

Full XYZ coordinates of QM/MM-optimized species (“QM(B3LYP)/MM” stands for the QM/MM-optimized structures obtained with the B3LYP functional (without dispersion), and “open-shell singlet” means that the open-shell singlet state was used in the QM/MM calculation)

(<i>R,R</i>)-1-RC	C	18.404876	3.417024	19.587993			
C	12.487000	7.261000	26.395000	C	17.639888	4.497025	20.008011
C	11.616000	6.503000	25.622000	C	17.550017	4.800019	21.362013
C	12.086000	5.395000	24.927000	C	16.783924	5.881020	21.784030
C	13.428000	5.043000	25.007000	C	16.107910	6.659026	20.850045
C	13.027000	3.179000	23.539000	C	16.197885	6.355032	19.497042
C	11.685000	3.529000	23.460000	C	16.963876	5.274031	19.076025
C	11.215000	4.638000	24.154000	O	15.523872	7.185038	18.539057
O	10.782000	2.793000	22.654000	O	18.565823	5.527821	24.111054
Cu	18.543436	6.084805	26.013443	O	18.017878	3.388039	24.573350
Cu	17.946107	3.697792	26.528166	C	18.263378	4.335537	23.745083
C	22.207131	3.939446	26.373350	C	14.301000	5.801000	25.782000
C	22.750745	3.181819	27.426208	C	13.829000	6.909000	26.476000
C	24.102685	2.863274	27.451108	C	27.928247	6.998486	26.482974
C	24.935196	3.290294	26.421893	C	27.095466	6.156473	25.754705
C	24.428234	4.024842	25.332608	C	27.608111	5.038435	25.064532
C	23.043407	4.335953	25.292337	C	29.002341	4.772680	25.125469
C	22.526771	5.001037	24.159562	C	13.900000	3.935000	24.313000
C	23.369981	5.389126	23.123287	C	28.681730	2.891464	23.623522
C	24.736466	5.129540	23.183135	C	27.315032	3.111346	23.592494
C	25.276748	4.437917	24.275765	C	26.753329	4.188862	24.313815
O	25.567939	5.524534	22.140947	O	26.550591	2.217255	22.845818
O	20.432955	5.514509	26.188006	O	16.596342	6.403264	25.847219
O	19.906511	3.369280	26.650012	O	16.053413	4.265038	26.319646
C	20.763546	4.295868	26.415403	C	15.735398	5.462569	25.983475
C	18.226927	4.022014	22.293999	C	17.902375	5.826218	30.223994
C	18.992915	2.941012	21.873981	C	18.892535	6.587126	30.871568
C	19.081890	2.638017	20.519979	C	16.745304	5.422980	30.947109

C	15.671461	4.756402	30.318978	O	33.615560	3.334182	24.570245
C	14.559884	4.358957	31.055653	C	33.845604	4.306591	23.763258
O	18.430525	6.404695	27.972755	C	29.839642	5.607422	25.916266
O	17.894331	4.260719	28.429047	C	29.287283	6.727681	26.562917
C	18.093368	5.475700	28.791378	C	43.550271	6.896540	26.586867
Cu	34.092656	5.990628	26.097501	C	42.720612	6.039220	25.875182
Cu	33.543847	3.581651	26.546007	C	43.239211	4.923049	25.186727
C	37.800760	3.886650	26.434447	C	44.638190	4.671101	25.236987
C	38.323963	3.139277	27.505531	C	29.525737	3.704713	24.368909
C	39.673247	2.814053	27.558137	C	44.316841	2.758408	23.777380
C	40.524388	3.218994	26.536008	C	42.949483	2.979485	23.737966
C	40.040464	3.943405	25.430121	C	42.385189	4.066573	24.442721
C	38.659011	4.271305	25.366949	O	42.186898	2.077597	22.998875
C	38.167912	4.939359	24.225872	O	32.126732	6.286133	25.981645
C	39.030750	5.303324	23.196503	O	31.641701	4.119836	26.379716
C	40.392246	5.018428	23.273573	C	31.288136	5.321677	26.101865
C	40.909472	4.330425	24.379978	C	33.562581	5.590818	30.325269
O	41.241891	5.388756	22.236984	C	34.586691	6.319230	30.958084
O	36.000575	5.441752	26.228960	C	32.420486	5.197687	31.080376
O	35.506918	3.281208	26.651787	C	31.326105	4.541203	30.480297
C	36.350800	4.224954	26.443216	C	30.218692	4.178906	31.242170
C	33.846855	4.021974	22.293721	O	34.009067	6.242306	28.073044
C	34.612832	2.940971	21.873686	O	33.496921	4.082036	28.472087
C	34.701783	2.637980	20.519681	C	33.700559	5.285250	28.871443
C	34.024755	3.416991	19.587710	Cu	49.695781	6.207181	25.981277
C	33.259777	4.496993	20.007743	Cu	49.343761	3.790233	26.564306
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.105898	5.497417	24.167795	C	53.770890	5.287820	24.113942

C	54.557834	5.591822	23.007903	O	49.296665	4.395920	28.455237
C	55.929834	5.377808	23.052827	C	49.388614	5.633100	28.784771
C	56.515890	4.858790	24.200790	C	11.158284	7.260965	41.959133
O	56.643771	5.617813	21.841791	C	10.287267	6.502972	41.186144
O	51.637646	5.837991	26.120883	C	10.757252	5.394972	40.491132
O	51.334207	3.662036	26.636203	C	12.099252	5.042967	40.571107
C	52.092790	4.667279	26.380273	C	11.698220	3.178974	39.103108
C	49.466780	4.021882	22.293161	C	10.356220	3.528979	39.024133
C	50.232747	2.940878	21.873109	C	9.886236	4.637978	39.718145
C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.233239	6.153749	41.467023
C	48.879663	4.496911	20.007197	Cu	16.692489	3.752870	41.967575
C	48.790739	4.799899	21.361205	C	20.956380	4.082772	41.826761
C	48.023773	5.880903	21.783256	C	21.479081	3.326417	42.891548
C	47.347732	6.658919	20.849300	C	22.832877	3.022660	42.956276
C	47.437657	6.354932	19.496292	C	23.691270	3.460103	41.953797
C	48.203622	5.273928	19.075240	C	23.211811	4.197274	40.855346
O	46.763615	7.184949	18.538336	C	21.824410	4.500278	40.777497
O	49.731242	5.591586	24.088742	C	21.338613	5.175888	39.638765
O	49.385064	3.426484	24.608743	C	22.211452	5.571651	38.629335
C	49.525274	4.368945	23.749559	C	23.576051	5.311696	38.723438
C	45.478031	5.539904	25.986921	C	24.086739	4.620341	39.827096
C	44.915028	6.653240	26.637668	O	24.431585	5.707130	37.703090
C	45.161977	3.587703	24.505092	O	19.142999	5.618941	41.598692
O	47.715720	6.340173	25.884775	O	18.662269	3.464140	42.061692
O	47.393477	4.172750	26.419204	C	19.501338	4.408619	41.831986
C	46.948604	5.334250	26.097989	C	16.881409	4.138507	37.721879
C	49.205884	5.999653	30.215095	C	17.590367	3.037663	37.209212
C	50.152497	6.843404	30.823881	C	17.596874	2.766955	35.847835
C	48.095336	5.533565	30.972590	C	16.894726	3.590057	34.974459
C	47.063362	4.772110	30.384013	C	16.146408	4.688895	35.446402
C	45.993283	4.322214	31.151186	C	16.118586	4.952860	36.841345
O	49.608513	6.569455	27.935238	C	15.305812	5.999342	37.321551

C	14.583692	6.790236	36.437014	O	16.662321	4.295640	43.878550
C	14.638902	6.573835	35.070237	C	16.857284	5.508540	44.251182
C	15.427414	5.522661	34.549843	Cu	32.876873	6.271331	41.544288
O	13.914380	7.449877	34.264871	Cu	32.328455	3.796075	42.176453
O	17.230064	5.617095	39.555659	C	36.508666	4.025501	41.807601
O	16.748081	3.458572	40.001404	C	37.005196	3.153221	42.759563
C	16.959574	4.420216	39.178876	C	38.382017	2.842239	42.786056
C	12.972269	5.800962	41.346096	C	39.239278	3.382733	41.851894
C	12.500284	6.908961	42.040108	C	38.771940	4.260050	40.819607
C	26.684752	7.068801	42.312817	C	37.366521	4.583411	40.801832
C	25.867293	6.289980	41.519705	C	36.877211	5.416093	39.754532
C	26.375937	5.197368	40.743341	C	37.724548	5.914975	38.794249
C	27.789637	4.934149	40.826066	C	39.116354	5.632108	38.825017
C	12.571236	3.934968	39.877095	C	39.644011	4.810665	39.819531
C	27.535341	3.120234	39.228602	O	39.935688	6.163060	37.875159
C	26.135957	3.357737	39.151571	O	34.730855	5.581134	41.711293
C	25.547345	4.375114	39.899060	O	34.251934	3.419380	42.122542
O	25.493171	2.494882	38.310525	C	35.053244	4.370770	41.879371
O	15.269282	6.440147	41.352713	C	32.362735	3.944990	37.961756
O	14.778878	4.286845	41.805654	C	32.993969	2.789627	37.536498
C	14.425678	5.484502	41.503139	C	33.057018	2.493295	36.158069
C	16.713324	5.841907	45.695717	C	32.478352	3.337537	35.233049
C	17.716063	6.613456	46.311376	C	31.774862	4.523574	35.623301
C	18.781304	6.903267	32.219181	C	31.710858	4.818417	37.031500
C	17.677331	6.468474	32.944032	C	30.956860	5.950671	37.456138
C	16.648206	5.728081	32.330248	C	30.332765	6.762888	36.545085
C	15.588299	5.421769	46.459920	C	30.427489	6.507584	35.150094
C	14.507438	4.731311	45.871751	C	31.136189	5.405067	34.680245
C	13.423996	4.326512	46.645422	O	29.773539	7.434783	34.389133
C	14.486992	4.608061	32.423671	O	32.786413	5.463153	39.711776
C	15.518704	5.300928	33.071185	O	32.181902	3.364168	40.249706
O	13.372282	4.201754	33.148588	C	32.439299	4.282950	39.417025
O	17.159031	6.450622	43.433320	C	28.606679	5.762473	41.659837

C	28.071702	6.815201	42.380840	C	54.401202	4.554601	40.869191
C	42.295393	7.232720	42.158116	C	53.028202	4.768621	40.826292
C	41.455484	6.431117	41.394305	C	52.442128	5.287645	39.677341
C	41.962071	5.356802	40.636650	C	53.229054	5.591649	38.571289
C	43.357137	5.082254	40.675525	C	54.601054	5.377629	38.616189
C	28.337598	3.876788	40.042658	C	55.187129	4.858606	39.764139
C	43.010326	3.266795	39.102380	O	55.314970	5.617636	37.405141
C	41.646354	3.507424	39.077729	O	50.372332	5.931473	41.729107
C	41.103372	4.559765	39.841045	O	49.973767	3.756088	42.179324
O	40.867908	2.659805	38.294298	C	50.775210	4.733646	41.957397
O	30.858559	6.455118	41.474383	C	48.267132	4.395455	37.817942
O	30.433954	4.354628	42.157350	C	49.053285	3.334876	37.333186
C	30.074275	5.502827	41.771640	C	49.116572	3.057477	35.974818
C	32.271732	6.061439	45.738783	C	48.390820	3.829969	35.075363
C	33.137188	6.975467	46.312448	C	47.567754	4.887132	35.516419
C	34.519867	6.619751	32.312799	C	47.492376	5.165572	36.907894
C	33.420897	6.212867	33.061084	C	46.620634	6.178530	37.354403
C	32.357585	5.508311	32.467443	C	45.881246	6.920925	36.442225
C	31.175969	5.513652	46.485239	C	45.970169	6.682368	35.080696
C	30.198457	4.661515	45.894997	C	46.817889	5.662289	34.592670
C	29.152089	4.168739	46.637028	O	45.215079	7.504644	34.246996
C	30.167439	4.458341	32.605396	O	48.478276	5.883205	39.668834
C	31.226087	5.128478	33.226619	O	48.096686	3.700340	40.090765
O	29.049973	4.100164	33.348289	C	48.279980	4.676554	39.278338
O	32.791453	6.588009	43.499787	C	44.206483	5.886142	41.485515
O	32.437219	4.430489	44.035064	C	43.657145	6.967346	42.198762
C	32.516706	5.661798	44.317996	C	43.867382	4.038344	39.879359
Cu	48.447196	6.400713	41.587749	O	46.473326	6.618921	41.476721
Cu	47.997314	3.974343	42.058479	O	46.067134	4.436507	41.875870
C	52.242277	4.464616	41.931345	C	45.668363	5.629201	41.614207
C	52.828352	3.947593	43.079296	C	47.873829	6.039511	45.796982
C	54.201352	3.732573	43.123194	C	48.830463	6.846344	46.440167
C	54.987277	4.036578	42.018142	C	50.045140	7.184662	32.166100

C	48.986589	6.695194	32.923586	O	17.304510	3.423555	57.670957
C	47.999893	5.871199	32.348890	C	18.146096	4.373755	57.482121
C	46.741103	5.582049	46.526458	C	15.685825	4.212374	53.322283
C	45.700259	4.858721	45.906057	C	16.411505	3.110369	52.835072
C	44.612287	4.410928	46.648765	C	16.472500	2.841207	51.474934
C	45.921713	4.611142	32.511612	C	15.802606	3.662325	50.575406
C	46.912593	5.392921	33.121153	C	15.040839	4.763639	51.017606
O	44.848358	4.152097	33.266807	C	14.970624	5.037012	52.410890
O	48.350750	6.676061	43.552918	C	14.159285	6.098985	52.857104
O	47.919535	4.501543	43.973004	C	13.475299	6.891630	51.943926
C	48.065561	5.718077	44.356971	C	13.559537	6.655582	50.581664
C	9.830844	7.260885	57.522289	C	14.344673	5.586714	50.093228
C	8.959813	6.502896	56.749314	O	12.860058	7.525851	49.748094
C	9.429780	5.394897	56.054290	O	15.947551	5.655519	55.205237
C	10.771780	5.042887	56.134240	O	15.439541	3.489646	55.578734
C	10.370715	3.178901	54.666241	C	15.689325	4.468918	54.788026
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.302315	7.076492	57.572741
Cu	15.893546	6.138020	57.133923	C	24.469313	6.248580	56.829465
Cu	15.341354	3.724228	57.551286	C	24.982422	5.148000	56.112113
C	19.594781	4.040745	57.437265	C	26.378070	4.884830	56.161273
C	20.147981	3.277401	58.480965	C	11.243748	3.934890	55.440215
C	21.500976	2.962924	58.494400	C	26.054773	3.033124	54.624233
C	22.324370	3.397233	57.461116	C	24.687529	3.252522	54.600473
C	21.808171	4.139930	56.381711	C	24.126037	4.313433	55.346343
C	20.423047	4.452287	56.356174	O	23.921921	2.371556	53.839452
C	19.897813	5.133193	55.237212	O	13.938891	6.431855	56.972272
C	20.732144	5.528433	54.196314	O	13.435047	4.270298	57.369153
C	22.098421	5.262935	54.239540	C	13.091675	5.475089	57.084547
C	22.647975	4.560495	55.320788	C	15.283042	5.695809	61.352094
O	22.920753	5.665212	53.193111	C	16.314083	6.385792	61.978046
O	17.795277	5.594841	57.299992	C	17.647087	6.928780	47.662112

C	16.569966	6.488273	48.422721	C	29.632458	6.033620	52.861408
C	15.528953	5.737359	47.844280	C	28.905473	6.791583	51.949863
C	14.198077	5.242813	62.095147	C	29.000031	6.565254	50.586314
C	13.166036	4.552830	61.469195	C	29.836771	5.541736	50.099612
C	12.083071	4.099834	62.213248	O	28.259375	7.398830	49.752931
C	13.382962	4.597621	48.010829	O	31.483903	5.671003	55.198654
C	14.421833	5.313967	48.620706	O	31.044426	3.490736	55.575504
O	12.291327	4.190867	48.770068	C	31.256689	4.477727	54.783028
O	15.758650	6.378514	59.108000	C	27.216886	5.707562	56.962999
O	15.278126	4.206425	59.477097	C	26.662718	6.810268	57.637869
C	15.446276	5.410044	59.891887	C	40.912875	6.952107	57.633069
Cu	31.463163	6.145044	57.131260	C	40.085536	6.136866	56.872109
Cu	30.955701	3.721442	57.550789	C	40.602244	5.045964	56.142568
C	35.200797	4.083059	57.439952	C	41.999422	4.783105	56.192452
C	35.740951	3.344957	58.509040	C	26.900422	3.832391	55.383165
C	37.087597	3.006708	58.535223	C	41.678514	2.944749	54.640452
C	37.919043	3.390986	57.489437	C	40.311381	3.168268	54.609604
C	37.418670	4.112408	56.388515	C	39.747177	4.224242	55.360891
C	36.039166	4.451819	56.351773	O	39.548310	2.293495	53.839116
C	35.529206	5.113803	55.215608	O	29.494735	6.411473	57.016995
C	36.372877	5.461260	54.164900	O	29.043249	4.232345	57.383570
C	37.733970	5.168749	54.217216	C	28.670487	5.433873	57.128604
C	38.269586	4.486391	55.318639	C	30.903116	5.695628	61.351271
O	38.565112	5.526440	53.161779	C	31.934171	6.385605	61.977208
O	33.381433	5.621887	57.260155	C	32.987090	7.334607	47.669904
O	32.919442	3.449770	57.661395	C	31.973326	6.790464	48.429685
C	33.748654	4.407286	57.461577	C	31.026052	5.870005	47.874009
C	31.252005	4.222725	53.316546	C	29.818163	5.242633	62.094342
C	32.031539	3.161969	52.821616	C	28.786109	4.552656	61.468406
C	32.109408	2.908831	51.459077	C	27.703155	4.099663	62.212477
C	31.400489	3.702438	50.564671	C	29.028995	4.466783	48.020746
C	30.578036	4.754456	51.014663	C	29.949699	5.308583	48.641929
C	30.494549	5.015083	52.409805	O	28.005178	3.929726	48.740412

O	31.365104	6.379846	59.106653	C	42.836611	5.605463	56.996305
O	30.899419	4.204633	59.477416	C	42.273479	6.691174	57.692987
C	31.063446	5.409408	59.891489	C	42.523299	3.736928	55.408569
Cu	47.050931	6.251388	57.151014	O	45.076797	6.400703	57.023778
Cu	46.686615	3.795058	57.532586	O	44.741042	4.194577	57.350054
C	50.914826	4.464382	57.493755	C	44.304163	5.381782	57.123597
C	51.500920	3.947352	58.641694	C	46.523192	5.695393	61.350166
C	52.873920	3.732327	58.685568	C	47.554258	6.385364	61.976087
C	53.659827	4.036331	57.580503	C	48.707517	7.164406	47.786106
C	53.073733	4.554362	56.431564	C	47.625095	6.685348	48.514770
C	51.700733	4.768387	56.388690	C	46.632280	5.891490	47.908315
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.530526	4.665274	48.015353
O	53.987443	5.617405	52.967501	C	45.527300	5.414240	48.655850
O	48.991607	5.859508	57.301162	O	43.440622	4.206414	48.746278
O	48.672392	3.655313	57.668263	O	46.921223	6.443748	59.124213
C	49.437846	4.672514	57.497813	O	46.573397	4.239341	59.461338
C	46.962186	4.367428	53.316311	C	46.675301	5.443884	59.890907
C	47.784108	3.348784	52.801771	C	16.262158	6.620778	63.347051
C	47.836269	3.095630	51.438619	C	15.179191	6.168782	64.090104
C	47.065825	3.852687	50.564016	C	14.147152	5.478800	63.465152
C	46.213442	4.873779	51.034620	C	12.031146	4.336820	63.582253
C	46.146744	5.124109	52.431560	C	13.063187	5.025805	64.207205
C	45.242747	6.093975	52.908362	O	10.943183	3.908824	64.361306
C	44.465669	6.826150	52.019770	C	31.882271	6.620587	63.346214
C	44.548613	6.619871	50.652664	C	30.799317	6.168593	64.089284
C	45.426925	5.640830	50.134519	C	29.767262	5.478616	63.464348
O	43.761980	7.438198	49.844729	C	27.651255	4.336645	63.581483
O	47.121732	5.803477	55.214922	C	28.683309	5.025622	64.206418
O	46.812529	3.595539	55.560886	O	26.563304	3.908650	64.360554
C	46.965262	4.604166	54.783520	C	47.502385	6.620342	63.345096

C	46.419443	6.168348	64.088184	H	37.116535	5.179340	24.106265
C	45.387375	5.478376	63.463264	H	38.630784	5.817281	22.332929
C	43.271365	4.336411	63.580432	H	35.146058	2.325290	22.590355
C	44.303433	5.025383	64.205353	H	35.297745	1.792953	20.190413
O	42.183428	3.908416	64.359522	H	34.099803	3.170470	18.536513
H	12.119254	8.127133	26.935666	H	32.267957	6.144862	22.826123
H	10.573032	6.786854	25.566333	H	31.125441	7.499989	21.165063
H	13.383763	2.323394	22.982316	H	29.921137	7.385836	27.146161
H	9.847446	3.169729	22.676912	H	43.132153	7.757364	27.099252
H	22.115784	2.849689	28.239717	H	41.664398	6.266861	25.854080
H	24.509703	2.285929	28.275398	H	30.587141	3.489108	24.325993
H	25.983279	3.028143	26.475247	H	44.726140	1.924889	23.222447
H	21.469865	5.218615	24.049312	H	35.450194	6.646231	30.389652
H	22.950491	5.901127	22.267826	H	31.302176	4.310944	29.419868
H	19.532040	2.329460	22.589907	H	29.391703	3.675890	30.758801
H	19.679264	1.794024	20.190520	H	31.291872	6.860973	17.596321
H	18.480489	3.170817	18.536724	H	40.762650	5.904749	21.514402
H	16.651512	6.145316	22.827135	H	41.205496	2.298119	23.000600
H	15.506946	7.501029	21.165187	H	53.552003	3.700202	28.381287
H	14.495591	7.508317	27.087429	H	55.987723	3.326161	28.455755
H	27.515324	7.862516	26.994084	H	57.384075	3.866347	26.497861
H	26.042652	6.398286	25.719286	H	52.703465	5.451763	24.014100
H	14.941519	3.634106	24.311133	H	54.081117	5.975897	22.116757
H	29.090976	2.069016	23.052181	H	50.777529	2.335081	22.589467
H	19.763787	6.924642	30.321714	H	50.920925	1.795288	20.189768
H	15.665798	4.545495	29.254934	H	49.720401	3.170977	18.535925
H	13.751339	3.846370	30.552277	H	47.862597	6.134555	22.823763
H	15.671692	6.861015	17.596372	H	46.741136	7.496768	21.164913
H	25.072102	6.039503	21.428862	H	45.548169	7.335162	27.193975
H	25.569095	2.436739	22.852331	H	46.223623	3.370662	24.471799
H	37.673663	2.816640	28.310760	H	50.986574	7.227494	30.247726
H	40.062844	2.245180	28.396730	H	47.058984	4.525022	29.327763
H	41.569245	2.948768	26.609055	H	45.215537	3.738459	30.677613

H	46.913313	6.862038	17.595733	H	35.815285	5.659183	39.708441
H	56.056209	5.977265	21.104179	H	37.325769	6.552014	37.995902
H	10.790982	8.128149	42.498338	H	33.460696	2.130963	38.273590
H	9.244447	6.787092	41.129966	H	33.575895	1.590588	35.820484
H	12.055455	2.324970	38.544175	H	32.556963	3.074166	34.173290
H	8.519403	3.171305	38.239510	H	30.868090	6.171417	38.520536
H	20.824964	2.982196	43.684838	H	29.741177	7.625206	36.864231
H	23.221176	2.446587	43.790651	H	28.714163	7.430514	43.016441
H	24.739966	3.204285	42.037243	H	41.886692	8.064809	42.723111
H	20.283976	5.393611	39.503147	H	40.400228	6.670177	41.387993
H	21.814254	6.087405	37.765189	H	29.406110	3.657830	40.089438
H	18.150975	2.393461	37.876894	H	43.408966	2.461914	38.498720
H	18.153499	1.917171	35.465284	H	33.941957	7.401888	45.708144
H	16.925109	3.347617	33.921665	H	35.325003	7.172680	32.786952
H	15.203057	6.214978	38.379019	H	33.401767	6.465792	34.113757
H	13.966217	7.594786	36.813520	H	30.269157	4.398514	44.839024
H	13.169370	7.511900	42.644912	H	28.403559	3.524524	46.160241
H	26.259133	7.893067	42.893632	H	28.381050	3.570388	32.808651
H	24.799339	6.528752	41.490396	H	29.794711	7.226221	33.442160
H	13.611949	3.633921	39.868251	H	39.418355	6.716261	37.267825
H	27.947986	2.313954	38.616593	H	39.884352	2.881789	38.323171
H	18.564705	6.961423	45.733293	H	52.223863	3.709906	43.947690
H	19.557715	7.484228	32.707139	H	54.659332	3.328160	44.019912
H	17.625082	6.729722	33.992320	H	56.055406	3.866631	42.061230
H	14.474489	4.505815	44.811293	H	51.374612	5.452702	39.579093
H	12.609926	3.794478	46.172030	H	52.752219	5.975683	37.680078
H	12.716350	3.682479	32.584410	H	49.630504	2.727632	38.021210
H	13.971696	7.223648	33.286681	H	49.733671	2.239967	35.615475
H	23.960312	6.246154	36.991284	H	48.465000	3.581708	34.026170
H	24.547195	2.689038	38.223119	H	46.485617	6.405093	38.405990
H	36.322056	2.724232	43.496936	H	45.217844	7.700138	36.793040
H	38.770177	2.168232	43.556109	H	44.296926	7.601416	42.802241
H	40.301160	3.122285	41.902454	H	44.926718	3.809019	39.834465

H	49.681887	7.224661	45.885903	H	12.954309	7.298460	48.772895
H	50.788394	7.829816	32.624093	H	22.420666	6.189215	52.490592
H	48.934929	6.978728	33.966221	H	22.941238	2.594305	53.847135
H	45.701837	4.639955	44.843860	H	35.104101	3.033456	59.329159
H	43.828921	3.855155	46.151367	H	37.489794	2.440412	59.369407
H	44.218565	3.575601	32.729032	H	38.961460	3.106885	57.539827
H	45.308053	7.270142	33.273427	H	34.477694	5.362436	55.117145
H	54.726518	5.972725	36.665982	H	35.958920	5.969372	53.304419
H	9.463382	8.127040	58.062938	H	32.593938	2.535875	53.505087
H	7.916937	6.786690	56.693565	H	32.724486	2.093006	51.092156
H	10.728186	2.325406	54.106682	H	31.487403	3.473237	49.510870
H	7.191576	3.170330	53.803812	H	29.497013	6.252034	53.915496
H	19.518893	2.934610	59.294488	H	28.247892	7.574692	52.304244
H	21.915542	2.380464	59.311234	H	27.296794	7.458201	58.232294
H	23.372988	3.135211	57.503723	H	40.496024	7.793120	58.178227
H	18.841088	5.359010	55.142669	H	39.032716	6.378355	56.845560
H	20.306176	6.050714	53.350309	H	27.961915	3.618324	55.334443
H	16.941353	2.461529	53.523153	H	42.088204	2.138947	54.046219
H	17.042838	1.990857	51.114370	H	32.787939	6.739530	61.409433
H	15.871852	3.418357	49.524834	H	33.685118	8.045585	48.122645
H	14.029356	6.326810	53.908989	H	31.889815	7.084782	49.480670
H	12.859674	7.709193	52.294409	H	28.748430	4.375670	60.399840
H	11.840563	7.509201	58.212320	H	26.897622	3.574758	61.718340
H	24.888817	7.926377	58.106509	H	27.470646	3.352504	48.171403
H	23.415628	6.487519	56.805255	H	28.374154	7.187975	48.772978
H	12.285083	3.636314	55.426780	H	38.075987	6.038984	52.443179
H	26.463352	2.223083	54.034971	H	38.568112	2.518200	53.843197
H	17.168294	6.739369	61.410620	H	50.894885	3.700084	59.506304
H	18.434582	7.516401	48.123853	H	53.331559	3.325528	59.581311
H	16.549267	6.750995	49.471789	H	54.727845	3.865735	57.623143
H	13.128808	4.376143	60.400560	H	50.047611	5.459292	55.145269
H	11.277806	3.574488	61.719256	H	51.424883	5.976993	53.243013
H	11.625158	3.659443	48.229875	H	48.392047	2.750795	53.471164

H	48.476825	2.307064	51.056422	H	44.238613	5.198840	65.267029
H	47.129270	3.620247	49.510665	H	48.274005	5.043193	18.026057
H	45.111748	6.294594	53.965694	C	32.766118	8.585356	39.331873
H	43.777950	7.572883	52.393704	C	33.208145	9.556260	40.357228
H	42.903973	7.338451	58.292031	C	34.531862	10.289463	40.224317
H	43.584712	3.522001	55.363261	C	35.171629	10.136374	38.831086
H	48.405659	6.744615	61.407908	C	35.064136	8.700645	38.298076
H	49.455983	7.784949	48.268900	C	33.595922	8.292855	38.104888
H	47.560418	6.953156	49.560686	O	33.329008	8.132781	40.573372
H	44.381318	4.364407	60.399389	C	30.038258	9.879727	42.631563
H	42.519309	3.571669	61.717702	C	29.336099	11.054848	42.970965
H	42.806376	3.655744	48.186960	C	29.423642	11.588770	44.259656
H	43.848703	7.225840	48.865735	C	30.203429	10.967052	45.242155
H	53.398691	5.970970	52.227763	C	30.902261	9.799464	44.909815
H	17.068265	7.157987	63.836008	C	30.829036	9.260555	43.623837
H	15.148107	6.357233	65.155559	N	29.997214	9.353294	41.340010
H	10.263169	3.421745	63.797076	H	34.376874	11.357585	40.459466
H	32.688224	7.158026	63.835097	H	32.428277	10.009033	40.982102
H	30.768021	6.357173	65.154687	H	31.688681	8.391958	39.252077
H	25.881770	3.424331	63.795669	H	36.227563	10.458280	38.872828
H	48.307513	7.159116	63.833759	H	34.662310	10.816583	38.119743
H	46.387752	6.357304	65.153493	H	35.601685	8.607366	37.336859
H	41.501161	3.425247	63.794418	H	35.547224	8.006168	39.008980
H	54.922549	4.682785	55.325786	H	33.150188	8.846194	37.255544
H	56.250090	4.683167	39.763715	H	33.503515	7.217682	37.874981
H	57.578895	4.683439	24.200639	H	35.209246	9.890417	41.002410
H	32.654274	5.043336	18.026522	H	28.719976	11.551847	42.212813
H	17.034867	5.043642	18.026671	H	28.869712	12.503833	44.498084
H	10.176549	4.915312	24.089625	H	30.264297	11.384960	46.251835
H	8.847993	4.915598	39.653310	H	31.514049	9.287711	45.660562
H	7.520561	4.915553	55.216445	H	31.391680	8.355677	43.382322
H	12.998950	5.198986	65.269020	H	30.218364	8.356639	41.272657
H	28.618763	5.198981	65.268146	H	29.180392	9.608607	40.791024

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C	12.487000	7.261000	26.395000	C	16.107910	6.659026	20.850045
C	11.616000	6.503000	25.622000	C	16.197885	6.355031	19.497042
C	12.086000	5.395000	24.927000	C	16.963875	5.274030	19.076025
C	13.428000	5.043000	25.007000	O	15.523872	7.185037	18.539057
C	13.027000	3.179000	23.539000	O	18.566867	5.529630	24.111016
C	11.685000	3.529000	23.460000	O	18.023068	3.388865	24.570326
C	11.215000	4.638000	24.154000	C	18.264899	4.337454	23.743465
O	10.782000	2.793000	22.654000	C	14.301000	5.801000	25.782000
Cu	18.541005	6.085547	26.019072	C	13.829000	6.909000	26.476000
Cu	17.952304	3.697441	26.526471	C	28.021199	7.174712	26.466282
C	22.218138	3.963576	26.392874	C	27.171709	6.306698	25.787129
C	22.749609	3.184297	27.436449	C	27.671539	5.165157	25.127232
C	24.106882	2.885553	27.482722	C	29.068273	4.899079	25.175052
C	24.958091	3.351830	26.485100	C	13.900000	3.935000	24.313000
C	24.464012	4.106708	25.403980	C	28.715845	2.960227	23.751745
C	23.074193	4.401754	25.343125	C	27.350933	3.185520	23.730352
C	22.576100	5.089841	24.215871	C	26.803103	4.292545	24.417520
C	23.436848	5.518355	23.208793	O	26.575441	2.270739	23.022203
C	24.804000	5.269994	23.287917	O	16.592685	6.402792	25.852021
C	25.329214	4.553561	24.372984	O	16.053524	4.263613	26.321043
O	25.651769	5.701147	22.273383	C	15.733683	5.460916	25.984876
O	20.435127	5.524410	26.197811	C	17.923420	5.802433	30.237103
O	19.918955	3.374875	26.645635	C	18.906488	6.584482	30.870694
C	20.771989	4.307335	26.419216	C	16.796475	5.357804	30.984231
C	18.226927	4.022014	22.293999	C	15.725262	4.668871	30.376182
C	18.992915	2.941012	21.873981	C	14.641583	4.232146	31.134056
C	19.081890	2.638017	20.519979	O	18.425286	6.399434	27.984244
C	18.404876	3.417023	19.587993	O	17.904642	4.251133	28.432477
C	17.639888	4.497024	20.008011	C	18.097412	5.464570	28.800139
C	17.550913	4.800019	21.362013	Cu	34.183736	6.119025	26.005245
C	16.783924	5.881020	21.784030	Cu	33.620026	3.737715	26.564834
				C	37.869834	3.986729	26.375881
				C	38.396831	3.282890	27.474228

