379648
Si	8.965691	12.2759	7.498212
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Si	15.34476	1.731437	12.89622
Si	4.714018	10.45191	9.754018
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Si	2.467429	1.701374	12.64311
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O	6.43365	2.093562	0.893224
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O	14.41878	2.743297	6.182292
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O	17.15235	6.658792	0.950059
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O	18.92453	15.84249	4.095781
O	18.93358	1.850827	3.688097
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O	12.26356	7.257954	3.64767
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O	19.32474	14.90719	1.67107
O	1.625044	2.77499	5.924347
O	19.36431	2.768128	6.10898
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O	5.286283	4.33208	7.615911
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O	18.30835	13.2968	7.358768
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O	2.540638	13.14739	14.87197
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F	6.007646	8.74603	4.12601
F	14.84038	9.09438	4.16412
F	6.007646	8.74603	11.71371
F	14.84038	9.09438	11.75182
C	9.736132	16.15486	0.957229
C	9.495646	16.54403	14.67758
C	8.870089	0.235658	14.78576
C	9.628716	0.887454	0.769517
C	11.17634	16.43073	3.482497
C	11.9248	16.60133	4.613003
C	11.81622	1.264229	4.404552
C	11.07409	1.160838	3.259882
C	10.73539	17.57208	2.737522
C	20.20458	10.70004	3.774232
C	20.0686	10.55093	5.289629
C	19.65366	9.0884	5.505627
C	20.26935	8.314421	4.339236
C	0.527278	10.08819	1.21676
C	1.326358	9.77299	0.15232
C	1.171837	7.466661	0.622058
C	0.407161	7.712365	1.729286
C	0.128815	9.059588	2.125124
C	9.736132	16.15486	8.544929
C	9.495646	16.54403	7.089883
C	8.870089	0.235658	7.198058
C	9.628716	0.887454	8.357217
C	11.17634	16.43073	11.0702
C	11.9248	16.60133	12.2007
C	11.81622	1.264229	11.99225
C	11.07409	1.160838	10.84758
C	10.73539	17.57208	10.32522
C	20.20458	10.70004	11.36193
C	20.0686	10.55093	12.87733
C	19.65366	9.0884	13.09333

C	20.26935	8.314421	11.92694
C	0.527278	10.08819	8.80446
C	1.326358	9.77299	7.74002
C	1.171837	7.466661	8.209758
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N	1.670834	8.489059	15.05125
N	20.48428	9.334643	3.299322
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N	1.670834	8.489059	7.463549
N	20.48428	9.334643	10.88702
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H	10.5918	9.522396	2.944208
H	8.832593	15.7223	1.419374
H	10.55985	15.43873	1.071405
H	10.46169	16.59189	6.571842
H	8.860103	15.81902	6.571298
H	8.9494	0.826976	6.276316
H	7.806549	0.1473	15.03856
H	10.51804	1.448198	0.431462
H	9.001182	1.577114	1.353296
H	10.94407	15.41904	3.157576
H	12.31712	15.77016	5.197094
H	12.13171	2.217616	4.827343
H	10.77059	2.0708	2.746316
H	12.85638	0.24301	5.864303
H	19.27847	11.07361	3.310834
H	0.105898	11.36965	3.498379
H	0.11018	10.7589	5.75967
H	19.32898	11.24536	5.705165
H	19.97124	8.692683	6.479217
H	18.56592	8.997579	5.460046
H	0.316243	7.859411	4.594544
H	19.59835	7.522683	3.971498
H	0.260106	11.12955	1.379085
H	1.742654	10.51956	14.65824
H	1.421275	6.457476	0.309257
H	0.035113	6.869846	2.307621
H	2.420275	8.324623	6.770673
H	10.23014	8.0521	10.36879
H	10.5918	9.522396	10.53191
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H	10.55985	15.43873	8.659104

H	10.46169	16.59189	14.15954
H	8.860103	15.81902	14.159
H	8.9494	0.826976	13.86402
H	7.806549	0.1473	7.45086
H	10.51804	1.448198	8.019162
H	9.001182	1.577114	8.940996
H	10.94407	15.41904	10.74528
H	12.31712	15.77016	12.7848
H	12.13171	2.217616	12.41504
H	10.77059	2.0708	10.33402
H	12.85638	0.24301	13.452
H	19.27847	11.07361	10.89853
H	0.105898	11.36965	11.08608
H	0.11018	10.7589	13.34737
H	19.32898	11.24536	13.29287
H	19.97124	8.692683	14.06692
H	18.56592	8.997579	13.04775
H	0.316243	7.859411	12.18224
H	19.59835	7.522683	11.5592
H	0.260106	11.12955	8.966784
H	1.742654	10.51956	7.070535
H	1.421275	6.457476	7.896957
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S14a_6, Rel. E = 0.44

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Ge	4.766261	10.07716	5.227879
Ge	4.670754	7.031025	4.966763
Ge	16.23252	7.051779	5.245936
Ge	16.18667	7.583053	2.123089
Ge	13.02754	7.045382	5.216609
Ge	7.938689	7.046553	5.050625
Ge	7.965554	10.22775	5.351861
Ge	12.96056	7.643096	2.042898
Ge	13.09646	10.7463	2.662584
Ge	12.96298	10.18314	5.807648
Ge	16.25264	10.75304	10.27767
Ge	16.08179	10.15813	13.32209
Ge	4.766261	10.07716	12.81558
Ge	4.670754	7.031025	12.55446
Ge	16.23252	7.051779	12.83364
Ge	16.18667	7.583053	9.710789
Ge	13.02754	7.045382	12.80431
Ge	7.938689	7.046553	12.63833

Ge	7.965554	10.22775	12.93956
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Ge	13.09646	10.7463	10.25028
Ge	12.96298	10.18314	13.39535
Si	5.664663	16.32183	5.441002
Si	15.36412	16.28001	5.614573
Si	5.638669	1.250777	1.983522
Si	15.31779	1.398014	2.260924
Si	4.733823	7.380659	1.900897
Si	5.645291	15.93543	2.399195
Si	15.3296	1.701027	5.330814
Si	4.730921	10.48435	2.186445
Si	15.30296	15.99827	2.533897
Si	5.681429	1.651984	5.050582
Si	2.438141	1.255343	2.053905
Si	2.479393	1.708353	5.066204
Si	18.46062	15.96617	2.530236
Si	18.48492	16.30765	5.573931
Si	7.788575	7.376589	1.890638
Si	2.449188	16.35186	5.518013
Si	18.47605	1.363858	2.214228
Si	7.795482	10.42845	2.169674
Si	18.45929	1.716553	5.247836
Si	2.425641	15.92515	2.531023
Si	3.914931	5.289458	7.351515
Si	17.06705	12.35718	0.257931
Si	17.08283	5.345833	0.022315
Si	3.907497	12.25198	14.99052
Si	14.44273	14.23195	0.197959
Si	6.492107	3.389501	7.397697
Si	6.451585	14.18599	0.000381
Si	14.45256	3.474255	0.100656
Si	1.516128	3.310719	7.482287
Si	19.48146	14.34181	0.139877
Si	19.49227	3.337734	0.038173
Si	1.512767	14.31149	0.114397
Si	11.89819	12.34792	0.317893
Si	8.983749	5.32329	7.391973
Si	8.992167	12.29662	7.525961
Si	11.92852	5.383221	-0.04182
Si	5.664663	16.32183	13.0287
Si	15.36412	16.28001	13.20227
Si	5.638669	1.250777	9.571222
Si	15.31779	1.398014	9.848623
Si	4.733823	7.380659	9.488597
Si	5.645291	15.93543	9.986895

Si	15.3296	1.701027	12.91851
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Si	5.681429	1.651984	12.63828
Si	2.438141	1.255343	9.641605
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Si	18.46062	15.96617	10.11794
Si	18.48492	16.30765	13.16163
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Si	2.449188	16.35186	13.10571
Si	18.47605	1.363858	9.801928
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Si	18.45929	1.716553	12.83554
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O	14.52736	10.99062	6.070795
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O	14.57307	6.84028	1.976805
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O	14.45182	2.733488	6.22047
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O	17.25938	11.97681	1.84062
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O	3.724841	11.1708	6.225165
O	17.17402	6.647222	0.980674
O	17.22201	5.788164	6.042959
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O	6.136692	17.40051	1.843687
O	15.1663	0.174933	5.906315
O	15.06173	17.5134	1.965069
O	6.175713	0.175154	5.584781
O	16.39242	9.293205	1.661737
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O	4.611647	8.971972	1.570354
O	16.3267	8.477357	6.321736
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O	14.84143	15.94097	4.099887
O	14.81978	1.738116	3.781462
O	6.084366	15.76666	3.96332
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O	17.04065	7.239708	3.669088
O	1.933734	17.41214	2.077514
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O	18.69276	17.47548	1.969803
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O	13.28324	9.335997	1.576666
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O	19.33644	14.92343	1.657012
O	1.692551	2.818647	5.937005
O	19.35178	2.741346	6.118609
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O	12.00258	11.93352	1.892561
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C	0.411914	7.69095	1.718753
C	0.155639	9.022741	2.175999
C	9.655847	16.30582	1.493985
C	9.015596	16.72175	0.360302
C	9.266218	1.295656	0.966706
C	9.879708	0.945113	2.136652
C	10.06574	17.26885	2.468446
C	10.84491	15.48812	4.010002
C	11.26571	15.56147	5.479644
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C	10.06574	17.26885	10.05615
C	10.84491	15.48812	11.5977
C	11.26571	15.56147	13.06735
C	11.82479	16.97997	13.22438
C	10.97663	0.131695	12.2876
N	1.651311	8.532768	15.05148
N	20.51786	9.258533	3.36127
N	8.814861	0.339657	0.108507
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N	1.651311	8.532768	7.463776
N	20.51786	9.258533	10.94897
N	8.814861	0.339657	7.696208
N	10.59286	16.8946	11.22475
H	10.27209	8.083384	2.827371
H	10.57436	9.567381	2.97874
H	19.33235	11.01006	3.388068
H	0.154261	11.27911	3.659101

H	0.058672	10.57479	5.892595
H	19.29117	11.09786	5.789165
H	19.82284	8.50717	6.491134
H	18.50719	8.875823	5.372288
H	0.313349	7.758911	4.653573
H	19.63129	7.41602	3.94342
H	0.317309	11.12219	1.529725
H	1.751397	10.57849	14.75371
H	1.372461	6.48783	0.220375
H	0.039222	6.82819	2.265703
H	2.385809	8.386815	6.751318
H	9.815811	15.23883	1.637757
H	8.625608	16.02772	14.797
H	9.106239	2.332716	0.679539
H	10.21563	1.738592	2.800244
H	9.936009	14.88559	3.85738
H	11.64256	15.07604	3.36909
H	10.39756	15.40255	6.132591
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H	11.81709	17.34557	6.6717
H	12.85734	17.01297	5.276803
H	11.53957	0.981677	4.286129
H	10.06766	0.528376	5.187997
H	8.217146	0.606	14.4994
H	10.27209	8.083384	10.41507
H	10.57436	9.567381	10.56644
H	19.33235	11.01006	10.97577
H	0.154261	11.27911	11.2468
H	0.058672	10.57479	13.4803
H	19.29117	11.09786	13.37686
H	19.82284	8.50717	14.07883
H	18.50719	8.875823	12.95999
H	0.313349	7.758911	12.24127
H	19.63129	7.41602	11.53112
H	0.317309	11.12219	9.117425
H	1.751397	10.57849	7.166007
H	1.372461	6.48783	7.808074
H	0.039222	6.82819	9.853403
H	2.385809	8.386815	14.33902
H	9.815811	15.23883	9.225457
H	8.625608	16.02772	7.209298
H	9.106239	2.332716	8.267239
H	10.21563	1.738592	10.38794
H	9.936009	14.88559	11.44508
H	11.64256	15.07604	10.95679
H	10.39756	15.40255	13.72029

H	12.00629	14.7959	13.32184
H	11.81709	17.34557	14.2594
H	12.85734	17.01297	12.8645
H	11.53957	0.981677	11.87383
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H	8.217146	0.606	6.911697

S14a_7, Rel. E = 1.71

Ge	16.30743	10.79661	2.576283
Ge	16.15549	10.18493	5.583705
Ge	4.847762	10.18108	5.382175
Ge	4.404917	6.963235	4.999653
Ge	16.31521	7.071911	5.195071
Ge	16.1216	7.60751	2.068138
Ge	13.07685	7.081316	5.242456
Ge	7.752129	6.93854	5.004327
Ge	7.993464	10.16774	5.390906
Ge	12.85722	7.710136	2.042818
Ge	13.13746	10.81836	2.606595
Ge	13.01496	10.2355	5.763228
Ge	16.30743	10.79661	10.16398
Ge	16.15549	10.18493	13.17141
Ge	4.847762	10.18108	12.96988
Ge	4.404917	6.963235	12.58735
Ge	16.31521	7.071911	12.78277
Ge	16.1216	7.60751	9.655838
Ge	13.07685	7.081316	12.83016
Ge	7.752129	6.93854	12.59203
Ge	7.993464	10.16774	12.97861
Ge	12.85722	7.710136	9.630518
Ge	13.13746	10.81836	10.1943
Ge	13.01496	10.2355	13.35093
Si	5.643741	16.2868	5.461989
Si	15.36034	16.3615	5.6117
Si	5.60386	1.220268	2.038961
Si	15.29129	1.397358	2.184055
Si	4.640976	7.362335	1.882841
Si	5.63796	15.87215	2.446378
Si	15.3232	1.783864	5.249145
Si	4.686728	10.46379	2.345298
Si	15.28139	16.00813	2.532863
Si	5.623453	1.632328	5.095094
Si	2.411247	1.204936	2.083948
Si	2.430752	1.644826	5.111906
Si	18.4571	15.97232	2.559633
Si	18.50048	16.39742	5.569205

Si	7.770654	7.376784	1.857476
Si	2.43371	16.29634	5.522841
Si	18.46927	1.380175	2.144827
Si	7.831754	10.38945	2.238286
Si	18.47127	1.830578	5.14647
Si	2.427588	15.86248	2.540803
Si	3.925539	5.205583	7.411294
Si	17.01722	12.44302	0.11801
Si	17.07554	5.35172	15.14711
Si	3.855469	12.20527	15.17247
Si	14.38983	14.30351	0.16372
Si	6.483963	3.335459	7.476743
Si	6.40463	14.15366	0.020742
Si	14.4308	3.497217	0.03915
Si	1.508967	3.267231	7.536969
Si	19.43039	14.43119	0.117237
Si	19.4824	3.363909	-0.01328
Si	1.464816	14.24663	0.135153
Si	11.88113	12.41852	0.270203
Si	8.93154	5.268612	7.371221
Si	8.949752	12.25451	7.573225
Si	11.90386	5.39787	-0.05138
Si	5.643741	16.2868	13.04969
Si	15.36034	16.3615	13.1994
Si	5.60386	1.220268	9.626661
Si	15.29129	1.397358	9.771754
Si	4.640976	7.362335	9.47054
Si	5.63796	15.87215	10.03408
Si	15.3232	1.783864	12.83685
Si	4.686728	10.46379	9.932998
Si	15.28139	16.00813	10.12056
Si	5.623453	1.632328	12.68279
Si	2.411247	1.204936	9.671648
Si	2.430752	1.644826	12.69961
Si	18.4571	15.97232	10.14733
Si	18.50048	16.39742	13.1569
Si	7.770654	7.376784	9.445176
Si	2.43371	16.29634	13.11054
Si	18.46927	1.380175	9.732527
Si	7.831754	10.38945	9.825986
Si	18.47127	1.830578	12.73417
Si	2.427588	15.86248	10.1285
Si	3.925539	5.205583	14.99899
Si	17.01722	12.44302	7.70571
Si	17.07554	5.35172	7.559413
Si	3.855469	12.20527	7.584769

Si	14.38983	14.30351	7.75142
Si	6.483963	3.335459	15.06444
Si	6.40463	14.15366	7.608441
Si	14.4308	3.497217	7.62685
Si	1.508967	3.267231	15.12467
Si	19.43039	14.43119	7.704937
Si	19.4824	3.363909	7.574417
Si	1.464816	14.24663	7.722853
Si	11.88113	12.41852	7.857903
Si	8.93154	5.268612	14.95892
Si	8.949752	12.25451	15.16093
Si	11.90386	5.39787	7.536324
O	4.005035	1.254256	1.751939
O	16.93102	16.03941	5.842233
O	16.86654	15.66562	2.383344
O	4.030167	1.74905	5.393938
O	16.8894	2.182968	5.351214
O	4.026192	15.73511	2.275517
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O	16.87667	1.661593	1.955405
O	14.7143	11.64089	2.666237
O	6.153308	6.18904	4.970513
O	6.213701	6.945643	1.848268
O	14.59847	11.00534	5.991792
O	6.422716	11.01921	5.598709
O	14.49332	6.910895	1.940614
O	14.68831	6.325048	5.258693
O	6.269508	10.85926	2.384375
O	6.404285	2.056668	0.915928
O	14.44988	15.56621	6.688846
O	14.40303	14.94795	1.676563
O	6.429892	2.735373	5.953863
O	14.39972	2.792493	6.127702
O	6.379592	14.73217	1.556649
O	6.39375	15.44612	6.616321
O	14.44923	2.253848	1.108526
O	17.2554	12.03754	1.687854
O	3.799642	5.453939	5.819418
O	3.918804	6.628708	0.623475
O	17.12187	11.1321	6.7902
O	3.755253	10.95864	6.550046
O	17.08493	6.678483	0.890049
O	17.27086	5.776021	5.992157
O	3.889233	11.61592	1.504208
O	6.116583	17.36222	1.967393
O	15.08422	0.26197	5.829805

O	14.96685	17.51305	1.973929
O	6.131952	0.133608	5.533885
O	16.41225	9.308581	1.58482
O	5.326665	8.49655	5.509798
O	4.48087	8.991526	1.681576
O	16.51453	8.535492	6.200692
O	5.93591	1.841524	3.509836
O	14.86885	15.93318	4.113347
O	14.83361	1.832459	3.695221
O	6.035103	15.64373	4.011075
O	17.11948	10.72429	4.154166
O	3.956467	6.86341	3.257008
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O	17.02403	7.189395	3.567038
O	1.925532	17.34539	2.107733
O	18.7224	0.296769	5.630102
O	18.76329	17.4871	2.063329
O	1.935308	0.138056	5.533566
O	13.28599	9.384385	1.555153
O	8.170447	8.469429	5.890544
O	7.862979	8.960887	1.464473
O	12.91306	8.53278	6.281112
O	2.115298	1.889237	3.533423
O	18.92391	15.79922	4.111293
O	18.92284	1.976883	3.592286
O	2.052355	15.57208	4.103368
O	12.26831	10.50425	4.142747
O	8.442351	7.136642	3.339562
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O	12.28577	7.265297	3.679747
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O	19.42023	15.72943	6.718101
O	19.31387	14.92461	1.668837
O	1.646007	2.745775	5.992603
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O	8.817309	5.744752	5.816029
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O	11.96832	11.13715	6.878033
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O	5.2749	4.356538	0.206144
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O	15.74431	4.420744	0.209933
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O	2.657683	4.320848	0.348522
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O	18.38501	4.469353	0.387847
O	2.447465	13.01098	7.335155
O	12.95268	13.60241	-0.11243
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O	7.787821	13.37771	7.330544
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O	10.37241	13.05987	0.104974
O	10.43082	4.682436	0.084541
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O	17.27086	5.776021	13.57986
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O	1.925532	17.34539	9.695434
O	18.7224	0.296769	13.2178
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O	10.43082	4.682436	7.672241
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C	9.490747	16.54245	7.243574
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C	11.88265	16.60072	4.771924
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C	20.41515	7.751923	0.136532
C	19.5215	8.930325	7.318738
C	20.03452	10.08419	0.589143
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C	1.059512	10.12853	5.074127
C	0.531294	12.17719	4.009674
C	0.035454	11.51698	2.918517
C	0.052417	10.08382	2.873786
C	9.659297	16.17366	8.713725
C	9.490747	16.54245	14.83127

C	8.932101	0.265849	14.88452
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C	1.059512	10.12853	12.66183
C	0.531294	12.17719	11.59737
C	0.035454	11.51698	10.50622
C	0.052417	10.08382	10.46149
N	12.20659	0.143943	5.216578
N	10.02533	17.45775	1.749571
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N	1.034115	11.48702	12.65519
N	20.55327	9.420127	9.383781
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H	8.839501	15.83942	6.713551
H	9.090996	0.834279	6.370876
H	7.853254	0.23788	15.07737
H	10.57228	1.443174	0.59765
H	9.018097	1.612925	1.447286
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H	12.14008	2.21401	4.966263
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H	12.84456	0.237015	6.007343
H	19.73511	7.509964	2.203923
H	0.593079	7.542054	2.037779
H	0.471432	7.804392	7.230243
H	19.96746	6.777007	7.49543
H	19.56526	9.167618	6.248332
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H	-0.07542	10.64659	0.102554

H	19.24199	10.79541	0.857835
H	0.639755	8.32379	4.065827
H	1.515576	9.652785	5.93824
H	0.561228	13.26406	4.076466
H	20.56827	12.09814	2.08984
H	1.460941	11.98855	5.850143
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H	10.4391	15.4173	8.868437
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H	9.018097	1.612925	9.034986
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H	0.471432	7.804392	14.81794
H	19.96746	6.777007	15.08313
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H	18.4751	8.723534	7.57467
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H	19.24199	10.79541	8.445535
H	0.639755	8.32379	11.65353
H	1.515576	9.652785	13.52594
H	0.561228	13.26406	11.66417
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H	1.460941	11.98855	13.43784

S14a_8, Rel. E = 1.75

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Ge	16.21263	10.22628	5.722302
Ge	4.767542	10.1459	5.374935
Ge	4.756578	6.894947	5.009017
Ge	16.33946	7.094846	5.240798
Ge	16.12015	7.654088	2.127397
Ge	13.11651	7.105654	5.250164
Ge	8.062481	6.925986	4.955747
Ge	8.057833	10.18261	5.311871
Ge	12.88833	7.747969	2.053717