C	39.742103	2.937671	27.520812	C	44.380974	2.748001	23.713349
C	40.585187	3.280940	26.469041	C	43.014643	2.962119	23.648518
C	40.095310	3.963911	25.338748	C	42.433023	4.050963	24.337522
C	38.716552	4.306855	25.279671	O	42.271368	2.048041	22.906111
C	38.218908	4.924438	24.113343	O	32.214143	6.427886	25.911281
C	39.071937	5.230465	23.055697	O	31.718911	4.286265	26.413948
C	40.431823	4.939539	23.130555	C	31.370527	5.476623	26.088518
C	40.956309	4.299452	24.263263	C	33.757985	5.920884	30.246000
O	41.273369	5.259549	22.070924	C	34.799065	6.690703	30.797714
O	36.090258	5.554975	26.130365	C	32.638904	5.580536	31.056704
O	35.579976	3.418910	26.647054	C	31.530366	4.880404	30.537105
C	36.428909	4.343684	26.387627	C	30.443217	4.572520	31.351618
C	33.846854	4.021972	22.293718	O	34.140415	6.459722	27.964015
C	34.612831	2.940969	21.873683	O	33.622380	4.324151	28.471587
C	34.701781	2.637978	20.519678	C	33.845740	5.542401	28.810118
C	34.024753	3.416989	19.587708	Cu	49.700141	6.207575	25.980832
C	33.259776	4.496991	20.007741	Cu	49.346534	3.791293	26.560551
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.162978	5.545891	24.103370	C	53.770890	5.287813	24.113936
O	33.652866	3.405857	24.595376	C	54.557834	5.591815	23.007897
C	33.879930	4.345752	23.750071	C	55.929834	5.377800	23.052821
C	29.922427	5.762612	25.916003	C	56.515889	4.858782	24.200784
C	29.383588	6.908012	26.529164	O	56.643771	5.617805	21.841785
C	43.549375	6.898537	26.487857	O	51.642672	5.838949	26.127013
C	42.735479	6.038763	25.759858	O	51.338324	3.661582	26.634248
C	43.270083	4.916598	25.092428	C	52.096362	4.667229	26.380447
C	44.668874	4.667356	25.175299	C	49.466779	4.021876	22.293156
C	29.574601	3.800110	24.451687	C	50.232745	2.940872	21.873104

C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.241501	6.036945	41.546083
C	48.879661	4.496905	20.007192	Cu	16.615839	3.659841	42.056808
C	48.790737	4.799893	21.361200	C	20.882005	3.859849	42.086796
C	48.023772	5.880897	21.783251	C	21.338337	3.174692	43.227660
C	47.347731	6.658913	20.849295	C	22.684318	2.861612	43.380907
C	47.437655	6.354926	19.496287	C	23.599134	3.217649	42.394810
C	48.203620	5.273922	19.075235	C	23.181620	3.873379	41.221634
O	46.763613	7.184943	18.538331	C	21.803501	4.184743	41.054190
O	49.738719	5.591850	24.085275	C	21.382646	4.778226	39.846567
O	49.388331	3.427566	24.604383	C	22.306485	5.078770	38.848020
C	49.528321	4.370170	23.746340	C	23.661212	4.812011	39.027049
C	45.489980	5.537977	25.942993	C	24.109894	4.211957	40.209666
C	44.912923	6.654505	26.575649	O	24.570478	5.118704	38.022835
C	45.209176	3.583603	24.455339	O	19.132926	5.439097	41.731471
O	47.720903	6.342657	25.876978	O	18.570283	3.307804	42.211888
O	47.395650	4.176003	26.411962	C	19.443563	4.223995	42.004420
C	46.954545	5.335584	26.081153	C	16.906896	4.010773	37.810476
C	49.193466	5.991037	30.213388	C	17.602708	2.896260	37.309653
C	50.127770	6.845494	30.826194	C	17.631427	2.630696	35.945859
C	48.091309	5.503492	30.969836	C	16.963172	3.469068	35.058456
C	47.066912	4.733823	30.378465	C	16.225487	4.579485	35.519129
C	46.004240	4.260397	31.143681	C	16.179739	4.842805	36.915763
O	49.604101	6.568142	27.938381	C	15.381740	5.907688	37.380758
O	49.297833	4.393382	28.453837	C	14.690933	6.714781	36.484084
C	49.382682	5.629761	28.784900	C	14.759440	6.494033	35.119777
C	11.158286	7.260970	41.959133	C	15.531763	5.424546	34.611418
C	10.287269	6.502976	41.186145	O	14.059371	7.380821	34.305508
C	10.757253	5.394976	40.491133	O	17.264824	5.485181	39.639212
C	12.099253	5.042971	40.571108	O	16.712277	3.345295	40.090198
C	11.698221	3.178978	39.103109	C	16.966393	4.295140	39.265832
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108

C	26.533421	7.057596	42.403616	C	37.394387	4.139684	40.728007
C	25.766348	6.116505	41.749316	C	36.887413	4.931877	39.658046
C	26.344264	4.963786	41.124995	C	37.725712	5.458146	38.703617
C	27.772531	4.795193	41.237840	C	39.128411	5.234507	38.765192
C	12.571237	3.934972	39.877096	C	39.668822	4.427088	39.766501
C	27.612666	2.750519	39.929658	O	39.945478	5.803709	37.835746
C	26.205987	2.910422	39.806734	O	34.991822	5.409547	41.821988
C	25.565888	3.999642	40.389745	O	34.220044	3.359834	42.228461
O	25.611122	1.914062	39.086308	C	35.151227	4.173034	41.935613
O	15.285141	6.385438	41.388429	C	32.721047	4.965344	38.041689
O	14.725657	4.250481	41.846590	C	33.467221	3.850650	37.695292
C	14.412868	5.454493	41.529824	C	33.599455	3.484383	36.340333
C	16.627454	5.788161	45.760711	C	32.951727	4.203667	35.357165
C	17.642660	6.538396	46.382440	C	32.142298	5.346404	35.660061
C	18.817970	6.880438	32.225938	C	32.046142	5.741902	37.043999
C	17.744556	6.406726	32.973664	C	31.233323	6.865717	37.374760
C	16.721284	5.646829	32.374439	C	30.562004	7.559136	36.401687
C	15.481144	5.407086	46.512151	C	30.651792	7.180210	35.035602
C	14.386278	4.746924	45.915329	C	31.427649	6.088898	34.653367
C	13.282441	4.373720	46.678102	O	29.924003	7.988404	34.208322
C	14.589532	4.470455	32.504475	O	32.764563	6.499318	39.850571
C	15.616346	5.187413	33.135249	O	32.449441	4.304020	40.272885
O	13.501162	4.029488	33.249154	C	32.627551	5.289046	39.502721
O	17.134179	6.356631	43.507081	C	28.541041	5.798795	41.914056
O	16.557842	4.224184	43.963201	C	27.933560	6.914646	42.466287
C	16.783951	5.434032	44.326317	C	42.205334	6.872666	42.214557
Cu	32.544664	7.264024	41.663507	C	41.399114	6.055545	41.428491
Cu	32.522556	4.342448	42.244788	C	41.955380	5.035491	40.630564
C	36.545037	3.631734	41.767309	C	43.363604	4.830664	40.656886
C	37.042673	2.760705	42.716594	C	28.373792	3.662259	40.614781
C	38.416188	2.421868	42.715707	C	43.100904	3.053685	39.021144
C	39.273905	2.963602	41.782677	C	41.727997	3.227796	39.005215
C	38.802718	3.842361	40.752768	C	41.135261	4.226477	39.804362

O	40.992804	2.372784	38.189582	C	50.772469	4.699939	41.949646
O	30.655887	6.799398	41.763502	C	48.256208	4.297270	37.816198
O	30.579259	4.635766	42.334775	C	49.051335	3.245871	37.325946
C	30.032407	5.727977	42.006917	C	49.121660	2.982032	35.964015
C	32.450026	6.542046	45.856840	C	48.396290	3.758355	35.066164
C	33.274217	7.436596	46.512533	C	47.563980	4.805628	35.513446
C	34.764470	7.092153	32.127464	C	47.478375	5.068312	36.908946
C	33.682863	6.747521	32.930425	C	46.591133	6.066838	37.358690
C	32.607937	5.996993	32.417815	C	45.851686	6.814648	36.449032
C	31.382580	5.878036	46.547943	C	45.954006	6.594122	35.086552
C	30.464531	5.015403	45.881153	C	46.812905	5.585569	34.592991
C	29.430079	4.421018	46.562176	O	45.196222	7.419344	34.259178
C	30.423302	4.956096	32.689268	O	48.435868	5.784696	39.665038
C	31.494130	5.677631	33.230242	O	48.119434	3.591930	40.086744
O	29.322051	4.659610	33.482073	C	48.269162	4.574157	39.274954
O	32.787067	7.282447	43.638204	C	44.175600	5.648201	41.489799
O	32.748948	5.062852	44.057839	C	43.579789	6.677772	42.239250
C	32.679978	6.276433	44.398717	C	43.921017	3.840327	39.824565
Cu	48.396665	6.300381	41.583816	O	46.412793	6.459851	41.480703
Cu	48.016682	3.863616	42.057702	O	46.074919	4.265097	41.876932
C	52.242278	4.464620	41.931334	C	45.641105	5.443950	41.616464
C	52.828353	3.947597	43.079285	C	47.861159	5.935822	45.792557
C	54.201353	3.732577	43.123183	C	48.824439	6.739398	46.429629
C	54.987278	4.036581	42.018131	C	50.016371	7.174395	32.172478
C	54.401203	4.554604	40.869180	C	48.967301	6.662746	32.930481
C	53.028203	4.768624	40.826281	C	47.992051	5.828605	32.350455
C	52.442128	5.287648	39.677330	C	46.725935	5.491793	46.524974
C	53.229054	5.591652	38.571278	C	45.680930	4.770082	45.910581
C	54.601054	5.377632	38.616177	C	44.583302	4.342631	46.653515
C	55.187129	4.858609	39.764128	C	45.930286	4.536226	32.506076
O	55.314970	5.617639	37.405129	C	46.911648	5.327656	33.120553
O	50.338489	5.886306	41.720010	O	44.865389	4.053960	33.259086
O	49.998209	3.702612	42.175703	O	48.299677	6.576451	43.548833

O	47.925684	4.392794	43.975672	C	13.380728	6.875095	52.012272
C	48.044583	5.613345	44.355332	C	13.439659	6.648478	50.648152
C	9.830848	7.260896	57.522290	C	14.221054	5.586363	50.137745
C	8.959816	6.502907	56.749315	O	12.723895	7.524711	49.836146
C	9.429783	5.394908	56.054291	O	15.941089	5.642761	55.206557
C	10.771783	5.042898	56.134241	O	15.428636	3.478859	55.584991
C	10.370718	3.178911	54.666243	C	15.671739	4.457959	54.793441
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.317185	7.079411	57.558387
Cu	15.892571	6.129113	57.135570	C	24.479463	6.245554	56.825708
Cu	15.336776	3.718257	57.557746	C	24.990069	5.137637	56.117911
C	19.590647	4.027466	57.441808	C	26.387662	4.874947	56.165058
C	20.139638	3.263088	58.486987	C	11.243751	3.934900	55.440217
C	21.493968	2.949361	58.504205	C	26.055805	3.009551	54.642730
C	22.323244	3.384055	57.474489	C	24.689322	3.227966	54.623157
C	21.810178	4.126905	56.393467	C	24.130456	4.296264	55.361240
C	20.423547	4.439838	56.364746	O	23.923249	2.340896	53.870891
C	19.903904	5.119991	55.242836	O	13.936631	6.427924	56.975039
C	20.741511	5.515351	54.203052	O	13.428930	4.268725	57.377123
C	22.107119	5.248878	54.249066	C	13.088397	5.472720	57.087646
C	22.653514	4.546746	55.333291	C	15.283046	5.695821	61.352095
O	22.932301	5.650852	53.204605	C	16.314087	6.385804	61.978046
O	17.796243	5.583138	57.300418	C	17.561855	6.869336	47.729617
O	17.302248	3.413307	57.672312	C	16.464285	6.463130	48.481202
C	18.144614	4.361982	57.482272	C	15.412745	5.732106	47.894850
C	15.640629	4.204372	53.331730	C	14.198081	5.242825	62.095148
C	16.359339	3.106164	52.826302	C	13.166040	4.552842	61.469196
C	16.385778	2.839322	51.463603	C	12.083075	4.099846	62.213249
C	15.690899	3.659043	50.580626	C	13.235852	4.644801	48.042867
C	14.938121	4.758670	51.043648	C	14.288800	5.333778	48.662236
C	14.898697	5.026302	52.440115	O	12.129439	4.262190	48.793123
C	14.089462	6.081285	52.907184	O	15.760635	6.374310	59.110960

O	15.280820	4.203286	59.484350	C	26.678842	6.813601	57.622880
C	15.446887	5.407598	59.895730	C	40.912483	6.945103	57.611651
Cu	31.474279	6.145566	57.138444	C	40.085211	6.123855	56.855795
Cu	30.968633	3.721595	57.552473	C	40.603974	5.025872	56.138085
C	35.209866	4.088117	57.458246	C	42.002767	4.764716	56.193007
C	35.751466	3.365493	58.536839	C	26.905259	3.816512	55.391698
C	37.099113	3.026789	58.562870	C	41.683130	2.912886	54.652960
C	37.929344	3.392877	57.508334	C	40.316577	3.133351	54.620195
C	37.425467	4.098170	56.398084	C	39.750285	4.195721	55.361781
C	36.045224	4.439937	56.362839	O	39.557673	2.250684	53.855690
C	35.533711	5.086211	55.218408	O	29.504281	6.409420	57.014829
C	36.373284	5.415849	54.157267	O	29.054305	4.229716	57.376541
C	37.733557	5.120847	54.206962	C	28.681571	5.430616	57.121563
C	38.272941	4.454988	55.317919	C	30.903120	5.695641	61.351269
O	38.560338	5.461562	53.142280	C	31.934175	6.385618	61.977205
O	33.394547	5.625351	57.276093	C	33.106267	7.665079	47.897083
O	32.933425	3.452123	57.671139	C	32.105506	7.025040	48.597334
C	33.761060	4.410980	57.475680	C	31.196960	6.120747	47.955832
C	31.295403	4.234979	53.324925	C	29.818167	5.242646	62.094340
C	32.099723	3.196107	52.823374	C	28.786113	4.552669	61.468405
C	32.210205	2.979291	51.455247	C	27.703159	4.099675	62.212476
C	31.515406	3.790221	50.563277	C	29.256995	4.628794	47.956525
C	30.668499	4.819163	51.022636	C	30.124504	5.467113	48.653993
C	30.543825	5.035507	52.422700	O	28.236605	4.007268	48.611685
C	29.649337	6.023479	52.880369	O	31.366724	6.380565	59.113218
C	28.932512	6.797924	51.973083	O	30.904188	4.204541	59.481237
C	29.073818	6.620915	50.607737	C	31.063894	5.409405	59.895328
C	29.945186	5.629581	50.113222	Cu	47.048987	6.244385	57.149430
O	28.339999	7.467450	49.782045	Cu	46.688733	3.789862	57.536779
O	31.507076	5.673086	55.206761	C	50.914829	4.464394	57.493750
O	31.070215	3.490891	55.575542	C	51.500923	3.947364	58.641689
C	31.285939	4.480646	54.788528	C	52.873923	3.732339	58.685563
C	27.230218	5.704126	56.956354	C	53.659830	4.036343	57.580498

C	53.073736	4.554373	56.431559	C	47.614518	6.605435	48.507003
C	51.700736	4.768398	56.388685	C	46.615308	5.815505	47.905011
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.497768	4.612753	48.016762
O	53.987445	5.617415	52.967495	C	45.502294	5.356012	48.654391
O	48.992472	5.856373	57.300794	O	43.398305	4.175656	48.746884
O	48.676948	3.652321	57.668811	O	46.917668	6.441386	59.125117
C	49.440179	4.670381	57.496804	O	46.577964	4.237028	59.466911
C	46.958343	4.348887	53.320600	C	46.674831	5.442384	59.893497
C	47.780011	3.327322	52.811093	C	16.262162	6.620790	63.347051
C	47.825382	3.063216	51.448779	C	15.179196	6.168795	64.090104
C	47.048804	3.809935	50.569659	C	14.147156	5.478812	63.465153
C	46.197873	4.834553	51.035646	C	12.031150	4.336833	63.582254
C	46.138101	5.096709	52.432497	C	13.063191	5.025817	64.207206
C	45.233668	6.069166	52.903219	O	10.943187	3.908837	64.361307
C	44.449602	6.792455	52.011117	C	31.882275	6.620600	63.346211
C	44.526507	6.574953	50.646234	C	30.799322	6.168606	64.089282
C	45.404706	5.592876	50.131766	C	29.767267	5.478629	63.464346
O	43.732712	7.384708	49.837444	C	27.651260	4.336658	63.581482
O	47.119184	5.792284	55.211222	C	28.683314	5.025635	64.206417
O	46.811675	3.585518	55.563773	O	26.563309	3.908663	64.360554
C	46.962128	4.591992	54.784206	C	47.502389	6.620356	63.345091
C	42.838408	5.593344	56.992114	C	46.419447	6.168363	64.088179
C	42.274027	6.685354	57.678079	C	45.387379	5.478391	63.463260
C	42.526894	3.713060	55.416331	C	43.271369	4.336426	63.580429
O	45.073265	6.391576	57.021074	C	44.303437	5.025398	64.205349
O	44.740521	4.186605	57.355219	O	42.183431	3.908432	64.359519
C	44.303101	5.371693	57.122718	H	12.119370	8.127103	26.935477
C	46.523195	5.695406	61.350162	H	10.572727	6.787268	25.566452
C	47.554262	6.385378	61.976082	H	13.377754	2.322876	22.980214
C	48.702647	7.067445	47.774274	H	9.846122	3.167855	22.675435

H	22.102474	2.821734	28.228025	H	41.681012	6.270420	25.708440
H	24.504043	2.292665	28.300132	H	30.634321	3.583016	24.399260
H	26.009213	3.104639	26.555995	H	44.798925	1.912701	23.168287
H	21.519485	5.291053	24.085747	H	35.645955	6.979279	30.183997
H	23.030247	6.048983	22.359269	H	31.478944	4.575232	29.498659
H	19.532148	2.329264	22.590171	H	29.606512	4.032809	30.929808
H	19.679021	1.794023	20.190610	H	31.291248	6.863217	17.594900
H	18.480548	3.170353	18.536430	H	40.796501	5.750651	21.329269
H	16.650249	6.140419	22.827024	H	41.288726	2.263069	22.885737
H	15.505628	7.501824	21.158911	H	53.552148	3.699851	28.381689
H	14.495782	7.508469	27.087682	H	55.987724	3.326094	28.455521
H	27.618183	8.056914	26.952720	H	57.384426	3.866088	26.498127
H	26.117482	6.545711	25.764969	H	52.704036	5.448100	24.015384
H	14.941677	3.638871	24.310055	H	54.083195	5.976006	22.116677
H	29.108464	2.114211	23.204351	H	50.778385	2.335037	22.589416
H	19.756287	6.952473	30.305618	H	50.920987	1.795422	20.189901
H	15.698463	4.474061	29.310672	H	49.720850	3.170558	18.535633
H	13.836722	3.701636	30.644881	H	47.862913	6.130289	22.823632
H	15.670377	6.862986	17.594960	H	46.740238	7.497712	21.158846
H	25.169504	6.227671	21.560124	H	45.533270	7.339930	27.143323
H	25.594119	2.493335	23.030786	H	46.271551	3.373026	24.442585
H	37.753609	3.008177	28.303520	H	50.956491	7.246041	30.251969
H	40.135207	2.400661	28.377825	H	47.062109	4.500907	29.320220
H	41.626244	2.994563	26.538326	H	45.234801	3.669170	30.667358
H	37.168790	5.166703	23.996965	H	46.912735	6.863905	17.594429
H	38.666968	5.706887	22.173891	H	56.063092	5.977865	21.099171
H	35.151422	2.330072	22.590899	H	10.790899	8.127462	42.499104
H	35.298699	1.793815	20.190412	H	9.244091	6.787402	41.130360
H	34.100181	3.170182	18.536189	H	12.049826	2.325142	38.541278
H	32.261822	6.137874	22.825956	H	8.517974	3.169198	38.238704
H	31.123245	7.500060	21.159045	H	20.640888	2.898646	44.011522
H	30.028761	7.587662	27.075446	H	23.023271	2.344811	44.272902
H	43.119565	7.763134	26.982939	H	24.640620	2.962839	42.549125

H	20.339150	5.000813	39.652300	H	40.332825	6.232831	41.443582
H	21.959578	5.530938	37.929141	H	29.453241	3.522154	40.676701
H	18.138062	2.239313	37.986620	H	43.532240	2.289896	38.387653
H	18.179153	1.771996	35.571806	H	34.062606	7.949857	45.954894
H	17.010888	3.230430	34.005029	H	35.578163	7.681075	32.538197
H	15.266442	6.122985	38.436023	H	33.685938	7.085654	33.959240
H	14.084172	7.533922	36.845217	H	30.573044	4.816173	44.814977
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H	14.358603	4.524213	44.855267	H	51.375279	5.450197	39.581159
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H	36.371321	2.372686	43.487306	H	45.177068	7.584170	36.798443
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H	35.815604	5.121802	39.586035	H	49.679106	7.108693	45.872720
H	37.310035	6.055390	37.883102	H	50.750262	7.827026	32.633846
H	33.944307	3.262554	38.483479	H	48.913766	6.937014	33.975833
H	34.205188	2.613818	36.069245	H	45.688679	4.538701	44.852005
H	33.061938	3.872062	34.319743	H	43.796488	3.789414	46.159993
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H 7.916605 6.787083 56.694063	H 32.843585 2.181437 51.081393
H 10.722410 2.324956 54.104727	H 31.631070 3.593129 49.505157
H 7.190376 3.168797 53.802850	H 29.480882 6.200760 53.936406
H 19.507729 2.919434 59.299049	H 28.248067 7.557075 52.327597
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H 23.371960 3.121702 57.520799	H 40.494279 7.790324 58.148336
H 18.847866 5.342427 55.145215	H 39.032387 6.365988 56.824472
H 20.319110 6.038024 53.356380	H 27.966437 3.606819 55.338434
H 16.908211 2.457548 53.500662	H 42.089228 2.101518 54.064583
H 16.947931 1.990822 51.087584	H 32.788421 6.739923 61.409690
H 15.732494 3.414271 49.528554	H 33.775067 8.358457 48.417075
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H 24.905777 7.934179 58.085088	H 27.739004 3.452013 47.989473
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H 16.435669 6.738015 49.527246	H 54.728193 3.865562 57.623768
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H 12.794754 7.302849 48.857450	H 48.464937 2.272584 51.070408
H 22.438971 6.174215 52.496703	H 47.106609 3.566435 49.518236
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H	44.382077	4.368277	60.399975	C	37.895022	7.061527	43.433889
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H	42.760239	3.619636	48.196860	C	39.518880	7.833953	45.069541
H	43.817511	7.167534	48.859142	C	38.945901	7.010323	46.045434
H	53.405536	5.972351	52.223367	C	37.836423	6.223214	45.711322
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H	15.148345	6.357534	65.155915	N	37.320125	7.137583	42.157692
H	10.258596	3.420391	63.803975	H	35.000331	9.413246	38.935267
H	32.688052	7.158042	63.835068	H	35.034046	7.299314	40.313730
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H	46.388350	6.357497	65.153875	H	37.628829	10.138744	41.585870
H	41.497299	3.423012	63.801422	H	36.799697	11.548508	42.272296
H	54.923364	4.683318	55.324879	H	35.011557	10.138270	43.216757
H	56.250908	4.683600	39.762528	H	36.549039	9.395563	43.668755
H	57.579678	4.683861	24.199224	H	36.632939	8.951492	39.471710
H	32.653505	5.044465	18.025502	H	39.430309	8.527851	43.016460
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H	10.175615	4.914249	24.088542	H	39.357445	6.986405	47.058975
H	8.847003	4.914442	39.652550	H	37.372878	5.578944	46.465364
H	7.519560	4.914412	55.215976	H	36.446080	5.624910	44.157474
H	12.997579	5.198435	65.269740	H	37.952290	7.400505	41.403756
H	28.617624	5.198373	65.268908	H	36.720217	6.343484	41.900708
H	44.237735	5.198152	65.267813				
H	48.273515	5.044295	18.025049	(R,R)-1-Int1			
C	35.444293	8.362606	42.178029	C	12.487000	7.261000	26.395000
C	35.054329	8.303079	40.761200	C	11.616000	6.503000	25.622000
C	35.654774	9.338588	39.821898	C	12.086000	5.395000	24.927000
C	35.838474	10.703514	40.498368	C	13.428000	5.043000	25.007000
C	36.628266	10.561451	41.807946	C	13.027000	3.179000	23.539000
C	35.907810	9.640745	42.803485	C	11.685000	3.529000	23.460000
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O	10.782000	2.793000	22.654000	C	28.021199	7.174712	26.466282
Cu	18.541005	6.085547	26.019072	C	27.171709	6.306698	25.787129
Cu	17.952304	3.697441	26.526471	C	27.671539	5.165157	25.127232
C	22.218138	3.963576	26.392874	C	29.068273	4.899079	25.175052
C	22.749609	3.184297	27.436449	C	13.900000	3.935000	24.313000
C	24.106882	2.885553	27.482722	C	28.715845	2.960227	23.751745
C	24.958091	3.351830	26.485100	C	27.350933	3.185520	23.730352
C	24.464012	4.106708	25.403980	C	26.803103	4.292545	24.417520
C	23.074193	4.401754	25.343125	O	26.575441	2.270739	23.022203
C	22.576100	5.089841	24.215871	O	16.592685	6.402792	25.852021
C	23.436848	5.518355	23.208793	O	16.053524	4.263613	26.321043
C	24.804000	5.269994	23.287917	C	15.733683	5.460916	25.984876
C	25.329214	4.553561	24.372984	C	17.923420	5.802433	30.237103
O	25.651769	5.701147	22.273383	C	18.906488	6.584482	30.870694
O	20.435127	5.524410	26.197811	C	16.796475	5.357804	30.984231
O	19.918955	3.374875	26.645635	C	15.725262	4.668871	30.376182
C	20.771989	4.307335	26.419216	C	14.641583	4.232146	31.134056
C	18.226927	4.022014	22.293999	O	18.425286	6.399434	27.984244
C	18.992915	2.941012	21.873981	O	17.904642	4.251133	28.432477
C	19.081890	2.638017	20.519979	C	18.097412	5.464570	28.800139
C	18.404876	3.417023	19.587993	Cu	34.183736	6.119025	26.005245
C	17.639888	4.497024	20.008011	Cu	33.620026	3.737715	26.564834
C	17.550913	4.800019	21.362013	C	37.869834	3.986729	26.375881
C	16.783924	5.881020	21.784030	C	38.396831	3.282890	27.474228
C	16.107910	6.659026	20.850045	C	39.742103	2.937671	27.520812
C	16.197885	6.355031	19.497042	C	40.585187	3.280940	26.469041
C	16.963875	5.274030	19.076025	C	40.095310	3.963911	25.338748
O	15.523872	7.185037	18.539057	C	38.716552	4.306855	25.279671
O	18.566867	5.529630	24.111016	C	38.218908	4.924438	24.113343
O	18.023068	3.388865	24.570326	C	39.071937	5.230465	23.055697
C	18.264899	4.337454	23.743465	C	40.431823	4.939539	23.130555
C	14.301000	5.801000	25.782000	C	40.956309	4.299452	24.263263
C	13.829000	6.909000	26.476000	O	41.273369	5.259549	22.070924

O	36.090258	5.554975	26.130365	C	32.638904	5.580536	31.056704
O	35.579976	3.418910	26.647054	C	31.530366	4.880404	30.537105
C	36.428909	4.343684	26.387627	C	30.443217	4.572520	31.351618
C	33.846854	4.021972	22.293718	O	34.140415	6.459722	27.964015
C	34.612831	2.940969	21.873683	O	33.622380	4.324151	28.471587
C	34.701781	2.637978	20.519678	C	33.845740	5.542401	28.810118
C	34.024753	3.416989	19.587708	Cu	49.700141	6.207575	25.980832
C	33.259776	4.496991	20.007741	Cu	49.346534	3.791293	26.560551
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.162978	5.545891	24.103370	C	53.770890	5.287813	24.113936
O	33.652866	3.405857	24.595376	C	54.557834	5.591815	23.007897
C	33.879930	4.345752	23.750071	C	55.929834	5.377800	23.052821
C	29.922427	5.762612	25.916003	C	56.515889	4.858782	24.200784
C	29.383588	6.908012	26.529164	O	56.643771	5.617805	21.841785
C	43.549375	6.898537	26.487857	O	51.642672	5.838949	26.127013
C	42.735479	6.038763	25.759858	O	51.338324	3.661582	26.634248
C	43.270083	4.916598	25.092428	C	52.096362	4.667229	26.380447
C	44.668874	4.667356	25.175299	C	49.466779	4.021876	22.293156
C	29.574601	3.800110	24.451687	C	50.232745	2.940872	21.873104
C	44.380974	2.748001	23.713349	C	50.321669	2.637885	20.519096
C	43.014643	2.962119	23.648518	C	49.644627	3.416901	19.587140
C	42.433023	4.050963	24.337522	C	48.879661	4.496905	20.007192
O	42.271368	2.048041	22.906111	C	48.790737	4.799893	21.361200
O	32.214143	6.427886	25.911281	C	48.023772	5.880897	21.783251
O	31.718911	4.286265	26.413948	C	47.347731	6.658913	20.849295
C	31.370527	5.476623	26.088518	C	47.437655	6.354926	19.496287
C	33.757985	5.920884	30.246000	C	48.203620	5.273922	19.075235
C	34.799065	6.690703	30.797714	O	46.763613	7.184943	18.538331

O	49.738719	5.591850	24.085275	C	21.382646	4.778226	39.846567
O	49.388331	3.427566	24.604383	C	22.306485	5.078770	38.848020
C	49.528321	4.370170	23.746340	C	23.661212	4.812011	39.027049
C	45.489980	5.537977	25.942993	C	24.109894	4.211957	40.209666
C	44.912923	6.654505	26.575649	O	24.570478	5.118704	38.022835
C	45.209176	3.583603	24.455339	O	19.132926	5.439097	41.731471
O	47.720903	6.342657	25.876978	O	18.570283	3.307804	42.211888
O	47.395650	4.176003	26.411962	C	19.443563	4.223995	42.004420
C	46.954545	5.335584	26.081153	C	16.906896	4.010773	37.810476
C	49.193466	5.991037	30.213388	C	17.602708	2.896260	37.309653
C	50.127770	6.845494	30.826194	C	17.631427	2.630696	35.945859
C	48.091309	5.503492	30.969836	C	16.963172	3.469068	35.058456
C	47.066912	4.733823	30.378465	C	16.225487	4.579485	35.519129
C	46.004240	4.260397	31.143681	C	16.179739	4.842805	36.915763
O	49.604101	6.568142	27.938381	C	15.381740	5.907688	37.380758
O	49.297833	4.393382	28.453837	C	14.690933	6.714781	36.484084
C	49.382682	5.629761	28.784900	C	14.759440	6.494033	35.119777
C	11.158286	7.260970	41.959133	C	15.531763	5.424546	34.611418
C	10.287269	6.502976	41.186145	O	14.059371	7.380821	34.305508
C	10.757253	5.394976	40.491133	O	17.264824	5.485181	39.639212
C	12.099253	5.042971	40.571108	O	16.712277	3.345295	40.090198
C	11.698221	3.178978	39.103109	C	16.966393	4.295140	39.265832
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.533421	7.057596	42.403616
Cu	17.241501	6.036945	41.546083	C	25.766348	6.116505	41.749316
Cu	16.615839	3.659841	42.056808	C	26.344264	4.963786	41.124995
C	20.882005	3.859849	42.086796	C	27.772531	4.795193	41.237840
C	21.338337	3.174692	43.227660	C	12.571237	3.934972	39.877096
C	22.684318	2.861612	43.380907	C	27.612666	2.750519	39.929658
C	23.599134	3.217649	42.394810	C	26.205987	2.910422	39.806734
C	23.181620	3.873379	41.221634	C	25.565888	3.999642	40.389745
C	21.803501	4.184743	41.054190	O	25.611122	1.914062	39.086308

O	15.285141	6.385438	41.388429	C	32.721047	4.965344	38.041689
O	14.725657	4.250481	41.846590	C	33.467221	3.850650	37.695292
C	14.412868	5.454493	41.529824	C	33.599455	3.484383	36.340333
C	16.627454	5.788161	45.760711	C	32.951727	4.203667	35.357165
C	17.642660	6.538396	46.382440	C	32.142298	5.346404	35.660061
C	18.817970	6.880438	32.225938	C	32.046142	5.741902	37.043999
C	17.744556	6.406726	32.973664	C	31.233323	6.865717	37.374760
C	16.721284	5.646829	32.374439	C	30.562004	7.559136	36.401687
C	15.481144	5.407086	46.512151	C	30.651792	7.180210	35.035602
C	14.386278	4.746924	45.915329	C	31.427649	6.088898	34.653367
C	13.282441	4.373720	46.678102	O	29.924003	7.988404	34.208322
C	14.589532	4.470455	32.504475	O	32.764563	6.499318	39.850571
C	15.616346	5.187413	33.135249	O	32.449441	4.304020	40.272885
O	13.501162	4.029488	33.249154	C	32.627551	5.289046	39.502721
O	17.134179	6.356631	43.507081	C	28.541041	5.798795	41.914056
O	16.557842	4.224184	43.963201	C	27.933560	6.914646	42.466287
C	16.783951	5.434032	44.326317	C	42.205334	6.872666	42.214557
Cu	32.544664	7.264024	41.663507	C	41.399114	6.055545	41.428491
Cu	32.522556	4.342448	42.244788	C	41.955380	5.035491	40.630564
C	36.545037	3.631734	41.767309	C	43.363604	4.830664	40.656886
C	37.042673	2.760705	42.716594	C	28.373792	3.662259	40.614781
C	38.416188	2.421868	42.715707	C	43.100904	3.053685	39.021144
C	39.273905	2.963602	41.782677	C	41.727997	3.227796	39.005215
C	38.802718	3.842361	40.752768	C	41.135261	4.226477	39.804362
C	37.394387	4.139684	40.728007	O	40.992804	2.372784	38.189582
C	36.887413	4.931877	39.658046	O	30.655887	6.799398	41.763502
C	37.725712	5.458146	38.703617	O	30.579259	4.635766	42.334775
C	39.128411	5.234507	38.765192	C	30.032407	5.727977	42.006917
C	39.668822	4.427088	39.766501	C	32.450026	6.542046	45.856840
O	39.945478	5.803709	37.835746	C	33.274217	7.436596	46.512533
O	34.991822	5.409547	41.821988	C	34.764470	7.092153	32.127464
O	34.220044	3.359834	42.228461	C	33.682863	6.747521	32.930425
C	35.151227	4.173034	41.935613	C	32.607937	5.996993	32.417815

C	31.382580	5.878036	46.547943	C	45.954006	6.594122	35.086552
C	30.464531	5.015403	45.881153	C	46.812905	5.585569	34.592991
C	29.430079	4.421018	46.562176	O	45.196222	7.419344	34.259178
C	30.423302	4.956096	32.689268	O	48.435868	5.784696	39.665038
C	31.494130	5.677631	33.230242	O	48.119434	3.591930	40.086744
O	29.322051	4.659610	33.482073	C	48.269162	4.574157	39.274954
O	32.787067	7.282447	43.638204	C	44.175600	5.648201	41.489799
O	32.748948	5.062852	44.057839	C	43.579789	6.677772	42.239250
C	32.679978	6.276433	44.398717	C	43.921017	3.840327	39.824565
Cu	48.396665	6.300381	41.583816	O	46.412793	6.459851	41.480703
Cu	48.016682	3.863616	42.057702	O	46.074919	4.265097	41.876932
C	52.242278	4.464620	41.931334	C	45.641105	5.443950	41.616464
C	52.828353	3.947597	43.079285	C	47.861159	5.935822	45.792557
C	54.201353	3.732577	43.123183	C	48.824439	6.739398	46.429629
C	54.987278	4.036581	42.018131	C	50.016371	7.174395	32.172478
C	54.401203	4.554604	40.869180	C	48.967301	6.662746	32.930481
C	53.028203	4.768624	40.826281	C	47.992051	5.828605	32.350455
C	52.442128	5.287648	39.677330	C	46.725935	5.491793	46.524974
C	53.229054	5.591652	38.571278	C	45.680930	4.770082	45.910581
C	54.601054	5.377632	38.616177	C	44.583302	4.342631	46.653515
C	55.187129	4.858609	39.764128	C	45.930286	4.536226	32.506076
O	55.314970	5.617639	37.405129	C	46.911648	5.327656	33.120553
O	50.338489	5.886306	41.720010	O	44.865389	4.053960	33.259086
O	49.998209	3.702612	42.175703	O	48.299677	6.576451	43.548833
C	50.772469	4.699939	41.949646	O	47.925684	4.392794	43.975672
C	48.256208	4.297270	37.816198	C	48.044583	5.613345	44.355332
C	49.051335	3.245871	37.325946	C	9.830848	7.260896	57.522290
C	49.121660	2.982032	35.964015	C	8.959816	6.502907	56.749315
C	48.396290	3.758355	35.066164	C	9.429783	5.394908	56.054291
C	47.563980	4.805628	35.513446	C	10.771783	5.042898	56.134241
C	47.478375	5.068312	36.908946	C	10.370718	3.178911	54.666243
C	46.591133	6.066838	37.358690	C	9.028718	3.528920	54.587293
C	45.851686	6.814648	36.449032	C	8.558750	4.637919	55.281317

O	8.125684	2.792932	53.781319	C	25.317185	7.079411	57.558387
Cu	15.892571	6.129113	57.135570	C	24.479463	6.245554	56.825708
Cu	15.336776	3.718257	57.557746	C	24.990069	5.137637	56.117911
C	19.590647	4.027466	57.441808	C	26.387662	4.874947	56.165058
C	20.139638	3.263088	58.486987	C	11.243751	3.934900	55.440217
C	21.493968	2.949361	58.504205	C	26.055805	3.009551	54.642730
C	22.323244	3.384055	57.474489	C	24.689322	3.227966	54.623157
C	21.810178	4.126905	56.393467	C	24.130456	4.296264	55.361240
C	20.423547	4.439838	56.364746	O	23.923249	2.340896	53.870891
C	19.903904	5.119991	55.242836	O	13.936631	6.427924	56.975039
C	20.741511	5.515351	54.203052	O	13.428930	4.268725	57.377123
C	22.107119	5.248878	54.249066	C	13.088397	5.472720	57.087646
C	22.653514	4.546746	55.333291	C	15.283046	5.695821	61.352095
O	22.932301	5.650852	53.204605	C	16.314087	6.385804	61.978046
O	17.796243	5.583138	57.300418	C	17.561855	6.869336	47.729617
O	17.302248	3.413307	57.672312	C	16.464285	6.463130	48.481202
C	18.144614	4.361982	57.482272	C	15.412745	5.732106	47.894850
C	15.640629	4.204372	53.331730	C	14.198081	5.242825	62.095148
C	16.359339	3.106164	52.826302	C	13.166040	4.552842	61.469196
C	16.385778	2.839322	51.463603	C	12.083075	4.099846	62.213249
C	15.690899	3.659043	50.580626	C	13.235852	4.644801	48.042867
C	14.938121	4.758670	51.043648	C	14.288800	5.333778	48.662236
C	14.898697	5.026302	52.440115	O	12.129439	4.262190	48.793123
C	14.089462	6.081285	52.907184	O	15.760635	6.374310	59.110960
C	13.380728	6.875095	52.012272	O	15.280820	4.203286	59.484350
C	13.439659	6.648478	50.648152	C	15.446887	5.407598	59.895730
C	14.221054	5.586363	50.137745	Cu	31.474279	6.145566	57.138444
O	12.723895	7.524711	49.836146	Cu	30.968633	3.721595	57.552473
O	15.941089	5.642761	55.206557	C	35.209866	4.088117	57.458246
O	15.428636	3.478859	55.584991	C	35.751466	3.365493	58.536839
C	15.671739	4.457959	54.793441	C	37.099113	3.026789	58.562870
C	11.644816	5.800887	56.909216	C	37.929344	3.392877	57.508334
C	11.172849	6.908886	57.603240	C	37.425467	4.098170	56.398084

C	36.045224	4.439937	56.362839	O	39.557673	2.250684	53.855690
C	35.533711	5.086211	55.218408	O	29.504281	6.409420	57.014829
C	36.373284	5.415849	54.157267	O	29.054305	4.229716	57.376541
C	37.733557	5.120847	54.206962	C	28.681571	5.430616	57.121563
C	38.272941	4.454988	55.317919	C	30.903120	5.695641	61.351269
O	38.560338	5.461562	53.142280	C	31.934175	6.385618	61.977205
O	33.394547	5.625351	57.276093	C	33.106267	7.665079	47.897083
O	32.933425	3.452123	57.671139	C	32.105506	7.025040	48.597334
C	33.761060	4.410980	57.475680	C	31.196960	6.120747	47.955832
C	31.295403	4.234979	53.324925	C	29.818167	5.242646	62.094340
C	32.099723	3.196107	52.823374	C	28.786113	4.552669	61.468405
C	32.210205	2.979291	51.455247	C	27.703159	4.099675	62.212476
C	31.515406	3.790221	50.563277	C	29.256995	4.628794	47.956525
C	30.668499	4.819163	51.022636	C	30.124504	5.467113	48.653993
C	30.543825	5.035507	52.422700	O	28.236605	4.007268	48.611685
C	29.649337	6.023479	52.880369	O	31.366724	6.380565	59.113218
C	28.932512	6.797924	51.973083	O	30.904188	4.204541	59.481237
C	29.073818	6.620915	50.607737	C	31.063894	5.409405	59.895328
C	29.945186	5.629581	50.113222	Cu	47.048987	6.244385	57.149430
O	28.339999	7.467450	49.782045	Cu	46.688733	3.789862	57.536779
O	31.507076	5.673086	55.206761	C	50.914829	4.464394	57.493750
O	31.070215	3.490891	55.575542	C	51.500923	3.947364	58.641689
C	31.285939	4.480646	54.788528	C	52.873923	3.732339	58.685563
C	27.230218	5.704126	56.956354	C	53.659830	4.036343	57.580498
C	26.678842	6.813601	57.622880	C	53.073736	4.554373	56.431559
C	40.912483	6.945103	57.611651	C	51.700736	4.768398	56.388685
C	40.085211	6.123855	56.855795	C	51.114643	5.287428	55.239746
C	40.603974	5.025872	56.138085	C	51.901549	5.591433	54.133681
C	42.002767	4.764716	56.193007	C	53.273549	5.377407	54.178555
C	26.905259	3.816512	55.391698	C	53.859642	4.858378	55.326493
C	41.683130	2.912886	54.652960	O	53.987445	5.617415	52.967495
C	40.316577	3.133351	54.620195	O	48.992472	5.856373	57.300794
C	39.750285	4.195721	55.361781	O	48.676948	3.652321	57.668811

C	49.440179	4.670381	57.496804	O	46.577964	4.237028	59.466911
C	46.958343	4.348887	53.320600	C	46.674831	5.442384	59.893497
C	47.780011	3.327322	52.811093	C	16.262162	6.620790	63.347051
C	47.825382	3.063216	51.448779	C	15.179196	6.168795	64.090104
C	47.048804	3.809935	50.569659	C	14.147156	5.478812	63.465153
C	46.197873	4.834553	51.035646	C	12.031150	4.336833	63.582254
C	46.138101	5.096709	52.432497	C	13.063191	5.025817	64.207206
C	45.233668	6.069166	52.903219	O	10.943187	3.908837	64.361307
C	44.449602	6.792455	52.011117	C	31.882275	6.620600	63.346211
C	44.526507	6.574953	50.646234	C	30.799322	6.168606	64.089282
C	45.404706	5.592876	50.131766	C	29.767267	5.478629	63.464346
O	43.732712	7.384708	49.837444	C	27.651260	4.336658	63.581482
O	47.119184	5.792284	55.211222	C	28.683314	5.025635	64.206417
O	46.811675	3.585518	55.563773	O	26.563309	3.908663	64.360554
C	46.962128	4.591992	54.784206	C	47.502389	6.620356	63.345091
C	42.838408	5.593344	56.992114	C	46.419447	6.168363	64.088179
C	42.274027	6.685354	57.678079	C	45.387379	5.478391	63.463260
C	42.526894	3.713060	55.416331	C	43.271369	4.336426	63.580429
O	45.073265	6.391576	57.021074	C	44.303437	5.025398	64.205349
O	44.740521	4.186605	57.355219	O	42.183431	3.908432	64.359519
C	44.303101	5.371693	57.122718	H	12.119370	8.127103	26.935477
C	46.523195	5.695406	61.350162	H	10.572727	6.787268	25.566452
C	47.554262	6.385378	61.976082	H	13.377754	2.322876	22.980214
C	48.702647	7.067445	47.774274	H	9.846122	3.167855	22.675435
C	47.614518	6.605435	48.507003	H	22.102474	2.821734	28.228025
C	46.615308	5.815505	47.905011	H	24.504043	2.292665	28.300132
C	45.438253	5.242413	62.093251	H	26.009213	3.104639	26.555995
C	44.406185	4.552442	61.467332	H	21.519485	5.291053	24.085747
C	43.323243	4.099449	62.211421	H	23.030247	6.048983	22.359269
C	44.497768	4.612753	48.016762	H	19.532148	2.329264	22.590171
C	45.502294	5.356012	48.654391	H	19.679021	1.794023	20.190610
O	43.398305	4.175656	48.746884	H	18.480548	3.170353	18.536430
O	46.917668	6.441386	59.125117	H	16.650249	6.140419	22.827024

H	15.505628	7.501824	21.158911	H	53.552148	3.699851	28.381689
H	14.495782	7.508469	27.087682	H	55.987724	3.326094	28.455521
H	27.618183	8.056914	26.952720	H	57.384426	3.866088	26.498127
H	26.117482	6.545711	25.764969	H	52.704036	5.448100	24.015384
H	14.941677	3.638871	24.310055	H	54.083195	5.976006	22.116677
H	29.108464	2.114211	23.204351	H	50.778385	2.335037	22.589416
H	19.756287	6.952473	30.305618	H	50.920987	1.795422	20.189901
H	15.698463	4.474061	29.310672	H	49.720850	3.170558	18.535633
H	13.836722	3.701636	30.644881	H	47.862913	6.130289	22.823632
H	15.670377	6.862986	17.594960	H	46.740238	7.497712	21.158846
H	25.169504	6.227671	21.560124	H	45.533270	7.339930	27.143323
H	25.594119	2.493335	23.030786	H	46.271551	3.373026	24.442585
H	37.753609	3.008177	28.303520	H	50.956491	7.246041	30.251969
H	40.135207	2.400661	28.377825	H	47.062109	4.500907	29.320220
H	41.626244	2.994563	26.538326	H	45.234801	3.669170	30.667358
H	37.168790	5.166703	23.996965	H	46.912735	6.863905	17.594429
H	38.666968	5.706887	22.173891	H	56.063092	5.977865	21.099171
H	35.151422	2.330072	22.590899	H	10.790899	8.127462	42.499104
H	35.298699	1.793815	20.190412	H	9.244091	6.787402	41.130360
H	34.100181	3.170182	18.536189	H	12.049826	2.325142	38.541278
H	32.261822	6.137874	22.825956	H	8.517974	3.169198	38.238704
H	31.123245	7.500060	21.159045	H	20.640888	2.898646	44.011522
H	30.028761	7.587662	27.075446	H	23.023271	2.344811	44.272902
H	43.119565	7.763134	26.982939	H	24.640620	2.962839	42.549125
H	41.681012	6.270420	25.708440	H	20.339150	5.000813	39.652300
H	30.634321	3.583016	24.399260	H	21.959578	5.530938	37.929141
H	44.798925	1.912701	23.168287	H	18.138062	2.239313	37.986620
H	35.645955	6.979279	30.183997	H	18.179153	1.771996	35.571806
H	31.478944	4.575232	29.498659	H	17.010888	3.230430	34.005029
H	29.606512	4.032809	30.929808	H	15.266442	6.122985	38.436023
H	31.291248	6.863217	17.594900	H	14.084172	7.533922	36.845217
H	40.796501	5.750651	21.329269	H	13.169252	7.508328	42.649159
H	41.288726	2.263069	22.885737	H	26.054240	7.927751	42.863351

H	24.684361	6.277134	41.708001	H	29.960940	7.710102	33.280328
H	13.612641	3.640435	39.863317	H	39.416184	6.294644	37.186283
H	28.068624	1.883439	39.444305	H	39.997555	2.532695	38.235350
H	18.509178	6.858050	45.813242	H	52.223642	3.704278	43.946438
H	19.589194	7.476647	32.702581	H	54.659165	3.326852	44.019235
H	17.710857	6.652999	34.026775	H	56.055723	3.866048	42.061517
H	14.358603	4.524213	44.855267	H	51.375279	5.450197	39.581159
H	12.458986	3.863865	46.198051	H	52.754484	5.976134	37.680116
H	12.840750	3.500867	32.698673	H	49.632256	2.637188	38.010803
H	14.128624	7.157653	33.326865	H	49.745884	2.172618	35.599941
H	24.146979	5.599568	37.242811	H	48.478342	3.521114	34.014661
H	24.655327	2.044177	38.986345	H	46.443070	6.274365	38.411344
H	36.371321	2.372686	43.487306	H	45.177068	7.584170	36.798443
H	38.805577	1.743596	43.481554	H	44.191222	7.320358	42.863983
H	40.336777	2.707456	41.831309	H	44.989987	3.668214	39.773240
H	35.815604	5.121802	39.586035	H	49.679106	7.108693	45.872720
H	37.310035	6.055390	37.883102	H	50.750262	7.827026	32.633846
H	33.944307	3.262554	38.483479	H	48.913766	6.937014	33.975833
H	34.205188	2.613818	36.069245	H	45.688679	4.538701	44.852005
H	33.061938	3.872062	34.319743	H	43.796488	3.789414	46.159993
H	31.142402	7.175639	38.415499	H	44.241647	3.469443	32.722654
H	29.931061	8.417059	36.649513	H	45.305348	7.205576	33.282013
H	28.550220	7.676128	42.949872	H	54.733421	5.973037	36.660950
H	41.762734	7.658933	42.814879	H	9.463506	8.126829	58.063134
H	40.332825	6.232831	41.443582	H	7.916605	6.787083	56.694063
H	29.453241	3.522154	40.676701	H	10.722410	2.324956	54.104727
H	43.532240	2.289896	38.387653	H	7.190376	3.168797	53.802850
H	34.062606	7.949857	45.954894	H	19.507729	2.919434	59.299049
H	35.578163	7.681075	32.538197	H	21.905318	2.366467	59.321703
H	33.685938	7.085654	33.959240	H	23.371960	3.121702	57.520799
H	30.573044	4.816173	44.814977	H	18.847866	5.342427	55.145215
H	28.730295	3.770235	46.024332	H	20.319110	6.038024	53.356380
H	28.639167	4.087164	33.007570	H	16.908211	2.457548	53.500662

H	16.947931	1.990822	51.087584	H	32.788421	6.739923	61.409690
H	15.732494	3.414271	49.528554	H	33.775067	8.358457	48.417075
H	13.980761	6.300379	53.962388	H	32.001760	7.228669	49.667866
H	12.766892	7.688281	52.374810	H	28.749314	4.379529	60.400407
H	11.840497	7.509056	58.213286	H	26.897626	3.574621	61.720244
H	24.905777	7.934179	58.085088	H	27.739004	3.452013	47.989473
H	23.425585	6.485198	56.802431	H	28.479278	7.284617	48.799238
H	12.285084	3.640674	55.426536	H	38.073877	5.967243	52.416946
H	26.456873	2.194068	54.056523	H	38.575402	2.467686	53.862477
H	17.168825	6.739444	61.410817	H	50.895049	3.699562	59.506766
H	18.356642	7.441993	48.196360	H	53.331422	3.325561	59.581254
H	16.435669	6.738015	49.527246	H	54.728193	3.865562	57.623768
H	13.128508	4.380832	60.401068	H	50.048142	5.455201	55.146464
H	11.277598	3.574663	61.721067	H	51.426938	5.977204	53.243093
H	11.453286	3.742541	48.253335	H	48.392173	2.734790	53.482802
H	12.794754	7.302849	48.857450	H	48.464937	2.272584	51.070408
H	22.438971	6.174215	52.496703	H	47.106609	3.566435	49.518236
H	22.941328	2.559820	53.882015	H	45.108848	6.276190	53.959179
H	35.116591	3.066232	59.364051	H	43.761295	7.542138	52.376858
H	37.503289	2.473202	59.403970	H	42.902941	7.338242	58.274127
H	38.971600	3.107165	57.559593	H	43.588195	3.501968	55.373732
H	34.483020	5.334704	55.122664	H	48.406274	6.744633	61.408085
H	35.957353	5.912580	53.291892	H	49.455858	7.684667	48.252912
H	32.659413	2.563509	53.504071	H	47.550999	6.883618	49.550597
H	32.843585	2.181437	51.081393	H	44.382077	4.368277	60.399975
H	31.631070	3.593129	49.505157	H	42.519429	3.571442	61.719562
H	29.480882	6.200760	53.936406	H	42.760239	3.619636	48.196860
H	28.248067	7.557075	52.327597	H	43.817511	7.167534	48.859142
H	27.314604	7.466896	58.211005	H	53.405536	5.972351	52.223367
H	40.494279	7.790324	58.148336	H	17.068094	7.157953	63.835986
H	39.032387	6.365988	56.824472	H	15.148345	6.357534	65.155915
H	27.966437	3.606819	55.338434	H	10.258596	3.420391	63.803975
H	42.089228	2.101518	54.064583	H	32.688052	7.158042	63.835068

H	30.768378	6.357485	65.155053	H	35.091866	7.556366	42.817679
H	25.877478	3.422597	63.802684	H	34.843569	11.133888	40.713960
H	48.307555	7.158926	63.833660	H	36.353253	11.399402	39.812276
H	46.388350	6.357497	65.153875	H	37.628829	10.138744	41.585870
H	41.497299	3.423012	63.801422	H	36.799697	11.548508	42.272296
H	54.923364	4.683318	55.324879	H	35.011557	10.138270	43.216757
H	56.250908	4.683600	39.762528	H	36.549039	9.395563	43.668755
H	57.579678	4.683861	24.199224	H	36.632939	8.951492	39.471710
H	32.653505	5.044465	18.025502	H	39.430309	8.527851	43.016460
H	17.033768	5.044633	18.025670	H	40.380462	8.462576	45.318211
H	10.175615	4.914249	24.088542	H	39.357445	6.986405	47.058975
H	8.847003	4.914442	39.652550	H	37.372878	5.578944	46.465364
H	7.519560	4.914412	55.215976	H	36.446080	5.624910	44.157474
H	12.997579	5.198435	65.269740	H	37.952290	7.400505	41.403756
H	28.617624	5.198373	65.268908	H	36.720217	6.343484	41.900708
H	44.237735	5.198152	65.267813				
H	48.273515	5.044295	18.025049				
C	35.444293	8.362606	42.178029	(R,R)-2-RC			
C	35.054329	8.303079	40.761200	C	12.487000	7.261000	26.395000
C	35.654774	9.338588	39.821898	C	11.616000	6.503000	25.622000
C	35.838474	10.703514	40.498368	C	12.086000	5.395000	24.927000
C	36.628266	10.561451	41.807946	C	13.428000	5.043000	25.007000
C	35.907810	9.640745	42.803485	C	13.027000	3.179000	23.539000
O	33.811435	8.689173	41.317916	C	11.685000	3.529000	23.460000
C	37.895022	7.061527	43.433889	C	11.215000	4.638000	24.154000
C	38.994145	7.868521	43.775285	O	10.782000	2.793000	22.654000
C	39.518880	7.833953	45.069541	Cu	18.543436	6.084805	26.013443
C	38.945901	7.010323	46.045434	Cu	17.946107	3.697792	26.528166
C	37.836423	6.223214	45.711322	C	22.207131	3.939446	26.373350
C	37.309458	6.243448	44.418383	C	22.750745	3.181819	27.426208
N	37.320125	7.137583	42.157692	C	24.102685	2.863274	27.451108
H	35.000331	9.413246	38.935267	C	24.935196	3.290294	26.421893
H	35.034046	7.299314	40.313730	C	24.428234	4.024842	25.332608
				C	23.043407	4.335953	25.292337

C	22.526771	5.001037	24.159562	O	16.596342	6.403264	25.847219
C	23.369981	5.389126	23.123287	O	16.053413	4.265038	26.319646
C	24.736466	5.129540	23.183135	C	15.735398	5.462569	25.983475
C	25.276748	4.437917	24.275765	C	17.902375	5.826218	30.223994
O	25.567939	5.524534	22.140947	C	18.892535	6.587126	30.871568
O	20.432955	5.514509	26.188006	C	16.745304	5.422980	30.947109
O	19.906511	3.369280	26.650012	C	15.671461	4.756402	30.318978
C	20.763546	4.295868	26.415403	C	14.559884	4.358957	31.055653
C	18.226927	4.022014	22.293999	O	18.430525	6.404695	27.972755
C	18.992915	2.941012	21.873981	O	17.894331	4.260719	28.429047
C	19.081890	2.638017	20.519979	C	18.093368	5.475700	28.791378
C	18.404876	3.417024	19.587993	Cu	34.092656	5.990628	26.097501
C	17.639888	4.497025	20.008011	Cu	33.543847	3.581651	26.546007
C	17.550017	4.800019	21.362013	C	37.800760	3.886650	26.434447
C	16.783924	5.881020	21.784030	C	38.323963	3.139277	27.505531
C	16.107910	6.659026	20.850045	C	39.673247	2.814053	27.558137
C	16.197885	6.355032	19.497042	C	40.524388	3.218994	26.536008
C	16.963876	5.274031	19.076025	C	40.040464	3.943405	25.430121
O	15.523872	7.185038	18.539057	C	38.659011	4.271305	25.366949
O	18.565823	5.527821	24.111054	C	38.167912	4.939359	24.225872
O	18.017878	3.388039	24.573350	C	39.030750	5.303324	23.196503
C	18.263378	4.335537	23.745083	C	40.392246	5.018428	23.273573
C	14.301000	5.801000	25.782000	C	40.909472	4.330425	24.379978
C	13.829000	6.909000	26.476000	O	41.241891	5.388756	22.236984
C	27.928247	6.998486	26.482974	O	36.000575	5.441752	26.228960
C	27.095466	6.156473	25.754705	O	35.506918	3.281208	26.651787
C	27.608111	5.038435	25.064532	C	36.350800	4.224954	26.443216
C	29.002341	4.772680	25.125469	C	33.846855	4.021974	22.293721
C	13.900000	3.935000	24.313000	C	34.612832	2.940971	21.873686
C	28.681730	2.891464	23.623522	C	34.701783	2.637980	20.519681
C	27.315032	3.111346	23.592494	C	34.024755	3.416991	19.587710
C	26.753329	4.188862	24.313815	C	33.259777	4.496993	20.007743
O	26.550591	2.217255	22.845818	C	33.170827	4.799985	21.361749

C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.105898	5.497417	24.167795	C	53.770890	5.287820	24.113942
O	33.615560	3.334182	24.570245	C	54.557834	5.591822	23.007903
C	33.845604	4.306591	23.763258	C	55.929834	5.377808	23.052827
C	29.839642	5.607422	25.916266	C	56.515890	4.858790	24.200790
C	29.287283	6.727681	26.562917	O	56.643771	5.617813	21.841791
C	43.550271	6.896540	26.586867	O	51.637646	5.837991	26.120883
C	42.720612	6.039220	25.875182	O	51.334207	3.662036	26.636203
C	43.239211	4.923049	25.186727	C	52.092790	4.667279	26.380273
C	44.638190	4.671101	25.236987	C	49.466780	4.021882	22.293161
C	29.525737	3.704713	24.368909	C	50.232747	2.940878	21.873109
C	44.316841	2.758408	23.777380	C	50.321671	2.637891	20.519101
C	42.949483	2.979485	23.737966	C	49.644629	3.416907	19.587145
C	42.385189	4.066573	24.442721	C	48.879663	4.496911	20.007197
O	42.186898	2.077597	22.998875	C	48.790739	4.799899	21.361205
O	32.126732	6.286133	25.981645	C	48.023773	5.880903	21.783256
O	31.641701	4.119836	26.379716	C	47.347732	6.658919	20.849300
C	31.288136	5.321677	26.101865	C	47.437657	6.354932	19.496292
C	33.562581	5.590818	30.325269	C	48.203622	5.273928	19.075240
C	34.586691	6.319230	30.958084	O	46.763615	7.184949	18.538336
C	32.420486	5.197687	31.080376	O	49.731242	5.591586	24.088742
C	31.326105	4.541203	30.480297	O	49.385064	3.426484	24.608743
C	30.218692	4.178906	31.242170	C	49.525274	4.368945	23.749559
O	34.009067	6.242306	28.073044	C	45.478031	5.539904	25.986921
O	33.496921	4.082036	28.472087	C	44.915028	6.653240	26.637668
C	33.700559	5.285250	28.871443	C	45.161977	3.587703	24.505092
Cu	49.695781	6.207181	25.981277	O	47.715720	6.340173	25.884775
Cu	49.343761	3.790233	26.564306	O	47.393477	4.172750	26.419204
C	53.571004	4.464799	26.367945	C	46.948604	5.334250	26.097989

C	49.205884	5.999653	30.215095	C	17.590367	3.037663	37.209212
C	50.152497	6.843404	30.823881	C	17.596874	2.766955	35.847835
C	48.095336	5.533565	30.972590	C	16.894726	3.590057	34.974459
C	47.063362	4.772110	30.384013	C	16.146408	4.688895	35.446402
C	45.993283	4.322214	31.151186	C	16.118586	4.952860	36.841345
O	49.608513	6.569455	27.935238	C	15.305812	5.999342	37.321551
O	49.296665	4.395920	28.455237	C	14.583692	6.790236	36.437014
C	49.388614	5.633100	28.784771	C	14.638902	6.573835	35.070237
C	11.158284	7.260965	41.959133	C	15.427414	5.522661	34.549843
C	10.287267	6.502972	41.186144	O	13.914380	7.449877	34.264871
C	10.757252	5.394972	40.491132	O	17.230064	5.617095	39.555659
C	12.099252	5.042967	40.571107	O	16.748081	3.458572	40.001404
C	11.698220	3.178974	39.103108	C	16.959574	4.420216	39.178876
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108
O	9.453203	2.792985	38.218146	C	26.684752	7.068801	42.312817
Cu	17.233239	6.153749	41.467023	C	25.867293	6.289980	41.519705
Cu	16.692489	3.752870	41.967575	C	26.375937	5.197368	40.743341
C	20.956380	4.082772	41.826761	C	27.789637	4.934149	40.826066
C	21.479081	3.326417	42.891548	C	12.571236	3.934968	39.877095
C	22.832877	3.022660	42.956276	C	27.535341	3.120234	39.228602
C	23.691270	3.460103	41.953797	C	26.135957	3.357737	39.151571
C	23.211811	4.197274	40.855346	C	25.547345	4.375114	39.899060
C	21.824410	4.500278	40.777497	O	25.493171	2.494882	38.310525
C	21.338613	5.175888	39.638765	O	15.269282	6.440147	41.352713
C	22.211452	5.571651	38.629335	O	14.778878	4.286845	41.805654
C	23.576051	5.311696	38.723438	C	14.425678	5.484502	41.503139
C	24.086739	4.620341	39.827096	C	16.713324	5.841907	45.695717
O	24.431585	5.707130	37.703090	C	17.716063	6.613456	46.311376
O	19.142999	5.618941	41.598692	C	18.781304	6.903267	32.219181
O	18.662269	3.464140	42.061692	C	17.677331	6.468474	32.944032
C	19.501338	4.408619	41.831986	C	16.648206	5.728081	32.330248
C	16.881409	4.138507	37.721879	C	15.588299	5.421769	46.459920