Ge	13.10568	10.84736	2.649546
Ge	13.03475	10.25713	5.800869
Ge	16.2217	10.78994	10.30549
Ge	16.2156	10.21053	13.30799
Ge	4.771942	10.1391	12.96841
Ge	4.750191	6.887583	12.60569
Ge	16.3511	7.074344	12.82561
Ge	16.13868	7.634782	9.70802
Ge	13.12314	7.07964	12.84506
Ge	8.060701	6.911233	12.55298
Ge	8.063214	10.17254	12.90692
Ge	12.90719	7.751362	9.65621
Ge	13.09672	10.84589	10.2453
Ge	13.04247	10.2359	13.39801
Si	5.454806	16.28189	5.285833
Si	15.3193	16.38442	5.634583
Si	5.646431	1.216122	2.074545
Si	15.33109	1.421789	2.236995
Si	4.746095	7.35902	1.92349
Si	5.629297	15.83748	2.347886
Si	15.29439	1.786872	5.284908
Si	4.75377	10.4123	2.263022
Si	15.29383	16.04792	2.567272
Si	5.646058	1.531687	5.138975
Si	2.524245	1.222322	2.134631
Si	2.542729	1.560773	5.194966
Si	18.4913	16.00667	2.631133
Si	18.49263	16.42341	5.652664
Si	7.853469	7.341863	1.829066
Si	2.491865	16.18008	5.539563
Si	18.52629	1.389905	2.228065
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Si	3.999488	5.167894	7.429407
Si	17.01602	12.43812	0.244202
Si	17.16615	5.434243	0.052919
Si	3.875165	12.27694	15.13499
Si	14.40955	14.3001	0.20995
Si	6.585663	3.258804	7.455966
Si	6.441817	14.2219	15.05799
Si	14.53975	3.567086	0.089993
Si	1.533872	3.212411	7.550549
Si	19.42071	14.42617	0.209805
Si	19.51228	3.422469	0.071062
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Si	11.88939	12.42106	0.303042
Si	9.031157	5.239717	7.362908
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Si	4.747919	10.40392	9.856311
Si	15.31312	16.06295	10.1693
Si	5.632337	1.550542	12.7244
Si	2.525154	1.23715	9.723132
Si	2.53824	1.581137	12.78262
Si	18.47923	16.02174	10.24055
Si	18.50722	16.46657	13.25512
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Si	2.499946	16.20108	13.12593
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Si	7.863906	10.37683	9.772017
Si	18.48734	1.835567	12.83289
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Si	3.991484	5.166104	15.02711
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Si	17.15906	5.413318	7.618031
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Si	14.39373	14.32189	7.816246
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Si	6.414995	14.21533	7.473732
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Si	1.528409	3.209675	15.14877
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Si	19.52408	3.403074	7.643692
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H	10.79597	1.255807	14.51367
H	12.23342	1.88085	7.832964
H	12.17864	16.66517	5.503283
H	12.14738	14.45107	10.7884
H	8.80826	15.62357	8.319296
H	13.37134	-0.04002	7.729852

S14a_9, Rel. E = 1.84

Ge	16.37486	10.77337	2.639955
Ge	16.16138	10.14981	5.645358
Ge	4.770497	10.16139	5.470366
Ge	4.676129	6.910485	5.009418
Ge	16.28375	7.034476	5.212491
Ge	16.171	7.591312	2.101353
Ge	13.05446	7.063395	5.22425
Ge	7.956722	6.930402	4.950528
Ge	8.016983	10.18673	5.386678
Ge	12.93103	7.703948	2.036961
Ge	13.21142	10.80261	2.61583
Ge	13.02485	10.21944	5.759604
Ge	16.35279	10.79033	10.21937
Ge	16.16916	10.17684	13.22558
Ge	4.775862	10.17076	13.05333
Ge	4.690215	6.915956	12.59457
Ge	16.2963	7.049684	12.7911
Ge	16.17098	7.612369	9.680142
Ge	13.07265	7.087769	12.79779
Ge	7.975809	6.943243	12.54226
Ge	8.028576	10.19745	12.97639
Ge	12.92837	7.721487	9.610105
Ge	13.19518	10.81376	10.19389
Ge	13.03874	10.24008	13.33673
Si	5.55865	16.29475	5.368728
Si	15.34685	16.34033	5.624963
Si	5.533516	1.328739	2.099653
Si	15.2692	1.388004	2.214952

Si	4.657618	7.425926	1.928447
Si	5.582604	15.9846	2.351285
Si	15.30586	1.748787	5.287874
Si	4.721324	10.46876	2.367595
Si	15.25685	16.00105	2.560904
Si	5.560615	1.591886	5.134651
Si	2.442734	1.291936	2.16125
Si	2.480838	1.620523	5.204758
Si	18.4388	15.96535	2.557997
Si	18.50213	16.37505	5.572495
Si	7.780509	7.385008	1.830687
Si	2.512185	16.26997	5.510243
Si	18.44423	1.365324	2.151089
Si	7.859457	10.40071	2.254703
Si	18.45527	1.792632	5.176715
Si	2.502014	15.94503	2.481745
Si	3.849228	5.274072	7.439174
Si	17.06087	12.3942	0.186884
Si	17.06386	5.335366	15.17072
Si	3.896487	12.2951	0.069149
Si	14.43125	14.25933	0.206724
Si	6.429975	3.364717	7.461076
Si	6.459292	14.24278	15.14129
Si	14.43491	3.473477	0.059302
Si	1.444212	3.261938	7.579844
Si	19.44617	14.38231	0.12838
Si	19.46985	3.353429	-0.00777
Si	1.445588	14.29575	0.140469
Si	11.92333	12.38588	0.273755
Si	8.943287	5.294901	7.368655
Si	8.955473	12.29117	7.584687
Si	11.9358	5.419203	-0.06044
Si	5.557203	16.25428	12.95562
Si	15.41488	16.30484	13.2248
Si	5.499399	1.308691	9.669981
Si	15.28754	1.359247	9.813352
Si	4.656827	7.447213	9.51307
Si	5.5538	15.96638	9.924975
Si	15.32276	1.720061	12.86392
Si	4.715726	10.49496	9.953982
Si	15.31684	15.96395	10.1366
Si	5.547536	1.582091	12.71672
Si	2.418498	1.265934	9.735466
Si	2.46226	1.587499	12.77571
Si	18.48037	15.94322	10.12797
Si	18.54384	16.35932	13.16377

Si	7.777951	7.415882	9.418972
Si	2.496177	16.23774	13.07686
Si	18.47045	1.341536	9.743093
Si	7.850407	10.4267	9.846031
Si	18.47614	1.777132	12.75253
Si	2.481013	15.93381	10.05877
Si	3.894866	5.246851	15.02227
Si	17.03887	12.40593	7.753351
Si	17.04452	5.328015	7.594869
Si	3.886756	12.30099	7.639152
Si	14.41474	14.27234	7.776961
Si	6.478059	3.339789	15.03972
Si	6.441485	14.24584	7.53778
Si	14.41607	3.465931	7.668926
Si	1.463568	3.246948	15.15089
Si	19.44182	14.37985	7.700882
Si	19.45301	3.347831	7.586527
Si	1.439383	14.30208	7.709129
Si	11.90867	12.39343	7.852485
Si	8.964412	5.266325	14.94274
Si	8.972978	12.28804	0.009381
Si	11.91701	5.397312	7.553008
O	3.979746	1.532915	1.672917
O	16.92286	16.02428	5.812349
O	16.84161	15.6593	2.431377
O	4.037826	1.941066	5.606986
O	16.87245	2.135736	5.396645
O	4.029537	15.63578	1.990051
O	4.060338	16.01001	5.95906
O	16.85044	1.656819	1.962335
O	14.78323	11.62795	2.717972
O	6.317319	6.211528	4.970732
O	6.217709	6.95996	1.974103
O	14.60375	10.99196	5.997477
O	6.38696	10.88574	5.61958
O	14.54519	6.881945	1.982382
O	14.65439	6.287148	5.217772
O	6.301418	10.84681	2.485106
O	6.390481	2.238529	1.048457
O	14.4715	15.52913	6.718439
O	14.39222	14.92476	1.708783
O	6.484984	2.652506	6.000649
O	14.40043	2.775635	6.168481
O	6.46414	14.92322	1.448651
O	6.480001	15.39204	6.39764
O	14.41363	2.274867	1.174839

O	17.35327	11.99314	1.755807
O	3.639991	5.769875	5.879852
O	3.876643	6.585614	0.794424
O	17.11285	11.05531	6.884945
O	3.734825	11.04427	6.590781
O	17.11647	6.671444	0.907526
O	17.2194	5.737677	6.020509
O	3.941654	11.64201	1.56521
O	6.051579	17.48794	1.888925
O	15.05238	0.232704	5.872792
O	14.9445	17.50421	1.996179
O	6.132004	0.121525	5.623627
O	16.48478	9.291124	1.637529
O	4.709114	8.445532	5.939709
O	4.537475	9.027997	1.609684
O	16.44317	8.481368	6.252304
O	5.912218	1.927063	3.576051
O	14.81852	15.92365	4.135849
O	14.81918	1.805946	3.735041
O	5.96401	15.66219	3.907769
O	17.15861	10.66918	4.232018
O	3.970231	7.126592	3.392625
O	4.051834	10.39124	3.859846
O	17.05107	7.165426	3.611606
O	1.996594	17.4321	2.074186
O	18.72905	0.272457	5.68562
O	18.72982	17.47342	2.031607
O	2.022643	0.113471	5.633791
O	13.37763	9.372823	1.555498
O	8.030817	8.4677	5.86995
O	7.851954	8.970938	1.473234
O	12.90428	8.513089	6.269589
O	2.165008	1.925774	3.637404
O	18.93433	15.81265	4.103388
O	18.88325	1.928364	3.61641
O	2.203275	15.59985	4.048172
O	12.30007	10.4831	4.129511
O	8.544317	7.10144	3.271495
O	8.597637	10.28341	3.711053
O	12.26751	7.289444	3.655692
O	1.510374	2.080101	1.094635
O	19.39907	15.6733	6.713844
O	19.26107	14.89876	1.663638
O	1.585186	2.674079	6.071668
O	19.30811	2.850975	6.040255
O	1.591784	14.87197	1.644568

O	1.605333	15.44285	6.583603
O	19.30322	2.083354	0.996923
O	12.09683	11.96048	1.839071
O	8.967098	5.748341	5.786813
O	8.533327	6.547024	0.685537
O	11.95664	11.11938	6.856214
O	9.066904	11.19435	6.370658
O	11.98208	6.717246	0.907119
O	12.03498	5.811913	5.981472
O	8.647712	11.51025	1.402097
O	5.305531	4.469212	0.032194
O	15.66177	13.27417	7.562575
O	15.73109	4.424675	0.25551
O	5.175109	13.22342	7.338988
O	2.632196	4.342758	0.262865
O	18.28277	13.3603	-0.29952
O	18.37445	4.462337	0.397361
O	2.479977	13.07369	7.422731
O	13.00664	13.54522	-0.1011
O	7.930089	4.055734	0.033918
O	7.826239	13.41399	7.321581
O	13.05392	4.288228	0.281968
O	0.025479	4.009488	0.13127
O	-0.04423	13.62445	7.540604
O	10.41603	13.03812	0.127549
O	10.45208	4.729044	0.143559
O	10.73371	8.819704	2.203841
O	3.949422	1.557266	9.24776
O	16.98556	15.97676	13.44717
O	16.89207	15.62059	9.940967
O	4.014876	1.942104	13.14438
O	16.89236	2.131373	12.91235
O	4.004341	15.57363	9.581564
O	4.045294	15.93352	13.48671
O	16.8715	1.634797	9.586064
O	14.76215	11.6484	10.27426
O	6.334436	6.231353	12.54147
O	6.216988	6.975625	9.538342
O	14.61356	11.02626	13.56568
O	6.394328	10.88796	13.20818
O	14.54438	6.905601	9.546539
O	14.6681	6.30182	12.77344
O	6.294785	10.87494	10.07958
O	6.355345	2.235714	8.619397
O	14.54284	15.48157	14.30331
O	14.41369	14.90706	9.291842

O	6.456655	2.647785	13.57376
O	14.4507	2.756985	13.75724
O	6.438486	14.90085	9.026872
O	6.480569	15.37114	13.98851
O	14.44368	2.229997	8.741811
O	17.31132	12.02409	9.328822
O	3.679837	5.755307	13.4667
O	3.863298	6.614818	8.380338
O	17.12959	11.05359	14.47648
O	3.744083	11.05756	14.17488
O	17.1124	6.66757	8.500193
O	17.23719	5.759448	13.59867
O	3.939706	11.66697	9.144046
O	5.996182	17.46748	9.42493
O	15.14064	0.197729	13.43744
O	14.97449	17.47061	9.591818
O	6.037534	0.096223	13.1973
O	16.48612	9.310658	9.212252
O	4.707098	8.454332	13.52114
O	4.537307	9.050637	9.199663
O	16.43451	8.502793	13.82292
O	5.895537	1.877642	11.14886
O	14.9509	15.85047	11.72053
O	14.79928	1.773649	11.31767
O	5.962592	15.66633	11.47879
O	17.15144	10.70922	11.8075
O	3.979349	7.139366	10.97955
O	4.049344	10.41818	11.44753
O	17.05934	7.205723	11.1904
O	1.976767	17.40704	9.588178
O	18.74578	0.260677	13.28176
O	18.75821	17.45259	9.601377
O	2.033408	0.084627	13.24727
O	13.35527	9.393162	9.116736
O	8.053537	8.479789	13.46291
O	7.837564	9.000806	9.057539
O	12.9594	8.534606	13.84886
O	2.098161	1.871113	11.21529
O	18.94969	15.80854	11.68145
O	18.94619	1.893858	11.19998
O	2.126391	15.59341	11.61757
O	12.29339	10.50587	11.71453
O	8.544426	7.13624	10.85741
O	8.598001	10.30304	11.29628
O	12.27669	7.345442	11.23927
O	1.487787	2.080929	8.679374

O	19.46508	15.65205	14.28575
O	19.3176	14.87231	9.250413
O	1.568315	2.638945	13.65089
O	19.31195	2.840401	13.62941
O	1.569421	14.85094	9.220972
O	1.600693	15.41336	14.16864
O	19.30174	2.063061	8.570763
O	12.08263	11.97993	9.419847
O	8.980538	5.751292	13.36695
O	8.550772	6.58972	8.276018
O	11.96684	11.11186	14.45018
O	9.078931	11.20877	13.95314
O	11.97378	6.699946	8.511302
O	12.03172	5.856253	13.54903
O	8.633718	11.5379	8.99036
O	5.251291	4.476507	7.605771
O	15.67222	13.24215	0.049045
O	15.69552	4.435302	7.854459
O	5.188539	13.21988	14.97529
O	2.588619	4.381175	7.878656
O	18.2747	13.36027	7.280378
O	18.33798	4.432523	8.002365
O	2.487908	13.06797	15.04187
O	12.98162	13.56762	7.475522
O	7.87001	4.114855	7.654603
O	7.835731	13.40373	14.9362
O	13.0159	4.245312	7.910347
O	0.001107	4.017187	7.728612
O	-0.04038	13.61339	0.025677
O	10.39995	13.04375	7.702071
O	10.42032	4.721478	7.743757
O	10.72104	8.829711	9.774265
F	4.1842	17.59102	3.888196
F	14.9375	9.105074	4.120619
F	4.061416	17.54812	11.37628
F	14.93601	9.152418	11.66612
C	9.617267	16.31903	1.157494
C	8.99989	16.71617	7.638578
C	9.698161	16.28462	8.73392
C	9.537012	1.059761	1.084831
C	10.97909	16.45239	3.736636
C	11.71647	16.55253	4.884503
C	11.7567	1.220399	4.71948
C	11.01633	1.187129	3.570295
C	10.61235	17.63374	3.011275
C	20.50057	7.807026	1.652978

C	20.34068	7.656851	0.138495
C	19.47799	8.889163	7.34908
C	20.03158	9.986654	0.658171
C	0.561956	9.185518	4.069247
C	1.06799	9.874542	5.137977
C	0.618979	11.95568	4.100241
C	0.109308	11.32996	2.995133
C	0.069465	9.89845	2.928766
C	9.141136	1.262218	8.353081
C	9.387731	16.78914	14.89944
C	8.77313	0.476237	15.06994
C	9.8225	0.896478	9.479756
C	10.08905	17.22099	9.740572
C	10.98263	15.41265	11.18173
C	11.66448	15.45712	12.557
C	12.12003	16.91641	12.70213
C	11.07628	0.027954	11.95178
C	20.48339	7.817822	9.240574
C	20.33069	7.672225	7.724885
C	19.49043	8.875337	14.93771
C	20.00674	9.999501	8.253504
C	0.554981	9.192912	11.65527
C	1.074004	9.880395	12.71889
C	0.627026	11.96361	11.68321
C	0.102204	11.33877	10.58424
C	0.057573	9.907193	10.51802
N	12.09134	0.068069	5.365884
N	9.945274	17.57227	1.859946
N	1.09031	11.23406	5.153169
N	20.538	9.270524	1.843674
N	8.708035	0.329512	7.464328
N	10.67812	16.82246	10.87122
N	1.105248	11.23978	12.73149
N	20.51811	9.28085	9.435313
H	10.28742	8.059443	2.633724
H	10.83316	9.448275	2.952281
H	8.710698	15.86754	1.59156
H	10.44663	15.60163	1.23837
H	13.07026	17.05887	12.18108
H	11.50142	0.956575	11.54556
H	10.19733	0.286857	12.5676
H	8.047691	0.592151	6.72532
H	10.43619	1.617442	0.770188
H	8.915938	1.72786	1.699797
H	10.69202	15.46507	3.381738
H	12.05125	15.68735	5.45548

H	12.13405	2.144059	5.156585
H	10.77469	2.123101	3.071419
H	12.72576	0.113156	6.163229
H	19.63261	7.382711	2.187191
H	0.492654	7.343363	2.039048
H	0.397372	7.715189	7.248561
H	19.86567	6.71626	7.45567
H	19.54019	9.163674	6.288413
H	18.42405	8.698784	7.58316
H	20.86103	10.55015	0.19373
H	19.25662	10.70577	0.954495
H	0.54695	8.097981	4.099838
H	1.474642	9.379987	6.018949
H	0.682446	13.04036	4.187565
H	20.66936	11.9405	2.173575
H	1.518169	11.72025	5.944499
H	10.28151	8.063823	10.2012
H	10.81591	9.452837	10.52754
H	9.90703	15.22119	8.832707
H	8.619074	16.03933	6.878288
H	10.36184	16.86799	14.40713
H	8.750895	16.10345	14.32962
H	8.869501	1.111801	14.17907
H	7.706904	0.38761	0.126815
H	8.91186	2.300155	8.133195
H	10.12574	1.676283	10.17395
H	10.05232	14.82237	11.18875
H	11.6455	14.99758	10.40531
H	10.95405	15.17776	13.34632
H	12.50993	14.76236	12.61344
H	12.25769	17.23878	13.74195
H	19.6137	7.390431	9.769452
H	0.474384	7.354492	9.629215
H	0.405403	7.695871	14.83315
H	19.8722	6.701177	15.05039
H	19.54849	9.144983	13.87561
H	18.43656	8.691621	0.00329
H	20.83076	10.57547	7.79478
H	19.22304	10.70829	8.552923
H	0.533724	8.105606	11.68746
H	1.484249	9.384488	13.59743
H	0.698473	13.04845	11.7669
H	20.65459	11.95098	9.767575
H	1.544015	11.72272	13.51887

S14a_10, Rel. E = 1.96

Ge	16.35046	10.75627	2.626305
Ge	16.10015	10.11742	5.658291
Ge	4.734006	10.26251	5.39061
Ge	4.668296	7.009161	4.980618
Ge	16.23455	7.017176	5.20288
Ge	16.17692	7.551275	2.080908
Ge	13.01147	7.047494	5.222254
Ge	7.964924	7.025945	4.986541
Ge	8.008888	10.26666	5.391346
Ge	12.93862	7.666086	2.033836
Ge	13.18105	10.76553	2.638859
Ge	12.98587	10.18626	5.803964
Ge	16.35046	10.75627	10.21401
Ge	16.10015	10.11742	13.24599
Ge	4.734006	10.26251	12.97831
Ge	4.668296	7.009161	12.56832
Ge	16.23455	7.017176	12.79058
Ge	16.17692	7.551275	9.668608
Ge	13.01147	7.047494	12.80995
Ge	7.964924	7.025945	12.57424
Ge	8.008888	10.26666	12.97905
Ge	12.93862	7.666086	9.621535
Ge	13.18105	10.76553	10.22656
Ge	12.98587	10.18626	13.39166
Si	5.630957	16.35969	5.363312
Si	15.34602	16.30072	5.602718
Si	5.583717	1.375484	2.077795
Si	15.29154	1.365934	2.210022
Si	4.752784	7.474399	1.894665
Si	5.595931	16.04257	2.344378
Si	15.30795	1.706753	5.281792
Si	4.789168	10.53242	2.3001
Si	15.2669	15.98096	2.546375
Si	5.658549	1.640551	5.093223
Si	2.492643	1.396647	2.184593
Si	2.589205	1.719942	5.222553
Si	18.44416	15.93443	2.537987
Si	18.49607	16.33031	5.557194
Si	7.834996	7.459892	1.863531
Si	2.570496	16.36133	5.553309
Si	18.46178	1.327053	2.147385
Si	7.883512	10.48071	2.267458
Si	18.45715	1.73688	5.178539
Si	2.498468	16.0415	2.512508
Si	3.872466	5.335319	7.387906
Si	17.10646	12.34617	0.176081

Si	17.04478	5.301289	15.15959
Si	3.93856	12.39099	15.15637
Si	14.47274	14.22399	0.189005
Si	6.461111	3.406991	7.417357
Si	6.496557	14.31079	15.12011
Si	14.41324	3.450889	0.059042
Si	1.481621	3.357971	7.589966
Si	19.47461	14.34043	0.119394
Si	19.46772	3.322029	-0.01353
Si	1.4861	14.4197	0.168111
Si	11.93219	12.35296	0.299888
Si	8.958267	5.360375	7.383849
Si	9.002298	12.35506	7.602003
Si	11.90898	5.379282	-0.04935
Si	5.630957	16.35969	12.95101
Si	15.34602	16.30072	13.19042
Si	5.583717	1.375484	9.665495
Si	15.29154	1.365934	9.797722
Si	4.752784	7.474399	9.482366
Si	5.595931	16.04257	9.932077
Si	15.30795	1.706753	12.86949
Si	4.789168	10.53242	9.8878
Si	15.2669	15.98096	10.13408
Si	5.658549	1.640551	12.68092
Si	2.492643	1.396647	9.772292
Si	2.589205	1.719942	12.81025
Si	18.44416	15.93443	10.12569
Si	18.49607	16.33031	13.14489
Si	7.834996	7.459892	9.451231
Si	2.570496	16.36133	13.14101
Si	18.46178	1.327053	9.735085
Si	7.883512	10.48071	9.855158
Si	18.45715	1.73688	12.76624
Si	2.498468	16.0415	10.10021
Si	3.872466	5.335319	14.97561
Si	17.10646	12.34617	7.763781
Si	17.04478	5.301289	7.571891
Si	3.93856	12.39099	7.568674
Si	14.47274	14.22399	7.776705
Si	6.461111	3.406991	15.00506
Si	6.496557	14.31079	7.532414
Si	14.41324	3.450889	7.646742
Si	1.481621	3.357971	0.002266
Si	19.47461	14.34043	7.707094
Si	19.46772	3.322029	7.574173
Si	1.4861	14.4197	7.755811