C	14.507438	4.731311	45.871751	C	31.136189	5.405067	34.680245
C	13.423996	4.326512	46.645422	O	29.773539	7.434783	34.389133
C	14.486992	4.608061	32.423671	O	32.786413	5.463153	39.711776
C	15.518704	5.300928	33.071185	O	32.181902	3.364168	40.249706
O	13.372282	4.201754	33.148588	C	32.439299	4.282950	39.417025
O	17.159031	6.450622	43.433320	C	28.606679	5.762473	41.659837
O	16.662321	4.295640	43.878550	C	28.071702	6.815201	42.380840
C	16.857284	5.508540	44.251182	C	42.295393	7.232720	42.158116
Cu	32.876873	6.271331	41.544288	C	41.455484	6.431117	41.394305
Cu	32.328455	3.796075	42.176453	C	41.962071	5.356802	40.636650
C	36.508666	4.025501	41.807601	C	43.357137	5.082254	40.675525
C	37.005196	3.153221	42.759563	C	28.337598	3.876788	40.042658
C	38.382017	2.842239	42.786056	C	43.010326	3.266795	39.102380
C	39.239278	3.382733	41.851894	C	41.646354	3.507424	39.077729
C	38.771940	4.260050	40.819607	C	41.103372	4.559765	39.841045
C	37.366521	4.583411	40.801832	O	40.867908	2.659805	38.294298
C	36.877211	5.416093	39.754532	O	30.858559	6.455118	41.474383
C	37.724548	5.914975	38.794249	O	30.433954	4.354628	42.157350
C	39.116354	5.632108	38.825017	C	30.074275	5.502827	41.771640
C	39.644011	4.810665	39.819531	C	32.271732	6.061439	45.738783
O	39.935688	6.163060	37.875159	C	33.137188	6.975467	46.312448
O	34.730855	5.581134	41.711293	C	34.519867	6.619751	32.312799
O	34.251934	3.419380	42.122542	C	33.420897	6.212867	33.061084
C	35.053244	4.370770	41.879371	C	32.357585	5.508311	32.467443
C	32.362735	3.944990	37.961756	C	31.175969	5.513652	46.485239
C	32.993969	2.789627	37.536498	C	30.198457	4.661515	45.894997
C	33.057018	2.493295	36.158069	C	29.152089	4.168739	46.637028
C	32.478352	3.337537	35.233049	C	30.167439	4.458341	32.605396
C	31.774862	4.523574	35.623301	C	31.226087	5.128478	33.226619
C	31.710858	4.818417	37.031500	O	29.049973	4.100164	33.348289
C	30.956860	5.950671	37.456138	O	32.791453	6.588009	43.499787
C	30.332765	6.762888	36.545085	O	32.437219	4.430489	44.035064
C	30.427489	6.507584	35.150094	C	32.516706	5.661798	44.317996

Cu	48.447196	6.400713	41.587749	O	46.473326	6.618921	41.476721
Cu	47.997314	3.974343	42.058479	O	46.067134	4.436507	41.875870
C	52.242277	4.464616	41.931345	C	45.668363	5.629201	41.614207
C	52.828352	3.947593	43.079296	C	47.873829	6.039511	45.796982
C	54.201352	3.732573	43.123194	C	48.830463	6.846344	46.440167
C	54.987277	4.036578	42.018142	C	50.045140	7.184662	32.166100
C	54.401202	4.554601	40.869191	C	48.986589	6.695194	32.923586
C	53.028202	4.768621	40.826292	C	47.999893	5.871199	32.348890
C	52.442128	5.287645	39.677341	C	46.741103	5.582049	46.526458
C	53.229054	5.591649	38.571289	C	45.700259	4.858721	45.906057
C	54.601054	5.377629	38.616189	C	44.612287	4.410928	46.648765
C	55.187129	4.858606	39.764139	C	45.921713	4.611142	32.511612
O	55.314970	5.617636	37.405141	C	46.912593	5.392921	33.121153
O	50.372332	5.931473	41.729107	O	44.848358	4.152097	33.266807
O	49.973767	3.756088	42.179324	O	48.350750	6.676061	43.552918
C	50.775210	4.733646	41.957397	O	47.919535	4.501543	43.973004
C	48.267132	4.395455	37.817942	C	48.065561	5.718077	44.356971
C	49.053285	3.334876	37.333186	C	9.830844	7.260885	57.522289
C	49.116572	3.057477	35.974818	C	8.959813	6.502896	56.749314
C	48.390820	3.829969	35.075363	C	9.429780	5.394897	56.054290
C	47.567754	4.887132	35.516419	C	10.771780	5.042887	56.134240
C	47.492376	5.165572	36.907894	C	10.370715	3.178901	54.666241
C	46.620634	6.178530	37.354403	C	9.028715	3.528910	54.587291
C	45.881246	6.920925	36.442225	C	8.558747	4.637908	55.281315
C	45.970169	6.682368	35.080696	O	8.125681	2.792922	53.781316
C	46.817889	5.662289	34.592670	Cu	15.893546	6.138020	57.133923
O	45.215079	7.504644	34.246996	Cu	15.341354	3.724228	57.551286
O	48.478276	5.883205	39.668834	C	19.594781	4.040745	57.437265
O	48.096686	3.700340	40.090765	C	20.147981	3.277401	58.480965
C	48.279980	4.676554	39.278338	C	21.500976	2.962924	58.494400
C	44.206483	5.886142	41.485515	C	22.324370	3.397233	57.461116
C	43.657145	6.967346	42.198762	C	21.808171	4.139930	56.381711
C	43.867382	4.038344	39.879359	C	20.423047	4.452287	56.356174

C	19.897813	5.133193	55.237212	O	13.938891	6.431855	56.972272
C	20.732144	5.528433	54.196314	O	13.435047	4.270298	57.369153
C	22.098421	5.262935	54.239540	C	13.091675	5.475089	57.084547
C	22.647975	4.560495	55.320788	C	15.283042	5.695809	61.352094
O	22.920753	5.665212	53.193111	C	16.314083	6.385792	61.978046
O	17.795277	5.594841	57.299992	C	17.647087	6.928780	47.662112
O	17.304510	3.423555	57.670957	C	16.569966	6.488273	48.422721
C	18.146096	4.373755	57.482121	C	15.528953	5.737359	47.844280
C	15.685825	4.212374	53.322283	C	14.198077	5.242813	62.095147
C	16.411505	3.110369	52.835072	C	13.166036	4.552830	61.469195
C	16.472500	2.841207	51.474934	C	12.083071	4.099834	62.213248
C	15.802606	3.662325	50.575406	C	13.382962	4.597621	48.010829
C	15.040839	4.763639	51.017606	C	14.421833	5.313967	48.620706
C	14.970624	5.037012	52.410890	O	12.291327	4.190867	48.770068
C	14.159285	6.098985	52.857104	O	15.758650	6.378514	59.108000
C	13.475299	6.891630	51.943926	O	15.278126	4.206425	59.477097
C	13.559537	6.655582	50.581664	C	15.446276	5.410044	59.891887
C	14.344673	5.586714	50.093228	Cu	31.463163	6.145044	57.131260
O	12.860058	7.525851	49.748094	Cu	30.955701	3.721442	57.550789
O	15.947551	5.655519	55.205237	C	35.200797	4.083059	57.439952
O	15.439541	3.489646	55.578734	C	35.740951	3.344957	58.509040
C	15.689325	4.468918	54.788026	C	37.087597	3.006708	58.535223
C	11.644813	5.800876	56.909215	C	37.919043	3.390986	57.489437
C	11.172845	6.908875	57.603239	C	37.418670	4.112408	56.388515
C	25.302315	7.076492	57.572741	C	36.039166	4.451819	56.351773
C	24.469313	6.248580	56.829465	C	35.529206	5.113803	55.215608
C	24.982422	5.148000	56.112113	C	36.372877	5.461260	54.164900
C	26.378070	4.884830	56.161273	C	37.733970	5.168749	54.217216
C	11.243748	3.934890	55.440215	C	38.269586	4.486391	55.318639
C	26.054773	3.033124	54.624233	O	38.565112	5.526440	53.161779
C	24.687529	3.252522	54.600473	O	33.381433	5.621887	57.260155
C	24.126037	4.313433	55.346343	O	32.919442	3.449770	57.661395
O	23.921921	2.371556	53.839452	C	33.748654	4.407286	57.461577

C	31.252005	4.222725	53.316546	C	29.818163	5.242633	62.094342
C	32.031539	3.161969	52.821616	C	28.786109	4.552656	61.468406
C	32.109408	2.908831	51.459077	C	27.703155	4.099663	62.212477
C	31.400489	3.702438	50.564671	C	29.028995	4.466783	48.020746
C	30.578036	4.754456	51.014663	C	29.949699	5.308583	48.641929
C	30.494549	5.015083	52.409805	O	28.005178	3.929726	48.740412
C	29.632458	6.033620	52.861408	O	31.365104	6.379846	59.106653
C	28.905473	6.791583	51.949863	O	30.899419	4.204633	59.477416
C	29.000031	6.565254	50.586314	C	31.063446	5.409408	59.891489
C	29.836771	5.541736	50.099612	Cu	47.050931	6.251388	57.151014
O	28.259375	7.398830	49.752931	Cu	46.686615	3.795058	57.532586
O	31.483903	5.671003	55.198654	C	50.914826	4.464382	57.493755
O	31.044426	3.490736	55.575504	C	51.500920	3.947352	58.641694
C	31.256689	4.477727	54.783028	C	52.873920	3.732327	58.685568
C	27.216886	5.707562	56.962999	C	53.659827	4.036331	57.580503
C	26.662718	6.810268	57.637869	C	53.073733	4.554362	56.431564
C	40.912875	6.952107	57.633069	C	51.700733	4.768387	56.388690
C	40.085536	6.136866	56.872109	C	51.114640	5.287417	55.239751
C	40.602244	5.045964	56.142568	C	51.901547	5.591423	54.133687
C	41.999422	4.783105	56.192452	C	53.273547	5.377397	54.178561
C	26.900422	3.832391	55.383165	C	53.859639	4.858367	55.326499
C	41.678514	2.944749	54.640452	O	53.987443	5.617405	52.967501
C	40.311381	3.168268	54.609604	O	48.991607	5.859508	57.301162
C	39.747177	4.224242	55.360891	O	48.672392	3.655313	57.668263
O	39.548310	2.293495	53.839116	C	49.437846	4.672514	57.497813
O	29.494735	6.411473	57.016995	C	46.962186	4.367428	53.316311
O	29.043249	4.232345	57.383570	C	47.784108	3.348784	52.801771
C	28.670487	5.433873	57.128604	C	47.836269	3.095630	51.438619
C	30.903116	5.695628	61.351271	C	47.065825	3.852687	50.564016
C	31.934171	6.385605	61.977208	C	46.213442	4.873779	51.034620
C	32.987090	7.334607	47.669904	C	46.146744	5.124109	52.431560
C	31.973326	6.790464	48.429685	C	45.242747	6.093975	52.908362
C	31.026052	5.870005	47.874009	C	44.465669	6.826150	52.019770

C	44.548613	6.619871	50.652664	C	30.799317	6.168593	64.089284
C	45.426925	5.640830	50.134519	C	29.767262	5.478616	63.464348
O	43.761980	7.438198	49.844729	C	27.651255	4.336645	63.581483
O	47.121732	5.803477	55.214922	C	28.683309	5.025622	64.206418
O	46.812529	3.595539	55.560886	O	26.563304	3.908650	64.360554
C	46.965262	4.604166	54.783520	C	47.502385	6.620342	63.345096
C	42.836611	5.605463	56.996305	C	46.419443	6.168348	64.088184
C	42.273479	6.691174	57.692987	C	45.387375	5.478376	63.463264
C	42.523299	3.736928	55.408569	C	43.271365	4.336411	63.580432
O	45.076797	6.400703	57.023778	C	44.303433	5.025383	64.205353
O	44.741042	4.194577	57.350054	O	42.183428	3.908416	64.359522
C	44.304163	5.381782	57.123597	H	12.119254	8.127133	26.935666
C	46.523192	5.695393	61.350166	H	10.573032	6.786854	25.566333
C	47.554258	6.385364	61.976087	H	13.383763	2.323394	22.982316
C	48.707517	7.164406	47.786106	H	9.847446	3.169729	22.676912
C	47.625095	6.685348	48.514770	H	22.115784	2.849689	28.239717
C	46.632280	5.891490	47.908315	H	24.509703	2.285929	28.275398
C	45.438249	5.242399	62.093255	H	25.983279	3.028143	26.475247
C	44.406182	4.552428	61.467335	H	21.469865	5.218615	24.049312
C	43.323240	4.099435	62.211424	H	22.950491	5.901127	22.267826
C	44.530526	4.665274	48.015353	H	19.532040	2.329460	22.589907
C	45.527300	5.414240	48.655850	H	19.679264	1.794024	20.190520
O	43.440622	4.206414	48.746278	H	18.480489	3.170817	18.536724
O	46.921223	6.443748	59.124213	H	16.651512	6.145316	22.827135
O	46.573397	4.239341	59.461338	H	15.506946	7.501029	21.165187
C	46.675301	5.443884	59.890907	H	14.495591	7.508317	27.087429
C	16.262158	6.620778	63.347051	H	27.515324	7.862516	26.994084
C	15.179191	6.168782	64.090104	H	26.042652	6.398286	25.719286
C	14.147152	5.478800	63.465152	H	14.941519	3.634106	24.311133
C	12.031146	4.336820	63.582253	H	29.090976	2.069016	23.052181
C	13.063187	5.025805	64.207205	H	19.763787	6.924642	30.321714
O	10.943183	3.908824	64.361306	H	15.665798	4.545495	29.254934
C	31.882271	6.620587	63.346214	H	13.751339	3.846370	30.552277

H	15.671692	6.861015	17.596372	H	46.741136	7.496768	21.164913
H	25.072102	6.039503	21.428862	H	45.548169	7.335162	27.193975
H	25.569095	2.436739	22.852331	H	46.223623	3.370662	24.471799
H	37.673663	2.816640	28.310760	H	50.986574	7.227494	30.247726
H	40.062844	2.245180	28.396730	H	47.058984	4.525022	29.327763
H	41.569245	2.948768	26.609055	H	45.215537	3.738459	30.677613
H	37.116535	5.179340	24.106265	H	46.913313	6.862038	17.595733
H	38.630784	5.817281	22.332929	H	56.056209	5.977265	21.104179
H	35.146058	2.325290	22.590355	H	10.790982	8.128149	42.498338
H	35.297745	1.792953	20.190413	H	9.244447	6.787092	41.129966
H	34.099803	3.170470	18.536513	H	12.055455	2.324970	38.544175
H	32.267957	6.144862	22.826123	H	8.519403	3.171305	38.239510
H	31.125441	7.499989	21.165063	H	20.824964	2.982196	43.684838
H	29.921137	7.385836	27.146161	H	23.221176	2.446587	43.790651
H	43.132153	7.757364	27.099252	H	24.739966	3.204285	42.037243
H	41.664398	6.266861	25.854080	H	20.283976	5.393611	39.503147
H	30.587141	3.489108	24.325993	H	21.814254	6.087405	37.765189
H	44.726140	1.924889	23.222447	H	18.150975	2.393461	37.876894
H	35.450194	6.646231	30.389652	H	18.153499	1.917171	35.465284
H	31.302176	4.310944	29.419868	H	16.925109	3.347617	33.921665
H	29.391703	3.675890	30.758801	H	15.203057	6.214978	38.379019
H	31.291872	6.860973	17.596321	H	13.966217	7.594786	36.813520
H	40.762650	5.904749	21.514402	H	13.169370	7.511900	42.644912
H	41.205496	2.298119	23.000600	H	26.259133	7.893067	42.893632
H	53.552003	3.700202	28.381287	H	24.799339	6.528752	41.490396
H	55.987723	3.326161	28.455755	H	13.611949	3.633921	39.868251
H	57.384075	3.866347	26.497861	H	27.947986	2.313954	38.616593
H	52.703465	5.451763	24.014100	H	18.564705	6.961423	45.733293
H	54.081117	5.975897	22.116757	H	19.557715	7.484228	32.707139
H	50.777529	2.335081	22.589467	H	17.625082	6.729722	33.992320
H	50.920925	1.795288	20.189768	H	14.474489	4.505815	44.811293
H	49.720401	3.170977	18.535925	H	12.609926	3.794478	46.172030
H	47.862597	6.134555	22.823763	H	12.716350	3.682479	32.584410

H	13.971696	7.223648	33.286681	H	49.733671	2.239967	35.615475
H	23.960312	6.246154	36.991284	H	48.465000	3.581708	34.026170
H	24.547195	2.689038	38.223119	H	46.485617	6.405093	38.405990
H	36.322056	2.724232	43.496936	H	45.217844	7.700138	36.793040
H	38.770177	2.168232	43.556109	H	44.296926	7.601416	42.802241
H	40.301160	3.122285	41.902454	H	44.926718	3.809019	39.834465
H	35.815285	5.659183	39.708441	H	49.681887	7.224661	45.885903
H	37.325769	6.552014	37.995902	H	50.788394	7.829816	32.624093
H	33.460696	2.130963	38.273590	H	48.934929	6.978728	33.966221
H	33.575895	1.590588	35.820484	H	45.701837	4.639955	44.843860
H	32.556963	3.074166	34.173290	H	43.828921	3.855155	46.151367
H	30.868090	6.171417	38.520536	H	44.218565	3.575601	32.729032
H	29.741177	7.625206	36.864231	H	45.308053	7.270142	33.273427
H	28.714163	7.430514	43.016441	H	54.726518	5.972725	36.665982
H	41.886692	8.064809	42.723111	H	9.463382	8.127040	58.062938
H	40.400228	6.670177	41.387993	H	7.916937	6.786690	56.693565
H	29.406110	3.657830	40.089438	H	10.728186	2.325406	54.106682
H	43.408966	2.461914	38.498720	H	7.191576	3.170330	53.803812
H	33.941957	7.401888	45.708144	H	19.518893	2.934610	59.294488
H	35.325003	7.172680	32.786952	H	21.915542	2.380464	59.311234
H	33.401767	6.465792	34.113757	H	23.372988	3.135211	57.503723
H	30.269157	4.398514	44.839024	H	18.841088	5.359010	55.142669
H	28.403559	3.524524	46.160241	H	20.306176	6.050714	53.350309
H	28.381050	3.570388	32.808651	H	16.941353	2.461529	53.523153
H	29.794711	7.226221	33.442160	H	17.042838	1.990857	51.114370
H	39.418355	6.716261	37.267825	H	15.871852	3.418357	49.524834
H	39.884352	2.881789	38.323171	H	14.029356	6.326810	53.908989
H	52.223863	3.709906	43.947690	H	12.859674	7.709193	52.294409
H	54.659332	3.328160	44.019912	H	11.840563	7.509201	58.212320
H	56.055406	3.866631	42.061230	H	24.888817	7.926377	58.106509
H	51.374612	5.452702	39.579093	H	23.415628	6.487519	56.805255
H	52.752219	5.975683	37.680078	H	12.285083	3.636314	55.426780
H	49.630504	2.727632	38.021210	H	26.463352	2.223083	54.034971

H	17.168294	6.739369	61.410620	H	50.894885	3.700084	59.506304
H	18.434582	7.516401	48.123853	H	53.331559	3.325528	59.581311
H	16.549267	6.750995	49.471789	H	54.727845	3.865735	57.623143
H	13.128808	4.376143	60.400560	H	50.047611	5.459292	55.145269
H	11.277806	3.574488	61.719256	H	51.424883	5.976993	53.243013
H	11.625158	3.659443	48.229875	H	48.392047	2.750795	53.471164
H	12.954309	7.298460	48.772895	H	48.476825	2.307064	51.056422
H	22.420666	6.189215	52.490592	H	47.129270	3.620247	49.510665
H	22.941238	2.594305	53.847135	H	45.111748	6.294594	53.965694
H	35.104101	3.033456	59.329159	H	43.777950	7.572883	52.393704
H	37.489794	2.440412	59.369407	H	42.903973	7.338451	58.292031
H	38.961460	3.106885	57.539827	H	43.584712	3.522001	55.363261
H	34.477694	5.362436	55.117145	H	48.405659	6.744615	61.407908
H	35.958920	5.969372	53.304419	H	49.455983	7.784949	48.268900
H	32.593938	2.535875	53.505087	H	47.560418	6.953156	49.560686
H	32.724486	2.093006	51.092156	H	44.381318	4.364407	60.399389
H	31.487403	3.473237	49.510870	H	42.519309	3.571669	61.717702
H	29.497013	6.252034	53.915496	H	42.806376	3.655744	48.186960
H	28.247892	7.574692	52.304244	H	43.848703	7.225840	48.865735
H	27.296794	7.458201	58.232294	H	53.398691	5.970970	52.227763
H	40.496024	7.793120	58.178227	H	17.068265	7.157987	63.836008
H	39.032716	6.378355	56.845560	H	15.148107	6.357233	65.155559
H	27.961915	3.618324	55.334443	H	10.263169	3.421745	63.797076
H	42.088204	2.138947	54.046219	H	32.688224	7.158026	63.835097
H	32.787939	6.739530	61.409433	H	30.768021	6.357173	65.154687
H	33.685118	8.045585	48.122645	H	25.881770	3.424331	63.795669
H	31.889815	7.084782	49.480670	H	48.307513	7.159116	63.833759
H	28.748430	4.375670	60.399840	H	46.387752	6.357304	65.153493
H	26.897622	3.574758	61.718340	H	41.501161	3.425247	63.794418
H	27.470646	3.352504	48.171403	H	54.922549	4.682785	55.325786
H	28.374154	7.187975	48.772978	H	56.250090	4.683167	39.763715
H	38.075987	6.038984	52.443179	H	57.578895	4.683439	24.200639
H	38.568112	2.518200	53.843197	H	32.654274	5.043336	18.026522

H	17.034867	5.043642	18.026671	H	28.869712	12.503833	44.498084
H	10.176549	4.915312	24.089625	H	30.264297	11.384960	46.251835
H	8.847993	4.915598	39.653310	H	31.514049	9.287711	45.660562
H	7.520561	4.915553	55.216445	H	31.391680	8.355677	43.382322
H	12.998950	5.198986	65.269020	H	30.218364	8.356639	41.272657
H	28.618763	5.198981	65.268146	H	29.180392	9.608607	40.791024
H	44.238613	5.198840	65.267029				
H	48.274005	5.043193	18.026057	(R,R)-2-TS1			
C	32.766118	8.585356	39.331873	C	12.487000	7.261000	26.395000
C	33.208145	9.556260	40.357228	C	11.616000	6.503000	25.622000
C	34.531862	10.289463	40.224317	C	12.086000	5.395000	24.927000
C	35.171629	10.136374	38.831086	C	13.428000	5.043000	25.007000
C	35.064136	8.700645	38.298076	C	13.027000	3.179000	23.539000
C	33.595922	8.292855	38.104888	C	11.685000	3.529000	23.460000
O	33.329008	8.132781	40.573372	C	11.215000	4.638000	24.154000
C	30.038258	9.879727	42.631563	O	10.782000	2.793000	22.654000
C	29.336099	11.054848	42.970965	Cu	18.544279	6.105772	26.008872
C	29.423642	11.588770	44.259656	Cu	17.964883	3.717377	26.532327
C	30.203429	10.967052	45.242155	C	22.233558	3.998725	26.386746
C	30.902261	9.799464	44.909815	C	22.771881	3.222610	27.429515
C	30.829036	9.260555	43.623837	C	24.127927	2.921829	27.468605
N	29.997214	9.353294	41.340010	C	24.971200	3.382753	26.463274
H	34.376874	11.357585	40.459466	C	24.472402	4.135232	25.383398
H	32.428277	10.009033	40.982102	C	23.084060	4.432948	25.329614
H	31.688681	8.391958	39.252077	C	22.579242	5.121731	24.205725
H	36.227563	10.458280	38.872828	C	23.434667	5.543637	23.192807
H	34.662310	10.816583	38.119743	C	24.801917	5.290963	23.264258
H	35.601685	8.607366	37.336859	C	25.332373	4.576757	24.347121
H	35.547224	8.006168	39.008980	O	25.643722	5.714771	22.241802
H	33.150188	8.846194	37.255544	O	20.439462	5.553167	26.186142
H	33.503515	7.217682	37.874981	O	19.932160	3.405924	26.655588
H	35.209246	9.890417	41.002410	C	20.782719	4.339131	26.418818
H	28.719976	11.551847	42.212813	C	18.226927	4.022014	22.293999

C	18.992915	2.941012	21.873981	O	17.908434	4.287658	28.432540
C	19.081890	2.638017	20.519979	C	18.101348	5.504580	28.792073
C	18.404876	3.417023	19.587993	Cu	34.187548	6.093276	26.027318
C	17.639888	4.497024	20.008011	Cu	33.609913	3.710292	26.569607
C	17.550913	4.800019	21.362013	C	37.866918	3.935413	26.370051
C	16.783924	5.881020	21.784030	C	38.394922	3.217954	27.459489
C	16.107910	6.659026	20.850045	C	39.738360	2.868015	27.500580
C	16.197885	6.355031	19.497042	C	40.578829	3.219777	26.450787
C	16.963875	5.274030	19.076025	C	40.089849	3.915293	25.328704
O	15.523872	7.185037	18.539057	C	38.713271	4.263529	25.274624
O	18.567471	5.538558	24.106503	C	38.214960	4.897556	24.117499
O	18.037486	3.396819	24.578821	C	39.067227	5.208344	23.061981
C	18.271757	4.342388	23.745259	C	40.426408	4.910501	23.132036
C	14.301000	5.801000	25.782000	C	40.950758	4.258831	24.257050
C	13.829000	6.909000	26.476000	O	41.267062	5.236618	22.073552
C	28.019067	7.171843	26.474936	O	36.089663	5.514958	26.135322
C	27.174123	6.314573	25.778627	O	35.568397	3.381422	26.651733
C	27.674326	5.177987	25.111498	C	36.423703	4.301173	26.390885
C	29.067943	4.904408	25.169325	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.720919	2.982015	23.725598	C	34.701781	2.637978	20.519678
C	27.356647	3.215586	23.692710	C	34.024753	3.416989	19.587708
C	26.807825	4.316792	24.387460	C	33.259776	4.496991	20.007741
O	26.581266	2.312584	22.968529	C	33.170826	4.799983	21.361747
O	16.594635	6.411418	25.842996	C	32.403848	5.880986	21.783781
O	16.064610	4.271166	26.319390	C	31.727821	6.658997	20.849810
C	15.738471	5.466732	25.981513	C	31.817771	6.355005	19.496805
C	17.910086	5.856767	30.225733	C	32.583748	5.274002	19.075771
C	18.902857	6.612656	30.875705	O	31.143743	7.185016	18.538835
C	16.751368	5.456168	30.948761	O	34.152235	5.537873	24.119680
C	15.677649	4.790230	30.320158	O	33.644559	3.393922	24.597186
C	14.561571	4.401028	31.054717	C	33.873505	4.338737	23.756522
O	18.431319	6.433100	27.969401	C	29.919504	5.757510	25.926917

C	29.378782	6.898541	26.546945	O	56.643771	5.617805	21.841785
C	43.529478	6.865261	26.484029	O	51.634074	5.835802	26.127230
C	42.722695	6.002781	25.753171	O	51.335868	3.657895	26.637289
C	43.262053	4.881830	25.088625	C	52.092240	4.665201	26.382380
C	44.659703	4.634858	25.177768	C	49.466779	4.021876	22.293156
C	29.576606	3.808359	24.443105	C	50.232745	2.940872	21.873104
C	44.382330	2.711600	23.721985	C	50.321669	2.637885	20.519096
C	43.015418	2.926235	23.647796	C	49.644627	3.416901	19.587140
C	42.429413	4.014766	24.332281	C	48.879661	4.496905	20.007192
O	42.274717	2.012634	22.901386	C	48.790737	4.799893	21.361200
O	32.219311	6.415075	25.945059	C	48.023772	5.880897	21.783251
O	31.713190	4.269309	26.418451	C	47.347731	6.658913	20.849295
C	31.369534	5.465473	26.107299	C	47.437655	6.354926	19.496287
C	33.811975	5.851962	30.275666	C	48.203620	5.273922	19.075235
C	34.921071	6.505028	30.844694	O	46.763613	7.184943	18.538331
C	32.665085	5.599474	31.078891	O	49.728359	5.589578	24.092935
C	31.501941	5.010897	30.542453	O	49.389168	3.422110	24.607358
C	30.384542	4.802522	31.347135	C	49.525403	4.367069	23.750354
O	34.163080	6.414926	27.989860	C	45.476464	5.510704	25.945967
O	33.610897	4.282988	28.480679	C	44.892587	6.625519	26.575781
C	33.866368	5.492470	28.830656	C	45.205602	3.548065	24.466716
Cu	49.690003	6.199630	25.988408	O	47.709961	6.326551	25.886620
Cu	49.344786	3.780131	26.563651	O	47.393679	4.156722	26.414087
C	53.571003	4.464792	26.367939	C	46.945985	5.315816	26.087740
C	54.157058	3.947774	27.515902	C	49.175747	5.975622	30.222929
C	55.530059	3.732759	27.559826	C	50.103586	6.833903	30.840988
C	56.316002	4.036762	26.454787	C	48.068143	5.488188	30.972883
C	55.729946	4.554780	25.305823	C	47.053164	4.709965	30.376409
C	54.356947	4.768795	25.262899	C	45.985693	4.240444	31.135521
C	53.770890	5.287813	24.113936	O	49.596260	6.555093	27.945647
C	54.557834	5.591815	23.007897	O	49.291365	4.378898	28.456735
C	55.929834	5.377800	23.052821	C	49.374026	5.615346	28.791494
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133

C	10.287269	6.502976	41.186145	O	13.987970	7.532259	34.281308
C	10.757253	5.394976	40.491133	O	17.230553	5.538035	39.567347
C	12.099253	5.042971	40.571108	O	16.678916	3.392468	39.992274
C	11.698221	3.178978	39.103109	C	16.921240	4.354646	39.178015
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.461310	6.338926	43.333452
Cu	17.248081	6.055394	41.484280	C	25.740205	5.784109	42.296583
Cu	16.643137	3.667183	41.964091	C	26.356407	4.967979	41.291703
C	20.919392	3.860886	41.813057	C	27.782358	4.768093	41.390557
C	21.377118	2.944990	42.779967	C	12.571237	3.934972	39.877096
C	22.715957	2.582320	42.848539	C	27.720357	3.417153	39.371909
C	23.629974	3.129913	41.956910	C	26.312730	3.590709	39.273627
C	23.223027	4.039731	40.964565	C	25.622234	4.360515	40.207957
C	21.845815	4.384529	40.863285	O	25.770057	2.929697	38.208811
C	21.431469	5.209431	39.797144	O	15.287806	6.397946	41.371978
C	22.363492	5.728491	38.903924	O	14.746126	4.256416	41.820550
C	23.719595	5.450165	39.045579	C	14.420799	5.461852	41.518367
C	24.162872	4.602370	40.067487	C	16.727156	5.732402	45.709607
O	24.634858	5.983805	38.146911	C	17.751289	6.473626	46.328023
O	19.145208	5.462202	41.614352	C	18.792060	6.925534	32.224572
O	18.602796	3.316424	42.039841	C	17.685588	6.494807	32.948109
C	19.471056	4.236996	41.821559	C	16.653387	5.761325	32.332266
C	16.833735	4.090722	37.716433	C	15.581851	5.358085	46.467876
C	17.500330	2.967935	37.193659	C	14.485833	4.693889	45.877949
C	17.500387	2.711436	35.829312	C	13.380497	4.338124	46.644975
C	16.831544	3.568158	34.962526	C	14.485449	4.654472	32.421980
C	16.123190	4.688800	35.443345	C	15.520627	5.340141	33.071817
C	16.105915	4.943424	36.840824	O	13.366491	4.255237	33.144324
C	15.338295	6.020645	37.327689	O	17.183825	6.339743	43.451193
C	14.645120	6.843486	36.448329	O	16.639291	4.193707	43.882958
C	14.685836	6.629625	35.080473	C	16.863040	5.399694	44.263600
C	15.434043	5.553483	34.552583	Cu	33.618497	6.712434	41.630936

Cu	32.470593	4.057403	42.255018	C	41.979173	5.098407	40.481403
C	36.597268	3.660813	41.553002	C	43.380785	4.872483	40.556648
C	37.072097	2.675562	42.398705	C	28.436176	3.986757	40.391949
C	38.429372	2.287579	42.338075	C	43.154309	3.121122	38.890303
C	39.289172	2.886537	41.442427	C	41.785048	3.320690	38.821850
C	38.837757	3.881313	40.514377	C	41.178405	4.310996	39.618327
C	37.446022	4.249273	40.555860	O	41.065431	2.495382	37.962341
C	36.959985	5.166664	39.579935	O	30.642309	6.396447	42.604005
C	37.801631	5.712434	38.640900	O	30.548040	4.166774	42.505847
C	39.190421	5.413214	38.640997	C	30.008696	5.324645	42.524841
C	39.713090	4.510519	39.564761	C	32.784170	6.339411	45.796364
O	40.012402	6.011713	37.734639	C	33.634502	7.231962	46.424398
O	35.056522	5.419571	41.712038	C	34.926880	6.868575	32.185250
O	34.288669	3.339829	42.029386	C	33.816819	6.606802	32.979731
C	35.206159	4.164839	41.772171	C	32.672267	5.985093	32.447667
C	32.446368	4.616371	38.042378	C	31.658334	5.785610	46.498493
C	32.827579	3.338011	37.666522	C	30.700278	4.942575	45.866165
C	32.835533	2.973089	36.304762	C	29.588024	4.497663	46.537217
C	32.429754	3.869955	35.339247	C	30.394792	5.166808	32.691756
C	31.980837	5.188361	35.672582	C	31.530709	5.761316	33.250140
C	32.003277	5.565331	37.063555	O	29.267835	4.963897	33.477801
C	31.536443	6.863273	37.418257	O	33.457109	6.919414	43.605263
C	31.079575	7.737436	36.465751	O	32.893780	4.777011	44.035281
C	31.065127	7.380022	35.090842	C	33.064089	5.982995	44.363788
C	31.512585	6.126479	34.685573	Cu	48.398154	6.310315	41.571648
O	30.591874	8.373163	34.279006	Cu	48.007877	3.874889	42.047292
O	33.002833	6.073360	39.841809	C	52.242278	4.464620	41.931334
O	32.211708	4.013874	40.297727	C	52.828353	3.947597	43.079285
C	32.551753	4.937095	39.504981	C	54.201353	3.732577	43.123183
C	28.507170	5.389297	42.457460	C	54.987278	4.036581	42.018131
C	27.856399	6.150880	43.413806	C	54.401203	4.554604	40.869180
C	42.192177	6.912323	42.097923	C	53.028203	4.768624	40.826281
C	41.408246	6.116717	41.270775	C	52.442128	5.287648	39.677330

C	53.229054	5.591652	38.571278	C	45.675202	4.762199	45.909410
C	54.601054	5.377632	38.616177	C	44.582809	4.330262	46.655820
C	55.187129	4.858609	39.764128	C	45.900461	4.524292	32.496118
O	55.314970	5.617639	37.405129	C	46.874955	5.319536	33.114515
O	50.337208	5.890237	41.714517	O	44.830022	4.045403	33.242954
O	49.989217	3.708926	42.176743	O	48.294948	6.588339	43.535566
C	50.768511	4.703398	41.950141	O	47.907060	4.407193	43.963012
C	48.250786	4.302200	37.801807	C	48.030533	5.627877	44.343561
C	49.041792	3.249427	37.307107	C	9.830848	7.260896	57.522290
C	49.098036	2.978794	35.946779	C	8.959816	6.502907	56.749315
C	48.361178	3.749636	35.055132	C	9.429783	5.394908	56.054291
C	47.533146	4.798482	35.505488	C	10.771783	5.042898	56.134241
C	47.463530	5.069875	36.898826	C	10.370718	3.178911	54.666243
C	46.586014	6.074498	37.353853	C	9.028718	3.528920	54.587293
C	45.836076	6.815168	36.448617	C	8.558750	4.637919	55.281317
C	45.919224	6.582684	35.085796	O	8.125684	2.792932	53.781319
C	46.773993	5.573048	34.588715	Cu	15.894143	6.147587	57.132322
O	45.151520	7.400853	34.259965	Cu	15.351076	3.731734	57.545932
O	48.442508	5.791079	39.654325	C	19.608464	4.066879	57.416480
O	48.119765	3.599565	40.078233	C	20.170150	3.290182	58.446140
C	48.272067	4.580234	39.264046	C	21.525232	2.982885	58.449278
C	44.173013	5.671311	41.427680	C	22.342913	3.437053	57.420009
C	43.561713	6.697562	42.170635	C	21.819348	4.193139	56.354115
C	43.955038	3.880887	39.737059	C	20.432260	4.499705	56.338930
O	46.416846	6.475908	41.457384	C	19.900772	5.196529	55.232747
O	46.068163	4.282389	41.851539	C	20.729402	5.609456	54.194080
C	45.639020	5.462938	41.585084	C	22.096537	5.346906	54.226591
C	47.841763	5.953645	45.783981	C	22.653604	4.632122	55.295866
C	48.797391	6.768842	46.418839	O	22.912181	5.765811	53.181337
C	49.980776	7.169112	32.183727	O	17.798908	5.612738	57.295522
C	48.926122	6.659137	32.933016	O	17.318597	3.438998	57.662624
C	47.957944	5.819851	32.349831	C	18.156538	4.392769	57.471730
C	46.710131	5.502035	46.519324	C	15.678686	4.225204	53.315541

C	16.386341	3.111902	52.826267	C	13.166040	4.552842	61.469196
C	16.426690	2.832797	51.467505	C	12.083075	4.099846	62.213249
C	15.754288	3.654306	50.570978	C	13.333891	4.629821	48.006028
C	15.013443	4.769259	51.013985	C	14.390451	5.318078	48.618205
C	14.963876	5.053798	52.406181	O	12.222115	4.268168	48.758798
C	14.173096	6.131017	52.853197	O	15.758320	6.383215	59.108266
C	13.489018	6.925889	51.941604	O	15.284104	4.209217	59.473737
C	13.553876	6.678244	50.580271	C	15.447778	5.412678	59.890865
C	14.319137	5.595490	50.090817	Cu	31.479086	6.226884	57.140298
O	12.859977	7.554270	49.748451	Cu	30.962413	3.797448	57.506110
O	15.948997	5.668044	55.201306	C	35.209395	4.147389	57.434250
O	15.448916	3.500442	55.573071	C	35.747677	3.405272	58.501644
C	15.691941	4.481433	54.782404	C	37.090783	3.051969	58.519725
C	11.644816	5.800887	56.909216	C	37.919468	3.422025	57.466747
C	11.172849	6.908886	57.603240	C	37.420703	4.146905	56.367600
C	25.312328	7.170930	57.515370	C	36.046014	4.506440	56.341165
C	24.478796	6.337172	56.779526	C	35.538352	5.179833	55.210751
C	24.991292	5.231474	56.070733	C	36.378320	5.509886	54.151212
C	26.387511	4.968632	56.120999	C	37.734441	5.192616	54.191004
C	11.243751	3.934900	55.440217	C	38.269083	4.506565	55.290725
C	26.060940	3.105185	54.597976	O	38.561705	5.532801	53.126744
C	24.693916	3.325408	54.573585	O	33.396202	5.697529	57.278200
C	24.133301	4.391032	55.313026	O	32.924631	3.519070	57.630800
O	23.927846	2.442012	53.816300	C	33.758398	4.477659	57.456888
O	13.938297	6.435880	56.971788	C	31.340812	4.382221	53.282075
O	13.441100	4.272178	57.364271	C	32.088409	3.293620	52.796331
C	13.093424	5.476896	57.082528	C	32.210042	3.061735	51.433347
C	15.283046	5.695821	61.352095	C	31.578269	3.904840	50.527458
C	16.314087	6.385804	61.978046	C	30.791366	4.988884	50.964508
C	17.679544	6.806793	47.674342	C	30.663200	5.229620	52.360006
C	16.578615	6.416457	48.427624	C	29.837149	6.285623	52.793765
C	15.518635	5.694203	47.847460	C	29.185122	7.092773	51.867079
C	14.198081	5.242825	62.095148	C	29.313877	6.875323	50.505353

C	30.126428	5.825714	50.035196	Cu	47.050074	6.251607	57.146971
O	28.625689	7.738707	49.657727	Cu	46.683736	3.796362	57.529837
O	31.526579	5.794363	55.199049	C	50.914829	4.464394	57.493750
O	31.074236	3.609339	55.524902	C	51.500923	3.947364	58.641689
C	31.305134	4.610600	54.754721	C	52.873923	3.732339	58.685563
C	27.228171	5.797078	56.917009	C	53.659830	4.036343	57.580498
C	26.673142	6.905537	57.582894	C	53.073736	4.554373	56.431559
C	40.913311	6.974770	57.594690	C	51.700736	4.768398	56.388685
C	40.087014	6.160764	56.831990	C	51.114643	5.287428	55.239746
C	40.601575	5.060472	56.115562	C	51.901549	5.591433	54.133681
C	41.996260	4.786809	56.180185	C	53.273549	5.377407	54.178555
C	26.908053	3.909740	55.350182	C	53.859642	4.858378	55.326493
C	41.672237	2.935676	54.643463	O	53.987445	5.617415	52.967495
C	40.307912	3.173333	54.595213	O	48.990976	5.858924	57.297802
C	39.746113	4.239582	55.333495	O	48.670697	3.655349	57.666847
O	39.544858	2.301675	53.821711	C	49.437093	4.672171	57.496541
O	29.509902	6.498540	57.007529	C	46.953008	4.362430	53.309956
O	29.052446	4.314301	57.329927	C	47.763687	3.333158	52.797366
C	28.682448	5.520120	57.091800	C	47.801229	3.066088	51.436327
C	30.903120	5.695641	61.351269	C	47.025892	3.817123	50.561507
C	31.934175	6.385618	61.977205	C	46.185672	4.849300	51.028730
C	33.445039	7.557159	47.785711	C	46.136836	5.117989	52.423509
C	32.392098	7.019087	48.495057	C	45.249653	6.105086	52.896552
C	31.445088	6.136668	47.880646	C	44.468351	6.831582	52.006417
C	29.818167	5.242646	62.094340	C	44.529623	6.602006	50.641666
C	28.786113	4.552669	61.468405	C	45.394615	5.609595	50.126684
C	27.703159	4.099675	62.212476	O	43.736056	7.411596	49.832213
C	29.381179	4.820830	47.903571	O	47.120095	5.802377	55.209090
C	30.301672	5.618514	48.580848	O	46.809448	3.595469	55.557561
O	28.283935	4.342916	48.554002	C	46.961139	4.602843	54.778147
O	31.360934	6.420496	59.119220	C	42.833750	5.611188	56.982872
O	30.887613	4.239967	59.444707	C	42.271687	6.705604	57.667574
C	31.055533	5.435393	59.884453	C	42.517340	3.727220	55.412448

O	45.075782	6.403046	57.018498	C	44.303437	5.025398	64.205349
O	44.737413	4.197816	57.345665	O	42.183431	3.908432	64.359519
C	44.301464	5.385081	57.116600	H	12.119185	8.126906	26.935985
C	46.523195	5.695406	61.350162	H	10.573009	6.786731	25.566619
C	47.554262	6.385378	61.976082	H	13.382333	2.322297	22.983053
C	48.672821	7.103220	47.760685	H	9.847342	3.169286	22.676731
C	47.588431	6.635847	48.493342	H	22.129661	2.863612	28.226095
C	46.596709	5.834146	47.896111	H	24.530380	2.331705	28.285723
C	45.438253	5.242413	62.093251	H	26.021968	3.133797	26.527965
C	44.406185	4.552442	61.467332	H	21.522341	5.331294	24.082143
C	43.323243	4.099449	62.211421	H	23.023437	6.073682	22.344493
C	44.493467	4.612606	48.016809	H	19.533554	2.330748	22.589829
C	45.489285	5.370291	48.648664	H	19.680116	1.794647	20.190449
O	43.398584	4.170436	48.750605	H	18.480939	3.171035	18.536732
O	46.920354	6.444545	59.122059	H	16.652667	6.146055	22.827010
O	46.570133	4.240719	59.459188	H	15.507071	7.501615	21.163912
C	46.673999	5.444889	59.889484	H	14.495540	7.508496	27.087300
C	16.262162	6.620790	63.347051	H	27.614503	8.050017	26.967606
C	15.179196	6.168795	64.090104	H	26.121418	6.557937	25.749444
C	14.147156	5.478812	63.465153	H	14.941022	3.632171	24.315868
C	12.031150	4.336833	63.582254	H	29.118764	2.138924	23.176548
C	13.063191	5.025817	64.207206	H	19.776788	6.946706	30.327542
O	10.943187	3.908837	64.361307	H	15.675724	4.573355	29.257184
C	31.882275	6.620600	63.346211	H	13.752556	3.890153	30.550568
C	30.799322	6.168606	64.089282	H	15.672568	6.862090	17.596212
C	29.767267	5.478629	63.464346	H	25.153578	6.240363	21.533417
C	27.651260	4.336658	63.581482	H	25.602410	2.543779	22.969498
C	28.683314	5.025635	64.206417	H	37.753154	2.937822	28.287515
O	26.563309	3.908663	64.360554	H	40.132415	2.322194	28.351896
C	47.502389	6.620356	63.345091	H	41.619234	2.930976	26.515630
C	46.419447	6.168363	64.088179	H	37.165867	5.151416	24.005886
C	45.387379	5.478391	63.463260	H	38.661923	5.695672	22.185675
C	43.271369	4.336426	63.580429	H	35.150390	2.329666	22.590745

H	35.299001	1.793872	20.190336	H	9.244445	6.787034	41.130187
H	34.100133	3.170613	18.536533	H	12.054315	2.324810	38.543621
H	32.266453	6.144287	22.826145	H	8.520586	3.174246	38.234839
H	31.125007	7.500137	21.163930	H	20.682548	2.517344	43.494774
H	30.021558	7.569531	27.105668	H	23.050704	1.877964	43.603602
H	43.094423	7.727737	26.978617	H	24.665918	2.826961	42.042846
H	41.667865	6.230554	25.698738	H	20.388588	5.449471	39.622201
H	30.635328	3.579665	24.402700	H	22.019833	6.360600	38.096161
H	44.807939	1.874820	23.184345	H	18.035361	2.296191	37.855582
H	35.791974	6.725074	30.237037	H	18.026254	1.846206	35.438801
H	31.435790	4.714621	29.499931	H	16.855995	3.335397	33.907408
H	29.502052	4.351883	30.913124	H	15.248503	6.236439	38.386341
H	31.288511	6.858988	17.596573	H	14.061028	7.670571	36.829470
H	40.785939	5.737824	21.341642	H	13.169561	7.508826	42.647560
H	41.293347	2.231138	22.875232	H	25.951448	6.942784	44.091220
H	53.552163	3.700132	28.381390	H	24.665185	5.984485	42.259921
H	55.987753	3.326329	28.455821	H	13.611819	3.634247	39.864799
H	57.384050	3.866374	26.497949	H	28.212125	2.816420	38.602191
H	52.703612	5.455003	24.016646	H	18.616474	6.787378	45.754480
H	54.081385	5.977075	22.117086	H	19.570815	7.500497	32.715205
H	50.777312	2.334731	22.589330	H	17.633926	6.753237	33.997203
H	50.920732	1.795127	20.189808	H	14.458461	4.450327	44.821303
H	49.720219	3.170699	18.535998	H	12.554651	3.825892	46.170335
H	47.864823	6.135689	22.823765	H	12.709393	3.737742	32.579618
H	46.741261	7.497332	21.163701	H	14.024142	7.300252	33.303363
H	45.508266	7.312671	27.145613	H	24.205734	6.611071	37.482229
H	46.267966	3.332399	24.463738	H	24.812208	3.058465	38.134265
H	50.935493	7.233800	30.271998	H	36.395100	2.230286	43.132427
H	47.059050	4.464380	29.319899	H	38.803744	1.518885	43.021512
H	45.221398	3.644203	30.655834	H	40.339819	2.579632	41.437690
H	46.906476	6.857497	17.596316	H	35.905007	5.441845	39.565748
H	56.056722	5.973371	21.101869	H	37.402645	6.405829	37.890672
H	10.790804	8.127563	42.499154	H	33.135431	2.626710	38.436441

H 33.163407 1.970123 36.013591	H 45.685857 4.517189 44.852772
H 32.447869 3.546661 34.293437	H 43.802715 3.763091 46.166322
H 31.546515 7.160106 38.464980	H 44.211766 3.461210 32.699898
H 30.713617 8.731807 36.736190	H 45.226474 7.158152 33.286926
H 28.424528 6.604204 44.230401	H 54.726433 5.965678 36.662652
H 41.733209 7.700464 42.686350	H 9.463473 8.127253 58.062682
H 40.345386 6.317151 41.241254	H 7.917045 6.786977 56.693388
H 29.515319 3.831343 40.443166	H 10.726902 2.324714 54.106889
H 43.601674 2.360189 38.264203	H 7.193629 3.175569 53.796225
H 34.459610 7.668477 45.856146	H 19.546308 2.931804 59.257358
H 35.795390 7.360515 32.611708	H 21.946438 2.390374 59.254977
H 33.855227 6.906371 34.019614	H 23.393031 3.179729 57.454618
H 30.848105 4.634332 44.835415	H 18.843264 5.421243 55.145257
H 28.857459 3.870446 46.012734	H 20.298129 6.143458 53.358249
H 28.530506 4.485465 32.981088	H 16.916148 2.460060 53.512006
H 30.548886 8.106040 33.347583	H 16.981550 1.973356 51.105228
H 39.504330 6.637403 37.193406	H 15.805565 3.399850 49.521965
H 40.079265 2.707245 37.941188	H 14.059800 6.370390 53.904366
H 52.223423 3.705219 43.946082	H 12.890110 7.755842 52.292181
H 54.659189 3.327090 44.019492	H 11.840652 7.509580 58.211824
H 56.055329 3.866298 42.061191	H 24.898086 8.023961 58.042922
H 51.374992 5.456018 39.580712	H 23.424881 6.575069 56.754263
H 52.752566 5.976914 37.680378	H 12.284714 3.635170 55.428892
H 49.629143 2.643909 37.988460	H 26.467891 2.290095 54.014417
H 49.719008 2.168378 35.579079	H 17.168373 6.739465 61.410792
H 48.430456 3.506558 34.004424	H 18.481695 7.371855 48.138167
H 46.453597 6.295812 38.406755	H 16.555048 6.695336 49.472419
H 45.168107 7.587742 36.805676	H 13.131933 4.372836 60.400895
H 44.158179 7.326822 42.821942	H 11.278243 3.573460 61.719598
H 45.022072 3.684781 39.728527	H 11.546059 3.747664 48.219925
H 49.648473 7.142819 45.860589	H 12.937878 7.316610 48.774375
H 50.709031 7.825404 32.649147	H 22.405513 6.291910 52.484986
H 48.862327 6.938763 33.976067	H 22.948829 2.672058 53.814284

H	35.112032	3.100896	59.325672	H	43.793553	7.591744	52.377009
H	37.492401	2.483129	59.352001	H	42.901469	7.354139	58.266501
H	38.958295	3.123858	57.509962	H	43.576727	3.500372	55.380781
H	34.491579	5.452185	55.124407	H	48.405415	6.744949	61.407787
H	35.966083	6.025804	53.294630	H	49.420118	7.729530	48.237022
H	32.593842	2.628871	53.488283	H	47.521327	6.919089	49.535036
H	32.799567	2.223932	51.074627	H	44.382152	4.362947	60.399651
H	31.696221	3.688454	49.473859	H	42.519470	3.571135	61.717957
H	29.667866	6.494110	53.844640	H	42.764826	3.611326	48.198779
H	28.551449	7.901141	52.207775	H	43.789414	7.166144	48.858627
H	27.306342	7.557372	58.174494	H	53.398482	5.963239	52.224232
H	40.497017	7.821866	58.130151	H	17.068392	7.157758	63.836081
H	39.036558	6.410600	56.793967	H	15.148237	6.357150	65.155560
H	27.969351	3.695063	55.300646	H	10.261813	3.422545	63.798034
H	42.079271	2.119364	54.061760	H	32.687856	7.158700	63.834996
H	32.786366	6.743099	61.409254	H	30.768036	6.357363	65.154634
H	34.139310	8.243720	48.280453	H	25.879052	3.427641	63.796130
H	32.270857	7.296407	49.547009	H	48.307446	7.159291	63.833705
H	28.751334	4.371811	60.400451	H	46.387793	6.357514	65.153432
H	26.898087	3.573613	61.718767	H	41.497826	3.429807	63.794561
H	27.767584	3.780090	47.954155	H	54.922507	4.682757	55.325512
H	28.665658	7.458920	48.689083	H	56.250046	4.683165	39.763409
H	38.074402	6.048062	52.408628	H	57.578867	4.683520	24.200343
H	38.570975	2.550701	53.794965	H	32.654209	5.043651	18.026503
H	50.894830	3.699832	59.506148	H	17.034665	5.043841	18.026657
H	53.331526	3.325381	59.581258	H	10.176533	4.915038	24.089435
H	54.727794	3.865558	57.623197	H	8.847931	4.915196	39.653322
H	50.047845	5.461044	55.146020	H	7.520482	4.915141	55.216550
H	51.425160	5.977887	53.243204	H	12.998694	5.198799	65.269003
H	48.372887	2.736121	53.466896	H	28.618525	5.198859	65.268118
H	48.432623	2.269887	51.055567	H	44.238379	5.198801	65.266981
H	47.076086	3.571289	49.510525	H	48.273938	5.043458	18.026037
H	45.135554	6.324597	53.952073	C	31.750921	8.755990	40.910124

C	31.743691	9.199883	42.312250	C	11.616000	6.503000	25.622000
C	32.061263	10.613501	42.684199	C	12.086000	5.395000	24.927000
C	31.654205	11.620618	41.600229	C	13.428000	5.043000	25.007000
C	32.132772	11.169742	40.212445	C	13.027000	3.179000	23.539000
C	31.521918	9.812346	39.837459	C	11.685000	3.529000	23.460000
O	33.117985	8.536899	41.209557	C	11.215000	4.638000	24.154000
C	29.364463	9.445402	44.177028	O	10.782000	2.793000	22.654000
C	28.653592	10.615383	44.496075	Cu	18.545211	6.099706	26.004396
C	28.559279	11.042126	45.824400	Cu	17.957621	3.712909	26.529586
C	29.180572	10.320728	46.850354	C	22.221207	3.972023	26.370636
C	29.897456	9.160678	46.531397	C	22.764886	3.214615	27.423776
C	29.985232	8.718032	45.210609	C	24.118096	2.901312	27.452650
N	29.549100	9.040941	42.844620	C	24.952702	3.333636	26.427392
H	31.581898	10.835191	43.654487	C	24.446952	4.068344	25.337960
H	31.828345	8.425025	43.069718	C	23.060449	4.373771	25.293200
H	31.194227	7.826765	40.710479	C	22.545304	5.036966	24.158835
H	32.054713	12.618811	41.850737	C	23.390644	5.428201	23.125328
H	30.550061	11.715286	41.593116	C	24.758122	5.174392	23.189753
H	31.869558	11.923887	39.449546	C	25.297986	4.485402	24.284302
H	33.234665	11.080650	40.214520	O	25.590849	5.570430	22.148912
H	30.428440	9.915772	39.688509	O	20.438399	5.538538	26.177222
H	31.943625	9.437701	38.888878	O	19.921198	3.393754	26.650254
H	33.150752	10.656827	42.867720	C	20.774832	4.322449	26.409936
H	28.170881	11.189206	43.697209	C	18.226927	4.022014	22.293999
H	27.994923	11.951350	46.056683	C	18.992915	2.941012	21.873981
H	29.109885	10.656803	47.888998	C	19.081890	2.638017	20.519979
H	30.410756	8.592797	47.312290	C	18.404876	3.417023	19.587993
H	30.543213	7.809259	44.973637	C	17.639888	4.497024	20.008011
H	29.663210	8.023321	42.709324	C	17.550913	4.800019	21.362013
H	28.898389	9.450774	42.176619	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
(<i>R,R</i>)-2-Int1				C	16.197885	6.355031	19.497042
C	12.487000	7.261000	26.395000	C	16.963875	5.274030	19.076025

O	15.523872	7.185037	18.539057	C	38.671631	4.201388	25.340775
O	18.566589	5.534636	24.104811	C	38.186422	4.862058	24.193079
O	18.028183	3.394469	24.576217	C	39.052885	5.208143	23.160384
C	18.267660	4.339912	23.743957	C	40.412770	4.916459	23.243236
C	14.301000	5.801000	25.782000	C	40.923900	4.237242	24.357851
C	13.829000	6.909000	26.476000	O	41.267492	5.275409	22.206798
C	27.956207	7.032197	26.505965	O	36.028958	5.413074	26.202683
C	27.120978	6.194168	25.775136	O	35.510847	3.260445	26.637283
C	27.631757	5.081004	25.076105	C	36.365085	4.192834	26.421274
C	29.026575	4.816167	25.131071	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.703912	2.946048	23.616103	C	34.701781	2.637978	20.519678
C	27.336646	3.163299	23.592046	C	34.024753	3.416989	19.587708
C	26.775183	4.235322	24.322233	C	33.259776	4.496991	20.007741
O	26.571630	2.272218	22.842322	C	33.170826	4.799983	21.361747
O	16.595625	6.409533	25.840243	C	32.403848	5.880986	21.783781
O	16.060871	4.270955	26.319640	C	31.727821	6.658997	20.849810
C	15.737715	5.466436	25.980565	C	31.817771	6.355005	19.496805
C	17.917761	5.856229	30.218759	C	32.583748	5.274002	19.075771
C	18.909843	6.621169	30.858682	O	31.143743	7.185016	18.538835
C	16.766136	5.452020	30.950082	O	34.116988	5.496104	24.161846
C	15.689591	4.782581	30.329903	O	33.609987	3.336919	24.568199
C	14.582923	4.385399	31.074233	C	33.846807	4.307023	23.760581
O	18.434937	6.427667	27.962775	C	29.866107	5.644536	25.926558
O	17.905256	4.284243	28.428683	C	29.315867	6.761068	26.581023
C	18.102646	5.501028	28.786111	C	43.530396	6.838114	26.562617
Cu	34.126310	5.987200	26.089034	C	42.711717	5.967643	25.854309
Cu	33.551789	3.584558	26.543220	C	43.243398	4.851571	25.175566
C	37.810428	3.836259	26.412284	C	44.644427	4.613480	25.232646
C	38.326233	3.092758	27.489711	C	29.549001	3.754989	24.364516
C	39.671868	2.753213	27.544445	C	44.345413	2.683258	23.790816
C	40.526980	3.141906	26.519435	C	42.976220	2.891150	23.744994
C	40.050108	3.862470	25.408047	C	42.400202	3.981432	24.434854

O	42.223734	1.973309	23.015316	C	48.790737	4.799893	21.361200
O	32.160923	6.305968	25.990791	C	48.023772	5.880897	21.783251
O	31.655912	4.144013	26.387837	C	47.347731	6.658913	20.849295
C	31.313109	5.349246	26.112288	C	47.437655	6.354926	19.496287
C	33.679966	5.584291	30.321158	C	48.203620	5.273922	19.075235
C	34.757805	6.253428	30.928931	O	46.763613	7.184943	18.538331
C	32.543840	5.236848	31.104830	O	49.726340	5.586859	24.092610
C	31.404135	4.637213	30.530862	O	49.389029	3.418936	24.606680
C	30.302143	4.321856	31.321453	C	49.524183	4.364848	23.750152
O	34.070108	6.238227	28.063068	C	45.473344	5.496586	25.978679
O	33.526563	4.086122	28.468262	C	44.897351	6.609138	26.619150
C	33.764130	5.283785	28.864875	C	45.180618	3.528702	24.511449
Cu	49.687381	6.194920	25.986368	O	47.705792	6.316031	25.888199
Cu	49.348200	3.774899	26.563795	O	47.397066	4.146344	26.421180
C	53.571003	4.464792	26.367939	C	46.945049	5.304226	26.098019
C	54.157058	3.947774	27.515902	C	49.185355	5.978101	30.217883
C	55.530059	3.732759	27.559826	C	50.110001	6.846905	30.825531
C	56.316002	4.036762	26.454787	C	48.082109	5.491956	30.973995
C	55.729946	4.554780	25.305823	C	47.068066	4.705994	30.386182
C	54.356947	4.768795	25.262899	C	46.006871	4.234803	31.152881
C	53.770890	5.287813	24.113936	O	49.595835	6.551878	27.940744
C	54.557834	5.591815	23.007897	O	49.299014	4.375419	28.456572
C	55.929834	5.377800	23.052821	C	49.379189	5.612948	28.788233
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.632356	5.833805	26.124940	C	10.757253	5.394976	40.491133
O	51.338020	3.655033	26.633752	C	12.099253	5.042971	40.571108
C	52.092332	4.663762	26.380332	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.238250	6.144506	41.487977
C	48.879661	4.496905	20.007192	Cu	16.685958	3.745008	41.980649

C	20.953443	4.060853	41.900959	C	27.834802	4.730012	41.021433
C	21.445223	3.295529	42.974305	C	12.571237	3.934972	39.877096
C	22.793830	2.977610	43.068240	C	27.541034	2.966359	39.378079
C	23.678262	3.406879	42.085480	C	26.152450	3.256672	39.287845
C	23.231855	4.154137	40.980045	C	25.585970	4.272205	40.055579
C	21.849956	4.476505	40.874940	O	25.494399	2.439809	38.411226
C	21.397685	5.166159	39.731351	O	15.273255	6.435570	41.361506
C	22.296788	5.556192	38.743161	O	14.774818	4.283092	41.808690
C	23.655036	5.272662	38.861409	C	14.425755	5.481886	41.506768
C	24.133517	4.564973	39.969602	C	16.702715	5.831146	45.712463
O	24.534096	5.652970	37.855413	C	17.713110	6.591735	46.329516
O	19.147040	5.603527	41.634548	C	18.806701	6.939091	32.206607
O	18.653556	3.450163	42.089667	C	17.708858	6.502278	32.939587
C	19.499042	4.392228	41.873887	C	16.677423	5.759050	32.333572
C	16.899511	4.145258	37.734453	C	15.568748	5.429531	46.472817
C	17.601230	3.040879	37.219520	C	14.483839	4.746711	45.883478
C	17.613679	2.778225	35.856494	C	13.390784	4.361319	46.653677
C	16.923257	3.611817	34.983605	C	14.518274	4.636774	32.442379
C	16.180920	4.713804	35.457279	C	15.553570	5.331175	33.082485
C	16.149545	4.971859	36.853511	O	13.408543	4.230460	33.174940
C	15.345288	6.024759	37.334322	O	17.153237	6.438814	43.452917
C	14.634411	6.826093	36.450112	O	16.646014	4.285245	43.893553
C	14.690586	6.612802	35.082957	C	16.846064	5.496846	44.268428
C	15.470091	5.555605	34.561398	Cu	32.932179	6.127311	41.585165
O	13.974650	7.496688	34.278418	Cu	32.420283	3.665814	42.252521
O	17.247008	5.613406	39.576156	C	36.607821	4.013075	41.741041
O	16.752861	3.455855	40.012386	C	37.128529	3.170998	42.706856
C	16.972908	4.419386	39.193754	C	38.507970	2.870573	42.714338
C	12.972270	5.800966	41.346096	C	39.342550	3.393840	41.750374
C	12.500286	6.908965	42.040108	C	38.848170	4.238928	40.703609
C	26.791182	6.874167	42.538323	C	37.439724	4.545786	40.701694
C	25.952682	6.135142	41.728368	C	36.918297	5.333091	39.634973
C	26.431519	5.043529	40.931598	C	37.741271	5.809345	38.642332

C	39.138687	5.551206	38.660834	C	30.136787	5.237077	41.961033
C	39.695579	4.771510	39.672750	C	32.422747	5.983127	45.791183
O	39.935305	6.063311	37.681396	C	33.293383	6.877113	46.387198
O	34.830659	5.571220	41.687303	C	34.749556	6.534389	32.288800
O	34.359537	3.402079	42.083045	C	33.655463	6.170745	33.065534
C	35.153774	4.356823	41.836129	C	32.537031	5.534830	32.495232
C	32.197823	3.843975	38.044160	C	31.291940	5.466349	46.505328
C	32.476637	2.550289	37.633444	C	30.306620	4.648065	45.881421
C	32.429067	2.217844	36.264357	C	29.215901	4.199286	46.584961
C	32.092602	3.171787	35.326630	C	30.300812	4.596505	32.687368
C	31.745770	4.511190	35.696415	C	31.408050	5.209656	33.282074
C	31.788746	4.845624	37.098335	O	29.189964	4.283820	33.460069
C	31.384488	6.155821	37.491871	O	32.934268	6.511297	43.549245
C	30.991933	7.082484	36.560973	O	32.615657	4.350620	44.095330
C	30.990384	6.776517	35.174232	C	32.678328	5.582609	44.371730
C	31.364258	5.510845	34.732415	Cu	48.451353	6.404301	41.573756
O	30.602108	7.827733	34.389990	Cu	47.998449	3.978766	42.047612
O	32.846551	5.307348	39.782158	C	52.242278	4.464620	41.931334
O	32.142968	3.247195	40.336703	C	52.828353	3.947597	43.079285
C	32.401064	4.158957	39.492371	C	54.201353	3.732577	43.123183
C	28.672783	5.519319	41.869946	C	54.987278	4.036581	42.018131
C	28.169512	6.578987	42.601170	C	54.401203	4.554604	40.869180
C	42.282457	7.206410	42.068224	C	53.028203	4.768624	40.826281
C	41.465250	6.409624	41.275173	C	52.442128	5.287648	39.677330
C	41.996081	5.350121	40.512769	C	53.229054	5.591652	38.571278
C	43.392410	5.089460	40.573136	C	54.601054	5.377632	38.616177
C	28.358074	3.673303	40.221409	C	55.187129	4.858609	39.764128
C	43.097067	3.304451	38.955828	O	55.314970	5.617639	37.405129
C	41.730132	3.526159	38.914782	O	50.375134	5.934729	41.729163
C	41.160287	4.554246	39.691961	O	49.973361	3.761190	42.185667
O	40.975892	2.680463	38.106088	C	50.776091	4.736728	41.959867
O	30.921104	6.174521	41.639619	C	48.304136	4.389376	37.810888
O	30.496317	4.088854	42.358931	C	49.127935	3.358473	37.325349