Si	11.93219	12.35296	7.887588
Si	8.958267	5.360375	14.97155
Si	9.002298	12.35506	0.014303
Si	11.90898	5.379282	7.53835
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O	16.84734	15.61818	2.441335
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O	16.88058	2.115516	5.362487
O	4.027841	15.71366	2.037619
O	4.129878	16.06961	5.947433
O	16.87413	1.662913	1.97091
O	14.75379	11.58994	2.728085
O	6.319705	6.328424	4.992153
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O	14.56548	10.94978	6.091607
O	6.369542	10.94594	5.579051
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O	14.61599	6.271235	5.234936
O	6.343216	10.97815	2.487358
O	6.413347	2.271538	0.983531
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O	14.41268	14.89935	1.68378
O	6.600997	2.700783	5.958972
O	14.42893	2.754207	6.159978
O	6.441099	14.96168	1.435159
O	6.559088	15.45249	6.387528
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O	14.82068	1.761953	3.726072
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O	17.02568	7.155039	3.614449
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O	18.70585	0.22716	5.725065
O	18.71312	17.43468	1.972085
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O	11.98543	5.802102	5.965888
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O	19.32446	2.794303	13.6256
O	1.555553	14.99959	9.269195
O	1.652316	15.58057	14.23439
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O	12.06638	11.92396	9.456745
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O	9.055632	11.29711	13.94018
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O	5.220242	4.451664	7.531337
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O	2.602868	13.27158	15.11481
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F	14.90504	9.051812	4.246475
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C	20.46555	10.08838	4.187352
C	19.64104	9.841393	5.249185
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C	-0.00174	9.005485	3.379325
C	0.788678	10.54793	1.605151
C	0.803483	10.23	0.114535
C	1.494555	8.86502	0.040582
C	0.967157	8.132061	1.278634
C	9.626328	16.42801	1.488301
C	8.950124	16.8837	0.388147
C	9.218001	1.429374	1.064269
C	9.864656	1.039049	2.204495
C	10.05698	17.35407	2.487557
C	10.84171	15.54267	4.000712
C	11.09744	15.58597	5.508879
C	11.66708	16.98925	5.750473
C	10.94842	0.172777	4.734129
C	20.46555	10.08838	11.77505
C	19.64104	9.841393	12.83689
C	19.81841	7.500831	12.51254
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C	-0.00174	9.005485	10.96703
C	0.788678	10.54793	9.192851
C	0.803483	10.23	7.702235
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H	19.17448	10.63176	5.833841
H	19.49373	6.519947	5.269774
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H	1.723726	11.01931	1.945745
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H	1.293	11.00599	14.69266
H	1.265024	8.31395	14.29329
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H	1.702391	7.444582	1.721835
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H	9.782031	15.3569	1.595865
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H	9.043401	2.47327	0.822508
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H	11.58838	0.989753	4.365808
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H	1.265024	8.31395	6.705592
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H	1.702391	7.444582	9.309535
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H	11.785	14.79798	13.42331
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S14a_11, Rel. E = 2.13

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Ge	16.234713	7.575466	2.116335
Ge	13.026360	7.059462	5.155796
Ge	8.003333	6.988544	4.996264
Ge	7.964024	10.213928	5.359010
Ge	13.048008	7.621248	1.991202
Ge	13.081776	10.711987	2.619300
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Si	15.293728	1.707421	5.309808
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Si	2.526023	1.267689	2.122564
Si	2.552916	1.652712	5.166337
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Si	18.449293	16.317480	5.575972
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Si	6.427450	14.272044	15.085605
Si	14.473821	3.511355	0.074431
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Si	19.416342	14.315093	0.14814
Si	19.500259	3.332114	0.023084
Si	1.405931	14.347052	0.155373
Si	11.861432	12.342434	0.286281
Si	8.987647	5.287369	7.396726
Si	8.919077	12.342745	7.540446
Si	11.947276	5.419806	-0.089242
Si	5.426600	16.342566	12.903763
Si	15.283021	16.316765	13.174208
Si	5.646880	1.233510	9.657164
Si	15.305781	1.418238	9.817794

Si	4.741239	7.373297	9.487018
Si	5.588760	15.862567	9.975994
Si	15.293728	1.707421	12.897509
Si	4.688113	10.445933	9.837079
Si	15.250463	16.021832	10.098321
Si	5.651879	1.594467	12.715266
Si	2.526023	1.267689	9.710264
Si	2.552916	1.652712	12.754037
Si	18.413980	15.950934	10.125524
Si	18.449293	16.317480	13.163671
Si	7.834592	7.411263	9.45423
Si	2.456202	16.272711	13.152729
Si	18.466566	1.353678	9.781016
Si	7.791171	10.443008	9.797493
Si	18.460562	1.710447	12.818818
Si	2.475841	15.896486	10.11371
Si	3.966450	5.175692	14.994312
Si	17.006987	12.355513	7.850549
Si	17.113754	5.358407	7.600427
Si	3.873711	12.341434	7.520884
Si	14.388343	14.240297	7.759978
Si	6.563484	3.277053	15.050445
Si	6.427450	14.272044	7.497905
Si	14.473821	3.511355	7.66213
Si	1.515967	3.245261	15.128794
Si	19.416342	14.315093	7.735839
Si	19.500259	3.332114	7.610784
Si	1.405931	14.347052	7.743073
Si	11.861432	12.342434	7.873981
Si	8.987647	5.287369	14.984426
Si	8.919077	12.342745	15.128145
Si	11.947276	5.419806	7.498458
O	4.083405	1.515021	1.719269
O	16.863934	15.995536	5.776691
O	16.821812	15.624291	2.384585
O	4.114969	2.023667	5.486269
O	16.878403	2.060885	5.407598
O	4.012149	15.50803	2.125222
O	3.987768	15.892034	5.990336
O	16.887239	1.723379	2.006916
O	14.643265	11.561644	2.757837
O	6.323023	6.381929	5.058962
O	6.289505	6.895855	1.999562
O	14.504613	10.981154	6.005066
O	6.276726	10.746685	5.608882
O	14.635172	6.794533	1.956997

O	14.614907	6.244275	5.178297
O	6.236397	10.89887	2.425093
O	6.516633	2.0997	0.990841
O	14.441107	15.412457	6.623915
O	14.355129	14.982464	1.639544
O	6.594546	2.658823	5.957656
O	14.457925	2.788057	6.188237
O	6.425128	14.801902	1.454009
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O	14.448739	2.318012	1.196078
O	17.224184	11.984801	1.846376
O	3.721821	5.670871	5.848783
O	4.013495	6.543186	0.717836
O	17.038839	11.006165	6.969635
O	3.606407	11.185403	6.375573
O	17.228897	6.669539	0.960741
O	17.224478	5.796722	6.029704
O	3.907842	11.553945	1.37007
O	6.030328	17.362055	1.875057
O	15.003448	0.200266	5.884561
O	15.002367	17.53899	1.942042
O	6.066373	0.124377	5.713617
O	16.4079	9.286931	1.664072
O	4.329865	8.466784	5.874917
O	4.596931	8.964381	1.544855
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O	14.78722	15.957842	4.071237
O	14.825423	1.784566	3.748536
O	6.020454	15.594594	3.947611
O	17.021313	10.607574	4.289732
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O	3.969501	10.360768	3.716755
O	17.063213	7.21769	3.66927
O	2.116726	17.408451	2.051058
O	18.72331	0.202229	5.770156
O	18.689911	17.460394	1.995311
O	2.129365	0.165602	5.670969
O	13.342082	9.317435	1.525819
O	8.16106	8.523722	5.896433
O	7.769836	8.988919	1.477351
O	12.853095	8.470737	6.243307
O	2.209423	1.891536	3.593619
O	18.891228	15.827098	4.086877
O	18.929386	1.833125	3.679481
O	2.097423	15.663811	4.091099

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O	5.313782	4.318891	0.043829
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O	15.771932	4.457553	0.275867
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O	2.644782	4.377064	0.286052
O	18.291622	13.228838	14.954606
O	18.423264	4.470045	0.378812
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O	7.950974	4.083743	7.69996
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C	8.99425	0.216739	5.152286
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C	12.061557	17.349997	0.017583
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C	20.275507	10.471992	4.354953
C	20.186424	10.266975	5.86551
C	19.652971	8.836699	6.032439
C	20.159321	8.067981	4.806408
C	0.675847	9.876339	1.806176
C	1.427698	9.539637	0.715723
C	1.051927	7.228412	1.080147
C	0.323834	7.496312	2.205345
C	0.159127	8.847431	2.657094
C	9.733581	0.56065	11.640447
C	8.99425	0.216739	12.739986
C	9.251821	15.616093	12.272641
C	9.985858	15.885996	11.148565
C	10.221595	17.244736	10.762085
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C	11.39098	1.025139	7.651472
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C	11.299362	16.534065	8.650494
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H	10.424808	16.011362	0.635659
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H	19.979746	8.366441	14.557006
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H	1.214188	6.216284	8.304853
H	-0.123678	6.666953	10.335646
H	2.292159	8.024464	7.214767
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S14a_12, Rel. E = 2.15

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Ge	16.27592	7.022811	5.183228
Ge	16.01889	7.627394	2.043068
Ge	13.02904	6.987977	5.264735
Ge	8.055175	7.076777	5.007025
Ge	8.094157	10.24547	5.232366
Ge	12.69558	7.756355	2.107588
Ge	13.0328	10.89275	2.713118
Ge	12.96761	10.19499	5.850046
Ge	16.24641	10.82352	10.21835
Ge	16.22294	10.23419	13.35062
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Si	15.2976	1.384501	2.246922
Si	4.701662	7.395753	1.999182
Si	5.593646	15.98387	2.355496
Si	15.27938	1.756624	5.292123
Si	4.786976	10.49704	2.262666
Si	15.33133	15.99882	2.564103
Si	5.519943	1.62258	5.128178
Si	2.453142	1.277268	2.106223
Si	2.435621	1.60815	5.143302

Si	18.49816	16.01455	2.591201
Si	18.50056	16.40974	5.649158
Si	7.766711	7.351335	1.860198
Si	2.490274	16.25932	5.44586
Si	18.47194	1.403949	2.222733
Si	7.847036	10.42412	2.086018
Si	18.41802	1.821584	5.249408
Si	2.527938	15.95197	2.430269
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Si	15.37956	16.33567	13.22768
Si	5.532831	1.332524	9.668243
Si	15.2976	1.384501	9.834621
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Si	5.593646	15.98387	9.943196
Si	15.27938	1.756624	12.87982
Si	4.786976	10.49704	9.850366
Si	15.33133	15.99882	10.1518
Si	5.519943	1.62258	12.71588
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Si	18.50056	16.40974	13.23686
Si	7.766711	7.351335	9.447899
Si	2.490274	16.25932	13.03356
Si	18.47194	1.403949	9.810433
Si	7.847036	10.42412	9.673717
Si	18.41802	1.821584	12.83711
Si	2.527938	15.95197	10.01797
Si	3.918129	5.27379	15.06139
Si	17.05437	12.49473	7.821092

Si	17.04969	5.35433	7.57008
Si	3.93381	12.28419	7.540639
Si	14.41529	14.2971	7.783761
Si	6.471133	3.348871	15.0582
Si	6.473242	14.27121	7.570841
Si	14.41624	3.462576	7.670057
Si	1.478006	3.262047	15.11379
Si	19.50893	14.43585	7.780786
Si	19.47748	3.424144	7.643378
Si	1.49648	14.28752	7.663039
Si	11.88148	12.4333	7.924821
Si	8.956651	5.281353	14.93718
Si	8.981836	12.30005	14.99953
Si	11.90398	5.353685	7.600629
O	3.986841	1.592021	1.637562
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O	16.90913	15.64147	2.422948
O	3.978376	1.980146	5.523735
O	16.82876	2.210746	5.369574
O	4.056977	15.58231	1.986426
O	4.031845	15.95586	5.880279
O	16.87277	1.712842	2.073201
O	14.65643	11.62606	2.862728
O	6.428814	6.385939	5.283282
O	6.239141	6.840367	1.967417
O	14.58928	10.94483	5.782158
O	6.532533	10.87857	5.849296
O	14.38091	6.983829	2.117322
O	14.66047	6.274355	5.132448
O	6.337009	11.01753	2.166429
O	6.447016	2.211733	1.043675
O	14.45284	15.5307	6.703729
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O	6.420932	2.682673	5.991233
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O	6.521072	14.94172	1.473054
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O	14.46868	2.241481	1.161673
O	17.21515	12.07255	1.814581
O	3.778298	5.793852	5.927967
O	3.862645	6.569246	0.88472
O	17.17465	11.12996	6.940069
O	3.891396	11.1706	6.356772
O	16.96299	6.723492	0.852823
O	17.27321	5.796293	5.995948
O	3.88407	11.53944	1.402477

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O	18.61382	0.313672	5.822919
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O	2.012069	0.104026	5.621261
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O	2.628521	4.360327	0.219368
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O	2.518927	13.06978	7.350986
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O	10.69821	8.638241	2.206828
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O	17.04048	10.49839	11.77984
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O	16.94364	7.354002	11.15882
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O	18.61382	0.313672	13.41062
O	18.73201	17.51646	9.608812
O	2.012069	0.104026	13.20896
O	13.25958	9.428115	9.310069
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O	7.818179	8.92312	9.045914
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O	2.076496	1.881253	11.16494
O	18.94066	15.9323	11.74267
O	18.92309	1.891975	11.29632
O	2.134651	15.61805	11.56911
O	12.20088	10.48504	11.83751
O	8.587642	7.09942	10.86701
O	8.621701	10.45331	11.11931
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O	1.512753	2.080945	8.628085
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O	19.35855	14.94692	9.32493
O	1.520873	2.657934	13.60318
O	19.2297	2.895347	13.71074
O	1.634818	14.86178	9.167562
O	1.579952	15.4253	14.10944
O	19.29515	2.183456	8.677266
O	11.98939	12.10456	9.534277

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O	12.06677	11.03783	14.68823
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O	11.94966	6.71882	8.472853
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O	5.196321	13.28349	15.00521
O	2.628521	4.360327	7.807068
O	18.29713	13.42541	7.410127
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O	2.518927	13.06978	14.93869
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O	7.929748	4.064157	7.585387
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C	9.428089	16.61605	7.155387
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C	9.551805	0.903074	0.92062
C	11.09569	16.31985	3.539487
C	11.85481	16.43581	4.668038
C	11.77265	1.106658	4.554176
C	11.0195	1.058894	3.415246
C	10.66546	17.49663	2.838509
C	20.40474	7.783352	1.545816
C	20.24919	7.722975	0.025395
C	19.45526	8.995301	7.297071
C	20.04771	10.03229	0.66358
C	0.627426	8.949153	3.96381
C	1.343192	9.52515	4.979803
C	1.018469	11.68822	4.083524
C	0.305171	11.1806	3.028048
C	0.127663	9.766501	2.904053

C	9.65024	16.16565	8.595292
C	9.428089	16.61605	14.74309
C	8.800874	0.300833	14.9059
C	9.551805	0.903074	8.508319
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C	11.85481	16.43581	12.25574
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C	20.40474	7.783352	9.133516
C	20.24919	7.722975	7.613095
C	19.45526	8.995301	14.88477
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H	10.40179	16.68632	6.654176
H	8.794486	15.92059	6.596015
H	8.882423	0.929671	6.422408
H	7.735841	0.20304	15.14756
H	10.44227	1.480941	0.613632
H	8.913168	1.557327	1.532184
H	10.82772	15.32593	3.188563
H	12.22488	15.5786	5.227805
H	12.09334	2.038985	5.016798
H	10.7076	1.990429	2.94812
H	12.79535	0.018709	5.977476
H	19.53055	7.346868	2.060038
H	0.385976	7.274436	1.897532
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H	18.39414	8.839974	7.533933
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H	10.44227	1.480941	8.201332
H	8.913168	1.557327	9.119884
H	10.82772	15.32593	10.77626
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H	10.7076	1.990429	10.53582
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H	0.385976	7.274436	9.485231
H	0.316624	7.754481	14.73036
H	19.74806	6.80292	14.87798
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S14a_13, Rel. E = 2.35

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Ge	4.711222	6.960364	4.955857
Ge	16.33918	6.974756	5.167269
Ge	16.08024	7.574722	2.058522
Ge	13.10982	6.94452	5.188501
Ge	8.010032	6.981181	4.944254

Ge	8.025919	10.23132	5.319041
Ge	12.84623	7.659453	2.026212
Ge	13.08388	10.72669	2.668555
Ge	13.03446	10.10216	5.813909
Ge	16.1362	10.68472	10.34064
Ge	16.2076	10.14788	13.35343
Ge	4.752314	10.20845	12.95707
Ge	4.711222	6.960364	12.54356
Ge	16.33918	6.974756	12.75497
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Ge	13.03446	10.10216	13.40161
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Si	15.34319	1.391093	2.267543
Si	4.738259	7.429368	1.87309
Si	5.584761	15.9997	2.293706
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Si	4.755463	10.48067	2.263697
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Si	18.51527	1.374531	2.314717
Si	7.867149	10.43392	2.189758
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Si	3.943997	12.35197	15.14076
Si	14.46425	14.15176	0.131337
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Si	6.508963	14.29001	15.09326
Si	14.45331	3.480139	0.081819
Si	1.479546	3.315379	7.488608
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Si	8.987929	12.32731	7.518609
Si	11.93748	5.351162	-0.04566
Si	5.556593	16.29653	12.91594
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Si	15.34319	1.391093	9.855243
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Si	15.3228	16.00302	10.04616
Si	5.573515	1.630297	12.62651
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Si	18.48648	15.98669	10.14332
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Si	18.3837	1.661412	12.95684
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Si	17.08045	12.31172	7.888222
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Si	1.479546	3.315379	15.07631
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O	16.78393	1.980039	5.473897
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O	6.365492	6.287189	4.960256
O	6.287099	6.927839	1.961984
O	14.60392	10.89829	6.075393
O	6.38699	10.89727	5.535116
O	14.47298	6.841059	1.925276
O	14.7265	6.202256	5.139555
O	6.322184	10.90673	2.414062
O	6.466104	2.208744	0.950877
O	14.35662	15.31389	6.550254
O	14.46919	14.95078	1.563157
O	6.520861	2.670977	5.897174
O	14.3447	2.693132	6.223002
O	6.486143	14.94065	1.408784
O	6.488966	15.42427	6.356672
O	14.54208	2.314646	1.219488
O	17.1621	11.91168	1.876605
O	3.708842	5.778254	5.810335
O	3.977779	6.603398	0.717435
O	17.20114	10.95982	7.002874
O	3.733696	11.17501	6.423092
O	17.07402	6.714854	0.853913
O	17.34779	5.747271	5.991345
O	3.961219	11.60677	1.423053
O	5.964306	17.48768	1.728837
O	14.88763	0.10513	5.891105
O	15.04887	17.52203	1.90822
O	5.966502	0.150836	5.616559
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O	4.660251	9.02264	1.522406
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O	14.77812	1.710204	3.769614
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O	17.04376	10.72879	4.292445
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O	11.92324	6.695593	0.858436
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O	2.614429	13.2382	7.428832
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O	18.62903	0.160765	13.52075
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O	18.87794	15.87972	11.71773
O	18.92164	1.762648	11.42871
O	2.0792	15.78395	11.55352
O	12.25177	10.38383	11.80517
O	8.602926	7.156179	10.84973
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O	12.26105	7.184566	11.24553
O	1.551697	2.140238	8.586246
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O	19.36319	14.91404	9.31001
O	1.608043	2.753234	13.56007
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O	19.40728	2.225846	8.868541
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O	11.94904	10.93139	14.52906
O	9.07378	11.27188	13.85491
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O	2.609251	4.448598	7.796933
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C	20.70375	9.15212	4.633377
C	0.754865	9.819021	6.80909
C	1.483389	8.982628	0.274626
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H	11.75802	15.06658	0.669358
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H	12.81828	16.90486	14.84813
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H	20.38815	7.093644	3.923206
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S14a_14, Rel. E = 2.36

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Ge	7.927219	6.943192	4.962286
Ge	7.966797	10.19365	5.419916
Ge	13.06403	7.589284	1.968259
Ge	13.13461	10.69173	2.543631
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Ge	16.30567	10.7252	10.21903
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Ge	4.660419	6.906835	12.55656
Ge	16.2305	7.051924	12.78241
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Si	15.46875	16.32126	5.537846

Si	5.602443	1.284754	2.013124
Si	15.37006	1.422929	2.257319
Si	4.670544	7.463672	1.902959
Si	5.637153	15.94892	2.388863
Si	15.42503	1.688844	5.328825
Si	4.71181	10.51881	2.348232
Si	15.3455	16.05657	2.489056
Si	5.635138	1.662127	5.060369
Si	2.388017	1.253553	2.075392
Si	2.424114	1.695556	5.082443
Si	18.43315	16.02369	2.501473
Si	18.49646	16.35052	5.520097
Si	7.781328	7.427517	1.843969
Si	2.435029	16.32535	5.529125
Si	18.46393	1.379763	2.208875
Si	7.835104	10.4395	2.265725
Si	18.48564	1.692974	5.247599
Si	2.423069	15.90592	2.525621
Si	3.882734	5.305967	7.425212
Si	17.02545	12.42591	0.223879
Si	17.08093	5.321068	15.14496
Si	3.863844	12.27704	0.026558
Si	14.42437	14.32578	0.136539
Si	6.475472	3.41522	7.415205
Si	6.441986	14.18919	15.17365
Si	14.45906	3.453043	0.075688
Si	1.487976	3.314054	7.508619
Si	19.44303	14.41615	0.105078
Si	19.49951	3.309554	0.018619
Si	1.445441	14.2856	0.140004
Si	11.93496	12.38767	0.212532
Si	8.975705	5.311327	7.374725
Si	8.979442	12.27907	7.603568
Si	11.95392	5.397168	-0.12544
Si	5.638462	16.31778	13.02798
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Si	18.43315	16.02369	10.08917
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Si	19.44303	14.41615	7.692778
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Si	11.93496	12.38767	7.800231
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Si	8.979442	12.27907	0.015868
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O	16.95787	2.090572	5.686221
O	4.031455	15.73289	2.2981
O	4.047273	16.13411	5.685585
O	16.91376	1.697095	1.811201
O	14.7022	11.51898	2.719143
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O	14.58302	10.95745	5.935332
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O	14.49865	15.46345	6.55847
O	14.40509	15.0333	1.611085
O	6.430756	2.791514	5.907804
O	14.46193	2.69827	6.204032
O	6.394491	14.79971	1.51804

O	6.426208	15.43316	6.538623
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O	3.878487	6.663903	0.743201
O	17.13193	11.08382	6.908204
O	3.704389	11.01866	6.582073
O	17.23265	6.633629	0.930245
O	17.21846	5.793829	5.99876
O	3.899843	11.67611	1.540959
O	6.049834	17.42337	1.804023
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O	14.91929	17.56948	2.029716
O	6.044092	0.182525	5.626582
O	16.43161	9.260571	1.604519
O	4.659713	8.442552	5.895614
O	4.550331	9.068172	1.607106
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O	17.08922	10.53375	4.217924
O	3.96104	7.129599	3.351635
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O	17.0742	7.230418	3.633934
O	1.982842	17.38113	2.016253
O	18.92677	0.201398	5.727337
O	18.86428	17.51659	2.027086
O	2.044197	0.195574	5.60392
O	13.32042	9.281413	1.459211
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O	7.76006	9.013162	1.484963
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O	1.628139	2.013906	0.885779
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O	19.4295	2.721621	6.097572
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O	19.42068	2.148195	1.138519
O	12.07928	11.89512	1.758992
O	8.944107	5.769727	5.794064
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O	11.9625	11.14974	6.759135
O	9.038729	11.17378	6.39839
O	12.02963	6.706842	0.832832
O	12.00564	5.822198	5.889378
O	8.643049	11.54818	1.427801
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O	15.6408	13.25189	7.604188
O	15.71546	4.472829	0.235683
O	5.154231	13.21822	7.331607
O	2.648799	4.386645	0.310678
O	18.29848	13.33571	-0.21147
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O	12.98594	13.58369	-0.11251
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O	7.822373	13.39784	7.331483
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O	18.92677	0.201398	13.31504
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O	18.84816	15.72753	11.63811
O	18.83285	1.971097	11.27106
O	2.014321	15.6842	11.6747
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O	12.02963	6.706842	8.420531
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O	8.643049	11.54818	9.015501
O	5.289163	4.509339	7.626064
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O	15.71546	4.472829	7.823383
O	5.154231	13.21822	14.91931
O	2.648799	4.386645	7.898378
O	18.29848	13.33571	7.376226
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O	7.918246	4.100015	7.65306
O	7.822373	13.39784	14.91918
O	13.04449	4.2527	7.823231
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O	10.41132	13.03707	7.678387
O	10.45122	4.743019	7.716066
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F	16.89353	17.6573	11.58136
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C	9.787583	16.18292	0.916197
C	9.530107	16.62826	7.066528
C	8.917263	0.321115	7.233225
C	9.702542	0.920005	0.814639
C	11.22387	16.35214	3.445059
C	12.01698	16.47259	4.554177
C	11.96218	1.137446	4.413238
C	11.1752	1.086598	3.293156

C	10.7983	17.52355	2.744023
C	20.44923	7.798532	1.621453
C	20.28981	7.684231	0.104079
C	19.4326	8.905184	7.341577
C	19.94014	9.998492	0.69077
C	0.534429	9.126505	4.057201
C	1.045087	9.795097	5.13642
C	0.474551	11.89329	4.196256
C	-0.03359	11.29001	3.078685
C	-0.01102	9.860839	2.953588
C	9.787583	16.18292	8.503897
C	9.530107	16.62826	14.65423
C	8.917263	0.321115	14.82093
C	9.702542	0.920005	8.402339
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C	12.01698	16.47259	12.14188
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H	10.48882	16.69291	6.537149
H	8.883156	15.92798	6.526895
H	8.99414	0.940605	6.330095
H	7.855783	0.23619	7.498296
H	10.60385	1.463872	0.480493
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H	10.96714	15.35621	3.091161
H	12.426	15.62047	5.095923
H	12.33555	2.06761	4.841233
H	10.89385	2.016774	2.804982
H	13.0956	0.057668	5.750475
H	19.5867	7.349984	2.144108
H	0.447073	7.336675	1.995469
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H	19.14379	10.68396	8.595499
H	0.555438	8.038778	11.63832
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S14a_15, Rel. E = 2.43

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Ge	16.27892	6.990759	5.201325
Ge	16.19457	7.55062	2.072751
Ge	13.06274	6.979273	5.194443
Ge	8.01739	6.970914	4.992366
Ge	8.021639	10.19868	5.316344
Ge	12.95724	7.603292	2.020169
Ge	13.12742	10.70905	2.610421
Ge	12.96945	10.12439	5.74483
Ge	16.28032	10.7425	10.186
Ge	16.06387	10.10635	13.21801
Ge	4.657895	10.17109	12.93794
Ge	4.630788	6.941582	12.57745
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Ge	8.01739	6.970914	12.58007
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Ge	12.96945	10.12439	13.33253
Si	5.541548	16.27183	5.386899
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Si	5.549119	1.271954	2.025373
Si	15.2959	1.305673	2.168088
Si	4.743083	7.351852	1.88864
Si	5.525762	15.92769	2.356169
Si	15.25108	1.670078	5.244305
Si	4.75152	10.42613	2.221303
Si	15.23418	15.95824	2.51117
Si	5.56797	1.60212	5.05083
Si	2.474569	1.295626	2.098592
Si	2.508418	1.662247	5.121609
Si	18.43486	15.87646	2.570959
Si	18.44613	16.30969	5.573523
Si	7.831142	7.341092	1.850968
Si	2.478739	16.31325	5.512237
Si	18.49518	1.255714	2.161587
Si	7.849809	10.38165	2.165671
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Si	2.445082	15.9595	2.484908

Si	3.917546	5.173607	7.384012
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Si	3.898553	12.34744	15.11189
Si	14.43585	14.18346	0.150028
Si	6.503475	3.256444	7.400902
Si	6.469035	14.26158	15.13356
Si	14.46393	3.463273	0.016471
Si	1.4557	3.250292	7.508285
Si	19.42443	14.30557	0.132774
Si	19.44674	3.269591	-0.00663
Si	1.431727	14.36506	0.135068
Si	11.89675	12.27346	0.255711
Si	8.96982	5.231954	7.366188
Si	8.972533	12.30617	7.515659
Si	11.9341	5.318986	-0.06577
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Si	15.2959	1.305673	9.755789
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Si	5.525762	15.92769	9.943868
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O	14.44712	2.789356	6.105083
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O	3.955044	11.52676	1.352048
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O	5.982371	0.125133	5.613222
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O	14.87717	1.816164	3.663973
O	5.966612	15.69271	3.912859
O	17.03971	10.63629	4.203329
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O	18.77554	15.6037	4.140563
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O	1.49374	14.91947	1.654855
O	1.571058	15.53443	6.619255
O	19.32652	1.987022	0.99028
O	11.99734	11.84915	1.826108
O	8.968917	5.719741	5.791509
O	8.610531	6.518428	0.71297
O	11.89127	10.98521	6.864489
O	9.024964	11.32815	6.202085
O	12.00725	6.624061	0.888548
O	12.04951	5.720717	5.947413
O	8.67148	11.42077	1.259806
O	5.263203	4.312451	15.16582
O	15.73501	13.2699	7.496251
O	15.70118	4.479981	0.208321
O	5.2414	13.20491	7.281577
O	2.572717	4.403545	0.243501
O	18.34981	13.19487	14.85256

O	18.33005	4.35368	0.415059
O	2.548919	13.20986	7.496963
O	13.04087	13.38976	-0.09807
O	7.903805	4.053278	0.043441
O	7.871243	13.46358	7.356167
O	13.03088	4.168355	0.304837
O	-0.00937	3.966087	0.097206
O	-0.027	13.64495	7.550565
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O	10.44584	4.644214	0.132568
O	10.64507	8.728438	2.188014
O	4.007484	1.627773	9.227383
O	16.83869	16.17472	13.44927
O	16.82763	15.74251	9.896482
O	4.058483	2.082744	13.03175
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O	3.970354	15.52032	9.668777
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O	16.88995	1.397867	9.488956
O	14.68157	11.57597	10.24451
O	6.324034	6.408959	12.66509
O	6.284349	6.8436	9.576095
O	14.52071	10.94892	13.60367
O	6.332897	10.7176	13.1765
O	14.57987	6.806458	9.560484
O	14.66919	6.207076	12.7583
O	6.307026	10.88454	9.949688
O	6.454778	2.101993	8.529794
O	14.40639	15.45264	14.26924
O	14.41139	14.85032	9.237741
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O	14.44712	2.789356	13.69278
O	6.405533	14.85349	9.058667
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O	17.06086	10.97581	14.44617
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O	14.78588	0.180596	13.36494
O	14.80719	17.45389	9.573491

O	5.982371	0.125133	13.20092
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O	2.053956	17.43975	9.530484
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O	13.32338	9.285554	9.129647
O	8.248362	8.51357	13.45817
O	7.802556	8.916936	9.046385
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O	18.77554	15.6037	11.72826
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O	2.060611	15.72398	11.63682
O	12.22777	10.41498	11.71917
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O	8.568244	10.30772	11.2195
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O	19.25108	2.766774	13.63333
O	1.49374	14.91947	9.242556
O	1.571058	15.53443	14.20696
O	19.32652	1.987022	8.57798
O	11.99734	11.84915	9.413808
O	8.968917	5.719741	13.37921
O	8.610531	6.518428	8.300671
O	11.89127	10.98521	14.45219
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O	15.73501	13.2699	15.08395
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O	-0.027	13.64495	15.13827
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O	10.64507	8.728438	9.775714
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F	14.82095	9.076658	4.139903
F	4.076078	-0.04344	11.37382
F	14.82095	9.076658	11.7276
C	20.28216	10.64943	4.244334
C	20.26072	10.46849	5.760554
C	19.6957	9.057089	5.973642
C	20.1273	8.257384	4.738611
C	0.65586	9.975074	1.692712
C	1.427571	9.600639	0.629083
C	1.047993	7.302906	1.066444
C	0.294789	7.610087	2.164977
C	0.12955	8.975571	2.57252
C	9.567879	1.538612	4.447646
C	9.781907	1.272823	5.934628
C	9.18411	17.5763	6.137641
C	9.442298	16.84405	4.80736
C	11.00225	1.024461	1.897472
C	11.82859	0.718413	0.851802
C	11.49205	16.10612	1.176316
C	10.67975	16.34189	2.251031
C	10.45613	17.68154	2.710442
C	20.28216	10.64943	11.83203
C	20.26072	10.46849	13.34825
C	19.6957	9.057089	13.56134
C	20.1273	8.257384	12.32631
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C	1.427571	9.600639	8.216783
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C	0.12955	8.975571	10.16022
C	9.567879	1.538612	12.03535
C	9.781907	1.272823	13.52233
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C	11.00225	1.024461	9.485172
C	11.82859	0.718413	8.439502
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H	0.360943	10.54651	6.138262
H	19.65522	11.23692	6.254758
H	20.05401	8.591002	6.901133
H	0.092056	7.634113	4.926622
H	19.32809	7.603611	4.356226
H	0.496907	11.03588	1.871085
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H	1.221738	6.278675	0.742762
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H	2.317315	8.049817	14.78702
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H	1.221738	6.278675	8.330462
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S14a_16, Rel. E = 4.10

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Ge	4.830677	10.157123	5.385183
Ge	4.384068	6.955665	4.991340
Ge	16.242649	7.086199	5.215679
Ge	16.060923	7.657332	2.032453
Ge	12.998053	7.061924	5.217719
Ge	7.733432	6.915951	4.975944
Ge	7.976567	10.149892	5.355000
Ge	12.760515	7.745725	2.007923
Ge	13.065881	10.875448	2.635472
Ge	12.967619	10.251788	5.789231
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Ge	16.225071	10.303083	13.343452
Ge	4.830677	10.157123	12.972883
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Ge	16.242649	7.086199	12.803380
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Ge	12.998053	7.061924	12.805420
Ge	7.733432	6.915951	12.563643
Ge	7.976567	10.149892	12.942700
Ge	12.760515	7.745725	9.595623
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Si	5.625468	16.266024	5.458065
Si	15.562676	16.113438	5.595409
Si	5.564944	1.206895	2.041888
Si	15.291332	1.448770	2.222114
Si	4.601681	7.344738	1.871123
Si	5.621845	15.861063	2.448623
Si	15.380186	1.568014	5.357573
Si	4.653934	10.444624	2.340370
Si	15.279726	16.122725	2.490582
Si	5.583070	1.612001	5.106025
Si	2.372956	1.179529	2.085771
Si	2.392409	1.609977	5.127441
Si	18.411457	16.068293	2.558724
Si	18.627552	16.561201	5.560334
Si	7.722373	7.347532	1.833529
Si	2.410743	16.257463	5.523508
Si	18.429327	1.501865	2.146613
Si	7.789488	10.367777	2.208571
Si	18.570850	1.848778	5.126698
Si	2.403485	15.836765	2.541325
Si	3.909278	5.188097	7.401938
Si	16.985693	12.572362	0.248390
Si	17.065098	5.396680	-0.002345
Si	3.813855	12.187485	0.001867
Si	14.346922	14.362677	0.232102
Si	6.459565	3.316638	7.479387
Si	6.363211	14.138875	0.019941
Si	14.458889	3.492487	0.053915
Si	1.479925	3.252135	7.540903
Si	19.427879	14.545258	0.128597
Si	19.469687	3.426382	-0.026583
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Si	15.380186	1.568014	12.945272
Si	4.653934	10.444624	9.928071
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Si	5.583070	1.612001	12.693726
Si	2.372956	1.179529	9.67347
Si	2.392409	1.609977	12.71514
Si	18.411457	16.068293	10.146423
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Si	7.722373	7.347532	9.421228
Si	2.410743	16.257463	13.111207
Si	18.429327	1.501865	9.734312
Si	7.789488	10.367777	9.79627
Si	18.570850	1.848778	12.714398
Si	2.403485	15.836765	10.129025
Si	3.909278	5.188097	14.989638
Si	16.985693	12.572362	7.83609
Si	17.065098	5.396680	7.585355
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Si	11.846948	12.476293	7.887963
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O	14.965911	0.116169	5.930812
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O	1.909336	17.312601	2.076648
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O	1.930578	0.101127	5.567667
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O	7.810635	8.934334	1.444387
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O	18.876556	2.183858	3.558297
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O	8.532839	10.282195	3.660396
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O	1.544662	1.957764	0.94665
O	19.532354	15.75423	6.647044
O	19.362268	15.10063	1.655498
O	1.596521	2.710564	6.001792
O	19.293213	3.002675	6.004349
O	1.678384	14.671394	1.678931
O	1.703318	15.448254	6.726704
O	19.288214	2.127947	0.929878
O	11.986315	12.065237	1.885704
O	8.793341	5.72174	5.793354
O	8.567245	6.497272	0.751526
O	12.012007	11.146212	6.961022
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O	18.399117	4.566549	0.401043
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O	12.893804	13.660031	-0.058876
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O	0.052982	4.011359	0.152
O	-0.105492	13.674746	7.580479
O	10.324991	13.041668	0.084441
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O	10.673518	8.668709	2.139712
O	3.967456	1.254799	9.341131
O	17.091009	16.635664	13.612087
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C	10.69596	17.46447	2.932409
C	20.57593	7.978941	1.619
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C	20.001471	10.10614	0.56904
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H	9.052931	1.593192	1.529015
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S14b_4, Rel. E = 1.56

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Ge	4.742275	7.068583	4.955347
Ge	16.28728	7.056195	5.133423
Ge	16.22525	7.58922	2.030422
Ge	13.08768	6.982511	5.11974
Ge	13.04464	7.540063	1.954858
Ge	18.56784	15.87205	2.622061
Ge	18.4876	16.35434	5.780319
Ge	12.99829	10.66285	2.583133
Ge	12.96196	10.12568	5.73546
Ge	16.17965	10.75166	10.1462
Ge	16.09861	10.15318	13.21132
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Si	5.656727	1.364146	2.045807
Si	15.36832	1.363759	2.162824
Si	4.78862	7.365183	1.890942
Si	5.619034	15.96839	2.315297
Si	15.33097	1.744403	5.208728
Si	4.691761	10.4813	2.209202
Si	15.27162	15.98161	2.501374
Si	5.656865	1.647522	5.131505

Si	2.495646	1.373641	2.051224
Si	2.488711	1.685875	5.125728
Si	7.84965	7.390707	2.074689
Si	7.905816	7.136452	5.179036
Si	7.871447	10.2167	5.430687
Si	2.429916	16.2953	5.404481
Si	18.55998	1.321831	2.179602
Si	7.759713	10.47246	2.323089
Si	18.43756	1.808061	5.230563
Si	2.453807	15.99344	2.335611
Si	3.970017	5.293772	7.319932
Si	16.97426	12.41542	0.129339
Si	17.08811	5.366743	15.0913
Si	3.877756	12.25024	15.02275
Si	14.34403	14.26992	0.123546
Si	6.546562	3.406251	7.459536
Si	6.450319	14.18031	15.14236
Si	14.45986	3.47132	15.16449
Si	1.493016	3.381049	7.476062
Si	19.47638	14.24736	0.249959
Si	19.48525	3.388586	0.015902
Si	1.44262	14.28743	-0.01437
Si	11.84783	12.30797	0.242448
Si	8.990766	5.444058	7.488213
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O	3.732026	11.17865	13.83483
O	17.18132	6.691354	8.428856
O	17.29052	5.797616	13.52699
O	3.821606	11.50025	8.873011
O	5.958169	17.47966	9.369262
O	15.17828	0.217373	13.40366
O	15.06198	17.48501	9.473884
O	5.93202	0.123774	13.24122
O	16.32561	9.294258	9.116954
O	4.030602	8.505477	13.39121
O	4.579004	8.961454	9.196277
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O	17.10295	7.24764	11.14608
O	2.179678	17.50327	9.390518
O	18.54145	0.391358	13.61351
O	18.88191	17.45235	9.464948
O	2.161429	0.178916	13.2417
O	13.20419	9.252598	9.088691
O	8.162637	8.643599	13.3386
O	7.817781	8.971767	9.301551
O	12.89202	8.402814	13.77795
O	2.076365	1.815504	11.14727
O	19.24982	15.83919	11.85193
O	19.00122	1.707117	11.29561
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O	12.18341	10.44271	11.74293
O	8.315104	7.056391	11.19125
O	8.255937	10.55786	11.46337
O	12.28884	7.134563	11.12047
O	1.620896	2.197032	8.574599
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O	19.42333	14.53204	9.450283
O	1.618793	2.751704	13.56494
O	19.31563	2.872043	13.65151
O	1.585256	14.94644	9.05711
O	1.530447	15.46024	14.03682

O	19.40651	2.167715	8.683949
O	11.95148	11.88251	9.401178
O	8.886867	6.126799	13.60088
O	8.814017	6.562078	8.651227
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O	12.10403	5.696366	13.45674
O	8.708092	11.46519	9.036162
O	5.226092	4.313509	7.63249
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O	15.71865	4.477817	7.695621
O	5.166933	13.23702	14.92825
O	2.605181	4.509781	7.741002
O	18.27117	13.32678	7.313324
O	18.34035	4.445605	7.979725
O	2.547905	13.16861	14.89624
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O	7.90436	4.242847	7.657683
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O	13.04001	4.194561	7.868245
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O	20.91036	13.55431	15.08667
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O	10.44795	4.709884	7.649435
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C	9.759998	16.12062	0.950606
C	9.500345	16.50449	14.67337
C	8.878186	0.19796	14.78165
C	9.658916	0.854226	0.747112
C	11.15676	16.40091	3.488055
C	11.88534	16.56681	4.631177
C	11.80437	1.23085	4.414677
C	11.08258	1.13098	3.256855
C	10.74085	17.54409	2.73284
C	20.20997	10.67269	3.778561
C	20.05644	10.53062	5.292588
C	19.65375	9.065074	5.503222
C	20.3384	8.298248	4.372732
C	0.558104	10.07002	1.2351
C	1.345395	9.759462	0.159405
C	1.214456	7.455595	0.635144

C	0.468667	7.695817	1.756408
C	0.176464	9.039477	2.146662
C	9.759998	16.12062	8.538306
C	9.500345	16.50449	7.085674
C	8.878186	0.19796	7.19395
C	9.658916	0.854226	8.334812
C	11.15676	16.40091	11.07576
C	11.88534	16.56681	12.21888
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C	11.08258	1.13098	10.84456
C	10.74085	17.54409	10.32054
C	20.20997	10.67269	11.36626
C	20.05644	10.53062	12.88029
C	19.65375	9.065074	13.09092
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C	1.345395	9.759462	7.747105
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H	10.46076	16.5521	6.558949
H	8.862889	15.77724	6.572834
H	8.942619	0.782353	6.266695
H	7.817914	0.117528	15.05392
H	10.55166	1.399191	0.391458
H	9.046037	1.557345	1.330389
H	10.91908	15.391	3.161749
H	12.25512	15.73361	5.225963
H	12.11991	2.182391	4.840853
H	10.79747	2.041855	2.734661
H	12.78913	0.205326	5.9085
H	19.27989	11.01674	3.299706
H	0.095995	11.36238	3.508805
H	0.091014	10.74446	5.774535

H	19.30863	11.2228	5.696435
H	19.92737	8.679657	6.494179
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H	19.719	7.466324	4.003739
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H	1.756814	10.50853	14.66501
H	1.46744	6.448415	0.322872
H	0.12369	6.850773	2.347374
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H	10.65385	8.091747	10.76915
H	10.41323	9.598241	10.86144
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H	8.862889	15.77724	14.16053
H	8.942619	0.782353	13.8544
H	7.817914	0.117528	7.466224
H	10.55166	1.399191	7.979158
H	9.046037	1.557345	8.918089
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H	10.79747	2.041855	10.32236
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H	0.095995	11.36238	11.09651
H	0.091014	10.74446	13.36224
H	19.30863	11.2228	13.28414
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H	19.719	7.466324	11.59144
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S14b_6, Rel. E = 1.59

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Ge	4.741356	10.08408	5.215421
Ge	4.716901	7.072863	4.955394
Ge	16.26096	7.030473	5.171298
Ge	16.25121	7.572511	2.063328

Ge	13.05406	6.984617	5.116967
Ge	13.05922	7.536689	1.955339
Ge	18.5399	15.84217	2.624733
Ge	18.49216	16.33402	5.75624
Ge	13.0402	10.66331	2.589278
Ge	12.97546	10.12957	5.740818
Ge	16.21674	10.73987	10.19266
Ge	16.09094	10.13637	13.25618
Ge	4.741356	10.08408	12.80312
Ge	4.716901	7.072863	12.54309
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Ge	16.25121	7.572511	9.651028
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Ge	13.05922	7.536689	9.543039
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Ge	13.0402	10.66331	10.17698
Ge	12.97546	10.12957	13.32852
Si	5.653985	16.26812	5.417278
Si	15.29591	16.27626	5.591693
Si	5.669682	1.324946	2.030922
Si	15.34549	1.338921	2.188851
Si	4.793073	7.373734	1.891321
Si	5.638933	15.96556	2.328483
Si	15.32639	1.710713	5.227211
Si	4.727578	10.48491	2.196681
Si	15.24991	15.95251	2.542574
Si	5.699153	1.629514	5.132728
Si	2.490996	1.346753	2.07164
Si	2.514713	1.698896	5.132928
Si	7.846853	7.396571	2.076604
Si	7.885414	7.139885	5.175347
Si	7.867581	10.22095	5.435144
Si	2.458238	16.31777	5.464801
Si	18.53027	1.286805	2.162936
Si	7.790848	10.47074	2.328853
Si	18.43636	1.776169	5.206836
Si	2.444238	15.97727	2.416062
Si	3.936833	5.30868	7.325525
Si	17.01784	12.36963	0.17911
Si	17.07652	5.337947	15.13215
Si	3.903356	12.24587	15.00187
Si	14.38623	14.23227	0.165192
Si	6.523816	3.423841	7.450446
Si	6.470853	14.1579	15.15317
Si	14.45491	3.449533	0.017003