C	49.194193	3.080256	35.967218	C	8.959816	6.502907	56.749315
C	48.434881	3.822889	35.070004	C	9.429783	5.394908	56.054291
C	47.577413	4.851848	35.512945	C	10.771783	5.042898	56.134241
C	47.498951	5.129879	36.903846	C	10.370718	3.178911	54.666243
C	46.595417	6.112902	37.353867	C	9.028718	3.528920	54.587293
C	45.823951	6.825744	36.444946	C	8.558750	4.637919	55.281317
C	45.914786	6.588728	35.083146	O	8.125684	2.792932	53.781319
C	46.797132	5.599655	34.591980	Cu	15.891522	6.155334	57.135290
O	45.128147	7.383745	34.252268	Cu	15.352118	3.737379	57.544434
O	48.497783	5.881555	39.657128	C	19.606139	4.079052	57.412957
O	48.118689	3.698481	40.082379	C	20.169417	3.302784	58.441645
C	48.307345	4.672820	39.269370	C	21.524003	2.994493	58.442266
C	44.216457	5.884090	41.416608	C	22.339706	3.448919	57.411476
C	43.644709	6.949596	42.135216	C	21.814518	4.206837	56.347207
C	43.929984	4.068068	39.765945	C	20.427205	4.511822	56.333763
O	46.479669	6.622603	41.444818	C	19.892913	5.206384	55.227518
O	46.070998	4.439867	41.841807	C	20.720276	5.624407	54.189930
C	45.675008	5.631729	41.572621	C	22.088438	5.367379	54.222861
C	47.843729	6.057421	45.781282	C	22.647293	4.649394	55.289004
C	48.785679	6.887232	46.417225	O	22.903312	5.792369	53.179590
C	49.988532	7.195259	32.164653	O	17.796353	5.623539	57.297908
C	48.938669	6.686084	32.921068	O	17.318956	3.448123	57.660625
C	47.974479	5.834587	32.348227	C	18.155017	4.403510	57.470893
C	46.720928	5.584278	46.517299	C	15.687578	4.242123	53.318160
C	45.690402	4.839643	45.905090	C	16.418874	3.147111	52.823636
C	44.612674	4.377822	46.654628	C	16.471812	2.881015	51.462663
C	45.926480	4.526204	32.512090	C	15.788830	3.698571	50.569936
C	46.897354	5.333352	33.120374	C	15.023693	4.794753	51.019639
O	44.863598	4.043889	33.267506	C	14.960636	5.063985	52.413830
O	48.337104	6.684857	43.537426	C	14.145010	6.119266	52.868151
O	47.900298	4.512357	43.960543	C	13.451891	6.911347	51.961506
C	48.042940	5.730098	44.342372	C	13.530613	6.680860	50.597910
C	9.830848	7.260896	57.522290	C	14.317809	5.616956	50.101782

O	12.825683	7.552960	49.770980	Cu	30.949634	3.749534	57.533970
O	15.948098	5.679682	55.205198	C	35.196960	4.101980	57.427724
O	15.451326	3.509931	55.571706	C	35.734129	3.349155	58.488031
C	15.694991	4.493172	54.784355	C	37.080459	3.009437	58.512937
C	11.644816	5.800887	56.909216	C	37.914730	3.406396	57.474164
C	11.172849	6.908886	57.603240	C	37.417613	4.142454	56.381571
C	25.305491	7.115481	57.593251	C	36.038544	4.484353	56.346321
C	24.472279	6.308731	56.827083	C	35.532607	5.163004	55.218113
C	24.983977	5.222865	56.086761	C	36.379735	5.525216	54.175141
C	26.378961	4.955324	56.132828	C	37.740100	5.229636	54.226568
C	11.243751	3.934900	55.440217	C	38.271473	4.529373	55.318590
C	26.056834	3.146973	54.545614	O	38.575038	5.603265	53.179625
C	24.689444	3.367450	54.526486	O	33.380608	5.645637	57.257414
C	24.127015	4.407257	55.301345	O	32.913254	3.472765	57.647288
O	23.924685	2.507377	53.741167	C	33.745062	4.429187	57.451881
O	13.936013	6.439336	56.974158	C	31.277411	4.265404	53.305162
O	13.441968	4.274243	57.363446	C	32.080221	3.217713	52.819404
C	13.093013	5.478540	57.082763	C	32.163922	2.954074	51.459439
C	15.283046	5.695821	61.352095	C	31.439582	3.725071	50.558135
C	16.314087	6.385804	61.978046	C	30.599642	4.767712	50.998096
C	17.640265	6.917722	47.677373	C	30.508812	5.037919	52.391012
C	16.552075	6.498336	48.433801	C	29.628915	6.044961	52.833033
C	15.505535	5.755631	47.854498	C	28.885628	6.778530	51.914183
C	14.198081	5.242825	62.095148	C	28.983003	6.539973	50.552581
C	13.166040	4.552842	61.469196	C	29.846230	5.534117	50.075022
C	12.083075	4.099846	62.213249	O	28.219999	7.345509	49.711536
C	13.345678	4.642201	48.017051	O	31.485947	5.712570	55.192979
C	14.390423	5.348848	48.628158	O	31.045828	3.530435	55.558667
O	12.246050	4.252167	48.773486	C	31.264397	4.519981	54.771534
O	15.754589	6.387479	59.110258	C	27.217349	5.754617	56.957700
O	15.284268	4.211934	59.472401	C	26.664535	6.841917	57.658102
C	15.446195	5.415018	59.890971	C	40.919690	6.964412	57.659376
Cu	31.463903	6.174286	57.130653	C	40.090252	6.158056	56.891158

C	40.604860	5.074970	56.148496	C	51.901549	5.591433	54.133681
C	42.001769	4.810587	56.192851	C	53.273549	5.377407	54.178555
C	26.901752	3.922815	55.329273	C	53.859642	4.858378	55.326493
C	41.677328	2.989238	54.621977	O	53.987445	5.617415	52.967495
C	40.310435	3.214753	54.595073	O	48.995154	5.863872	57.303430
C	39.748177	4.262802	55.358949	O	48.671314	3.659467	57.665666
O	39.545715	2.350364	53.814639	C	49.438696	4.675517	57.498128
O	29.497139	6.448322	57.017112	C	46.976219	4.387862	53.312763
O	29.037956	4.267274	57.363193	C	47.814338	3.383025	52.797313
C	28.669601	5.472829	57.119907	C	47.871936	3.133393	51.433674
C	30.903120	5.695641	61.351269	C	47.089466	3.878803	50.559757
C	31.934175	6.385618	61.977205	C	46.220531	4.885378	51.031219
C	33.115304	7.239235	47.740611	C	46.151263	5.134491	52.428401
C	32.066876	6.721432	48.471264	C	45.235352	6.092407	52.906168
C	31.109922	5.828549	47.887734	C	44.444823	6.811264	52.018520
C	29.818167	5.242646	62.094340	C	44.526305	6.603282	50.651372
C	28.786113	4.552669	61.468405	C	45.419405	5.638222	50.131841
C	27.703159	4.099675	62.212476	O	43.722357	7.405826	49.844686
C	29.056891	4.503162	47.963631	O	47.127066	5.819006	55.215411
C	29.987639	5.307894	48.618504	O	46.816133	3.610217	55.554876
O	27.987963	4.007364	48.646322	C	46.972439	4.620725	54.780567
O	31.364873	6.394423	59.109265	C	42.840918	5.624034	57.003065
O	30.889773	4.218924	59.464405	C	42.280310	6.702261	57.713121
C	31.059477	5.419578	59.887835	C	42.523728	3.772130	55.397558
Cu	47.055651	6.260771	57.153125	O	45.082212	6.414828	57.026493
Cu	46.686572	3.803902	57.527529	O	44.742469	4.207977	57.344661
C	50.914829	4.464394	57.493750	C	44.307878	5.397128	57.124541
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.661418	7.210315	47.761676
C	53.073736	4.554373	56.431559	C	47.591475	6.714339	48.496981
C	51.700736	4.768398	56.388685	C	46.611011	5.899901	47.898233
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251

C	44.406185	4.552442	61.467332	H	21.487785	5.249430	24.044641
C	43.323243	4.099449	62.211421	H	22.971879	5.937283	22.267790
C	44.531205	4.638665	48.020107	H	19.532717	2.330044	22.589896
C	45.517142	5.408043	48.652918	H	19.679477	1.794178	20.190515
O	43.451858	4.165480	48.757601	H	18.480499	3.170813	18.536728
O	46.924761	6.447470	59.126507	H	16.649980	6.144787	22.827018
O	46.571188	4.243086	59.457644	H	15.506631	7.500795	21.165206
C	46.675333	5.446344	59.890404	H	14.495691	7.508802	27.086848
C	16.262162	6.620790	63.347051	H	27.544390	7.892515	27.024129
C	15.179196	6.168795	64.090104	H	26.067709	6.434857	25.745019
C	14.147156	5.478812	63.465153	H	14.941446	3.633620	24.312812
C	12.031150	4.336833	63.582254	H	29.112826	2.128754	23.037196
C	13.063191	5.025817	64.207206	H	19.776906	6.959637	30.302797
O	10.943187	3.908837	64.361307	H	15.678100	4.569578	29.266264
C	31.882275	6.620600	63.346211	H	13.771745	3.871103	30.576881
C	30.799322	6.168606	64.089282	H	15.671866	6.861099	17.596378
C	29.767267	5.478629	63.464346	H	25.094740	6.080172	21.433310
C	27.651260	4.336658	63.581482	H	25.588912	2.485300	22.858991
C	28.683314	5.025635	64.206417	H	37.673078	2.784603	28.298330
O	26.563309	3.908663	64.360554	H	40.055700	2.186978	28.387465
C	47.502389	6.620356	63.345091	H	41.569179	2.861991	26.594490
C	46.419447	6.168363	64.088179	H	37.136923	5.109780	24.071672
C	45.387379	5.478391	63.463260	H	38.657766	5.715916	22.290953
C	43.271369	4.336426	63.580429	H	35.146104	2.325240	22.590313
C	44.303437	5.025398	64.205349	H	35.297709	1.792927	20.190421
O	42.183431	3.908432	64.359519	H	34.099756	3.170442	18.536518
H	12.119292	8.127223	26.935541	H	32.269117	6.145226	22.826304
H	10.573036	6.786857	25.566326	H	31.125577	7.500075	21.165083
H	13.383710	2.323187	22.982608	H	29.951149	7.414422	27.168037
H	9.847384	3.169534	22.677183	H	43.101768	7.697636	27.068403
H	22.128855	2.878336	28.234723	H	41.653339	6.184394	25.829323
H	24.524568	2.323825	28.277132	H	30.610683	3.541548	24.316365
H	26.001623	3.075333	26.483803	H	44.764150	1.847360	23.246573

H	35.618886	6.544135	30.337422	H	18.165768	1.926271	35.472286
H	31.343147	4.414637	29.469908	H	16.958184	3.375320	33.929601
H	29.439700	3.860781	30.858716	H	15.240148	6.237771	38.392000
H	31.291693	6.860811	17.596363	H	14.023748	7.635428	36.827431
H	40.793345	5.790108	21.479982	H	13.169313	7.511492	42.645374
H	41.239475	2.180964	23.018429	H	26.396714	7.704135	43.132981
H	53.552011	3.699701	28.381160	H	24.892876	6.408004	41.696563
H	55.987694	3.325991	28.455688	H	13.612084	3.634289	39.867747
H	57.384069	3.866316	26.497848	H	27.933432	2.162732	38.749412
H	52.703450	5.452774	24.015157	H	18.569613	6.924724	45.754180
H	54.081129	5.976133	22.116856	H	19.585040	7.522457	32.688588
H	50.777290	2.334582	22.589267	H	17.663033	6.764077	33.988093
H	50.920785	1.795180	20.189773	H	14.456045	4.511393	44.824975
H	49.720358	3.170933	18.535926	H	12.573515	3.834708	46.179744
H	47.862763	6.134480	22.823774	H	12.749227	3.710299	32.615608
H	46.741177	7.496787	21.164899	H	14.034985	7.274631	33.299417
H	45.521778	7.300979	27.173038	H	24.084777	6.200632	37.136190
H	46.244308	3.321880	24.481606	H	24.560908	2.677904	38.303713
H	50.937041	7.247183	30.250249	H	36.463121	2.757711	43.469068
H	47.070039	4.455635	29.330869	H	38.916422	2.218605	43.492934
H	45.243476	3.631840	30.680101	H	40.406936	3.141905	41.786961
H	46.913204	6.861936	17.595746	H	35.850234	5.552248	39.594788
H	56.056144	5.976916	21.104057	H	37.318859	6.403114	37.822523
H	10.790976	8.128083	42.498432	H	32.758413	1.805389	38.381304
H	9.244443	6.787065	41.130005	H	32.673317	1.200342	35.943357
H	12.055519	2.325066	38.544075	H	32.084660	2.878167	34.272063
H	8.519278	3.170935	38.240000	H	31.384089	6.424628	38.546901
H	20.770376	2.953700	43.751062	H	30.670725	8.084076	36.860271
H	23.157589	2.394848	43.908935	H	28.832680	7.176160	43.229277
H	24.721539	3.137374	42.190245	H	41.855562	8.027251	42.635993
H	20.349332	5.398995	39.575118	H	40.408878	6.641785	41.248934
H	21.924656	6.082910	37.874542	H	29.419300	3.420240	40.275445
H	18.152750	2.388272	37.886631	H	43.516743	2.517995	38.342242

H	34.124896	7.284059	45.805712	H	19.546867	2.944509	59.253514
H	35.597364	7.035897	32.745155	H	21.945941	2.401007	59.247280
H	33.686526	6.399718	34.123299	H	23.389597	3.190561	57.443891
H	30.403710	4.375521	44.830303	H	18.834307	5.425560	55.139833
H	28.459762	3.586512	46.080007	H	20.287161	6.157377	53.354275
H	28.473481	3.807963	32.931790	H	16.958459	2.500826	53.506541
H	30.549859	7.595362	33.449733	H	17.045805	2.035745	51.096013
H	39.400334	6.584743	37.061327	H	15.851557	3.455999	49.518668
H	39.988635	2.885986	38.125797	H	14.019583	6.342893	53.921468
H	52.223991	3.710387	43.947918	H	12.834374	7.724776	52.318247
H	54.659345	3.328203	44.019913	H	11.840450	7.509607	58.212083
H	56.055412	3.866650	42.061230	H	24.893213	7.954395	58.144987
H	51.374685	5.452690	39.579208	H	23.419820	6.553045	56.802796
H	52.752229	5.975719	37.680067	H	12.285038	3.636243	55.427117
H	49.730733	2.775141	38.012136	H	26.465838	2.353649	53.934267
H	49.839076	2.285199	35.606290	H	17.168075	6.740032	61.410658
H	48.511046	3.573621	34.021224	H	18.432707	7.498032	48.139878
H	46.461430	6.338365	38.405927	H	16.527597	6.770590	49.480349
H	45.134243	7.580601	36.798354	H	13.130836	4.374522	60.400654
H	44.266979	7.578081	42.762289	H	11.278104	3.573997	61.719325
H	44.992662	3.850969	39.738280	H	11.577010	3.724193	48.233474
H	49.627670	7.279455	45.858211	H	12.919154	7.331415	48.794389
H	50.713735	7.861854	32.620936	H	22.396462	6.323929	52.487671
H	48.875268	6.976365	33.961186	H	22.944468	2.731769	53.751071
H	45.691475	4.615231	44.844110	H	35.095294	3.027806	59.302801
H	43.837034	3.805848	46.163547	H	37.480289	2.432389	59.340859
H	44.248710	3.450076	32.731348	H	38.956913	3.121122	57.523539
H	45.224024	7.150726	33.278671	H	34.481833	5.414363	55.119876
H	54.726531	5.972693	36.665929	H	35.969074	6.047131	53.321417
H	9.463399	8.127109	58.062853	H	32.652952	2.607315	53.508492
H	7.916946	6.786720	56.693530	H	32.793476	2.145999	51.099975
H	10.728169	2.325384	54.106726	H	31.527592	3.483826	49.507089
H	7.191740	3.170751	53.803257	H	29.492057	6.271848	53.885316

H	28.211233	7.550381	52.261461	H	43.806724	7.190193	48.866223
H	27.298698	7.472282	58.271042	H	53.398692	5.970814	52.227674
H	40.504528	7.799350	58.215008	H	17.068201	7.158110	63.835991
H	39.037476	6.400209	56.869686	H	15.148083	6.357292	65.155550
H	27.963229	3.707903	55.279749	H	10.263157	3.421775	63.797076
H	42.085653	2.189801	54.018283	H	32.688068	7.158307	63.835060
H	32.787217	6.740914	61.409196	H	30.767941	6.357329	65.154661
H	33.817424	7.933123	48.213317	H	25.881862	3.424130	63.795740
H	31.960153	7.020767	49.518578	H	48.307513	7.159135	63.833759
H	28.748062	4.375542	60.400007	H	46.387765	6.357309	65.153493
H	26.897525	3.574889	61.718378	H	41.501220	3.425122	63.794463
H	27.451200	3.451790	48.057936	H	54.922556	4.682785	55.325779
H	28.292391	7.085807	48.739468	H	56.250097	4.683171	39.763700
H	38.089230	6.128903	52.468364	H	57.578892	4.683412	24.200625
H	38.565764	2.575991	53.822527	H	32.654232	5.043308	18.026530
H	50.894922	3.700529	59.506444	H	17.034810	5.043582	18.026682
H	53.331584	3.325647	59.581346	H	10.176547	4.915299	24.089643
H	54.727848	3.865728	57.623137	H	8.847999	4.915598	39.653310
H	50.047651	5.459410	55.145286	H	7.520561	4.915556	55.216444
H	51.424893	5.977051	53.243021	H	12.998950	5.198991	65.269024
H	48.430558	2.793083	53.466230	H	28.618759	5.198985	65.268152
H	48.525350	2.355945	51.050520	H	44.238629	5.198825	65.267036
H	47.156979	3.648561	49.506201	H	48.273990	5.043163	18.026055
H	45.105638	6.293333	53.963699	C	31.784209	8.965730	40.986375
H	43.746553	7.547705	52.393414	C	31.549297	9.257704	42.482529
H	42.912671	7.342219	58.318057	C	32.565751	10.299555	43.005129
H	43.584912	3.556439	55.349055	C	32.556105	11.579479	42.156702
H	48.405614	6.744907	61.407981	C	32.834566	11.270500	40.676436
H	49.399651	7.847671	48.238216	C	31.845086	10.230306	40.124822
H	47.526217	6.985589	49.541973	O	32.995076	8.190427	40.836636
H	44.381439	4.364306	60.399424	C	29.553236	9.558112	43.952943
H	42.519341	3.571630	61.717714	C	28.277752	10.139703	44.139612
H	42.826712	3.598181	48.204694	C	27.618403	10.044646	45.364646

C	28.203052	9.370033	46.445213	C	22.228265	4.003088	26.389201
C	29.460960	8.786187	46.266366	C	22.763047	3.225299	27.432155
C	30.133145	8.871427	45.043599	C	24.119380	2.927885	27.477528
N	30.167670	9.637581	42.711270	C	24.966474	3.395532	26.478366
H	32.340305	10.520713	44.062654	C	24.470809	4.150354	25.398301
H	31.717145	8.304799	42.998534	C	23.081862	4.442418	25.337354
H	30.993409	8.290254	40.636370	C	22.579760	5.129758	24.211259
H	33.293131	12.305449	42.544441	C	23.439172	5.560413	23.205483
H	31.564508	12.064499	42.247204	C	24.807283	5.315371	23.285212
H	32.789126	12.191874	40.068750	C	25.334213	4.598597	24.367964
H	33.872044	10.892442	40.570247	O	25.653503	5.746106	22.269284
H	30.831301	10.674254	40.085680	O	20.435279	5.555770	26.184768
H	32.099433	9.941567	39.089462	O	19.928313	3.407796	26.652593
H	33.579480	9.850563	42.998684	C	20.778131	4.341825	26.417223
H	27.803644	10.664901	43.302432	C	18.226927	4.022014	22.293999
H	26.632672	10.509360	45.476593	C	18.992915	2.941012	21.873981
H	27.688335	9.310627	47.409065	C	19.081890	2.638017	20.519979
H	29.948162	8.252587	47.088630	C	18.404876	3.417023	19.587993
H	31.108925	8.392313	44.948320	C	17.639888	4.497024	20.008011
H	33.766798	8.698218	41.139702	C	17.550913	4.800019	21.362013
H	29.758177	10.302918	42.065783	C	16.783924	5.881020	21.784030
(R,R)-2-Int2				C	16.107910	6.659026	20.850045
C	12.487000	7.261000	26.395000	C	16.197885	6.355031	19.497042
C	11.616000	6.503000	25.622000	C	16.963875	5.274030	19.076025
C	12.086000	5.395000	24.927000	O	15.523872	7.185037	18.539057
C	13.428000	5.043000	25.007000	O	18.567269	5.538612	24.104762
C	13.027000	3.179000	23.539000	O	18.034240	3.397557	24.577574
C	11.685000	3.529000	23.460000	C	18.270582	4.342619	23.744333
C	11.215000	4.638000	24.154000	C	14.301000	5.801000	25.782000
O	10.782000	2.793000	22.654000	C	13.829000	6.909000	26.476000
Cu	18.541625	6.107269	26.005391	C	28.029639	7.162013	26.527427
Cu	17.962155	3.718468	26.529898	C	27.180829	6.314278	25.823543
				C	27.677609	5.186382	25.138689

C	29.071297	4.912981	25.184716	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.719464	3.013514	23.712766	C	34.701781	2.637978	20.519678
C	27.354347	3.242941	23.694605	C	34.024753	3.416989	19.587708
C	26.808343	4.334154	24.407433	C	33.259776	4.496991	20.007741
O	26.575596	2.347142	22.964713	C	33.170826	4.799983	21.361747
O	16.593188	6.411731	25.837881	C	32.403848	5.880986	21.783781
O	16.063321	4.272116	26.318279	C	31.727821	6.658997	20.849810
C	15.737658	5.467200	25.979170	C	31.817771	6.355005	19.496805
C	17.905774	5.857939	30.218855	C	32.583748	5.274002	19.075771
C	18.903789	6.602800	30.872671	O	31.143743	7.185016	18.538835
C	16.742626	5.464458	30.937303	O	34.146496	5.527849	24.129439
C	15.663202	4.813570	30.302657	O	33.632400	3.381728	24.590629
C	14.543288	4.428658	31.033587	C	33.866277	4.331704	23.757589
O	18.426459	6.435404	27.964416	C	29.925474	5.752904	25.952593
O	17.905278	4.289262	28.428409	C	29.389119	6.885623	26.590593
C	18.097266	5.506499	28.786591	C	43.531837	6.835130	26.527230
Cu	34.192881	6.065185	26.042523	C	42.723550	5.978122	25.791099
Cu	33.603626	3.679943	26.564557	C	43.263526	4.868449	25.107727
C	37.860303	3.889291	26.360018	C	44.662544	4.626763	25.184101
C	38.384937	3.162063	27.444263	C	29.577856	3.831136	24.436256
C	39.729369	2.817176	27.489201	C	44.385718	2.722749	23.703793
C	40.574336	3.186231	26.448757	C	43.017244	2.930834	23.642248
C	40.088075	3.891743	25.331396	C	42.430771	4.008182	24.343915
C	38.709954	4.231586	25.272225	O	42.275832	2.023514	22.888521
C	38.213594	4.871516	24.117430	O	32.227139	6.399553	25.972598
C	39.070301	5.201082	23.071414	O	31.710823	4.251088	26.423529
C	40.431417	4.914209	23.148192	C	31.373405	5.452444	26.126537
C	40.952775	4.252847	24.268862	C	33.893198	5.763467	30.292880
O	41.276815	5.257925	22.099097	C	35.059433	6.314927	30.853181
O	36.090591	5.475572	26.136075	C	32.752354	5.560776	31.116720
O	35.560442	3.340435	26.637412	C	31.540332	5.074673	30.588510
C	36.419042	4.258619	26.382212	C	30.429722	4.915160	31.413100

O	34.184739	6.365294	28.008974	C	45.479666	5.495033	25.958908
O	33.615705	4.232810	28.480309	C	44.896328	6.599475	26.606439
C	33.895769	5.433081	28.841618	C	45.209571	3.553784	24.453431
Cu	49.688918	6.190776	25.990786	O	47.709987	6.313670	25.889990
Cu	49.349268	3.768085	26.558576	O	47.398316	4.141631	26.412965
C	53.571003	4.464792	26.367939	C	46.948793	5.301299	26.091674
C	54.157058	3.947774	27.515902	C	49.175928	5.947707	30.221737
C	55.530059	3.732759	27.559826	C	50.097755	6.809746	30.842717
C	56.316002	4.036762	26.454787	C	48.074594	5.445360	30.970197
C	55.729946	4.554780	25.305823	C	47.062622	4.666037	30.369607
C	54.356947	4.768795	25.262899	C	46.004603	4.176346	31.128959
C	53.770890	5.287813	24.113936	O	49.594491	6.538984	27.948227
C	54.557834	5.591815	23.007897	O	49.298099	4.359523	28.451654
C	55.929834	5.377800	23.052821	C	49.375980	5.594933	28.790054
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.632511	5.831162	26.128908	C	10.757253	5.394976	40.491133
O	51.339369	3.650122	26.629469	C	12.099253	5.042971	40.571108
C	52.092776	4.660790	26.380081	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.241781	6.037628	41.460397
C	48.879661	4.496905	20.007192	Cu	16.627561	3.652360	41.948810
C	48.790737	4.799893	21.361200	C	20.895043	3.821224	41.738203
C	48.023772	5.880897	21.783251	C	21.365823	2.911062	42.703407
C	47.347731	6.658913	20.849295	C	22.704679	2.548126	42.753781
C	47.437655	6.354926	19.496287	C	23.604737	3.092037	41.845881
C	48.203620	5.273922	19.075235	C	23.182259	3.995458	40.853151
O	46.763613	7.184943	18.538331	C	21.804175	4.336066	40.768424
O	49.728037	5.586509	24.094321	C	21.371882	5.149890	39.700598
O	49.391355	3.417099	24.603279	C	22.290401	5.665278	38.790844
C	49.525626	4.364773	23.749433	C	23.649596	5.395258	38.919112

C	24.108837	4.558795	39.942764	C	16.757458	5.719333	45.688738
O	24.552687	5.924640	38.006272	C	17.791097	6.453773	46.298759
O	19.133643	5.433324	41.571082	C	18.794387	6.910353	32.222689
O	18.582919	3.289958	42.002231	C	17.684075	6.483621	32.943191
C	19.452426	4.205531	41.771536	C	16.646237	5.761855	32.322187
C	16.792469	4.069114	37.701462	C	15.616465	5.351058	46.455486
C	17.455306	2.944462	37.178805	C	14.510002	4.697740	45.872692
C	17.460639	2.692063	35.813858	C	13.410013	4.345215	46.648590
C	16.802509	3.557005	34.946664	C	14.468994	4.672388	32.402689
C	16.097228	4.679642	35.428388	C	15.509253	5.345237	33.057585
C	16.071237	4.926743	36.826653	O	13.346451	4.277840	33.122073
C	15.301586	6.001597	37.315126	O	17.197194	6.323814	43.427031
C	14.618921	6.833086	36.436172	O	16.647113	4.180307	43.865845
C	14.671952	6.630019	35.067100	C	16.879276	5.385673	44.242680
C	15.419347	5.553640	34.538266	Cu	33.464608	6.627629	41.371161
O	13.985794	7.542100	34.268261	Cu	32.396139	3.839335	42.152902
O	17.203863	5.517655	39.545648	C	36.548831	3.649783	41.296777
O	16.641438	3.376016	39.977897	C	36.992464	2.719815	42.220336
C	16.885039	4.335363	39.161029	C	38.352733	2.340588	42.251198
C	12.972270	5.800966	41.346096	C	39.252760	2.892241	41.365317
C	12.500286	6.908965	42.040108	C	38.841528	3.828674	40.361363
C	26.307283	6.334268	43.235126	C	37.446538	4.188984	40.313493
C	25.636186	5.801633	42.154444	C	37.010843	5.050555	39.266321
C	26.276288	4.945993	41.198199	C	37.897445	5.553941	38.345040
C	27.686218	4.692228	41.376592	C	39.284305	5.260620	38.428461
C	12.571237	3.934972	39.877096	C	39.761313	4.406944	39.421432
C	27.677268	3.352265	39.350592	O	40.148757	5.814009	37.532827
C	26.282097	3.565109	39.182802	O	34.932989	5.365262	41.209470
C	25.571427	4.346988	40.091411	O	34.263183	3.310497	41.815252
O	25.772537	2.917805	38.097366	C	35.138013	4.140133	41.437385
O	15.285868	6.391096	41.364764	C	31.965957	4.203448	38.116411
O	14.736418	4.253380	41.824540	C	31.999188	2.885147	37.676352
C	14.416810	5.458928	41.518656	C	31.979572	2.580914	36.303973

C	31.899200	3.592374	35.371378	C	30.495281	5.228651	32.769886
C	31.833906	4.970676	35.750585	C	31.684837	5.715079	33.324475
C	31.897614	5.282736	37.162325	O	29.375498	5.068090	33.576059
C	31.889339	6.659407	37.539419	O	33.380580	6.662456	43.422856
C	31.772852	7.648901	36.596166	O	32.868096	4.522829	43.901184
C	31.668154	7.348490	35.213007	C	33.025823	5.743063	44.207436
C	31.722553	6.028006	34.775971	Cu	48.388604	6.278306	41.557617
O	31.537013	8.460475	34.426628	Cu	48.017308	3.841627	42.045029
O	32.168964	5.528950	40.133876	C	52.242278	4.464620	41.931334
O	31.932041	3.337250	40.317473	C	52.828353	3.947597	43.079285
C	32.027292	4.391505	39.604137	C	54.201353	3.732577	43.123183
C	28.361834	5.284899	42.496109	C	54.987278	4.036581	42.018131
C	27.678694	6.076445	43.411103	C	54.401203	4.554604	40.869180
C	42.176254	6.840887	41.990123	C	53.028203	4.768624	40.826281
C	41.411992	6.028513	41.160601	C	52.442128	5.287648	39.677330
C	42.002235	4.999112	40.400318	C	53.229054	5.591652	38.571278
C	43.403172	4.781025	40.506465	C	54.601054	5.377632	38.616177
C	28.359695	3.887032	40.412056	C	55.187129	4.858609	39.764128
C	43.217616	3.001815	38.865195	O	55.314970	5.617639	37.405129
C	41.848608	3.191336	38.768984	O	50.329191	5.876361	41.709867
C	41.222320	4.195535	39.532719	O	49.997570	3.693563	42.178355
O	41.149600	2.343421	37.914199	C	50.768537	4.693403	41.948492
O	30.478693	6.127502	43.192745	C	48.273395	4.250346	37.801998
O	30.404408	4.036190	42.502260	C	49.090296	3.216619	37.310694
C	29.821528	5.112452	42.721439	C	49.158359	2.948297	35.950532
C	32.762618	6.114113	45.644699	C	48.409030	3.704873	35.056447
C	33.541338	7.113757	46.202111	C	47.555280	4.734243	35.505008
C	35.128787	6.614218	32.207384	C	47.471131	4.999165	36.898154
C	34.025978	6.391705	33.024135	C	46.564957	5.978100	37.352719
C	32.821542	5.886537	32.499646	C	45.803010	6.704543	36.446656
C	31.712984	5.499220	46.415326	C	45.903340	6.483435	35.083234
C	30.833996	4.517183	45.875469	C	46.784483	5.495840	34.587305
C	29.794110	4.002734	46.609669	O	45.125688	7.291023	34.255888