Si	1.501574	3.373129	7.497985
Si	19.49136	14.22431	0.241598
Si	19.47467	3.343536	-0.00081
Si	1.476681	14.29127	0.049942
Si	11.87848	12.28747	0.251683
Si	8.984326	5.456792	7.491854
Si	8.948611	12.18652	0.019879
Si	11.94175	5.333775	15.04044
Si	5.653985	16.26812	13.00498
Si	15.29591	16.27626	13.17939
Si	5.669682	1.324946	9.618622
Si	15.34549	1.338921	9.77655
Si	4.793073	7.373734	9.47902
Si	5.638933	15.96556	9.916183
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Si	4.727578	10.48491	9.784381
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Si	5.699153	1.629514	12.72043
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Si	2.514713	1.698896	12.72063
Si	7.846853	7.396571	9.664304
Si	7.885414	7.139885	12.76305
Si	7.867581	10.22095	13.02284
Si	2.458238	16.31777	13.0525
Si	18.53027	1.286805	9.750635
Si	7.790848	10.47074	9.916553
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Si	2.444238	15.97727	10.00376
Si	3.936833	5.30868	14.91323
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Si	19.49136	14.22431	7.829298
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O	6.604949	2.675188	5.987332
O	14.44122	2.733794	6.123385
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O	15.22651	0.190974	5.843838
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O	6.125828	0.124525	5.641382
O	16.37327	9.278719	1.578567
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O	19.31693	2.847429	6.039554
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O	14.54693	2.244323	8.706792
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O	4.018286	6.625061	8.260771
O	17.07494	11.03467	14.45547
O	3.7236	11.18594	13.80921
O	17.20906	6.656111	8.478253
O	17.25427	5.775584	13.56634
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O	6.08034	17.4583	9.39345
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O	15.07705	17.45259	9.494273
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O	2.176883	1.921355	11.14835
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O	12.21113	10.48167	11.74906
O	8.315198	7.068437	11.1926
O	8.267092	10.55641	11.473
O	12.26852	7.171202	11.11456
O	1.648074	2.157298	8.560946
O	19.42237	15.6769	14.67316
O	19.4134	14.52221	9.43637
O	1.683054	2.786794	13.57508
O	19.31693	2.847429	13.62725
O	1.608294	14.89995	9.144485
O	1.613225	15.51461	14.1604
O	19.38668	2.114867	8.65571
O	11.97386	11.86916	9.411012
O	8.858517	6.123727	13.60099
O	8.818626	6.570882	8.657211
O	11.92332	10.98372	14.46888
O	8.835359	11.12728	13.97203
O	12.05661	6.65953	8.383224
O	12.06432	5.711937	13.45964
O	8.74082	11.46374	9.046522
O	5.196186	4.311909	7.587686
O	15.68586	13.29406	15.13139
O	15.69936	4.47839	7.767867
O	5.209379	13.20883	14.87065
O	2.588636	4.523785	7.799396
O	18.31741	13.25898	7.312405
O	18.33777	4.406406	7.971106
O	2.586992	13.18592	14.92361
O	13.00001	13.42725	7.493877

O	7.882865	4.256565	7.673485
O	7.876197	13.39881	14.99259
O	13.031	4.1867	7.856689
O	0.026516	4.030998	7.680853
O	0.023184	13.56202	15.10726
O	10.39397	12.95506	7.610154
O	10.43249	4.709402	7.654524
O	10.42383	8.961679	10.24226
F	5.869359	8.751179	4.069474
F	14.76682	9.008272	4.066192
F	5.869359	8.751179	11.65717
F	14.76682	9.008272	11.65389
C	20.2577	10.6118	3.89125
C	20.0385	10.40315	5.388428
C	19.59611	8.939883	5.512812
C	20.31831	8.210705	4.381479
C	0.588779	10.09842	1.33063
C	1.350251	9.82904	0.227704
C	1.194788	7.507506	0.596453
C	0.471286	7.70358	1.740401
C	0.198382	9.031444	2.195488
C	9.62049	16.34006	1.495136
C	8.988711	16.75818	0.356633
C	9.296984	1.333088	0.934283
C	9.899072	0.980501	2.110237
C	10.05118	17.30383	2.460213
C	10.79298	15.52292	4.021288
C	11.22957	15.5971	5.487436
C	11.77497	17.02145	5.650455
C	10.93683	0.169149	4.70141
C	20.2577	10.6118	11.47895
C	20.0385	10.40315	12.97613
C	19.59611	8.939883	13.10051
C	20.31831	8.210705	11.96918
C	0.588779	10.09842	8.91833
C	1.350251	9.82904	7.815404
C	1.194788	7.507506	8.184154
C	0.471286	7.70358	9.3281
C	0.198382	9.031444	9.783189
C	9.62049	16.34006	9.082836
C	8.988711	16.75818	7.944333
C	9.296984	1.333088	8.521983
C	9.899072	0.980501	9.697937
C	10.05118	17.30383	10.04791
C	10.79298	15.52292	11.60899
C	11.22957	15.5971	13.07514

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N	1.670754	8.558146	15.05171
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H	10.50261	9.673588	3.319152
H	19.35904	11.0089	3.392947
H	0.175981	11.28601	3.687707
H	0.056512	10.56802	5.916443
H	19.29241	11.09405	5.796686
H	19.80591	8.50261	6.497927
H	18.51968	8.863527	5.339405
H	0.362877	7.788163	4.69549
H	19.70397	7.402085	3.957076
H	0.343875	11.13322	1.556472
H	1.746734	10.60514	14.75618
H	1.426565	6.512822	0.231158
H	0.125379	6.835073	2.295839
H	2.399376	8.417022	6.740971
H	9.747556	15.27155	1.657
H	8.578285	16.06646	14.80253
H	9.167112	2.370473	0.63365
H	10.24964	1.774447	2.765539
H	9.870605	14.93683	3.88374
H	11.57503	15.09037	3.374886
H	10.37191	15.42076	6.14961
H	11.98302	14.83967	5.728292
H	11.74771	17.38557	6.685775
H	12.81289	17.06348	5.307492
H	11.50525	1.018135	4.293978
H	10.02225	0.56697	5.177896
H	8.230212	0.651308	14.4768
H	10.67089	8.16483	10.756
H	10.50261	9.673588	10.90685
H	19.35904	11.0089	10.98065
H	0.175981	11.28601	11.27541
H	0.056512	10.56802	13.50414
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H	19.80591	8.50261	14.08563
H	18.51968	8.863527	12.9271

H	0.362877	7.788163	12.28319
H	19.70397	7.402085	11.54478
H	0.343875	11.13322	9.144172
H	1.746734	10.60514	7.16848
H	1.426565	6.512822	7.818857
H	0.125379	6.835073	9.883539
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H	9.747556	15.27155	9.244699
H	8.578285	16.06646	7.214825
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H	10.24964	1.774447	10.35324
H	9.870605	14.93683	11.47144
H	11.57503	15.09037	10.96259
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H	11.98302	14.83967	13.31599
H	11.74771	17.38557	14.27348
H	12.81289	17.06348	12.89519
H	11.50525	1.018135	11.88168
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S14b_17, Rel. E = 2.56

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Ge	16.030012	10.133834	5.725080
Ge	4.539271	10.247611	5.283396
Ge	4.678082	7.093129	5.149754
Ge	16.193211	6.966577	5.172110
Ge	16.220169	7.481675	2.017678
Ge	13.045027	6.981101	5.004802
Ge	13.034546	7.398287	1.868748
Ge	18.445980	15.875074	2.669083
Ge	18.480303	16.330070	5.646338
Ge	12.901902	10.534741	2.522090
Ge	12.822622	10.034522	5.630741
Ge	16.128502	10.668187	10.149912
Ge	16.030012	10.133834	13.312779
Ge	4.539271	10.247611	12.871095
Ge	4.678082	7.093129	12.737454
Ge	16.193211	6.966577	12.759809
Ge	16.220169	7.481675	9.605378
Ge	13.045027	6.981101	12.592502
Ge	13.034546	7.398287	9.456447
Ge	18.445980	15.875074	10.256783
Ge	18.480303	16.330070	13.234038
Ge	12.901902	10.534741	10.109790
Ge	12.822622	10.034522	13.218441

Si	5.622319	16.367035	5.528675
Si	15.346567	16.225576	5.550171
Si	5.668263	1.313416	2.085333
Si	15.460919	1.275695	2.100592
Si	5.090072	7.399915	1.892698
Si	5.552949	15.989160	2.466662
Si	15.450667	1.626622	5.174203
Si	4.806096	10.499951	2.178503
Si	15.316450	15.889718	2.453783
Si	5.755903	1.695887	5.147790
Si	2.495564	1.393471	2.171663
Si	2.581945	1.806072	5.187169
Si	8.157120	7.468621	2.214561
Si	7.871199	7.220583	5.383562
Si	7.888885	10.274159	5.457510
Si	2.449835	16.450851	5.615017
Si	18.613451	1.212122	2.093979
Si	7.856245	10.574567	2.386872
Si	18.590723	1.690235	5.143860
Si	2.378948	16.052446	2.593066
Si	3.954068	5.307426	7.477263
Si	17.010494	12.394334	0.197961
Si	17.100752	5.275666	15.113075
Si	3.909326	12.401465	15.060689
Si	14.374983	14.239518	0.104444
Si	6.549717	3.403196	7.505226
Si	6.463176	14.267596	0.087538
Si	14.514871	3.361799	15.108596
Si	1.524375	3.416562	7.58408
Si	19.474312	14.277108	0.253637
Si	19.512882	3.282073	-0.060683
Si	1.440207	14.435225	0.203051
Si	11.873780	12.261878	0.160706
Si	9.033259	5.403853	7.622208
Si	8.934478	12.338769	0.081616
Si	11.970207	5.222989	14.900504
Si	5.622319	16.367035	13.116375
Si	15.346567	16.225576	13.137871
Si	5.668263	1.313416	9.673034
Si	15.460919	1.275695	9.688293
Si	5.090072	7.399915	9.480398
Si	5.552949	15.989160	10.054362
Si	15.450667	1.626622	12.761904
Si	4.806096	10.499951	9.766203
Si	15.316450	15.889718	10.041483
Si	5.755903	1.695887	12.73549

Si	2.495564	1.393471	9.759363
Si	2.581945	1.806072	12.774869
Si	8.157120	7.468621	9.802261
Si	7.871199	7.220583	12.971262
Si	7.888885	10.274159	13.045209
Si	2.449835	16.450851	13.202717
Si	18.613451	1.212122	9.681679
Si	7.856245	10.574567	9.974572
Si	18.590723	1.690235	12.73156
Si	2.378948	16.052446	10.180766
Si	3.954068	5.307426	15.064962
Si	17.010494	12.394334	7.78566
Si	17.100752	5.275666	7.525375
Si	3.909326	12.401465	7.472989
Si	14.374983	14.239518	7.692144
Si	6.549717	3.403196	15.092925
Si	6.463176	14.267596	7.675237
Si	14.514871	3.361799	7.520896
Si	1.524375	3.416562	-0.00362
Si	19.474312	14.277108	7.841338
Si	19.512882	3.282073	7.527017
Si	1.440207	14.435225	7.790751
Si	11.873780	12.261878	7.748406
Si	9.033259	5.403853	0.034507
Si	8.934478	12.338769	7.669316
Si	11.970207	5.222989	7.312804
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O	17.013763	1.925951	5.502162
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O	4.059054	16.373755	5.937294
O	17.033751	1.395192	1.706223
O	14.481787	11.351693	2.67496
O	6.306129	6.951518	5.826354
O	6.613108	6.944135	1.698752
O	14.401348	10.848166	5.820695
O	6.264402	10.463507	5.588875
O	14.648334	6.66534	1.811507
O	14.61886	6.128648	5.144167
O	6.308358	11.107841	2.337863
O	6.488017	2.157299	0.972736
O	14.336614	15.41308	6.558634
O	14.301437	14.907071	1.599533
O	6.670399	2.742757	6.001685

O	14.564745	2.699281	6.028413
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O	6.4541	15.51087	6.620829
O	14.603863	2.174352	1.04676
O	17.117117	11.925586	1.777581
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O	4.145294	6.619522	0.820945
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O	3.608643	11.439504	6.182508
O	17.258696	6.586063	0.905681
O	17.268675	5.788002	5.973568
O	3.946278	11.473237	1.215748
O	6.149469	17.451931	2.023876
O	14.988608	0.121632	5.624456
O	14.952229	17.428083	2.012831
O	6.25016	0.182433	5.562268
O	16.218845	9.20036	1.539962
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O	4.841804	8.990708	1.583428
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O	6.016236	1.934706	3.558789
O	15.00067	15.659306	4.04702
O	15.141252	1.86375	3.591909
O	5.866347	15.727642	4.047568
O	16.868111	10.419982	4.163761
O	4.504968	7.040751	3.395653
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O	17.008413	7.25954	3.610408
O	1.931614	17.579489	2.26425
O	19.128456	0.283694	5.761774
O	19.14719	17.378935	1.974764
O	2.038025	0.320643	5.564663
O	12.926324	9.123758	1.422614
O	8.29621	8.74131	5.815609
O	7.915041	9.06421	1.817376
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O	2.338065	2.138819	3.613739
O	19.059971	15.351477	4.274059
O	18.915873	1.892716	3.558068
O	2.182465	15.736406	4.17647
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O	12.191884	6.949535	3.404554
O	1.691359	2.173722	1.022147
O	19.428505	15.641743	6.991045

O	19.391401	14.572495	1.835707
O	1.827268	2.928445	6.061559
O	19.423262	2.839317	5.965238
O	1.532137	14.985714	1.736713
O	1.634569	15.695113	6.774588
O	19.47632	2.045867	0.982859
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O	13.018991	13.359029	15.023804
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O	10.449137	4.599099	-0.024438
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O	6.4541	15.51087	14.208529
O	14.603863	2.174352	8.634459
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O	4.145294	6.619522	8.408645
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O	17.008413	7.25954	11.198108
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O	19.128456	0.283694	13.349474
O	19.14719	17.378935	9.562464
O	2.038025	0.320643	13.152364
O	12.926324	9.123758	9.010314
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O	1.634569	15.695113	14.362288
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O	11.908308	11.773706	9.304549
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O	12.03763	5.673907	13.342381
O	8.761086	11.596082	9.10787
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O	15.716419	4.444701	7.740404
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O	2.589595	4.591237	7.973334
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O	18.365561	4.345268	7.908216
O	2.6748	13.408973	15.13357
O	13.018991	13.359029	7.436103
O	7.881895	4.249833	7.821138
O	7.923748	13.605771	15.140942
O	13.058372	4.078331	7.702457
O	0.042217	4.04468	7.697856
O	0.060876	13.617728	15.160308
O	10.407701	13.004619	7.56416
O	10.449137	4.599099	7.563262
O	10.018106	8.189399	10.359492
F	17.318813	17.23374	3.893321
F	14.265888	8.558825	3.990645
F	17.318813	17.23374	11.48102
F	14.265888	8.558825	11.578345
C	20.028431	10.762294	3.89371
C	20.007072	10.592472	5.411602
C	19.582178	9.134207	5.641016
C	20.08617	8.366272	4.41611
C	0.405717	10.178019	1.338256
C	1.234624	9.868279	0.297147

C	1.080319	7.553546	0.759058
C	0.278359	7.794964	1.838957
C	-0.015566	9.141956	2.232639
C	9.825048	16.358351	1.265165
C	9.12979	16.797356	0.173487
C	9.430896	1.359332	0.799231
C	10.083261	0.984579	1.939697
C	10.264573	17.300322	2.249263
C	11.108395	15.521742	3.775077
C	11.227758	15.561717	5.298501
C	11.703217	16.989185	5.597056
C	11.07009	0.154823	4.51166
C	20.028431	10.762294	11.48141
C	20.007072	10.592472	12.999302
C	19.582178	9.134207	13.228717
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C	0.405717	10.178019	8.925956
C	1.234624	9.868279	7.884847
C	1.080319	7.553546	8.346758
C	0.278359	7.794964	9.426657
C	-0.015566	9.141956	9.820338
C	9.825048	16.358351	8.852864
C	9.12979	16.797356	7.761187
C	9.430896	1.359332	8.386931
C	10.083261	0.984579	9.527396
C	10.264573	17.300322	9.836963
C	11.108395	15.521742	11.362778
C	11.227758	15.561717	12.886202
C	11.703217	16.989185	13.184755
C	11.07009	0.154823	12.09936
N	1.594249	8.583116	0.029938
N	20.312929	9.405274	3.393691
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H	10.06518	8.985955	3.338608
H	19.063108	11.11302	3.50086
H	-0.116614	11.460971	3.565851
H	0.091037	10.769425	5.800452
H	19.331446	11.306916	5.89607
H	19.981508	8.717777	6.574955
H	18.493937	9.050196	5.702541

H	0.116479	7.849067	4.605204
H	19.356583	7.623396	4.060184
H	0.116289	11.216991	1.483117
H	1.646322	10.623379	14.808843
H	1.342333	6.545642	0.447245
H	-0.125389	6.948476	2.390354
H	2.308299	8.411862	6.900145
H	10.002841	15.290272	1.369166
H	8.710086	16.116879	14.614455
H	9.29857	2.401878	0.520084
H	10.478703	1.761817	2.589851
H	10.30673	14.851326	3.432302
H	12.051954	15.217131	3.291447
H	10.24694	15.360209	5.753098
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H	11.443048	17.328873	6.607439
H	12.789645	17.053432	5.51231
H	11.740171	0.965551	4.185906
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H	8.321882	0.706796	14.355074
H	10.72764	7.563233	10.710888
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H	0.116479	7.849067	12.192904
H	19.356583	7.623396	11.647883
H	0.116289	11.216991	9.070817
H	1.646322	10.623379	7.221143
H	1.342333	6.545642	8.034945
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H	10.002841	15.290272	8.956865
H	8.710086	16.116879	7.026756
H	9.29857	2.401878	8.107784
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H	12.051954	15.217131	10.879148
H	10.24694	15.360209	13.340797
H	11.931431	14.811824	13.264804
H	11.443048	17.328873	14.195139
H	12.789645	17.053432	13.10001
H	11.740171	0.965551	11.773606

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S14e_4, Rel. E = 3.63

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Ge	15.42558	16.07216	5.522645
Ge	16.06562	10.42408	2.749005
Ge	5.102553	7.170209	4.931887
Ge	16.33669	7.087144	5.137217
Ge	5.792033	15.88781	2.34391
Ge	7.997298	10.12164	5.340896
Ge	18.85724	1.383382	2.484673
Ge	18.81055	15.86906	2.661022
Ge	2.448012	1.698646	4.908587
Ge	8.174805	7.578263	1.926352
Ge	13.13613	10.06834	5.580441
Ge	5.826509	1.437871	9.642687
Ge	15.42558	16.07216	13.11035
Ge	16.06562	10.42408	10.33671
Ge	5.102553	7.170209	12.51959
Ge	16.33669	7.087144	12.72492
Ge	5.792033	15.88781	9.93161
Ge	7.997298	10.12164	12.9286
Ge	18.85724	1.383382	10.07237
Ge	18.81055	15.86906	10.24872
Ge	2.448012	1.698646	12.49629
Ge	8.174805	7.578263	9.514051
Ge	13.13613	10.06834	13.16814
Si	5.587859	16.30877	5.467256
Si	15.62086	1.36804	2.247573
Si	4.98991	7.423341	1.865249
Si	16.25111	10.17342	5.770583
Si	4.790955	10.16169	5.418965
Si	16.31875	7.451223	2.0702
Si	15.47695	1.570013	5.336343
Si	4.766173	10.5017	2.385613
Si	15.5467	15.97449	2.389316
Si	5.730536	1.649055	5.181484
Si	2.682675	1.433233	1.816533
Si	18.55786	16.09464	5.798384
Si	13.0126	10.42339	2.476522
Si	8.169689	6.978451	5.063401
Si	2.411067	16.28698	5.200922
Si	13.22706	7.383263	2.106416
Si	13.19133	6.952477	5.154743
Si	7.827212	10.68729	2.238231

Si	18.54259	1.477306	5.620102
Si	2.651934	16.03479	2.156125
Si	4.144198	5.399382	7.305288
Si	17.10484	12.16874	0.361833
Si	17.19952	5.352578	15.10827
Si	4.034793	12.2184	0.026262
Si	14.52668	14.05261	0.139669
Si	6.708633	3.525388	7.462572
Si	6.616383	14.13317	15.15406
Si	14.62818	3.380182	0.034797
Si	1.636063	3.448539	7.279448
Si	19.64413	14.06851	0.325751
Si	19.6866	3.408104	0.272705
Si	1.586538	14.27953	7.429692
Si	11.9667	12.09947	0.217183
Si	9.24791	5.450447	7.342044
Si	9.035631	12.30561	7.49704
Si	12.16648	5.33335	-0.06
Si	5.587859	16.30877	13.05496
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Si	4.98991	7.423341	9.452949
Si	16.25111	10.17342	13.35828
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Si	16.31875	7.451223	9.657899
Si	15.47695	1.570013	12.92404
Si	4.766173	10.5017	9.973313
Si	15.5467	15.97449	9.977016
Si	5.730536	1.649055	12.76918
Si	2.682675	1.433233	9.404233
Si	18.55786	16.09464	13.38609
Si	13.0126	10.42339	10.06422
Si	8.169689	6.978451	12.6511
Si	2.411067	16.28698	12.78862
Si	13.22706	7.383263	9.694117
Si	13.19133	6.952477	12.74244
Si	7.827212	10.68729	9.825931
Si	18.54259	1.477306	13.2078
Si	2.651934	16.03479	9.743825
Si	4.144198	5.399382	14.89299
Si	17.10484	12.16874	7.949533
Si	17.19952	5.352578	7.52057
Si	4.034793	12.2184	7.613962
Si	14.52668	14.05261	7.727368
Si	6.708633	3.525388	15.05027
Si	6.616383	14.13317	7.566359
Si	14.62818	3.380182	7.622496

Si	1.636063	3.448539	14.86715
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Si	11.9667	12.09947	7.804883
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O	6.336631	10.61234	5.752087
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O	14.71713	6.361242	5.166208
O	6.26964	11.12782	2.354732
O	6.897816	2.407355	1.066695
O	14.29924	15.08748	6.449811
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O	6.582246	2.713171	6.046371
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O	6.819521	14.70792	1.515241
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O	14.75021	2.255409	1.216831
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O	4.656953	9.030486	1.704672
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O	16.902	10.62619	4.330076
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O	17.04708	7.102007	3.511696
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O	18.42658	17.66389	6.188843
O	19.16928	17.43633	1.867206
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O	12.62498	7.061267	3.614748
O	1.85899	2.109482	0.602278
O	19.38961	15.37303	6.969685
O	19.72277	14.5723	1.890229
O	1.55194	2.982278	5.711621
O	19.39071	2.362415	6.653065
O	1.684715	15.18317	1.190483
O	1.571066	15.25289	6.120162
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O	11.95571	11.37762	1.674983
O	9.220296	5.955385	5.794733
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O	9.013103	11.11373	6.409091
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O	12.33259	5.84372	5.986824
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O	10.55513	12.91444	0.012643
O	10.674	4.685925	0.052349
O	10.23296	8.508827	2.594898
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O	17.05914	15.43482	13.31539
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O	7.977065	9.287037	9.019255
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O	19.31755	1.484122	11.77818
O	1.985869	16.08833	11.22733
O	12.39715	10.34514	11.57848
O	8.443431	6.740146	11.06858
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O	1.85899	2.109482	8.189978
O	19.38961	15.37303	14.55738
O	19.72277	14.5723	9.477929
O	1.55194	2.982278	13.29932
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O	1.571066	15.25289	13.70786
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O	9.220296	5.955385	13.38243
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O	18.52438	4.510609	7.939776
O	2.8017	13.23522	14.93055
O	13.1597	13.2094	7.771431
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O	0.1785	13.44956	15.10298
O	10.55513	12.91444	7.600343
O	10.674	4.685925	7.640049
O	10.23296	8.508827	10.1826
F	6.298414	8.590138	3.989021
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F	6.298414	8.590138	11.57672
F	14.93456	9.016035	11.43377
C	9.842177	16.14183	0.908877
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C	9.742102	0.878579	0.725355
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C	11.88411	1.217707	4.398507
C	11.1397	1.131093	3.253915
C	10.79878	17.54954	2.715438
C	20.19693	10.63746	3.729984
C	20.10197	10.51677	5.250757
C	19.71261	9.051887	5.4863
C	20.38893	8.27714	4.356134
C	0.603999	10.0112	1.192996
C	1.404403	9.685627	0.13139
C	1.278009	7.387915	0.647856
C	0.517888	7.647343	1.754371
C	0.21693	8.995953	2.121352
C	9.842177	16.14183	8.496576
C	9.541481	16.53972	7.053363
C	8.935009	0.237721	7.182481
C	9.742102	0.878579	8.313055
C	11.21011	16.3992	11.05046
C	11.9627	16.55216	12.18063