O	48.445905	5.748729	39.644863	C	19.604357	4.067200	57.439091
O	48.137096	3.556645	40.078962	C	20.158667	3.297375	58.477471
C	48.286705	4.534420	39.261265	C	21.513717	2.991243	58.493165
C	44.174447	5.597727	41.379393	C	22.338528	3.439547	57.466833
C	43.544673	6.632865	42.093297	C	21.821889	4.188147	56.391998
C	43.998347	3.781690	39.711475	C	20.434958	4.494142	56.365137
O	46.407959	6.424903	41.432000	C	19.910429	5.183499	55.251054
O	46.076152	4.231463	41.841809	C	20.746274	5.592756	54.216806
C	45.639069	5.405373	41.560081	C	22.113156	5.330395	54.260084
C	47.833662	5.935421	45.769951	C	22.662502	4.619082	55.335566
C	48.781552	6.764656	46.397650	O	22.936277	5.745056	53.218914
C	49.976785	7.133575	32.188163	O	17.796844	5.612558	57.303818
C	48.929795	6.606998	32.937017	O	17.314679	3.438621	57.669198
C	47.967149	5.763309	32.350157	C	18.152989	4.392735	57.483051
C	46.713823	5.467935	46.512384	C	15.692704	4.220745	53.322437
C	45.683384	4.717163	45.908231	C	16.398889	3.103504	52.840819
C	44.604970	4.265207	46.662824	C	16.454093	2.825125	51.482579
C	45.924020	4.444334	32.492840	C	15.798140	3.652391	50.578880
C	46.891655	5.245758	33.113748	C	15.057691	4.770754	51.014702
O	44.863218	3.945706	33.240520	C	14.992516	5.053433	52.406427
O	48.276015	6.565638	43.518943	C	14.199252	6.131789	52.846107
O	47.909253	4.382669	43.956688	C	13.532535	6.933323	51.928008
C	48.021444	5.606150	44.331059	C	13.613828	6.688827	50.567178
C	9.830848	7.260896	57.522290	C	14.376876	5.601077	50.085322
C	8.959816	6.502907	56.749315	O	12.934873	7.570206	49.728355
C	9.429783	5.394908	56.054291	O	15.952841	5.665883	55.206051
C	10.771783	5.042898	56.134241	O	15.447573	3.499312	55.578248
C	10.370718	3.178911	54.666243	C	15.695842	4.479147	54.788046
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.348630	7.149027	57.534293
Cu	15.893280	6.147322	57.135184	C	24.504937	6.314119	56.811421
Cu	15.348564	3.731586	57.549803	C	25.007308	5.205053	56.100117

C	26.403450	4.939607	56.134867	C	37.737348	5.119933	54.202336
C	11.243751	3.934900	55.440217	C	38.279219	4.461690	55.315437
C	26.056935	3.073348	54.620597	O	38.560752	5.446350	53.130836
C	24.689793	3.294506	54.612774	O	33.416938	5.673621	57.298388
C	24.139693	4.364655	55.353710	O	32.947218	3.497517	57.670172
O	23.913149	2.408837	53.868591	C	33.779345	4.456344	57.491600
O	13.938059	6.435217	56.970712	C	31.465317	4.305094	53.305864
O	13.439516	4.272459	57.367275	C	32.282304	3.247297	52.867053
C	13.092886	5.476698	57.083123	C	32.459144	2.994816	51.514045
C	15.283046	5.695821	61.352095	C	31.811055	3.783852	50.571516
C	16.314087	6.385804	61.978046	C	30.953601	4.831983	50.961425
C	17.733656	6.784962	47.646135	C	30.777371	5.099534	52.347007
C	16.637604	6.398186	48.408724	C	29.892004	6.123969	52.735046
C	15.567958	5.683658	47.836259	C	29.218736	6.869833	51.772980
C	14.198081	5.242825	62.095148	C	29.383655	6.618382	50.420493
C	13.166040	4.552842	61.469196	C	30.261182	5.602389	49.995511
C	12.083075	4.099846	62.213249	O	28.655001	7.407373	49.535436
C	13.377935	4.632397	48.010907	O	31.569202	5.749400	55.203135
C	14.443543	5.313613	48.615030	O	31.126141	3.564546	55.546776
O	12.270540	4.276334	48.772771	C	31.371775	4.557139	54.770474
O	15.754281	6.384465	59.109317	C	27.253978	5.768460	56.918456
O	15.282340	4.209919	59.475667	C	26.709097	6.880269	57.586728
C	15.445746	5.413468	59.891783	C	40.918022	6.954579	57.602495
Cu	31.501874	6.198601	57.140650	C	40.092847	6.133364	56.845946
Cu	30.986946	3.770681	57.523001	C	40.610550	5.033334	56.130466
C	35.229289	4.129315	57.473723	C	42.006975	4.769916	56.186969
C	35.773302	3.415037	58.556456	C	26.913852	3.878932	55.360209
C	37.118155	3.069217	58.579204	C	41.689517	2.917056	54.651460
C	37.942130	3.420746	57.515832	C	40.322448	3.139647	54.616455
C	37.436258	4.118106	56.401669	C	39.756961	4.202799	55.356668
C	36.059459	4.466448	56.369791	O	39.560836	2.256064	53.854725
C	35.543111	5.107108	55.224202	O	29.534989	6.466273	56.993046
C	36.378044	5.421436	54.156346	O	29.077583	4.283129	57.324628

C	28.707974	5.488441	57.082992	C	47.867453	3.068662	51.453953
C	30.903120	5.695641	61.351269	C	47.083472	3.803691	50.572785
C	31.934175	6.385618	61.977205	C	46.217612	4.817864	51.033611
C	33.348452	7.508042	47.544907	C	46.152373	5.085127	52.427665
C	32.363427	6.923398	48.312971	C	45.239655	6.051053	52.895282
C	31.496984	5.915572	47.780622	C	44.449101	6.760695	52.000216
C	29.818167	5.242646	62.094340	C	44.527009	6.535154	50.635647
C	28.786113	4.552669	61.468405	C	45.415999	5.560848	50.126623
C	27.703159	4.099675	62.212476	O	43.724614	7.330627	49.820513
C	29.584920	4.396803	47.956168	O	47.125564	5.794003	55.212512
C	30.434066	5.328368	48.550787	O	46.818226	3.586791	55.565462
O	28.558777	3.852989	48.668881	C	46.972992	4.592571	54.785061
O	31.368344	6.407235	59.116762	C	42.841612	5.598641	56.986571
O	30.892652	4.229091	59.455379	C	42.277522	6.691544	57.671107
C	31.059325	5.427315	59.887100	C	42.532599	3.716624	55.413648
Cu	47.052392	6.246823	57.148427	O	45.079825	6.394824	57.018696
Cu	46.689696	3.790934	57.535764	O	44.744733	4.189432	57.351165
C	50.914829	4.464394	57.493750	C	44.308004	5.375661	57.119728
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.662675	7.096597	47.740407
C	53.073736	4.554373	56.431559	C	47.591644	6.611218	48.481229
C	51.700736	4.768398	56.388685	C	46.607049	5.795526	47.890553
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.524011	4.541057	48.025580
O	53.987445	5.617415	52.967495	C	45.512381	5.314059	48.650428
O	48.992071	5.857440	57.300410	O	43.443525	4.078498	48.768124
O	48.674657	3.653577	57.672182	O	46.920681	6.442166	59.122346
C	49.438787	4.671146	57.498581	O	46.574869	4.238004	59.463156
C	46.977932	4.347980	53.319264	C	46.675608	5.443126	59.890825
C	47.813668	3.335779	52.814279	C	16.262162	6.620790	63.347051

C	15.179196	6.168795	64.090104	H	26.128118	6.558552	25.802270
C	14.147156	5.478812	63.465153	H	14.941464	3.633615	24.312815
C	12.031150	4.336833	63.582254	H	29.116241	2.180973	23.147279
C	13.063191	5.025817	64.207206	H	19.780483	6.932119	30.326511
O	10.943187	3.908837	64.361307	H	15.660656	4.605597	29.237826
C	31.882275	6.620600	63.346211	H	13.729706	3.929264	30.525093
C	30.799322	6.168606	64.089282	H	15.672185	6.861350	17.596330
C	29.767267	5.478629	63.464346	H	25.164790	6.270450	21.559206
C	27.651260	4.336658	63.581482	H	25.594895	2.569538	22.984166
C	28.683314	5.025635	64.206417	H	37.740022	2.871680	28.266009
O	26.563309	3.908663	64.360554	H	40.120492	2.263452	28.337184
C	47.502389	6.620356	63.345091	H	41.616036	2.903067	26.517093
C	46.419447	6.168363	64.088179	H	37.162633	5.115069	24.000513
C	45.387379	5.478391	63.463260	H	38.666668	5.693265	22.196955
C	43.271369	4.336426	63.580429	H	35.149084	2.328493	22.590754
C	44.303437	5.025398	64.205349	H	35.298504	1.793509	20.190378
O	42.183431	3.908432	64.359519	H	34.099935	3.170577	18.536510
H	12.119316	8.127320	26.935403	H	32.265803	6.143753	22.826270
H	10.573062	6.786924	25.566212	H	31.124962	7.499641	21.165105
H	13.383644	2.323186	22.982549	H	30.035105	7.547351	27.156130
H	9.847515	3.169908	22.676554	H	43.097347	7.689919	27.036116
H	22.117625	2.862301	28.223982	H	41.667235	6.201408	25.747514
H	24.518638	2.335815	28.295218	H	30.637086	3.607498	24.382941
H	26.017717	3.150019	26.548043	H	44.812518	1.896346	23.151407
H	21.522125	5.331194	24.080745	H	35.927656	6.496534	30.229583
H	23.030277	6.089958	22.355612	H	31.434092	4.821180	29.537372
H	19.533121	2.330426	22.589880	H	29.508614	4.542578	30.985171
H	19.679653	1.794311	20.190480	H	31.292333	6.861283	17.596307
H	18.480621	3.170892	18.536721	H	40.796242	5.762597	21.369409
H	16.649657	6.144518	22.827030	H	41.292472	2.234358	22.875468
H	15.506576	7.500787	21.165127	H	53.552028	3.699311	28.381080
H	14.495706	7.508990	27.086640	H	55.987677	3.325963	28.455687
H	27.628753	8.034556	27.033581	H	57.384056	3.866290	26.497852

H 52.703418 5.453306 24.015720	H 18.652249 6.763746 45.717690
H 54.081165 5.976315 22.116909	H 19.577584 7.477445 32.716054
H 50.777540 2.334604 22.589108	H 17.633611 6.736611 33.993623
H 50.920824 1.795210 20.189775	H 14.470451 4.460795 44.814930
H 49.720320 3.170916 18.535938	H 12.576104 3.840726 46.179617
H 47.863464 6.134602 22.823904	H 12.684859 3.771415 32.552838
H 46.741165 7.496801 21.164858	H 14.034118 7.320728 33.288326
H 45.513441 7.281406 27.180494	H 24.115494 6.559622 37.353651
H 46.273334 3.345463 24.438748	H 24.835615 3.113925 37.944159
H 50.923915 7.220945 30.273909	H 36.282437 2.311442 42.943586
H 47.063622 4.435260 29.309842	H 38.696136 1.616980 42.997343
H 45.243185 3.578527 30.646515	H 40.304327 2.595197 41.430033
H 46.912816 6.861653 17.595795	H 35.956690 5.313281 39.187956
H 56.056214 5.977061 21.104074	H 37.536142 6.206665 37.541105
H 10.790772 8.127608 42.499069	H 32.052895 2.087923 38.418996
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H 20.681650 2.488553 43.430962	H 31.760755 8.703349 36.885773
H 23.049835 1.847037 43.507654	H 28.197351 6.490082 44.278966
H 24.640958 2.787621 41.917957	H 41.703407 7.638082 42.555326
H 20.324902 5.382720 39.537931	H 40.349364 6.224642 41.105529
H 21.933375 6.288143 37.981397	H 29.422881 3.674441 40.520446
H 17.984134 2.268690 37.841189	H 43.681528 2.233612 38.260421
H 17.983604 1.824594 35.423594	H 34.308604 7.590330 45.587161
H 16.832123 3.328747 33.890653	H 36.043602 7.020292 32.628138
H 15.201542 6.208101 38.374757	H 34.120945 6.626889 34.076446
H 14.033258 7.658180 36.818979	H 30.993346 4.159770 44.864291
H 13.169553 7.508714 42.647679	H 29.126345 3.260212 46.156140
H 25.778744 6.965293 43.956101	H 28.593515 4.671471 33.076323
H 24.576837 6.052467 42.043987	H 31.432476 8.245577 33.486624
H 13.612098 3.635448 39.861497	H 39.666469 6.406527 36.933821
H 28.190952 2.740234 38.604639	H 40.159269 2.534062 37.887597

H	52.223352	3.703704	43.945662	H	12.932475	7.764484	52.273515
H	54.659108	3.326668	44.019334	H	11.840552	7.509343	58.212198
H	56.055338	3.866232	42.061068	H	24.943270	8.005409	58.063932
H	51.374822	5.453943	39.579447	H	23.451159	6.553629	56.798531
H	52.752290	5.975929	37.680128	H	12.285047	3.636113	55.427474
H	49.688609	2.625181	37.994423	H	26.456526	2.257062	54.033786
H	49.799026	2.151788	35.585393	H	17.168134	6.739851	61.410666
H	48.488996	3.465792	34.005574	H	18.543415	7.345310	48.103132
H	46.419333	6.189179	38.406026	H	16.625303	6.674028	49.454522
H	45.112687	7.457073	36.803828	H	13.129947	4.375206	60.400605
H	44.126156	7.276702	42.743431	H	11.277940	3.574218	61.719337
H	45.066693	3.593922	39.721263	H	11.585478	3.763946	48.237800
H	49.622794	7.150613	45.833167	H	13.028957	7.338531	48.754213
H	50.701216	7.793112	32.655715	H	22.434230	6.269301	52.518116
H	48.867771	6.876841	33.982715	H	22.931726	2.627231	53.894703
H	45.686775	4.479547	44.849835	H	35.141021	3.126922	59.388505
H	43.828450	3.689165	46.177903	H	37.524552	2.521625	59.423760
H	44.250820	3.357430	32.695539	H	38.982934	3.130404	57.563530
H	45.227807	7.069368	33.280325	H	34.493468	5.366035	55.133004
H	54.726416	5.972044	36.665708	H	35.959362	5.912585	53.288300
H	9.463366	8.127025	58.062977	H	32.798558	2.623754	53.588360
H	7.916921	6.786659	56.693646	H	33.102739	2.181847	51.192261
H	10.728046	2.325206	54.106911	H	31.973406	3.553669	49.526856
H	7.191285	3.169589	53.804726	H	29.692254	6.351182	53.777102
H	19.528862	2.943556	59.285752	H	28.534371	7.650237	52.078951
H	21.928762	2.404201	59.306498	H	27.350481	7.532105	58.169010
H	23.388717	3.184056	57.511297	H	40.500410	7.801817	58.137302
H	18.853015	5.405168	55.154742	H	39.040993	6.377602	56.811827
H	20.320539	6.122112	53.375128	H	27.974547	3.664298	55.297874
H	16.916326	2.448196	53.532289	H	42.100463	2.105749	54.065622
H	17.008162	1.962092	51.126828	H	32.786996	6.741941	61.409440
H	15.861553	3.399684	49.530092	H	33.984564	8.287078	47.977048
H	14.069778	6.366499	53.896397	H	32.235656	7.254528	49.348621

H	28.750045	4.374172	60.400051	H	46.387793	6.357284	65.153489
H	26.897865	3.574261	61.718511	H	41.501393	3.424782	63.794566
H	28.091749	3.199885	48.122918	H	54.922545	4.682791	55.325743
H	28.742896	7.107722	48.575226	H	56.250070	4.683137	39.763668
H	38.068434	5.944280	52.404113	H	57.578882	4.683431	24.200630
H	38.581389	2.483594	53.850670	H	32.654283	5.043367	18.026539
H	50.894985	3.699885	59.506326	H	17.034862	5.043626	18.026680
H	53.331560	3.325478	59.581279	H	10.176560	4.915306	24.089557
H	54.727841	3.865719	57.623124	H	8.847971	4.915534	39.653308
H	50.047609	5.459177	55.145227	H	7.520542	4.915509	55.216501
H	51.424912	5.976971	53.242965	H	12.998928	5.198976	65.269026
H	48.429822	2.752556	53.489170	H	28.618789	5.198940	65.268159
H	48.518427	2.285063	51.079240	H	44.238642	5.198816	65.267024
H	47.147421	3.559420	49.522179	H	48.273932	5.043147	18.026074
H	45.112900	6.265989	53.950382	C	31.379495	8.439326	41.181451
H	43.754087	7.504252	52.366950	C	31.208252	8.931644	42.646400
H	42.906656	7.343576	58.266462	C	31.612195	10.401545	42.808779
H	43.594056	3.501462	55.371689	C	30.937256	11.331841	41.793587
H	48.405712	6.744479	61.407889	C	31.220664	10.859891	40.360398
H	49.404832	7.733953	48.210848	C	30.745418	9.417067	40.167322
H	47.529300	6.891257	49.524040	O	32.726362	8.264278	40.919292
H	44.381451	4.364402	60.399357	C	29.397079	8.974938	44.406531
H	42.519354	3.571600	61.717716	C	28.098031	9.468290	44.604395
H	42.814529	3.510717	48.220001	C	27.645817	9.771066	45.892091
H	43.806804	7.103226	48.844482	C	28.487882	9.598039	46.996191
H	53.398719	5.970593	52.227534	C	29.784193	9.108586	46.796593
H	17.068210	7.158077	63.836024	C	30.239019	8.789458	45.514314
H	15.148100	6.357250	65.155561	N	29.824206	8.592486	43.098723
H	10.263098	3.421682	63.797232	H	31.422955	10.734290	43.844697
H	32.687960	7.158510	63.835035	H	31.886705	8.311845	43.246688
H	30.767994	6.357266	65.154673	H	30.836702	7.475553	41.068413
H	25.881948	3.423843	63.795914	H	31.291080	12.368439	41.942466
H	48.307556	7.159072	63.833758	H	29.841602	11.350645	41.968335

H	30.731315	11.525590	39.625547	C	25.305882	4.529409	24.319477
H	32.308448	10.905175	40.168901	O	25.606538	5.647080	22.202108
H	29.640456	9.375343	40.268291	O	20.433876	5.529557	26.189389
H	30.976962	9.049116	39.154078	O	19.918112	3.381507	26.648373
H	32.705427	10.434224	42.653119	C	20.771331	4.312867	26.415445
H	27.436146	9.608513	43.742448	C	18.226927	4.022014	22.293999
H	26.628843	10.152707	46.029416	C	18.992915	2.941012	21.873981
H	28.138979	9.835930	48.005303	C	19.081890	2.638017	20.519979
H	30.457235	8.960656	47.646309	C	18.404876	3.417023	19.587993
H	31.245867	8.389306	45.383579	C	17.639888	4.497024	20.008011
H	30.022368	7.099090	43.131578	C	17.550913	4.800019	21.362013
H	29.130156	8.865322	42.401950	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
(<i>R,R</i>)-2-Int3				C	16.963875	5.274030	19.076025
C	12.487000	7.261000	26.395000	O	15.523872	7.185037	18.539057
C	11.616000	6.503000	25.622000	O	18.565044	5.532083	24.111142
C	12.086000	5.395000	24.927000	O	18.024977	3.390631	24.574154
C	13.428000	5.043000	25.007000	C	18.266031	4.338278	23.745298
C	13.027000	3.179000	23.539000	C	14.301000	5.801000	25.782000
C	11.685000	3.529000	23.460000	C	13.829000	6.909000	26.476000
C	11.215000	4.638000	24.154000	C	27.978551	7.141444	26.445114
O	10.782000	2.793000	22.654000	C	27.137806	6.279499	25.749181
Cu	18.542292	6.090788	26.015348	C	27.644039	5.145859	25.080731
Cu	17.953626	3.701648	26.527818	C	29.039201	4.881929	25.134854
C	22.219064	3.967301	26.378334	C	13.900000	3.935000	24.313000
C	22.761183	3.200327	27.425304	C	28.704411	2.962992	23.684318
C	24.116793	2.897851	27.460051	C	27.337850	3.183819	23.658327
C	24.955346	3.350309	26.446609	C	26.782440	4.278701	24.358007
C	24.451311	4.094170	25.362695	O	26.567359	2.275848	22.934874
C	23.062947	4.389963	25.312325	O	16.595232	6.404862	25.849336
C	22.551170	5.065708	24.183667	O	16.057300	4.264936	26.318891
C	23.401058	5.478842	23.162499	C	15.736237	5.462567	25.983972
C	24.769388	5.231391	23.231709				

C	17.912051	5.817553	30.230894	C	32.583748	5.274002	19.075771
C	18.907194	6.569497	30.881146	O	31.143743	7.185016	18.538835
C	16.760120	5.405607	30.957722	O	34.138470	5.532560	24.126684
C	15.681108	4.748751	30.328479	O	33.629797	3.386288	24.592552
C	14.572923	4.345443	31.067266	C	33.864657	4.334107	23.757375
O	18.429063	6.407867	27.977330	C	29.885001	5.736625	25.895630
O	17.900257	4.261265	28.429230	C	29.339160	6.873955	26.517199
C	18.097185	5.475390	28.794784	C	43.542355	6.861997	26.540780
Cu	34.148507	6.084025	26.035817	C	42.722661	6.001107	25.822248
Cu	33.572342	3.697193	26.564103	C	43.249961	4.879532	25.148763
C	37.829226	3.940189	26.411588	C	44.648160	4.629096	25.217400
C	38.349905	3.226552	27.506629	C	29.555172	3.794272	24.401552
C	39.694397	2.883231	27.561310	C	44.345756	2.706796	23.766015
C	40.543201	3.238755	26.519264	C	42.978515	2.924416	23.711513
C	40.061358	3.930624	25.391613	C	42.405313	4.016215	24.401694
C	38.683757	4.271769	25.324039	O	42.224903	2.012793	22.975222
C	38.192649	4.901116	24.161170	O	32.181503	6.399259	25.930844
C	39.053610	5.218474	23.114786	O	31.676679	4.250436	26.392818
C	40.413409	4.927102	23.197762	C	31.333342	5.446830	26.082883
C	40.929580	4.275201	24.326358	C	33.728830	5.822923	30.279624
O	41.262479	5.255536	22.146678	C	34.837518	6.461864	30.864060
O	36.050188	5.513140	26.164358	C	32.576937	5.563043	31.073097
O	35.530878	3.375594	26.666907	C	31.412013	4.995778	30.518965
C	36.385242	4.299691	26.418597	C	30.291387	4.774560	31.315454
C	33.846854	4.021972	22.293718	O	34.098469	6.399523	27.999373
C	34.612831	2.940969	21.873683	O	33.547961	4.263769	28.476082
C	34.701781	2.637978	20.519678	C	33.795495	5.472645	28.833144
C	34.024753	3.416989	19.587708	Cu	49.689080	6.190571	25.991185
C	33.259776	4.496991	20.007741	Cu	49.348574	3.768191	26.558982
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787

C	55.729946	4.554780	25.305823	C	47.070895	4.659764	30.375752
C	54.356947	4.768795	25.262899	C	46.014883	4.169057	31.137203
C	53.770890	5.287813	24.113936	O	49.595697	6.538499	27.948800
C	54.557834	5.591815	23.007897	O	49.300543	4.358918	28.452256
C	55.929834	5.377800	23.052821	C	49.378680	5.594243	28.790796
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.632463	5.830731	26.128880	C	10.757253	5.394976	40.491133
O	51.339037	3.649386	26.627826	C	12.099253	5.042971	40.571108
C	52.092636	4.660279	26.379538	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.246726	6.014777	41.482660
C	48.879661	4.496905	20.007192	Cu	16.613427	3.639518	41.998620
C	48.790737	4.799893	21.361200	C	20.882007	3.796822	41.908770
C	48.023772	5.880897	21.783251	C	21.355267	3.061651	43.011071
C	47.347731	6.658913	20.849295	C	22.699529	2.731860	43.126385
C	47.437655	6.354926	19.496287	C	23.597386	3.126605	42.141090
C	48.203620	5.273922	19.075235	C	23.165470	3.837033	41.005986
O	46.763613	7.184943	18.538331	C	21.786787	4.155183	40.870986
O	49.727742	5.586277	24.094643	C	21.346477	4.792978	39.693412
O	49.388653	3.417223	24.603474	C	22.256661	5.134624	38.696891
C	49.524596	4.364672	23.749624	C	23.615687	4.871926	38.851587
C	45.477639	5.502497	25.973483	C	24.082345	4.228708	40.003219
C	44.905924	6.618716	26.611583	O	24.511405	5.224617	37.850557
C	45.181623	3.542626	24.496801	O	19.134813	5.398547	41.618837
O	47.710175	6.314478	25.891723	O	18.565241	3.269252	42.101044
O	47.396858	4.143456	26.416996	C	19.442204	4.177862	41.873938
C	46.947680	5.303752	26.096877	C	16.817670	4.006592	37.744767
C	49.180817	5.946713	30.222891	C	17.487215	2.882460	37.230014
C	50.102283	6.810657	30.841826	C	17.502099	2.626293	35.865446
C	48.081643	5.442859	30.973590	C	16.846880	3.486732	34.990992

C	16.133747	4.607506	35.464811	C	15.546775	5.259958	33.088372
C	16.098413	4.858554	36.862281	O	13.395657	4.169795	33.164792
C	15.321905	5.932146	37.342765	O	17.186831	6.327073	43.444960
C	14.641871	6.758816	36.457542	O	16.605201	4.196689	43.906433
C	14.704005	6.552243	35.089598	C	16.847624	5.404270	44.269368
C	15.457001	5.476021	34.568102	Cu	33.565939	6.658432	41.200527
O	14.019709	7.460243	34.284352	Cu	32.407896	3.935425	42.125893
O	17.221221	5.470866	39.575724	C	36.538277	3.577736	41.380220
O	16.657497	3.334257	40.029766	C	36.986880	2.641825	42.295215
C	16.905022	4.284657	39.202930	C	38.350401	2.272544	42.322487
C	12.972270	5.800966	41.346096	C	39.246979	2.841351	41.443694
C	12.500286	6.908965	42.040108	C	38.829763	3.782373	40.446284
C	26.340749	6.875255	42.579675	C	37.431827	4.130688	40.399364
C	25.638135	6.015334	41.761938	C	36.990040	4.992026	39.354634
C	26.269240	4.937473	41.057729	C	37.872692	5.508526	38.436931
C	27.690298	4.766553	41.240614	C	39.262012	5.228160	38.520798
C	12.571237	3.934972	39.877096	C	39.745040	4.373717	39.510630
C	27.638334	2.907006	39.674364	O	40.122214	5.791044	37.628402
C	26.236776	3.056098	39.497691	O	34.937001	5.301534	41.311785
C	25.544715	4.052742	40.179656	O	34.238592	3.251572	41.883668
O	25.701048	2.143064	38.637332	C	35.131318	4.071319	41.522756
O	15.291468	6.378827	41.368293	C	31.957845	4.310292	38.053643
O	14.727026	4.246962	41.836577	C	32.194867	3.005056	37.638443
C	14.415682	5.452844	41.523679	C	32.209395	2.676941	36.270857
C	16.714205	5.757779	45.709369	C	31.968672	3.647533	35.322371
C	17.744732	6.496890	46.319081	C	31.687350	5.004625	35.679530
C	18.807171	6.865584	32.234480	C	31.692204	5.343434	37.085010
C	17.709030	6.420437	32.962401	C	31.413146	6.695103	37.444765
C	16.673479	5.691877	32.345875	C	31.142503	7.640849	36.488734
C	15.569230	5.395476	46.472683	C	31.134606	7.315235	35.107007
C	14.462570	4.744331	45.887665	C	31.412435	6.016539	34.691205
C	13.361402	4.391775	46.661848	O	30.845340	8.381291	34.301557
C	14.508431	4.579244	32.438547	O	32.208194	5.711643	40.000532

O	31.986351	3.517794	40.278054	C	52.828353	3.947597	43.079285
C	32.049927	4.549781	39.529738	C	54.201353	3.732577	43.123183
C	28.392122	5.686036	42.094432	C	54.987278	4.036581	42.018131
C	27.728966	6.723749	42.739520	C	54.401203	4.554604	40.869180
C	42.182161	6.870769	41.998177	C	53.028203	4.768624	40.826281
C	41.410107	6.036287	41.198075	C	52.442128	5.287648	39.677330
C	41.994974	4.993707	40.451863	C	53.229054	5.591652	38.571278
C	43.398288	4.784331	40.543354	C	54.601054	5.377632	38.616177
C	28.344810	3.728206	40.516381	C	55.187129	4.858609	39.764128
C	43.199334	2.971924	38.940252	O	55.314970	5.617639	37.405129
C	41.828278	3.151827	38.860295	O	50.334486	5.883989	41.712603
C	41.207312	4.168035	39.612357	O	49.996265	3.702368	42.182229
O	41.122314	2.285170	38.030416	C	50.769990	4.699336	41.950768
O	30.409776	6.769493	42.516068	C	48.277234	4.260882	37.809598
O	30.475296	4.527911	42.369416	C	49.095754	3.226998	37.321531
C	29.849029	5.601011	42.324146	C	49.166378	2.956564	35.962011
C	32.538951	6.125212	45.618444	C	48.417726	3.710960	35.065535
C	33.303763	7.157247	46.132235	C	47.563042	4.740960	35.510992
C	34.841827	6.796156	32.212079	C	47.477091	5.008765	36.903361
C	33.730375	6.517733	32.999508	C	46.571630	5.989885	37.354792
C	32.582324	5.917086	32.450856	C	45.810920	6.714584	36.446294
C	31.501269	5.516338	46.404333	C	45.911890	6.489525	35.083560
C	30.598826	4.554227	45.867769	C	46.793054	5.500326	34.590953
C	29.586240	4.026853	46.631150	O	45.134012	7.294129	34.253547
C	30.299451	5.106378	32.669043	O	48.450062	5.761198	39.649827
C	31.437005	5.680815	33.246161	O	48.133446	3.570688	40.086761
O	29.171115	4.883098	33.447731	C	48.287783	4.546844	39.268042
O	32.916836	6.581356	43.313459	C	44.177325	5.620652	41.390810
O	32.789860	4.447572	43.970899	C	43.552648	6.669753	42.088731
C	32.788429	5.686096	44.212140	C	43.987679	3.773256	39.758832
Cu	48.395021	6.293165	41.561333	O	46.413812	6.445175	41.436520
Cu	48.017635	3.858048	42.052459	O	46.077945	4.253798	41.853218
C	52.242278	4.464620	41.931334	C	45.642755	5.427547	41.568473

C	47.841250	5.956925	45.773494	C	22.657528	4.632802	55.331525
C	48.787719	6.787680	46.401366	O	22.932534	5.775964	53.224425
C	49.982769	7.135642	32.187103	O	17.794927	5.618914	57.306102
C	48.937202	6.608850	32.937760	O	17.313602	3.443693	57.665482
C	47.975008	5.763113	32.353069	C	18.151242	4.398612	57.481531
C	46.721472	5.488410	46.515042	C	15.678818	4.239758	53.320920
C	45.692243	4.736326	45.910177	C	16.384596	3.127284	52.828133
C	44.614549	4.281990	46.664048	C	16.428670	2.855487	51.468175
C	45.934391	4.440664	32.500285	C	15.762128	3.684952	50.574261
C	46.900637	5.245811	33.118392	C	15.022481	4.799375	51.021815
O	44.874985	3.941821	33.249915	C	14.968149	5.074852	52.415170
O	48.284712	6.583929	43.521976	C	14.175608	6.149019	52.866768
O	47.915598	4.401973	43.962943	C	13.498458	6.952896	51.958340
C	48.029762	5.625817	44.335453	C	13.569538	6.715726	50.595716
C	9.830848	7.260896	57.522290	C	14.332255	5.633027	50.102421
C	8.959816	6.502907	56.749315	O	12.881988	7.599734	49.766719
C	9.429783	5.394908	56.054291	O	15.951176	5.675970	55.208144
C	10.771783	5.042898	56.134241	O	15.445899	3.508359	55.574951
C	10.370718	3.178911	54.666243	C	15.691585	4.491015	54.787284
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.332555	7.141068	57.566990
Cu	15.891611	6.152894	57.137415	C	24.492269	6.313842	56.831324
Cu	15.348382	3.735769	57.547375	C	24.998238	5.213185	56.109252
C	19.601825	4.072637	57.434791	C	26.394079	4.948330	56.146359
C	20.155608	3.294434	58.467213	C	11.243751	3.934900	55.440217
C	21.509389	2.983213	58.477845	C	26.055011	3.097215	54.611853
C	22.333447	3.435902	57.452964	C	24.688018	3.318659	54.599735
C	21.817245	4.194759	56.384978	C	24.134546	4.380446	55.350061
C	20.431381	4.504601	56.362272	O	23.914803	2.440745	53.842909
C	19.906994	5.202954	55.253539	O	13.936446	6.438135	56.972630
C	20.742605	5.618456	54.221627	O	13.439727	4.274325	57.366427
C	22.109000	5.353815	54.262184	C	13.092448	5.478316	57.083157