C	11.88411	1.217707	11.98621
C	11.1397	1.131093	10.84162
C	10.79878	17.54954	10.30314
C	20.19693	10.63746	11.31768
C	20.10197	10.51677	12.83846
C	19.71261	9.051887	13.074
C	20.38893	8.27714	11.94383
C	0.603999	10.0112	8.780696
C	1.404403	9.685627	7.71909
C	1.278009	7.387915	8.235556
C	0.517888	7.647343	9.342071
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N	12.29205	0.091419	5.047696
N	10.14948	17.43157	1.556979
N	1.75839	8.400153	15.05175
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N	10.14948	17.43157	9.144678
N	1.75839	8.400153	7.464052
N	20.56174	9.279683	10.87784
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H	10.06571	9.319399	3.123294
H	8.971215	15.67528	1.396101
H	10.69184	15.44913	0.989186
H	10.48306	16.58073	6.492883
H	8.884997	15.81833	6.55564
H	8.991574	0.826208	6.257071
H	7.878585	0.166723	15.06002
H	10.64277	1.402088	0.357547
H	9.149999	1.595528	1.310889
H	10.9515	15.39409	3.137096
H	12.33722	15.71144	5.175319
H	12.20308	2.164139	4.832909
H	10.83492	2.047336	2.752517
H	12.91482	0.177746	5.851568
H	19.2333	10.92833	3.280737
H	0.040417	11.35726	3.418047
H	0.151946	10.73829	5.699826
H	19.36545	11.20964	5.673899
H	19.99794	8.68043	6.479168
H	18.62964	8.939757	5.393593
H	0.455459	7.887171	4.641479
H	19.77288	7.434464	4.005912
H	0.334037	11.05407	1.337864
H	1.815355	10.42934	14.63109
H	1.539663	6.377284	0.354816

H	0.167866	6.809755	2.352975
H	2.501451	8.216263	6.776803
H	10.69022	7.888162	10.78718
H	10.06571	9.319399	10.711
H	8.971215	15.67528	8.983801
H	10.69184	15.44913	8.576886
H	10.48306	16.58073	14.08058
H	8.884997	15.81833	14.14334
H	8.991574	0.826208	13.84477
H	7.878585	0.166723	7.472318
H	10.64277	1.402088	7.945247
H	9.149999	1.595528	8.898588
H	10.9515	15.39409	10.7248
H	12.33722	15.71144	12.76302
H	12.20308	2.164139	12.42061
H	10.83492	2.047336	10.34022
H	12.91482	0.177746	13.43927
H	19.2333	10.92833	10.86844
H	0.040417	11.35726	11.00575
H	0.151946	10.73829	13.28753
H	19.36545	11.20964	13.2616
H	19.99794	8.68043	14.06687
H	18.62964	8.939757	12.98129
H	0.455459	7.887171	12.22918
H	19.77288	7.434464	11.59361
H	0.334037	11.05407	8.925564
H	1.815355	10.42934	7.043391
H	1.539663	6.377284	7.942516
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S14e_6, Rel. E = 3.64

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Ge	16.07343	10.40447	2.756424
Ge	5.076103	7.168533	4.927126
Ge	16.30563	7.057458	5.192144
Ge	5.806616	15.85815	2.400704
Ge	7.982243	10.13608	5.371618
Ge	18.81522	1.305521	2.413786
Ge	18.76042	15.80642	2.652863
Ge	2.468553	1.719286	4.952267
Ge	8.205959	7.593342	1.967546
Ge	13.10873	10.05593	5.547202
Ge	5.839812	1.406595	9.645839
Ge	15.43992	16.08524	13.1457

Ge	16.07343	10.40447	10.34413
Ge	5.076103	7.168533	12.51483
Ge	16.30563	7.057458	12.77984
Ge	5.806616	15.85815	9.988404
Ge	7.982243	10.13608	12.95932
Ge	18.81522	1.305521	10.00149
Ge	18.76042	15.80642	10.24056
Ge	2.468553	1.719286	12.53997
Ge	8.205959	7.593342	9.555245
Ge	13.10873	10.05593	13.1349
Si	5.638329	16.34039	5.519123
Si	15.58752	1.325356	2.258296
Si	5.022555	7.437197	1.851259
Si	16.21909	10.15484	5.788625
Si	4.769241	10.16323	5.418235
Si	16.34024	7.417352	2.117546
Si	15.51892	1.559384	5.34294
Si	4.777529	10.51086	2.393248
Si	15.50341	15.93372	2.436896
Si	5.806864	1.645547	5.183945
Si	2.683371	1.430326	1.858095
Si	18.58817	16.08046	5.779771
Si	13.01868	10.39438	2.441753
Si	8.13308	6.990078	5.097611
Si	2.414081	16.34826	5.271639
Si	13.23976	7.346839	2.096616
Si	13.15154	6.932683	5.151958
Si	7.859375	10.70756	2.266851
Si	18.59796	1.452093	5.546221
Si	2.641684	16.0284	2.230976
Si	4.130095	5.422453	7.300731
Si	17.11964	12.14604	0.380099
Si	17.18998	5.312901	0.000235
Si	4.051723	12.21457	0.028911
Si	14.54315	14.03742	0.174936
Si	6.699176	3.543663	7.454687
Si	6.620229	14.11912	0.021491
Si	14.62655	3.351912	0.066099
Si	1.653803	3.473517	7.328501
Si	19.65392	14.03098	0.309217
Si	19.69113	3.356468	0.2157
Si	1.61114	14.28512	7.49035
Si	11.97719	12.08515	0.181978
Si	9.243704	5.465591	7.380261
Si	9.043981	12.33526	7.529087
Si	12.15937	5.296683	-0.07194

Si	5.638329	16.34039	13.10682
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Si	5.022555	7.437197	9.438959
Si	16.21909	10.15484	13.37633
Si	4.769241	10.16323	13.00594
Si	16.34024	7.417352	9.705246
Si	15.51892	1.559384	12.93064
Si	4.777529	10.51086	9.980948
Si	15.50341	15.93372	10.0246
Si	5.806864	1.645547	12.77165
Si	2.683371	1.430326	9.445794
Si	18.58817	16.08046	13.36747
Si	13.01868	10.39438	10.02945
Si	8.13308	6.990078	12.68531
Si	2.414081	16.34826	12.85934
Si	13.23976	7.346839	9.684316
Si	13.15154	6.932683	12.73966
Si	7.859375	10.70756	9.854551
Si	18.59796	1.452093	13.13392
Si	2.641684	16.0284	9.818676
Si	4.130095	5.422453	14.88843
Si	17.11964	12.14604	7.967798
Si	17.18998	5.312901	7.587935
Si	4.051723	12.21457	7.616611
Si	14.54315	14.03742	7.762636
Si	6.699176	3.543663	15.04239
Si	6.620229	14.11912	7.609191
Si	14.62655	3.351912	7.653798
Si	1.653803	3.473517	14.9162
Si	19.65392	14.03098	7.896917
Si	19.69113	3.356468	7.8034
Si	1.61114	14.28512	15.07805
Si	11.97719	12.08515	7.769678
Si	9.243704	5.465591	14.96796
Si	9.043981	12.33526	15.11679
Si	12.15937	5.296683	7.515764
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O	17.13765	1.841442	2.167365
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O	6.312859	10.58896	5.783392
O	14.79717	6.878786	2.019492
O	14.67829	6.353614	5.200921
O	6.288161	11.10971	2.347853
O	6.854337	2.372623	1.009973
O	14.356	15.09158	6.513188
O	14.59909	14.94117	1.538779
O	6.66082	2.7451	6.015646
O	14.6303	2.618476	6.186444
O	6.800832	14.65055	1.573843
O	6.239377	15.40981	6.687891
O	14.70103	2.214777	1.241044
O	17.10228	11.67183	1.925189
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O	4.112554	6.699935	0.70875
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O	3.900143	11.09014	6.45724
O	17.19101	6.559114	1.029653
O	17.31132	5.850564	6.051051
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O	15.34518	0.089122	6.052023
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O	6.035661	0.181305	5.903237
O	16.53928	8.991485	1.746065
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O	4.640697	9.034813	1.73179
O	16.39013	8.555396	6.140419
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O	14.79979	15.95159	3.911376
O	15.02122	1.515342	3.78656
O	6.350911	15.93793	4.092968
O	16.88007	10.6059	4.352765
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O	2.776424	17.52662	1.605224
O	18.52742	17.65574	6.174457
O	19.08326	17.35015	1.803525
O	2.013966	0.171635	5.710392
O	13.0666	8.920682	1.734278
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O	1.918656	1.745629	3.267843
O	19.33011	15.87152	4.333562
O	19.34402	1.40533	4.099709
O	1.991661	16.08554	3.720111
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O	12.61262	7.023468	3.598103
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O	1.640764	3.048111	5.745614
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F	6.277272	8.593477	11.5853
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C	9.527144	1.41029	0.937672
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C	10.82371	15.48948	3.995296
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C	11.8496	16.91782	5.65382
C	11.09279	0.1205	4.686459
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H	0.175167	10.61094	5.720193
H	19.40134	11.1278	5.760506
H	19.9952	8.551915	6.446609
H	18.6014	8.888553	5.417503
H	0.359627	7.763478	4.551441
H	19.64913	7.435448	3.909182
H	0.308288	11.10236	1.39067
H	1.810356	10.54399	14.68356
H	1.581777	6.468026	0.302484
H	0.17197	6.831218	2.285923
H	2.535971	8.347702	6.777515
H	9.680059	15.32248	1.651798
H	8.562624	16.20992	14.80605
H	9.464725	2.45656	0.644552
H	10.51657	1.768426	2.766481
H	9.888539	14.93535	3.821959
H	11.61546	15.04161	3.371159
H	10.32427	15.41722	6.107295
H	11.91114	14.72977	5.740004
H	11.82093	17.28324	6.688468
H	12.89602	16.88837	5.336522
H	11.73134	0.920233	4.282863
H	10.20602	0.592394	5.146813
H	8.394838	0.822689	14.49435
H	10.74599	7.783002	10.82153
H	10.11624	9.219875	10.86714
H	19.20519	10.91918	10.94038
H	0.015588	11.33833	11.06323
H	0.175167	10.61094	13.30789
H	19.40134	11.1278	13.34821
H	19.9952	8.551915	14.03431
H	18.6014	8.888553	13.0052
H	0.359627	7.763478	12.13914
H	19.64913	7.435448	11.49688
H	0.308288	11.10236	8.97837
H	1.810356	10.54399	7.095864
H	1.581777	6.468026	7.890183
H	0.17197	6.831218	9.873623
H	2.535971	8.347702	14.36521
H	9.680059	15.32248	9.239498

H	8.562624	16.20992	7.218348
H	9.464725	2.45656	8.232251
H	10.51657	1.768426	10.35418
H	9.888539	14.93535	11.40966
H	11.61546	15.04161	10.95886
H	10.32427	15.41722	13.695
H	11.91114	14.72977	13.3277
H	11.82093	17.28324	14.27617
H	12.89602	16.88837	12.92422
H	11.73134	0.920233	11.87056
H	10.20602	0.592394	12.73451
H	8.394838	0.822689	6.906651

S14e_17, Rel. E = 4.01

Ge	5.832320	1.388261	2.121007
Ge	15.561481	16.071209	5.466079
Ge	16.098463	10.478716	2.628568
Ge	4.936648	7.024787	5.075817
Ge	16.218708	7.059715	5.245349
Ge	5.806883	15.851389	2.496153
Ge	8.107227	10.168332	5.422009
Ge	18.767878	1.190345	2.424249
Ge	18.658796	15.871560	2.647564
Ge	2.443774	1.733902	5.036117
Ge	8.318918	7.663369	1.971599
Ge	13.102571	10.014065	5.299535
Ge	5.832320	1.388261	9.708706
Ge	15.561481	16.071209	13.05378
Ge	16.098463	10.478716	10.21627
Ge	4.936648	7.024787	12.66352
Ge	16.218708	7.059715	12.83305
Ge	5.806883	15.851389	10.08385
Ge	8.107227	10.168332	13.00971
Ge	18.767878	1.190345	10.01195
Ge	18.658796	15.871560	10.23526
Ge	2.443774	1.733902	12.62382
Ge	8.318918	7.663369	9.559299
Ge	13.102571	10.014065	12.88724
Si	5.639828	16.379190	5.584125
Si	15.616819	1.291825	2.188686
Si	5.135292	7.462238	1.847352
Si	16.126339	10.170045	5.763872
Si	4.720506	10.096000	5.402682
Si	16.304585	7.374225	2.152072
Si	15.611506	1.522628	5.287143
Si	4.822189	10.564233	2.437767

Si	15.525364	15.908383	2.305742
Si	5.793755	1.674263	5.246443
Si	2.665863	1.405998	1.922573
Si	18.694355	16.054041	5.726589
Si	13.003371	10.331927	2.270066
Si	8.109982	7.078823	5.152404
Si	2.404055	16.370232	5.347998
Si	13.222683	7.264798	2.047078
Si	13.044165	6.952731	5.108875
Si	7.958830	10.825715	2.366541
Si	18.704315	1.437476	5.487645
Si	2.632484	16.007406	2.319809
Si	4.091135	5.347810	7.471937
Si	17.145216	12.195668	0.28659
Si	17.153471	5.287507	0.030212
Si	4.096644	12.223425	0.039537
Si	14.540007	14.066555	0.078694
Si	6.689794	3.519884	7.550081
Si	6.622854	14.161804	0.078488
Si	14.631090	3.299997	0.015402
Si	1.599251	3.462068	7.434253
Si	19.663013	14.060657	0.318442
Si	19.647995	3.297647	0.231179
Si	1.620794	14.248812	7.553397
Si	12.018653	12.057692	-0.05422
Si	9.222099	5.450431	7.399949
Si	9.059361	12.433696	7.616683
Si	12.147498	5.226714	-0.15889
Si	5.639828	16.37919	13.17182
Si	15.616819	1.291825	9.776385
Si	5.135292	7.462238	9.435052
Si	16.126339	10.170045	13.35157
Si	4.720506	10.096	12.99038
Si	16.304585	7.374225	9.739772
Si	15.611506	1.522628	12.87484
Si	4.822189	10.564233	10.02547
Si	15.525364	15.908383	9.893442
Si	5.793755	1.674263	12.83414
Si	2.665863	1.405998	9.510274
Si	18.694355	16.054041	13.31429
Si	13.003371	10.331927	9.857765
Si	8.109982	7.078823	12.7401
Si	2.404055	16.370232	12.9357
Si	13.222683	7.264798	9.634779
Si	13.044165	6.952731	12.69658
Si	7.958830	10.825715	9.95424

Si	18.704315	1.437476	13.07534
Si	2.632484	16.007406	9.907509
Si	4.091135	5.34781	15.05964
Si	17.145216	12.195668	7.87429
Si	17.153471	5.287507	7.617912
Si	4.096644	12.223425	7.627237
Si	14.540007	14.066555	7.666394
Si	6.689794	3.519884	15.13778
Si	6.622854	14.161804	7.666188
Si	14.631090	3.299997	7.603102
Si	1.599251	3.462068	15.02195
Si	19.663013	14.060657	7.906142
Si	19.647995	3.297647	7.818879
Si	1.620794	14.248812	15.1411
Si	12.018653	12.057692	7.533477
Si	9.222099	5.450431	14.98765
Si	9.059361	12.433696	0.028983
Si	12.147498	5.226714	7.428815
O	4.193336	2.016412	1.940352
O	17.168245	15.45843	5.850267
O	17.027895	15.277317	2.131732
O	4.209764	1.998898	5.204905
O	17.163435	1.978735	5.444776
O	4.124134	15.313585	2.402921
O	4.037969	16.236616	5.44564
O	17.149069	1.806855	1.9401
O	14.459077	11.097581	2.275514
O	6.575962	6.937202	5.742703
O	6.647075	7.237702	1.347597
O	14.603216	10.739627	5.974357
O	6.333778	10.121421	5.516474
O	14.775617	6.80169	2.07598
O	14.575646	6.393054	5.226313
O	6.35427	11.101944	2.46825
O	6.870991	2.324653	1.058852
O	14.424123	15.076382	6.389461
O	14.510786	14.950035	1.449096
O	6.624832	2.804125	6.075981
O	14.720972	2.593506	6.136078
O	6.765432	14.623817	1.649551
O	6.198563	15.452431	6.780297
O	14.671799	2.211632	1.222018
O	17.177542	11.66171	1.833075
O	4.010284	5.737758	5.873384
O	4.148594	6.711392	0.776255
O	17.069263	10.937101	6.843005

O	4.021067	11.011758	6.538409
O	17.189451	6.527473	1.089797
O	17.24979	5.885788	6.095263
O	3.933989	11.572264	1.522057
O	6.064729	17.392696	1.626867
O	15.331494	0.058754	5.966793
O	15.372606	17.441059	1.74751
O	6.075812	0.214414	5.9557
O	16.409651	8.952403	1.761522
O	4.154219	8.558111	5.608188
O	4.715958	9.048605	1.857524
O	16.301445	8.580072	6.152555
O	6.465371	1.641423	3.756808
O	14.935366	15.821818	3.830209
O	15.117364	1.55226	3.731712
O	6.375968	15.931583	4.181136
O	16.757702	10.532499	4.283556
O	4.797189	6.811199	3.327722
O	4.216061	10.635355	3.948847
O	16.96335	7.128458	3.63605
O	2.764661	17.501253	1.6808
O	18.78466	17.635336	6.094188
O	19.308458	17.312777	1.774044
O	1.992376	0.189167	5.790611
O	13.07143	8.826435	1.631795
O	8.740211	8.530807	5.585802
O	8.21353	9.417154	1.603847
O	12.69102	8.359163	5.863589
O	1.945077	1.766799	3.34029
O	19.344812	15.626621	4.289571
O	19.427204	1.576657	4.038236
O	1.978517	16.089186	3.802891
O	12.264774	10.342897	3.734208
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O	8.628028	10.831475	3.863721
O	12.51762	6.96461	3.528606
O	1.876012	2.095816	0.696638
O	19.552839	15.302049	6.876574
O	19.626547	14.545792	1.85762
O	1.695663	3.107466	5.834142
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O	1.757208	15.051888	1.372321
O	1.687269	15.307434	6.317954
O	19.789526	2.365863	1.53311
O	12.001421	11.208591	1.335278
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O	9.267304	6.716771	0.821031
O	11.975254	11.08117	6.249172
O	8.774828	11.126963	6.705382
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O	12.178063	5.818793	5.90978
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O	5.35952	4.395537	0.221054
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O	15.791063	4.420468	0.223764
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O	18.471907	4.400681	0.315231
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O	8.092478	13.684392	7.153571
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O	0.157446	4.129415	0.148784
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O	14.575646	6.393054	12.81401
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O	6.870991	2.324653	8.646552
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O	14.671799	2.211632	8.809718
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C	20.162849	8.271911	4.318854
C	0.499899	10.101914	1.256149
C	1.308155	9.797778	0.197285
C	1.143942	7.479663	0.640281
C	0.367896	7.716082	1.740437
C	0.076715	9.060852	2.143396
C	9.749393	16.408588	1.466308
C	9.119331	16.882034	0.349241
C	9.616144	1.423663	0.934588
C	10.218572	1.01707	2.091406
C	10.282174	17.328726	2.425982

C	10.977085	15.49944	3.959418
C	11.29744	15.54958	5.454287
C	11.946136	16.924669	5.647738
C	11.245062	0.133549	4.644785
C	20.060398	10.663018	11.38424
C	20.037867	10.493149	12.90096
C	19.609877	9.034516	13.11381
C	20.162849	8.271911	11.90656
C	0.499899	10.101914	8.843848
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C	0.367896	7.716082	9.328136
C	0.076715	9.060852	9.731096
C	9.749393	16.408588	9.054008
C	9.119331	16.882034	7.93694
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C	10.282174	17.328726	10.01368
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C	11.29744	15.54958	13.04199
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N	1.646679	8.51169	15.08196
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H	0.120032	10.667523	5.709287
H	19.357666	11.201322	5.799725
H	19.964968	8.61601	6.477192
H	18.519897	8.960627	5.5338
H	0.194925	7.76812	4.534593
H	19.454502	7.517165	3.943301
H	0.231613	11.143472	1.416147
H	1.719853	10.559231	14.71731
H	1.388753	6.471974	0.31591
H	-0.022823	6.865432	2.29471
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H	9.803279	15.333639	1.621015

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H	19.080872	10.968256	10.98525
H	-0.114229	11.393052	11.05646
H	0.120032	10.667523	13.29699
H	19.357666	11.201322	13.38742
H	19.964968	8.61601	14.06489
H	18.519897	8.960627	13.1215
H	0.194925	7.76812	12.12229
H	19.454502	7.517165	11.531
H	0.231613	11.143472	9.003847
H	1.719853	10.559231	7.129611
H	1.388753	6.471974	7.90361
H	-0.022823	6.865432	9.88241
H	2.345694	8.334359	14.35492
H	9.803279	15.333639	9.208715
H	8.640691	16.226187	7.213819
H	9.554346	2.470347	8.231878
H	10.650669	1.77229	10.33098
H	10.061345	14.929543	11.32812
H	11.809047	15.073986	10.96109
H	10.373118	15.454276	13.6292
H	11.971142	14.740172	13.34445
H	11.882683	17.298628	14.26564
H	13.004918	16.873531	12.97201
H	11.922669	0.900262	11.82713
H	10.362372	0.645843	12.658
H	8.468873	0.83797	6.910178

S14i_4, Rel. E = 3.73

Ge	4.917165	7.546698	2.262368
Ge	16.09846	10.20154	5.305293
Ge	5.683074	1.369557	2.170512
Ge	16.14715	7.54366	1.996154

Ge	16.19674	7.119281	5.043221
Ge	15.30353	16.29595	5.521152
Ge	8.011558	7.540663	1.997556
Ge	12.98048	7.344788	2.23429
Ge	18.56096	15.9148	2.514768
Ge	18.5343	16.36671	5.694915
Ge	18.46919	1.85272	5.054924
Ge	2.48095	15.88299	2.503746
Ge	4.917165	7.546698	9.850068
Ge	16.09846	10.20154	12.89299
Ge	5.683074	1.369557	9.758212
Ge	16.14715	7.54366	9.583854
Ge	16.19674	7.119281	12.63092
Ge	15.30353	16.29595	13.10885
Ge	8.011558	7.540663	9.585256
Ge	12.98048	7.344788	9.82199
Ge	18.56096	15.9148	10.10247
Ge	18.5343	16.36671	13.28262
Ge	18.46919	1.85272	12.64262
Ge	2.48095	15.88299	10.09145
Si	5.587281	16.32851	5.549459
Si	5.607001	1.710289	5.27757
Si	15.28679	15.94055	2.426837
Si	5.729145	15.89502	2.507803
Si	4.770755	10.15658	5.50856
Si	4.81576	7.084761	5.304971
Si	15.30736	1.808221	5.047892
Si	4.616443	10.59933	2.488625
Si	16.06925	10.65485	2.265338
Si	15.34978	1.312718	2.015324
Si	2.430356	16.30836	5.578651
Si	2.448303	1.666424	5.188946
Si	13.07183	7.16969	5.366159
Si	7.922548	7.110082	5.132147
Si	7.932954	10.19135	5.38051
Si	18.51819	1.292708	1.949673
Si	12.98252	10.46852	2.396092
Si	7.72338	10.65802	2.324622
Si	2.452008	1.348003	2.117807
Si	12.99843	10.24146	5.468094
Si	3.961243	5.391404	7.723734
Si	16.92995	12.39502	15.06861
Si	17.01433	5.369293	14.98217
Si	3.945824	12.25716	0.131317
Si	14.33073	14.22838	0.059455
Si	6.524702	3.511174	0.033116

Si	6.503095	14.22741	0.121303
Si	14.43818	3.425238	15.03849
Si	1.485858	3.372825	7.549514
Si	19.51675	14.21474	0.176186
Si	19.48376	3.455976	15.05976
Si	1.495536	14.17525	0.086902
Si	11.88179	12.17292	0.081783
Si	9.034222	5.460597	7.41828
Si	8.888752	12.26628	-0.01193
Si	11.91897	5.330105	0.041265
Si	5.587281	16.32851	13.13716
Si	5.607001	1.710289	12.86527
Si	15.28679	15.94055	10.01454
Si	5.729145	15.89502	10.0955
Si	4.770755	10.15658	13.09626
Si	4.81576	7.084761	12.89267
Si	15.30736	1.808221	12.63559
Si	4.616443	10.59933	10.07632
Si	16.06925	10.65485	9.853038
Si	15.34978	1.312718	9.603024
Si	2.430356	16.30836	13.16635
Si	2.448303	1.666424	12.77665
Si	13.07183	7.16969	12.95386
Si	7.922548	7.110082	12.71985
Si	7.932954	10.19135	12.96821
Si	18.51819	1.292708	9.537374
Si	12.98252	10.46852	9.983792
Si	7.72338	10.65802	9.912322
Si	2.452008	1.348003	9.705507
Si	12.99843	10.24146	13.05579
Si	3.961243	5.391404	0.136034
Si	16.92995	12.39502	7.480911
Si	17.01433	5.369293	7.394467
Si	3.945824	12.25716	7.719017
Si	14.33073	14.22838	7.647154
Si	6.524702	3.511174	7.620815
Si	6.503095	14.22741	7.709003
Si	14.43818	3.425238	7.450787
Si	1.485858	3.372825	15.13722
Si	19.51675	14.21474	7.763886
Si	19.48376	3.455976	7.472061
Si	1.495536	14.17525	7.674602
Si	11.88179	12.17292	7.669483
Si	9.034222	5.460597	15.00598
Si	8.888752	12.26628	7.575773
Si	11.91897	5.330105	7.628964

O	3.998677	1.856238	1.950318
O	16.91544	15.60373	5.770959
O	16.84068	15.4716	2.577718
O	4.024785	2.080457	5.214034
O	16.79917	2.457218	5.024525
O	4.181784	15.37821	2.443086
O	4.012759	15.92532	5.560506
O	16.93287	1.675894	1.960681
O	14.49236	11.09559	2.333508
O	6.391694	6.861041	5.643123
O	6.391603	7.014625	1.392205
O	14.48551	10.89727	5.6094
O	6.358675	10.39988	5.713853
O	14.58799	6.662528	1.914149
O	14.5517	6.477878	5.365625
O	6.157695	11.09358	2.240155
O	6.731504	2.279441	1.103087
O	14.15853	15.53188	6.634782
O	14.45785	14.84269	1.570944
O	6.403673	2.80975	6.146921
O	14.3427	2.788628	5.922076
O	6.626724	14.82734	1.653271
O	6.349369	15.49169	6.693685
O	14.54119	2.152728	0.899446
O	16.85746	11.80247	1.405497
O	3.973102	6.026789	6.219944
O	3.782289	6.555864	1.221726
O	17.08941	11.25028	6.368322
O	4.031832	11.02215	6.675762
O	17.04424	6.699712	0.719713
O	17.15341	5.805573	5.833392
O	3.739842	11.72616	1.655056
O	5.918865	17.35185	1.780172
O	15.24892	0.349086	5.814179
O	15.15213	17.41439	1.726543
O	5.774066	0.205963	5.905467
O	16.268	9.2393	1.469115
O	4.317013	8.602049	5.756794
O	4.189621	9.159141	1.847543
O	16.52374	8.609804	5.994609
O	6.288643	1.717773	3.795481
O	14.6097	15.98124	3.916867
O	14.76119	1.65528	3.513114
O	6.215443	15.98434	4.070295
O	16.79632	10.67994	3.729848
O	4.361516	6.745974	3.782477

O	4.22217	10.72319	4.075867
O	17.05231	7.068077	3.465961
O	2.310616	17.46716	1.724349
O	18.43403	0.389989	6.07927
O	18.71917	17.41327	1.576439
O	2.251069	0.194259	5.867468
O	12.92036	9.018382	1.647893
O	8.393322	8.638129	5.511709
O	8.041831	9.272207	1.549206
O	12.99311	8.689118	5.956659
O	1.934499	1.62159	3.642678
O	19.31001	16.08975	4.11686
O	19.14537	1.591539	3.439334
O	1.784146	15.90499	4.130466
O	12.42738	10.39989	3.935193
O	8.154146	6.720221	3.575468
O	8.285866	10.71072	3.864709
O	12.35961	7.142889	3.892344
O	1.556804	2.177009	1.065953
O	19.53658	15.6184	6.922368
O	19.44304	14.58243	1.774156
O	1.59431	2.738585	6.045352
O	19.46596	3.032887	5.884425
O	1.578278	14.63845	1.651733
O	1.657968	15.48838	6.731782
O	19.31057	2.141599	0.835789
O	12.01556	11.48025	1.54901
O	8.883903	6.056843	5.916347
O	9.093592	6.668169	0.89655
O	12.04003	11.10368	6.460946
O	8.76262	11.10636	6.446126
O	11.9025	6.246206	1.375743
O	12.15551	6.219007	6.300286
O	8.574516	11.78566	1.502765
O	5.205188	4.364137	0.378506
O	15.63467	13.37075	7.237065
O	15.7119	4.394408	0.051163
O	5.238843	13.23258	-0.01117
O	2.605283	4.482016	7.806629
O	18.29134	13.28122	-0.25821
O	18.33108	4.508194	0.243355
O	2.606067	13.07584	7.283663
O	12.95837	13.39148	-0.05826
O	7.875176	4.363831	0.12044
O	7.881384	13.51264	7.253663
O	13.01898	4.130512	0.152759

O	0.032338	4.103432	0.12637
O	0.024374	13.47991	7.488575
O	10.40924	12.86673	15.12909
O	10.45114	4.62553	7.50282
O	10.16533	8.414362	2.845672
O	3.998677	1.856238	9.538018
O	16.91544	15.60373	13.35866
O	16.84068	15.4716	10.16542
O	4.024785	2.080457	12.80173
O	16.79917	2.457218	12.61223
O	4.181784	15.37821	10.03079
O	4.012759	15.92532	13.14821
O	16.93287	1.675894	9.548381
O	14.49236	11.09559	9.921208
O	6.391694	6.861041	13.23082
O	6.391603	7.014625	8.979905
O	14.48551	10.89727	13.1971
O	6.358675	10.39988	13.30155
O	14.58799	6.662528	9.501849
O	14.5517	6.477878	12.95333
O	6.157695	11.09358	9.827855
O	6.731504	2.279441	8.690787
O	14.15853	15.53188	14.22248
O	14.45785	14.84269	9.158645
O	6.403673	2.80975	13.73462
O	14.3427	2.788628	13.50978
O	6.626724	14.82734	9.240971
O	6.349369	15.49169	14.28139
O	14.54119	2.152728	8.487146
O	16.85746	11.80247	8.993196
O	3.973102	6.026789	13.80764
O	3.782289	6.555864	8.809426
O	17.08941	11.25028	13.95602
O	4.031832	11.02215	14.26346
O	17.04424	6.699712	8.307414
O	17.15341	5.805573	13.42109
O	3.739842	11.72616	9.242756
O	5.918865	17.35185	9.367871
O	15.24892	0.349086	13.40188
O	15.15213	17.41439	9.314243
O	5.774066	0.205963	13.49317
O	16.268	9.2393	9.056815
O	4.317013	8.602049	13.34449
O	4.189621	9.159141	9.435244
O	16.52374	8.609804	13.58231
O	6.288643	1.717773	11.38318

O	14.6097	15.98124	11.50457
O	14.76119	1.65528	11.10081
O	6.215443	15.98434	11.658
O	16.79632	10.67994	11.31755
O	4.361516	6.745974	11.37018
O	4.22217	10.72319	11.66357
O	17.05231	7.068077	11.05366
O	2.310616	17.46716	9.312049
O	18.43403	0.389989	13.66697
O	18.71917	17.41327	9.164139
O	2.251069	0.194259	13.45517
O	12.92036	9.018382	9.235592
O	8.393322	8.638129	13.09941
O	8.041831	9.272207	9.136906
O	12.99311	8.689118	13.54436
O	1.934499	1.62159	11.23038
O	19.31001	16.08975	11.70456
O	19.14537	1.591539	11.02703
O	1.784146	15.90499	11.71817
O	12.42738	10.39989	11.52289
O	8.154146	6.720221	11.16317
O	8.285866	10.71072	11.45241
O	12.35961	7.142889	11.48004
O	1.556804	2.177009	8.653654
O	19.53658	15.6184	14.51007
O	19.44304	14.58243	9.361856
O	1.59431	2.738585	13.63305
O	19.46596	3.032887	13.47213
O	1.578278	14.63845	9.239432
O	1.657968	15.48838	14.31948
O	19.31057	2.141599	8.423489
O	12.01556	11.48025	9.136709
O	8.883903	6.056843	13.50405
O	9.093592	6.668169	8.48425
O	12.04003	11.10368	14.04865
O	8.76262	11.10636	14.03383
O	11.9025	6.246206	8.963443
O	12.15551	6.219007	13.88799
O	8.574516	11.78566	9.090465
O	5.205188	4.364137	7.966206
O	15.63467	13.37075	14.82476
O	15.7119	4.394408	7.638863
O	5.238843	13.23258	7.576532
O	2.605283	4.482016	0.21893
O	18.29134	13.28122	7.32949
O	18.33108	4.508194	7.831055

O	2.606067	13.07584	14.87136
O	12.95837	13.39148	7.529442
O	7.875176	4.363831	7.708139
O	7.881384	13.51264	14.84136
O	13.01898	4.130512	7.740459
O	0.032338	4.103432	7.71407
O	0.024374	13.47991	15.07627
O	10.40924	12.86673	7.541388
O	10.45114	4.62553	15.09052
O	10.16533	8.414362	10.43337
F	6.12547	8.636947	3.496684
F	14.95031	8.678408	3.860283
F	6.12547	8.636947	11.08438
F	14.95031	8.678408	11.44798
C	9.7825	16.14868	0.916946
C	9.474707	16.52532	14.64624
C	8.865714	0.223496	14.7615
C	9.685455	0.882542	0.696358
C	11.12201	16.43409	3.474131
C	11.84445	16.5954	4.621789
C	11.77115	1.259071	4.407141
C	11.05834	1.163304	3.243807
C	10.72629	17.5781	2.710223
C	20.19134	10.67625	3.764795
C	20.16228	10.53564	5.285434
C	19.73642	9.08058	5.521157
C	20.31364	8.299489	4.338684
C	0.59199	10.0683	1.22046
C	1.378893	9.737397	0.152289
C	1.139011	7.432481	0.59462
C	0.393619	7.694273	1.710725
C	0.157989	9.044247	2.116969
C	9.7825	16.14868	8.504646
C	9.474707	16.52532	7.058543
C	8.865714	0.223496	7.173798
C	9.685455	0.882542	8.284058
C	11.12201	16.43409	11.06183
C	11.84445	16.5954	12.20949
C	11.77115	1.259071	11.99484
C	11.05834	1.163304	10.83151
C	10.72629	17.5781	10.29792
C	20.19134	10.67625	11.35249
C	20.16228	10.53564	12.87313
C	19.73642	9.08058	13.10886
C	20.31364	8.299489	11.92639
C	0.59199	10.0683	8.808159

C	1.378893	9.737397	7.739989
C	1.139011	7.432481	8.18232
C	0.393619	7.694273	9.298425
C	0.157989	9.044247	9.704668
N	12.16261	0.137553	5.07569
N	10.09337	17.44755	1.544019
N	1.66497	8.445018	15.03181
N	20.5132	9.320165	3.293308
N	12.16261	0.137553	12.66339
N	10.09337	17.44755	9.131719
N	1.66497	8.445018	7.444108
N	20.5132	9.320165	10.88101
H	10.60029	7.860865	3.530147
H	10.0743	9.300688	3.243036
H	8.914296	15.69034	1.41807
H	10.63434	15.45858	1.001572
H	10.41445	16.56183	6.496232
H	8.817502	15.7964	6.574116
H	8.908285	0.798604	6.239102
H	7.814148	0.154838	15.06876
H	10.58481	1.395884	0.31126
H	9.100533	1.611634	1.274763
H	10.87467	15.42641	3.148439
H	12.20573	15.76143	5.2198
H	12.08012	2.207843	4.843357
H	10.77069	2.075936	2.725911
H	12.74787	0.230582	5.905901
H	19.21031	10.98164	3.366057
H	0.027065	11.39281	3.429572
H	0.240004	10.72466	5.684012
H	19.4687	11.2465	5.749576
H	20.08084	8.683589	6.484679
H	18.64596	8.99664	5.520528
H	0.364168	7.839123	4.568429
H	19.63033	7.508835	3.991045
H	0.373086	11.11825	1.396107
H	1.820241	10.48266	14.67507
H	1.341171	6.420019	0.262306
H	0.00059	6.858405	2.283763
H	2.384015	8.247074	6.741465
H	10.60029	7.860865	11.11785
H	10.0743	9.300688	10.83074
H	8.914296	15.69034	9.00577
H	10.63434	15.45858	8.589272
H	10.41445	16.56183	14.08393
H	8.817502	15.7964	14.16182

H	8.908285	0.798604	13.8268
H	7.814148	0.154838	7.481063
H	10.58481	1.395884	7.89896
H	9.100533	1.611634	8.862463
H	10.87467	15.42641	10.73614
H	12.20573	15.76143	12.8075
H	12.08012	2.207843	12.43106
H	10.77069	2.075936	10.31361
H	12.74787	0.230582	13.4936
H	19.21031	10.98164	10.95376
H	0.027065	11.39281	11.01727
H	0.240004	10.72466	13.27171
H	19.4687	11.2465	13.33728
H	20.08084	8.683589	14.07238
H	18.64596	8.99664	13.10823
H	0.364168	7.839123	12.15613
H	19.63033	7.508835	11.57875
H	0.373086	11.11825	8.983807
H	1.820241	10.48266	7.087366
H	1.341171	6.420019	7.850006
H	0.00059	6.858405	9.871463
H	2.384015	8.247074	14.32917

S14i_6, Rel. E = 3.91

Ge	4.941182	7.569949	2.261117
Ge	16.0905	10.18249	5.351824
Ge	5.665136	1.363506	2.129502
Ge	16.16015	7.522791	2.014583
Ge	16.15221	7.090594	5.056445
Ge	15.31464	16.28415	5.554888
Ge	8.040073	7.563778	2.040686
Ge	12.99813	7.331817	2.22421
Ge	18.54485	15.90367	2.518178
Ge	18.53602	16.3494	5.680876
Ge	18.47176	1.833911	5.029656
Ge	2.481911	15.87623	2.540053
Ge	4.941182	7.569949	9.848817
Ge	16.0905	10.18249	12.93953
Ge	5.665136	1.363506	9.717201
Ge	16.16015	7.522791	9.602283
Ge	16.15221	7.090594	12.64415
Ge	15.31464	16.28415	13.14259
Ge	8.040073	7.563778	9.628386
Ge	12.99813	7.331817	9.811911
Ge	18.54485	15.90367	10.10588
Ge	18.53602	16.3494	13.26858

Ge	18.47176	1.833911	12.61736
Ge	2.481911	15.87623	10.12775
Si	5.660672	16.37856	5.540751
Si	5.678993	1.71571	5.246449
Si	15.26024	15.91607	2.480315
Si	5.733922	15.88524	2.503331
Si	4.763914	10.15767	5.515684
Si	4.78429	7.088099	5.300247
Si	15.32114	1.789294	5.059234
Si	4.633683	10.62136	2.503916
Si	16.10326	10.63001	2.300081
Si	15.32136	1.282527	2.039404
Si	2.437132	16.36147	5.613814
Si	2.453846	1.671499	5.211285
Si	13.03492	7.149054	5.352796
Si	7.887644	7.110242	5.166086
Si	7.926098	10.19305	5.411018
Si	18.49893	1.268157	1.932939
Si	13.00865	10.45591	2.400802
Si	7.739957	10.68063	2.353615
Si	2.436666	1.356016	2.130371
Si	12.98908	10.2234	5.471925
Si	3.932964	5.426153	7.717806
Si	16.96516	12.36236	15.11977
Si	17.00009	5.347536	15.00459
Si	3.96316	12.25507	0.132989
Si	14.36936	14.20482	0.112038
Si	6.500853	3.542074	-0.00712
Si	6.520164	14.2156	0.114172
Si	14.43483	3.400172	15.0559
Si	1.490273	3.392951	7.575495
Si	19.52664	14.20613	0.17124
Si	19.47705	3.42714	15.03665
Si	1.519357	14.18263	0.116328
Si	11.91091	12.16362	0.087099
Si	9.027917	5.463768	7.457292
Si	8.913934	12.27248	0.012917
Si	11.91496	5.317097	0.030034
Si	5.660672	16.37856	13.12845
Si	5.678993	1.71571	12.83415
Si	15.26024	15.91607	10.06802
Si	5.733922	15.88524	10.09103
Si	4.763914	10.15767	13.10338
Si	4.78429	7.088099	12.88795
Si	15.32114	1.789294	12.64694
Si	4.633683	10.62136	10.09162

Si	16.10326	10.63001	9.88778
Si	15.32136	1.282527	9.627104
Si	2.437132	16.36147	13.20151
Si	2.453846	1.671499	12.79899
Si	13.03492	7.149054	12.9405
Si	7.887644	7.110242	12.75379
Si	7.926098	10.19305	12.99872
Si	18.49893	1.268157	9.520639
Si	13.00865	10.45591	9.988502
Si	7.739957	10.68063	9.941316
Si	2.436666	1.356016	9.718072
Si	12.98908	10.2234	13.05963
Si	3.932964	5.426153	0.130106
Si	16.96516	12.36236	7.532067
Si	17.00009	5.347536	7.416894
Si	3.96316	12.25507	7.720688
Si	14.36936	14.20482	7.699738
Si	6.500853	3.542074	7.580582
Si	6.520164	14.2156	7.701872
Si	14.43483	3.400172	7.468204
Si	1.490273	3.392951	15.1632
Si	19.52664	14.20613	7.75894
Si	19.47705	3.42714	7.448949
Si	1.519357	14.18263	7.704028
Si	11.91091	12.16362	7.674799
Si	9.027917	5.463768	15.04499
Si	8.913934	12.27248	7.600616
Si	11.91496	5.317097	7.617733
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O	4.185716	15.37649	2.461218
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O	16.91102	1.635	1.965585
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O	6.349801	10.40225	5.739312
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O	14.50554	6.441335	5.359072
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O	4.024195	11.00923	6.691078
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O	17.11046	5.789116	5.855515
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O	15.36412	0.333966	5.82239
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O	4.215953	9.185236	1.851059
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O	18.70727	17.38845	1.560964
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O	19.15038	1.573349	10.99989

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O	12.33399	7.136843	11.45817
O	1.540658	2.170194	8.65498
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O	19.42091	14.57277	9.352578
O	1.693368	2.812326	13.64673
O	19.48841	3.005863	13.44806
O	1.583107	14.62792	9.277259
O	1.748012	15.50712	14.37743
O	19.29067	2.116275	8.402447
O	12.04762	11.47434	9.142674
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O	9.100251	6.657024	8.532916
O	12.02894	11.08727	14.0528
O	8.751706	11.10476	14.07237
O	11.90952	6.256572	8.937381
O	12.10033	6.203877	13.86376
O	8.589471	11.81794	9.124599
O	5.189755	4.399601	7.91031
O	15.67337	13.33723	14.89896
O	15.69971	4.382736	7.690242
O	5.27326	13.2067	7.536443
O	2.588264	4.514572	0.301468
O	18.33304	13.22834	7.32751
O	18.32674	4.480055	7.806481
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O	13.00385	13.35993	7.519248
O	7.876885	4.345699	7.753004
O	7.928911	13.54384	14.85381
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O	0.052303	13.49535	15.08299
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C	0.194268	9.015596	2.153125
C	9.619568	16.38397	1.496159
C	9.003574	16.8154	0.353882
C	9.365933	1.384658	0.928095
C	9.950937	1.018725	2.108622
C	10.0644	17.33976	2.46196
C	10.75853	15.54559	4.02924
C	11.19414	15.6108	5.496481
C	11.74686	17.03125	5.668464
C	10.92051	0.187362	4.718615
C	20.24341	10.59151	11.44397
C	20.12351	10.38518	12.95168
C	19.67014	8.927489	13.09859
C	20.32152	8.191336	11.92764
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C	1.390009	9.795372	7.793733
C	1.143765	7.474421	8.131263
C	0.420512	7.684975	9.271176
C	0.194268	9.015596	9.740825
C	9.619568	16.38397	9.083859
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H	19.93621	8.486327	6.480464
H	18.58282	8.857665	5.420146
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H	0.419865	11.12044	1.535946
H	1.819504	10.56868	14.75458
H	1.334871	6.478292	0.158977
H	0.036462	6.823031	2.224624
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H	0.419865	11.12044	9.123647
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S14i_17, Rel. E = 3.23

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Ge	16.09114	7.007561	4.995926
Ge	15.43139	16.32666	5.448439
Ge	8.188073	7.572318	2.205497
Ge	13.09966	7.462365	2.127305
Ge	18.4999	15.87584	2.440045
Ge	18.5571	16.36706	5.512375
Ge	18.60841	1.759429	4.955286
Ge	2.445851	15.81055	2.624923
Ge	4.995109	7.4483	9.800363
Ge	16.03411	10.22413	12.99523
Ge	5.636887	1.334278	9.778872
Ge	16.15127	7.534237	9.433225
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Ge	15.43139	16.32666	13.03614
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Si	2.440328	1.605894	5.251663
Si	12.95128	7.086109	5.202847
Si	7.878857	7.156438	5.401249
Si	7.989266	10.17004	5.585112
Si	18.56403	1.286573	1.85485

Si	12.934	10.51321	2.373642
Si	7.870233	10.75562	2.591179
Si	2.407019	1.297373	2.180318
Si	12.90175	10.19977	5.436684
Si	3.929526	5.37106	7.745524
Si	16.96946	12.38646	-0.03067
Si	17.07235	5.350706	14.96646
Si	4.002945	12.23813	0.2834
Si	14.36113	14.23773	-0.0369
Si	6.507085	3.509314	0.04895
Si	6.515179	14.24989	0.234148
Si	14.50631	3.43736	15.02579
Si	1.495981	3.348293	7.613903
Si	19.54369	14.22505	0.057767
Si	19.51526	3.407491	14.93155
Si	1.52124	14.10929	0.190159
Si	11.91559	12.18641	0.041367
Si	9.069963	5.395697	7.570946
Si	8.918426	12.3208	0.175013
Si	11.97375	5.362289	-0.02821
Si	5.676546	16.39859	13.21984
Si	5.680696	1.699301	12.87132
Si	15.31108	15.90603	9.890656
Si	5.708907	15.87094	10.20926
Si	4.746407	10.12936	13.2418
Si	4.81882	7.09439	13.01645
Si	15.37963	1.776862	12.65326
Si	4.741258	10.68938	10.32247
Si	16.06295	10.63587	9.861395
Si	15.39361	1.317322	9.573039
Si	2.439255	16.32696	13.288
Si	2.440328	1.605894	12.83936
Si	12.95128	7.086109	12.79055
Si	7.878857	7.156438	12.98895
Si	7.989266	10.17004	13.17281
Si	18.56403	1.286573	9.44255
Si	12.934	10.51321	9.961343
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Si	2.407019	1.297373	9.768018
Si	12.90175	10.19977	13.02438
Si	3.929526	5.37106	0.157824
Si	16.96946	12.38646	7.557033
Si	17.07235	5.350706	7.378757
Si	4.002945	12.23813	7.8711
Si	14.36113	14.23773	7.550797
Si	6.507085	3.509314	7.63665

Si	6.515179	14.24989	7.821848
Si	14.50631	3.43736	7.438086
Si	1.495981	3.348293	0.026203
Si	19.54369	14.22505	7.645466
Si	19.51526	3.407491	7.343852
Si	1.52124	14.10929	7.777859
Si	11.91559	12.18641	7.629067
Si	9.069963	5.395697	15.15865
Si	8.918426	12.3208	7.762712
Si	11.97375	5.362289	7.559494
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Si	2.527471	16.06439	9.669475
Si	3.977237	5.262751	14.92705
Si	16.9724	12.35774	7.552761
Si	17.01532	5.436579	7.530658
Si	3.878989	12.20811	7.489755
Si	14.37954	14.26339	7.741151
Si	6.564122	3.430496	15.12463
Si	6.488785	14.09087	7.567319
Si	14.45246	3.437859	7.620454
Si	1.439288	3.348006	15.03801
Si	19.47912	14.25145	7.97114
Si	19.42455	3.505998	7.701267
Si	1.381116	14.21297	14.98926
Si	11.88728	12.32904	7.8307
Si	9.042272	5.428557	14.926
Si	8.960496	12.16956	15.09232
Si	11.96311	5.340507	7.664426
O	4.057889	2.145755	1.961534
O	16.84433	15.80848	5.87879
O	16.90155	15.59982	2.518803
O	3.936984	2.055031	5.237425
O	16.81671	2.240796	5.31081
O	3.984648	15.32518	2.199741
O	3.950909	15.57498	5.38894
O	16.95464	1.577462	2.164098

O	14.68941	11.38966	2.475255
O	6.513715	6.503978	5.366009
O	6.307391	6.89136	1.774259
O	14.59779	10.96637	6.03538
O	6.427164	10.62469	5.806799
O	14.50153	6.921098	2.01934
O	14.64877	6.490139	5.438549
O	6.242047	10.92836	2.09551
O	6.816674	2.474525	1.266714
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O	6.679836	14.70714	1.499605
O	6.340392	15.35301	6.547801
O	14.61224	2.206569	1.094797
O	17.0421	11.59095	1.397471
O	3.945098	5.70491	5.783515
O	3.936545	6.566573	0.718271
O	17.18945	11.34086	6.328662
O	3.794464	11.132	6.298337
O	16.83808	6.7409	0.877303
O	17.26844	5.878825	5.975085
O	3.786049	11.46623	1.341397
O	5.876568	17.48904	1.514678
O	15.14226	0.209476	5.841321
O	15.03073	17.45779	1.952671
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O	16.09256	9.124177	1.716056
O	4.157667	8.464713	5.853
O	4.500009	8.929244	1.624803
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O	6.200576	1.501826	3.839795
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O	16.89586	10.63298	3.804918
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O	16.79968	7.160518	3.45284
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O	18.97929	17.52713	1.954829
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O	13.04558	9.228612	1.593801
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O	1.465396	2.672533	5.958599
O	19.19465	2.952448	6.185182
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O	12.00121	11.95203	1.830689
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O	8.758499	6.531996	0.90838
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O	8.946236	11.07758	6.300846
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O	18.24955	13.36659	-0.10245
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O	12.26073	5.897935	13.76643
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O	5.252893	4.342799	7.746177
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O	2.608729	4.434832	7.638738
O	18.24955	13.36659	7.485253
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O	2.543473	13.1201	14.93553
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O	7.91911	4.261332	14.95159
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C	9.652011	0.845721	0.7024
C	11.1819	16.42336	3.454207
C	11.89243	16.60013	4.608131
C	11.7648	1.262148	4.396361
C	11.06114	1.15164	3.228156
C	10.74973	17.56006	2.697037
C	20.20179	10.78682	3.717473
C	20.32888	10.6453	5.232713
C	19.80871	9.230042	5.515026
C	20.1916	8.409474	4.27793
C	0.556815	10.1061	1.155751
C	1.38563	9.742992	0.131843
C	1.144767	7.454792	0.63801
C	0.340947	7.747548	1.704826
C	0.09723	9.111	2.070945
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C	9.445375	16.48708	7.066844
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C	11.89243	16.60013	12.19583
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C	20.20179	10.78682	11.30517
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H	8.785568	15.74848	6.60089
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H	7.770339	0.085323	15.11939
H	10.53225	1.372621	0.291636
H	9.074717	1.566781	1.298303
H	10.96962	15.4102	3.120223
H	12.27256	15.77234	5.204561
H	12.05706	2.217589	4.829709
H	10.76704	2.058912	2.704529
H	12.75567	0.25223	5.897945
H	19.19366	11.11807	3.423894
H	0.021596	11.47442	3.299742
H	0.460676	10.74341	5.507008
H	19.75194	11.40854	5.768411
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H	7.770339	0.085323	7.531685
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H	9.074717	1.566781	8.886003
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H	12.05706	2.217589	12.41741
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H	18.72326	9.243262	13.22322
H	0.192971	7.830009	12.0137
H	19.39567	7.711544	11.55727
H	0.315841	11.15913	8.86564
H	1.844208	10.46051	7.048038
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S14c_6, Rel. E = 3.04

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Ge	16.252	7.117507	5.212673
Ge	5.671812	15.91052	2.300128
Ge	2.281226	16.18907	5.17791
Ge	12.95313	7.489201	2.242586
Ge	18.61172	15.9063	2.746338
Ge	18.5248	16.3662	5.901361
Ge	13.05547	10.64985	2.578922
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Ge	5.678864	1.461814	9.709026
Ge	16.11196	10.22135	13.01078
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Ge	12.95313	7.489201	9.830286
Ge	18.61172	15.9063	10.33404
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Ge	13.05536	10.14407	13.34551
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Si	16.1013	7.484204	2.111788

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Si	2.574672	1.485017	2.037704
Si	2.386171	1.646112	5.116437
Si	7.838581	7.411757	1.958775
Si	7.943592	7.129944	5.068167
Si	7.911597	10.22907	5.372165
Si	18.52739	1.330667	2.284292
Si	13.08362	7.043202	5.384598
Si	7.781617	10.50274	2.269855
Si	18.38423	1.802136	5.320987
Si	2.537621	16.08316	2.088032
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Si	1.394395	14.24921	7.403856
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Si	9.023093	5.489165	7.352159
Si	8.97385	12.18668	7.523462
Si	11.95401	5.326795	0.0683
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Si	15.30952	15.91569	10.21296
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Si	18.38423	1.802136	12.90869
Si	2.537621	16.08316	9.675732
Si	3.928663	5.300416	14.89079
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Si	14.40819	14.22864	7.814968
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Si	14.43035	3.395454	7.658857
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Si	1.394395	14.24921	14.99156
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O	6.226351	10.96757	2.083266
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O	14.42097	15.49954	6.773185
O	14.44799	14.84698	1.752996
O	6.453437	2.489796	6.197933
O	14.36793	2.693327	6.171871
O	6.67187	14.70276	1.484259
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O	14.56	2.176127	1.151367
O	17.09614	11.53856	1.452037
O	3.854591	5.742262	5.747984

O	3.927144	6.600476	0.681943
O	17.19576	11.30669	6.383097
O	3.759568	11.16073	6.273662
O	16.92994	6.686898	0.961418
O	17.21753	5.849168	6.040916
O	3.788183	11.51469	1.315896
O	5.895892	17.49946	1.49384
O	15.23251	0.176707	5.897981
O	15.08002	17.40718	1.989331
O	5.560263	0.041675	5.894945
O	16.13346	9.074778	1.75874
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O	4.475664	8.965971	1.608157
O	16.56829	8.621695	6.11854
O	6.213704	1.528903	3.807097
O	14.78415	15.89823	4.176899
O	14.73008	1.669081	3.740054
O	6.233047	16.00093	3.982182
O	16.89836	10.5951	3.85473
O	4.162157	6.816001	3.281026
O	4.086251	10.65703	3.708051
O	16.86374	7.166507	3.53976
O	2.774268	17.6259	1.641569
O	18.52432	0.408864	6.160862
O	18.88325	17.47331	1.948572
O	2.137791	0.158995	5.765283
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O	12.27237	10.54537	4.186355
O	8.276352	6.985848	3.475438
O	8.213693	10.65799	3.828873
O	12.42886	7.109146	3.895719
O	1.593792	2.173733	0.966071
O	19.45745	15.68858	7.225164
O	19.49727	14.57134	2.004284
O	1.495492	2.712885	5.94978
O	19.20236	2.910524	6.162978
O	1.627374	15.33388	1.002555
O	1.212777	15.07595	6.004681
O	19.32305	2.231131	1.20106

O	12.00502	11.88307	1.837251
O	8.99709	6.164584	5.87001
O	8.78014	6.596646	0.919702
O	11.99681	11.0026	6.897111
O	8.915864	11.08496	6.333447
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O	12.22122	5.912661	6.173025
O	8.67869	11.53464	1.391896
O	5.202776	4.348077	0.059772
O	15.66896	13.2616	7.554924
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O	5.230152	13.15311	7.366473
O	2.570239	4.475421	0.069468
O	18.28466	13.32154	-0.0707
O	18.32302	4.560105	0.481732
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O	4.060713	2.172598	9.535807
O	16.86873	15.7357	13.45698
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O	16.81525	2.233679	12.85488
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O	16.92994	6.686898	8.549118
O	17.21753	5.849168	13.62862
O	3.788183	11.51469	8.903597
O	5.895892	17.49946	9.08154
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O	5.560263	0.041675	13.48264
O	16.13346	9.074778	9.346439
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O	4.475664	8.965971	9.195857
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O	4.162157	6.816001	10.86873
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O	16.86374	7.166507	11.12746
O	2.774268	17.6259	9.229269
O	18.52432	0.408864	13.74856
O	18.88325	17.47331	9.536272
O	2.137791	0.158995	13.35298
O	13.01625	9.150653	9.200724
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O	7.944198	9.00127	9.267785
O	12.87177	8.43699	13.80666
O	1.963704	1.651872	11.12884
O	19.32673	15.93859	11.963
O	18.99694	1.689384	11.40129
O	1.73894	16.06151	11.09111
O	12.27237	10.54537	11.77406
O	8.276352	6.985848	11.06314
O	8.213693	10.65799	11.41657
O	12.42886	7.109146	11.48342
O	1.593792	2.173733	8.553771
O	19.45745	15.68858	14.81286
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O	1.495492	2.712885	13.53748
O	19.20236	2.910524	13.75068
O	1.627374	15.33388	8.590255
O	1.212777	15.07595	13.59238
O	19.32305	2.231131	8.78876
O	12.00502	11.88307	9.424951
O	8.99709	6.164584	13.45771
O	8.78014	6.596646	8.507401
O	11.99681	11.0026	14.48481
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O	11.93648	6.471995	8.801263
O	12.22122	5.912661	13.76073
O	8.67869	11.53464	8.979595
O	5.202776	4.348077	7.647472
O	15.66896	13.2616	15.14262
O	15.69225	4.407649	7.773034
O	5.230152	13.15311	14.95417
O	2.570239	4.475421	7.657167
O	18.28466	13.32154	7.517003
O	18.32302	4.560105	8.069432
O	2.591067	13.19755	14.91269
O	12.99639	13.48025	7.544791
O	7.897055	4.315591	14.98862
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O	13.01379	4.124745	7.969793
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C	20.22725	10.43498	5.341154
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C	20.325	8.228889	4.32625
C	0.589898	10.08266	1.25674
C	1.379282	9.786155	0.181871
C	1.153314	7.471714	0.551359
C	0.407398	7.694462	1.675912
C	0.16616	9.032101	2.125123
C	9.590628	16.39205	1.465837
C	8.974731	16.84009	0.329526
C	9.40444	1.399264	0.903015

C	9.98778	1.016771	2.078605
C	10.07776	17.33416	2.426733
C	10.78516	15.52619	3.981329
C	11.20753	15.58894	5.452421
C	11.79452	16.99588	5.619586
C	10.99221	0.167902	4.662049
C	20.24257	10.62448	11.41505
C	20.22725	10.43498	12.92885
C	19.76691	8.98486	13.12194
C	20.325	8.228889	11.91395
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C	1.379282	9.786155	7.769571
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C	10.78516	15.52619	11.56903
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H	18.67451	8.936227	5.528399
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H	19.63041	7.457263	3.957714
H	0.361879	11.12532	1.460706
H	1.820909	10.54561	14.7217
H	1.361139	6.470116	0.189689
H	0.01465	6.839961	2.221892

H	2.422694	8.351226	6.729452
H	9.659646	15.31903	1.633317
H	8.521742	16.16826	14.78002
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H	10.33682	15.44047	6.105303
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H	1.820909	10.54561	7.134
H	1.361139	6.470116	7.777389
H	0.01465	6.839961	9.809591
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H	11.76673	17.36194	14.24177
H	12.83686	17.00471	12.87627
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H	10.09035	0.601864	12.7188
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S14c_17, Rel. E = 3.63

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Ge	4.746189	10.267256	5.424623
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Ge	16.228775	7.048559	5.125432
Ge	5.720190	16.074585	2.127241
Ge	2.345469	16.037033	5.079258
Ge	12.916076	7.396377	2.232396
Ge	18.497652	15.979932	2.819962
Ge	18.521587	16.370884	5.830763
Ge	12.958741	10.546047	2.662239
Ge	13.041466	10.058062	5.724332
Ge	5.702804	1.627399	9.852907
Ge	16.164087	10.267992	13.076779
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Ge	4.801760	7.022769	12.682714
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Ge	5.720190	16.074585	9.714941
Ge	2.345469	16.037033	12.666959
Ge	12.916076	7.396377	9.820096
Ge	18.497652	15.979932	10.407662
Ge	18.521587	16.370884	13.418464
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Ge	13.041466	10.058062	13.312032
Si	5.565955	16.088572	5.278850
Si	15.367432	16.185213	5.635300
Si	16.074440	10.543485	2.347492
Si	15.420102	1.229450	2.194552
Si	4.818786	7.402628	1.861487
Si	16.079288	7.458215	2.030137
Si	15.323835	1.583459	5.252144
Si	4.760970	10.436299	2.232180
Si	15.383293	15.836096	2.529756
Si	5.543224	1.460703	5.431744
Si	2.603011	1.592983	2.242684
Si	2.432888	1.497584	5.323359
Si	7.925245	7.377495	1.990750
Si	7.906376	7.116480	5.072494
Si	7.873375	10.269576	5.380708
Si	18.573397	1.299823	2.231755
Si	13.058465	6.963255	5.319510
Si	7.908432	10.498615	2.337132
Si	18.467010	1.742791	5.276673
Si	2.589386	16.200979	1.967897
Si	3.866347	5.280584	7.384494
Si	17.054163	12.340966	0.066108
Si	16.961851	5.326140	-0.051353
Si	3.891136	12.347037	0.024526

Si	14.415976	14.177848	0.161537
Si	6.546994	3.499648	7.575906
Si	6.587904	14.103065	15.042563
Si	14.437381	3.289244	0.013365
Si	1.375850	3.327840	7.605985
Si	19.498026	14.325897	0.457207
Si	19.384211	3.406040	0.052399
Si	1.386487	14.330300	7.416917
Si	11.956549	12.182959	0.285454
Si	9.049672	5.490943	7.351404
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Si	11.976622	5.218050	0.030436
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Si	15.367432	16.185213	13.223
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Si	15.420102	1.229450	9.782252
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Si	16.079288	7.458215	9.617837
Si	15.323835	1.583459	12.839844
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Si	15.383293	15.836096	10.117456
Si	5.543224	1.460703	13.019444
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Si	7.873375	10.269576	12.968409
Si	18.573397	1.299823	9.819454
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Si	7.908432	10.498615	9.924832
Si	18.467010	1.742791	12.864372
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Si	3.866347	5.280584	14.972195
Si	17.054163	12.340966	7.653808
Si	16.961851	5.326140	7.536346
Si	3.891136	12.347037	7.612226
Si	14.415976	14.177848	7.749236
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Si	6.587904	14.103065	7.454863
Si	14.437381	3.289244	7.601065
Si	1.375850	3.327840	0.018285
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Si	19.384211	3.406040	7.640099
Si	1.386487	14.330300	15.004617
Si	11.956549	12.182959	7.873154
Si	9.049672	5.490943	14.939104

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O	16.912519	15.416459	2.150501
O	4.00443	1.977637	5.488278
O	16.872869	1.958645	5.551751
O	4.062222	15.453288	1.95872
O	4.052218	15.498551	5.221319
O	16.990126	1.466112	1.860731
O	14.581757	11.215706	2.314287
O	6.435493	6.39649	5.37883
O	6.369977	7.002497	1.62418
O	14.58967	10.905379	6.002267
O	6.373525	10.901403	5.703021
O	14.575639	6.823909	2.020027
O	14.581043	6.402944	5.17224
O	6.319699	10.866524	2.180192
O	6.765194	2.782616	1.446266
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O	14.57849	2.10154	1.108732
O	17.043447	11.51261	1.473493
O	3.691969	5.868881	5.861041
O	3.917189	6.531084	0.837086
O	17.280914	11.276394	6.428541
O	3.661735	11.298898	6.364994
O	16.891726	6.659425	0.878527
O	17.189644	5.808968	5.978674
O	3.882741	11.525787	1.426745
O	5.947159	0.03392	1.474652
O	14.957299	0.067641	5.727833
O	14.995584	17.364393	2.065814
O	5.609017	-0.099623	5.887915
O	16.092983	9.046282	1.684881
O	4.436153	8.572289	5.939638
O	4.555771	8.975641	1.529059
O	16.441751	8.576671	6.021421
O	6.231166	1.604506	3.956867
O	15.049039	15.629223	4.123259
O	14.984236	1.78764	3.671519
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O	16.755562	10.518199	3.834878
O	4.33103	7.085078	3.389704
O	4.179203	10.385809	3.752241
O	16.847015	7.161715	3.460621
O	2.872887	0.078883	1.730199
O	19.020227	0.374684	5.969825
O	19.149426	17.486536	2.067266
O	2.25037	-0.048711	5.821998
O	12.545475	9.05605	1.737363
O	7.661801	8.662003	5.518322
O	8.132263	8.975044	1.817814
O	12.90881	8.33967	6.187944
O	2.022695	1.61968	3.75755
O	19.167578	15.505079	4.421898
O	18.876001	1.938291	3.711625
O	1.83165	15.992435	3.391404
O	12.158917	10.668582	4.274801
O	8.218212	6.884364	3.503823
O	8.305712	10.737534	3.889756
O	12.28951	7.008212	3.865024
O	1.54963	2.333123	1.287198
O	19.49309	15.678473	7.154042
O	19.498299	14.685739	2.024756
O	1.524456	2.489505	6.215981
O	19.210672	2.945912	6.097133
O	1.675882	15.628631	0.776584
O	1.342107	14.831677	5.859082
O	19.379501	2.204915	1.132352
O	11.941868	11.80709	1.870539
O	9.013227	6.323057	5.948589
O	8.860701	6.542552	0.982931
O	12.060809	10.825578	6.999872
O	8.894135	10.895153	6.462673
O	11.938729	6.339548	1.19724
O	12.256412	5.821413	6.146847
O	8.759422	11.529592	1.445589
O	5.1883	4.363931	-0.062494
O	15.705956	13.225772	7.495028
O	15.634821	4.394421	0.122705
O	5.273999	13.166479	7.458076
O	2.527693	4.464326	0.122205
O	18.373947	13.260695	0.000235
O	18.287664	4.529493	0.445431
O	2.615182	13.301599	7.630335
O	13.038794	13.337782	-0.060566
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O	7.933077	13.265762	7.194689
O	12.991859	3.991217	0.330483
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O	10.423027	4.644168	7.53981
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O	1.342107	14.831677	13.446781
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O	11.941868	11.80709	9.458239
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O	8.860701	6.542552	8.570631
O	12.060809	10.825578	14.587571
O	8.894135	10.895153	14.050373
O	11.938729	6.339548	8.784939
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O	5.1883	4.363931	7.525206
O	15.705956	13.225772	15.082728
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O	18.373947	13.260695	7.587934
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C	0.441743	10.119019	1.258902
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C	0.117813	7.759384	1.7811
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H	10.097467	14.905158	3.348456
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