C	15.283046	5.695821	61.352095	C	31.688948	3.782151	50.563921
C	16.314087	6.385804	61.978046	C	30.849610	4.839348	50.968608
C	17.681759	6.835298	47.664372	C	30.704822	5.112558	52.356673
C	16.584664	6.448554	48.425464	C	29.839472	6.148630	52.759285
C	15.517682	5.730381	47.852413	C	29.158462	6.902060	51.808646
C	14.198081	5.242825	62.095148	C	29.294403	6.646903	50.453796
C	13.166040	4.552842	61.469196	C	30.146184	5.614813	50.014764
C	12.083075	4.099846	62.213249	O	28.564505	7.448144	49.580521
C	13.329244	4.675437	48.024859	O	31.541844	5.753107	55.202053
C	14.394013	5.356768	48.630241	O	31.097183	3.568852	55.547261
O	12.223467	4.314067	48.786551	C	31.334644	4.562356	54.769754
O	15.752325	6.386956	59.110894	C	27.240995	5.770095	56.940649
O	15.282648	4.211316	59.474280	C	26.693240	6.873455	57.620313
C	15.445157	5.414622	59.891863	C	40.919201	6.957055	57.637256
Cu	31.488470	6.201132	57.140331	C	40.092268	6.148865	56.868506
Cu	30.975593	3.772872	57.524069	C	40.608333	5.060845	56.133859
C	35.219199	4.131858	57.450457	C	42.004606	4.795000	56.185073
C	35.761603	3.398419	58.521257	C	26.908228	3.895335	55.363551
C	37.106569	3.053211	58.541163	C	41.684097	2.966766	54.621269
C	37.933118	3.425214	57.486965	C	40.317341	3.192473	54.589387
C	37.429755	4.142739	56.384663	C	39.753373	4.244570	55.346464
C	36.052325	4.489830	56.354918	O	39.554305	2.322671	53.813291
C	35.538828	5.149872	55.219097	O	29.521141	6.469209	57.005914
C	36.377419	5.486692	54.160867	O	29.065478	4.286032	57.340976
C	37.737155	5.186875	54.206118	C	28.694925	5.491420	57.101043
C	38.275953	4.507178	55.307711	C	30.903120	5.695641	61.351269
O	38.563878	5.535706	53.144250	C	31.934175	6.385618	61.977205
O	33.404636	5.676056	57.285434	C	33.123873	7.571523	47.470457
O	32.937303	3.499310	57.655509	C	32.173696	6.969835	48.268998
C	33.768579	4.458471	57.473690	C	31.316127	5.936156	47.771047
C	31.403076	4.312333	53.303475	C	29.818167	5.242646	62.094340
C	32.199834	3.245027	52.850691	C	28.786113	4.552669	61.468405
C	32.347780	2.988562	51.495087	C	27.703159	4.099675	62.212476

C	29.430312	4.393382	47.993579	O	47.125684	5.802060	55.214260
C	30.284346	5.333864	48.568174	O	46.817705	3.594260	55.563566
O	28.444010	3.824696	48.739045	C	46.973684	4.601245	54.785098
O	31.365997	6.407858	59.117030	C	42.841120	5.610648	56.995833
O	30.894502	4.228860	59.456791	C	42.278906	6.692742	57.698716
C	31.059512	5.427450	59.887716	C	42.528522	3.752656	55.396185
Cu	47.053556	6.251890	57.150511	O	45.080812	6.402857	57.022746
Cu	46.687893	3.795713	57.533723	O	44.742933	4.196785	57.348630
C	50.914829	4.464394	57.493750	C	44.307582	5.384668	57.122697
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.667707	7.119483	47.744106
C	53.073736	4.554373	56.431559	C	47.596885	6.632558	48.484339
C	51.700736	4.768398	56.388685	C	46.613685	5.815596	47.892968
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.532580	4.557535	48.026653
O	53.987445	5.617415	52.967495	C	45.519526	5.331948	48.651931
O	48.993096	5.859600	57.301232	O	43.452515	4.093082	48.768610
O	48.673082	3.655857	57.671134	O	46.922718	6.444253	59.124141
C	49.438590	4.672668	57.498686	O	46.572545	4.240223	59.461513
C	46.981066	4.359166	53.319385	C	46.675379	5.444555	59.890881
C	47.820976	3.350924	52.813548	C	16.262162	6.620790	63.347051
C	47.878774	3.088120	51.452608	C	15.179196	6.168795	64.090104
C	47.094477	3.823458	50.571951	C	14.147156	5.478812	63.465153
C	46.224366	4.833592	51.034022	C	12.031150	4.336833	63.582254
C	46.155195	5.096401	52.428499	C	13.063191	5.025817	64.207206
C	45.238566	6.058170	52.897214	O	10.943187	3.908837	64.361307
C	44.448474	6.768928	52.002613	C	31.882275	6.620600	63.346211
C	44.530536	6.548199	50.637588	C	30.799322	6.168606	64.089282
C	45.422470	5.577034	50.127870	C	29.767267	5.478629	63.464346
O	43.729045	7.344900	49.822700	C	27.651260	4.336658	63.581482

C	28.683314	5.025635	64.206417	H	37.701428	2.944376	28.328382
O	26.563309	3.908663	64.360554	H	40.082321	2.339926	28.417429
C	47.502389	6.620356	63.345091	H	41.584542	2.956210	26.594873
C	46.419447	6.168363	64.088179	H	37.142769	5.146525	24.038523
C	45.387379	5.478391	63.463260	H	38.654192	5.703758	22.234532
C	43.271369	4.336426	63.580429	H	35.148926	2.328658	22.590961
C	44.303437	5.025398	64.205349	H	35.298495	1.793509	20.190361
O	42.183431	3.908432	64.359519	H	34.100014	3.170646	18.536493
H	12.119261	8.127156	26.935637	H	32.263219	6.143371	22.825845
H	10.573047	6.786885	25.566293	H	31.124508	7.499335	21.165091
H	13.383695	2.323362	22.982316	H	29.978628	7.546482	27.077427
H	9.847481	3.169829	22.676730	H	43.117562	7.726029	27.042232
H	22.122362	2.849899	28.228042	H	41.667397	6.230444	25.784519
H	24.522199	2.313810	28.280447	H	30.616077	3.577103	24.354616
H	26.006180	3.100901	26.507866	H	44.762196	1.869693	23.221904
H	21.492997	5.271672	24.064027	H	35.711190	6.689358	30.263508
H	22.984895	5.998736	22.310196	H	31.347974	4.726518	29.468664
H	19.532377	2.329791	22.589909	H	29.407934	4.339263	30.867694
H	19.679416	1.794137	20.190503	H	31.292319	6.861337	17.596277
H	18.480536	3.170847	18.536725	H	40.784957	5.750658	21.408512
H	16.650844	6.145023	22.827103	H	41.242762	2.229551	22.967861
H	15.506775	7.500935	21.165124	H	53.552002	3.699229	28.381025
H	14.495563	7.508342	27.087417	H	55.987690	3.325955	28.455676
H	27.570455	8.018045	26.938367	H	57.384061	3.866295	26.497843
H	26.083891	6.517671	25.720596	H	52.703436	5.453370	24.015659
H	14.941549	3.634141	24.311438	H	54.081178	5.976339	22.116911
H	29.108443	2.126652	23.129657	H	50.777423	2.334581	22.589167
H	19.775048	6.912954	30.329592	H	50.920848	1.795227	20.189768
H	15.668802	4.551122	29.261812	H	49.720380	3.170955	18.535929
H	13.759613	3.841721	30.562629	H	47.863576	6.134732	22.823889
H	15.672013	6.861269	17.596333	H	46.741273	7.496888	21.164843
H	25.111961	6.163893	21.490531	H	45.531744	7.304385	27.171609
H	25.586646	2.499046	22.939460	H	46.243740	3.327113	24.475131

H 50.927023 7.222578 30.271467	H 36.280617 2.222830 43.016374
H 47.071176 4.426539 29.316571	H 38.699564 1.544316 43.061290
H 45.254762 3.567937 30.656865	H 40.301237 2.553939 41.507829
H 46.913295 6.862043 17.595725	H 35.933662 5.243653 39.270625
H 56.056245 5.977134 21.104084	H 37.505452 6.159596 37.634535
H 10.790779 8.127541 42.499181	H 32.388461 2.240361 38.392473
H 9.244406 6.786971 41.130131	H 32.417867 1.648304 35.960497
H 12.055582 2.325670 38.543149	H 31.995902 3.352774 34.268470
H 8.519316 3.171092 38.239705	H 31.427780 6.978569 38.494648
H 20.670767 2.758589 43.795511	H 30.925480 8.675936 36.766753
H 23.050345 2.174047 43.989242	H 28.281579 7.417387 43.375446
H 24.638441 2.856830 42.265608	H 41.713650 7.678545 42.551959
H 20.298841 5.019713 39.519562	H 40.345821 6.225811 41.154029
H 21.894569 5.618820 37.799624	H 29.419382 3.579764 40.619567
H 18.014905 2.211272 37.897864	H 43.659275 2.195501 38.342987
H 18.030870 1.759784 35.480990	H 34.054498 7.635212 45.497335
H 16.884915 3.256818 33.935583	H 35.712141 7.274892 32.650423
H 15.214779 6.141831 38.400996	H 33.771308 6.787283 34.047332
H 14.051245 7.583051 36.834561	H 30.696084 4.233155 44.832373
H 13.169664 7.508077 42.648176	H 28.892802 3.302180 46.188230
H 25.827040 7.688590 43.100419	H 28.429490 4.432660 32.932105
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H 13.612234 3.635575 39.862035	H 39.638400 6.386801 37.033788
H 28.140619 2.118881 39.107464	H 40.131480 2.473292 38.008582
H 18.608645 6.803328 45.740081	H 52.223536 3.704744 43.946086
H 19.588477 7.438036 32.724710	H 54.659171 3.326962 44.019441
H 17.666100 6.664557 34.015294	H 56.055358 3.866319 42.061099
H 14.423687 4.509708 44.829365	H 51.374793 5.453812 39.579512
H 12.527508 3.888712 46.191331	H 52.752290 5.975901 37.680118
H 12.732320 3.663711 32.597356	H 49.693585 2.637377 38.007277
H 14.082666 7.242878 33.304403	H 49.808527 2.160135 35.599292
H 24.070301 5.738159 37.101233	H 48.499440 3.470024 34.015232
H 24.757130 2.292250 38.472555	H 46.426021 6.204333 38.407449

H	45.121391	7.469054	36.800886	H	13.130156	4.374967	60.400624
H	44.139578	7.328647	42.718665	H	11.277971	3.574178	61.719332
H	45.057469	3.593596	39.753793	H	11.541391	3.797859	48.251450
H	49.628838	7.174559	45.837305	H	12.970102	7.373865	48.790637
H	50.707036	7.796590	32.652991	H	22.432523	6.312040	52.531041
H	48.876116	6.879983	33.983175	H	22.933871	2.662047	53.863046
H	45.695877	4.499186	44.851774	H	35.127799	3.095257	59.346797
H	43.839762	3.703996	46.178785	H	37.511163	2.490620	59.376680
H	44.263588	3.351108	32.706461	H	38.974118	3.135253	57.532446
H	45.237837	7.070734	33.278506	H	34.488695	5.406855	55.127832
H	54.726571	5.972541	36.665832	H	35.961074	5.993667	53.300844
H	9.463395	8.127098	58.062878	H	32.722022	2.616218	53.563151
H	7.916948	6.786723	56.693559	H	32.976625	2.168406	51.162649
H	10.728094	2.325312	54.106791	H	31.828985	3.548735	49.516906
H	7.191493	3.170138	53.804085	H	29.662788	6.381855	53.804088
H	19.526153	2.937081	59.274234	H	28.493010	7.694434	52.125763
H	21.923948	2.388608	59.285887	H	27.332476	7.519964	58.210800
H	23.382649	3.175743	57.493055	H	40.502816	7.795286	58.187034
H	18.850014	5.427345	55.159407	H	39.040340	6.393690	56.840487
H	20.317221	6.154882	53.384230	H	27.969116	3.680943	55.304476
H	16.910223	2.470637	53.512068	H	42.093704	2.163899	54.023021
H	16.982317	1.995966	51.103391	H	32.786972	6.742028	61.409450
H	15.816946	3.437115	49.523841	H	33.744126	8.376619	47.875887
H	14.055075	6.379089	53.919089	H	32.061694	7.313118	49.302174
H	12.899279	7.780877	52.312901	H	28.750139	4.374093	60.400036
H	11.840426	7.509559	58.212158	H	26.897802	3.574388	61.718471
H	24.924478	7.991132	58.104736	H	27.954482	3.180001	48.202920
H	23.438440	6.553099	56.816910	H	28.649805	7.165723	48.616007
H	12.285092	3.636258	55.427417	H	38.073919	6.049752	52.427276
H	26.457415	2.286941	54.018741	H	38.574746	2.549784	53.815888
H	17.168032	6.740075	61.410633	H	50.894986	3.700168	59.506400
H	18.489127	7.399113	48.121429	H	53.331574	3.325571	59.581317
H	16.569254	6.727730	49.470335	H	54.727850	3.865774	57.623152

H	50.047627	5.459282	55.145273	H	7.520566	4.915566	55.216450
H	51.424909	5.976997	53.242980	H	12.998924	5.199012	65.269015
H	48.437628	2.767939	53.488212	H	28.618755	5.199002	65.268145
H	48.533420	2.307979	51.077036	H	44.238627	5.198840	65.267025
H	47.162066	3.582891	49.520746	H	48.273987	5.043191	18.026061
H	45.108719	6.269109	53.952769	C	32.011617	9.050811	40.865779
H	43.750745	7.509600	52.370049	C	31.863091	9.612237	42.305607
H	42.909549	7.334852	58.303197	C	32.902641	10.723093	42.555623
H	43.589700	3.535872	55.352618	C	32.807571	11.838116	41.504705
H	48.405664	6.744700	61.407943	C	32.966124	11.273870	40.083204
H	49.408952	7.757581	48.215089	C	31.936488	10.170074	39.806225
H	47.533752	6.912101	49.527266	O	33.223077	8.386123	40.740465
H	44.381214	4.364582	60.399365	C	29.763498	9.765791	43.699176
H	42.519299	3.571684	61.717718	C	28.402872	10.157433	43.762413
H	42.823777	3.525826	48.219777	C	27.622723	9.877750	44.883599
H	43.818675	7.124639	48.845709	C	28.161192	9.199476	45.985938
H	53.398846	5.971261	52.227764	C	29.506861	8.817713	45.936781
H	17.068190	7.158131	63.835998	C	30.301954	9.095150	44.823096
H	15.148064	6.357335	65.155541	N	30.497332	10.033866	42.565848
H	10.262991	3.421938	63.797143	H	32.765933	11.126896	43.575364
H	32.687889	7.158639	63.835006	H	32.091848	8.774795	42.974716
H	30.767919	6.357402	65.154645	H	31.172727	8.345112	40.683817
H	25.881470	3.424746	63.795710	H	33.572943	12.611908	41.698830
H	48.307505	7.159160	63.833750	H	31.823734	12.341183	41.594819
H	46.387772	6.357321	65.153486	H	32.872940	12.080998	39.332864
H	41.501118	3.425241	63.794509	H	33.978146	10.842601	39.974293
H	54.922554	4.682827	55.325772	H	30.914332	10.599863	39.797443
H	56.250085	4.683170	39.763679	H	32.099153	9.712296	38.814329
H	57.578888	4.683442	24.200623	H	33.905646	10.261072	42.508972
H	32.654288	5.043390	18.026527	H	27.959624	10.678987	42.906235
H	17.034821	5.043621	18.026679	H	26.574387	10.196430	44.894325
H	10.176558	4.915311	24.089595	H	27.546838	8.988565	46.866422
H	8.847995	4.915583	39.653294	H	29.968847	8.294962	46.780629

H	31.345603	8.778620	44.833313	C	17.639888	4.497024	20.008011
H	31.377714	6.711067	42.767637	C	17.550913	4.800019	21.362013
H	30.011954	10.518397	41.821286	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
				C	16.963875	5.274030	19.076025
				O	15.523872	7.185037	18.539057
				O	18.563859	5.528167	24.115476
				O	18.018906	3.386346	24.571118
				C	18.263246	4.335812	23.745673
				C	14.301000	5.801000	25.782000
				C	13.829000	6.909000	26.476000
				C	27.990830	7.117834	26.500668
				C	27.149305	6.263947	25.795649
				C	27.655099	5.139498	25.111794
				C	29.050401	4.874319	25.162711
				C	13.900000	3.935000	24.313000
				C	28.713628	2.970006	23.693390
				C	27.347542	3.193831	23.667285
				C	26.792871	4.282427	24.377425
				O	26.576665	2.294766	22.933125
				O	16.597365	6.399706	25.858723
				O	16.054996	4.259538	26.320887
				C	15.736084	5.458837	25.988396
				C	17.930646	5.782632	30.242919
				C	18.919686	6.550408	30.884483
				C	16.796807	5.344681	30.983825
				C	15.722305	4.668938	30.366831
				C	14.633195	4.239683	31.118945
				O	18.433995	6.387090	27.987830
				O	17.905541	4.238735	28.429534
				C	18.105105	5.450198	28.801968
				Cu	34.164765	6.056132	26.048024

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C	12.487000	7.261000	26.395000
C	11.616000	6.503000	25.622000
C	12.086000	5.395000	24.927000
C	13.428000	5.043000	25.007000
C	13.027000	3.179000	23.539000
C	11.685000	3.529000	23.460000
C	11.215000	4.638000	24.154000
O	10.782000	2.793000	22.654000
Cu	18.544060	6.079470	26.022704
Cu	17.951638	3.689634	26.525167
C	22.219287	3.948707	26.373785
C	22.757839	3.171446	27.415060
C	24.114139	2.872554	27.454487
C	24.957128	3.337924	26.450809
C	24.457045	4.090412	25.371224
C	23.068020	4.383432	25.316214
C	22.560827	5.068367	24.191133
C	23.415458	5.493121	23.178609
C	24.784140	5.248143	23.252893
C	25.316495	4.536884	24.336751
O	25.625524	5.674316	22.231075
O	20.435186	5.513732	26.191515
O	19.916385	3.364366	26.639954
C	20.771223	4.295417	26.410908
C	18.226927	4.022014	22.293999
C	18.992915	2.941012	21.873981
C	19.081890	2.638017	20.519979
C	18.404876	3.417023	19.587993

Cu	33.582834	3.667539	26.562612	C	43.256628	4.858706	25.148136
C	37.838150	3.893076	26.394198	C	44.655771	4.615609	25.216513
C	38.355045	3.165282	27.481935	C	29.565073	3.792996	24.419101
C	39.698630	2.818183	27.535232	C	44.364071	2.693302	23.762658
C	40.550383	3.185716	26.499807	C	42.995878	2.904243	23.707811
C	40.071494	3.890929	25.379063	C	42.417399	3.992531	24.398753
C	38.694635	4.233959	25.311899	O	42.246603	1.990264	22.970020
C	38.205861	4.873877	24.153868	O	32.196833	6.380367	25.964028
C	39.068658	5.199777	23.111980	O	31.688515	4.229453	26.412044
C	40.428342	4.908709	23.195952	C	31.346674	5.428831	26.112688
C	40.941799	4.246870	24.319851	C	33.852177	5.746628	30.295110
O	41.280225	5.249172	22.151121	C	35.000371	6.344770	30.845751
O	36.064735	5.474148	26.156333	C	32.728160	5.497222	31.128978
O	35.539193	3.335543	26.647969	C	31.528602	4.969526	30.611530
C	36.395947	4.257944	26.403425	C	30.433618	4.765581	31.447388
C	33.846854	4.021972	22.293718	O	34.142187	6.353760	28.013472
C	34.612831	2.940969	21.873683	O	33.583963	4.217247	28.479132
C	34.701781	2.637978	20.519678	C	33.856217	5.418517	28.843443
C	34.024753	3.416989	19.587708	Cu	49.689242	6.188410	25.992639
C	33.259776	4.496991	20.007741	Cu	49.351337	3.765307	26.559661
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.135289	5.522642	24.134588	C	53.770890	5.287813	24.113936
O	33.624115	3.374181	24.587966	C	54.557834	5.591815	23.007897
C	33.859834	4.326995	23.758453	C	55.929834	5.377800	23.052821
C	29.897588	5.721152	25.931331	C	56.515889	4.858782	24.200784
C	29.352187	6.851410	26.565952	O	56.643771	5.617805	21.841785
C	43.538296	6.841821	26.541692	O	51.632520	5.829756	26.129138
C	42.723014	5.976128	25.823850	O	51.340879	3.647867	26.627325

C	52.093284	4.659485	26.379349	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.239126	5.946272	41.544520
C	48.879661	4.496905	20.007192	Cu	16.556875	3.582656	42.056324
C	48.790737	4.799893	21.361200	C	20.820018	3.660263	42.002157
C	48.023772	5.880897	21.783251	C	21.286897	2.928097	43.108474
C	47.347731	6.658913	20.849295	C	22.626515	2.577680	43.217892
C	47.437655	6.354926	19.496287	C	23.524464	2.950964	42.223406
C	48.203620	5.273922	19.075235	C	23.095145	3.656846	41.084355
O	46.763613	7.184943	18.538331	C	21.721027	3.992122	40.954358
O	49.727068	5.585619	24.095564	C	21.279843	4.621791	39.772218
O	49.390246	3.416036	24.603499	C	22.186843	4.943145	38.767417
C	49.524711	4.364091	23.749954	C	23.543452	4.668858	38.918504
C	45.480162	5.492754	25.973398	C	24.009155	4.029476	40.073198
C	44.903264	6.606362	26.611150	O	24.437595	5.007008	37.910955
C	45.195193	3.532674	24.494664	O	19.109679	5.294665	41.711139
O	47.710440	6.310491	25.894285	O	18.496418	3.175437	42.186931
O	47.400418	4.138828	26.419402	C	19.390580	4.068203	41.968106
C	46.949846	5.298281	26.099017	C	16.831942	3.936479	37.804671
C	49.182794	5.942522	30.223917	C	17.496995	2.804223	37.302160
C	50.108352	6.800085	30.845400	C	17.526889	2.543245	35.938660
C	48.077525	5.446813	30.970979	C	16.889676	3.405930	35.053025
C	47.065951	4.666749	30.370826	C	16.181816	4.535185	35.514027
C	46.004363	4.183213	31.128951	C	16.134452	4.793751	36.910016
O	49.597091	6.534905	27.950404	C	15.368026	5.880641	37.376660
O	49.303978	4.354827	28.453386	C	14.708786	6.711713	36.480033
C	49.381380	5.590126	28.792131	C	14.779927	6.495040	35.114098
C	11.158286	7.260970	41.959133	C	15.522461	5.405217	34.606185
C	10.287269	6.502976	41.186145	O	14.112816	7.405108	34.296756
C	10.757253	5.394976	40.491133	O	17.232738	5.398082	39.638383
C	12.099253	5.042971	40.571108	O	16.623933	3.272976	40.088480

C	16.901155	4.216727	39.263429	C	38.506151	2.505695	42.360486
C	12.972270	5.800966	41.346096	C	39.358995	3.044676	41.421117
C	12.500286	6.908965	42.040108	C	38.903512	3.992483	40.446862
C	26.367588	6.713793	42.540958	C	37.518236	4.378510	40.490210
C	25.616604	5.811624	41.816888	C	37.021376	5.240001	39.470554
C	26.216418	4.750797	41.059513	C	37.847795	5.714235	38.480452
C	27.648600	4.633890	41.121061	C	39.234487	5.402999	38.476297
C	12.571237	3.934972	39.877096	C	39.767025	4.558226	39.447992
C	27.556556	2.711077	39.640091	O	40.046023	5.934682	37.520392
C	26.144557	2.839869	39.534350	O	35.180065	5.653800	41.696780
C	25.468775	3.835431	40.235509	O	34.373992	3.561182	41.948770
O	25.581581	1.909008	38.710257	C	35.298439	4.395469	41.733597
O	15.295834	6.345723	41.399238	C	32.242651	4.129244	38.116617
O	14.689103	4.224575	41.866618	C	32.338119	2.811390	37.689646
C	14.404268	5.434164	41.545154	C	32.293574	2.500714	36.318204
C	16.639330	5.707738	45.761994	C	32.112799	3.501214	35.386855
C	17.674075	6.429337	46.385101	C	31.958133	4.873937	35.763284
C	18.832283	6.837921	32.240660	C	32.052666	5.197406	37.168623
C	17.752357	6.369202	32.980813	C	31.926905	6.567121	37.549170
C	16.722367	5.624904	32.374342	C	31.688300	7.540472	36.613025
C	15.479548	5.362417	46.510341	C	31.573760	7.229128	35.233370
C	14.369349	4.731160	45.910475	C	31.723864	5.915799	34.796178
C	13.255348	4.390845	46.671713	O	31.332268	8.323238	34.449956
C	14.580187	4.471088	32.491007	O	32.726131	5.466406	40.057341
C	15.611406	5.173395	33.128804	O	32.056396	3.384458	40.363788
O	13.484483	4.038674	33.229763	C	32.351587	4.351571	39.587075
O	17.154375	6.264424	43.504309	C	28.391283	5.618025	41.845302
O	16.530586	4.144888	43.961803	C	27.778123	6.646591	42.532019
C	16.787355	5.349287	44.325260	C	42.206205	6.953767	42.024547
Cu	33.656430	6.831931	41.551278	C	41.437217	6.171174	41.171274
Cu	32.492641	4.087829	42.153242	C	42.019799	5.154159	40.387796
C	36.680837	3.859654	41.531439	C	43.419291	4.927741	40.483884
C	37.154490	2.913780	42.420618	C	28.289851	3.582532	40.403164

C	43.224773	3.202855	38.786968	O	55.314970	5.617639	37.405129
C	41.854231	3.390985	38.709166	O	50.347716	5.899910	41.715331
C	41.233077	4.369852	39.508912	O	49.987692	3.721068	42.181252
O	41.147799	2.561814	37.842333	C	50.771540	4.711010	41.952475
O	30.336906	6.524549	40.942593	C	48.284029	4.305873	37.802880
O	30.563225	4.737482	42.300944	C	49.102507	3.271184	37.316045
C	29.873472	5.589895	41.731263	C	49.162773	2.989424	35.958341
C	32.554817	6.305209	45.701172	C	48.405035	3.734253	35.061840
C	33.360009	7.268832	46.283445	C	47.552973	4.767141	35.505332
C	35.070192	6.646313	32.199175	C	47.476557	5.045752	36.896469
C	33.985996	6.376601	33.025680	C	46.572252	6.028132	37.346607
C	32.799245	5.821131	32.511706	C	45.799491	6.740102	36.438050
C	31.485866	5.696451	46.442146	C	45.891812	6.505356	35.076028
C	30.550085	4.805696	45.842589	C	46.775956	5.518254	34.584280
C	29.521866	4.262590	46.573637	O	45.105153	7.300953	34.245617
C	30.503128	5.074292	32.804900	O	48.463793	5.804122	39.647327
C	31.680193	5.601359	33.347351	O	48.131106	3.614838	40.077983
O	29.397715	4.875707	33.622058	C	48.293940	4.591590	39.261905
O	33.114133	6.869525	43.478202	C	44.193973	5.710313	41.383325
O	32.753832	4.707350	43.969558	C	43.571611	6.727820	42.128186
C	32.828552	5.932541	44.276428	C	44.009960	3.953124	39.655836
Cu	48.413818	6.330096	41.563304	O	46.436703	6.506031	41.438634
Cu	48.009807	3.897063	42.043577	O	46.074532	4.314677	41.835837
C	52.242278	4.464620	41.931334	C	45.654437	5.496681	41.562078
C	52.828353	3.947597	43.079285	C	47.841311	5.981193	45.774837
C	54.201353	3.732577	43.123183	C	48.788426	6.807087	46.408285
C	54.987278	4.036581	42.018131	C	49.984722	7.129377	32.189207
C	54.401203	4.554604	40.869180	C	48.930969	6.613236	32.935776
C	53.028203	4.768624	40.826281	C	47.966214	5.771697	32.349108
C	52.442128	5.287648	39.677330	C	46.721911	5.507962	46.514678
C	53.229054	5.591652	38.571278	C	45.688479	4.766089	45.904555
C	54.601054	5.377632	38.616177	C	44.614075	4.302389	46.657437
C	55.187129	4.858609	39.764128	C	45.919037	4.459052	32.491037

C	46.885734	5.262062	33.111436	C	14.931578	4.757753	51.039674
O	44.854892	3.965760	33.237353	C	14.899945	5.034023	52.433241
O	48.303216	6.613588	43.526439	C	14.099714	6.095957	52.899523
O	47.904472	4.434785	43.955878	C	13.393282	6.888670	52.003896
C	48.031934	5.655305	44.334855	C	13.447708	6.656131	50.639549
C	9.830848	7.260896	57.522290	C	14.219257	5.586010	50.132028
C	8.959816	6.502907	56.749315	O	12.739629	7.535723	49.823307
C	9.429783	5.394908	56.054291	O	15.941650	5.653466	55.204662
C	10.771783	5.042898	56.134241	O	15.435937	3.487672	55.582702
C	10.370718	3.178911	54.666243	C	15.676110	4.467340	54.790241
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.326798	7.125686	57.546934
Cu	15.893784	6.138006	57.133117	C	24.489943	6.292293	56.814204
Cu	15.344289	3.724228	57.553376	C	24.999947	5.189199	56.099008
C	19.601744	4.048102	57.428959	C	26.397303	4.930867	56.136770
C	20.155710	3.276830	58.466509	C	11.243751	3.934900	55.440217
C	21.509769	2.965973	58.479792	C	26.066138	3.073241	54.608708
C	22.334714	3.412983	57.453022	C	24.697598	3.286176	54.598815
C	21.818929	4.163968	56.379548	C	24.138960	4.348123	55.345375
C	20.432172	4.471897	56.353421	O	23.928289	2.400327	53.847289
C	19.907766	5.159815	55.238497	O	13.938937	6.431005	56.974115
C	20.743493	5.565725	54.202704	O	13.436010	4.269632	57.372521
C	22.110528	5.304092	54.246780	C	13.091918	5.474231	57.086496
C	22.660208	4.595355	55.323686	C	15.283046	5.695821	61.352095
O	22.933666	5.716264	53.204749	C	16.314087	6.385804	61.978046
O	17.797199	5.598254	57.294689	C	17.600160	6.766947	47.729801
O	17.310463	3.426855	57.668464	C	16.488529	6.395445	48.476941
C	18.150916	4.377989	57.476066	C	15.418174	5.692768	47.890512
C	15.641877	4.212455	53.325542	C	14.198081	5.242825	62.095148
C	16.352053	3.107924	52.821685	C	13.166040	4.552842	61.469196
C	16.368901	2.830998	51.462079	C	12.083075	4.099846	62.213249
C	15.673278	3.649388	50.580095	C	13.215137	4.664734	48.036626

C	14.283415	5.327539	48.656388	O	31.107774	3.569981	55.542855
O	12.098011	4.312685	48.785806	C	31.339300	4.567078	54.768106
O	15.761019	6.378471	59.107941	C	27.240767	5.758306	56.929354
O	15.282229	4.206237	59.478393	C	26.688135	6.862045	57.604264
C	15.448074	5.410185	59.892228	C	40.920248	6.960255	57.612719
Cu	31.487819	6.203012	57.141025	C	40.093739	6.143753	56.852709
Cu	30.980973	3.772873	57.521057	C	40.609806	5.046711	56.131532
C	35.222770	4.142037	57.460753	C	42.005694	4.780179	56.187370
C	35.764545	3.419923	58.539533	C	26.916129	3.878769	55.356082
C	37.109434	3.074878	58.563830	C	41.685284	2.935607	54.642695
C	37.935742	3.433109	57.504769	C	40.318658	3.161722	54.607437
C	37.432391	4.137292	56.393792	C	39.754979	4.222351	55.352669
C	36.055962	4.487939	56.361689	O	39.555537	2.284233	53.840171
C	35.543553	5.139892	55.220757	O	29.519101	6.465310	57.004286
C	36.381627	5.461612	54.157462	O	29.069666	4.280045	57.332946
C	37.739795	5.154665	54.202704	C	28.695618	5.484460	57.094254
C	38.277901	4.485807	55.311146	C	30.903120	5.695641	61.351269
O	38.565859	5.487055	53.135104	C	31.934175	6.385618	61.977205
O	33.405587	5.682511	57.287755	C	33.183987	7.613997	47.641321
O	32.942527	3.504797	57.658021	C	32.199928	7.010153	48.394811
C	33.771790	4.465905	57.478402	C	31.306431	6.043195	47.830381
C	31.397162	4.328509	53.299808	C	29.818167	5.242646	62.094340
C	32.219674	3.291182	52.825037	C	28.786113	4.552669	61.468405
C	32.365181	3.061823	51.463657	C	27.703159	4.099675	62.212476
C	31.680643	3.854730	50.549537	C	29.375442	4.546961	47.957406
C	30.816953	4.882592	50.977484	C	30.248461	5.433213	48.587534
C	30.669568	5.122883	52.371263	O	28.376984	3.954294	48.667101
C	29.775539	6.123586	52.799055	O	31.364333	6.408930	59.117302
C	29.073816	6.880466	51.867600	O	30.894563	4.229283	59.454872
C	29.222890	6.668495	50.506899	C	31.058872	5.427777	59.887165
C	30.096041	5.665053	50.042113	Cu	47.053252	6.247208	57.149476
O	28.491504	7.490859	49.654980	Cu	46.688901	3.791481	57.536874
O	31.542751	5.757270	55.203401	C	50.914829	4.464394	57.493750

C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.671348	7.126643	47.754407
C	53.073736	4.554373	56.431559	C	47.603270	6.631524	48.493190
C	51.700736	4.768398	56.388685	C	46.618159	5.820924	47.896510
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.538455	4.560018	48.023913
O	53.987445	5.617415	52.967495	C	45.525419	5.330636	48.653631
O	48.992439	5.857445	57.301387	O	43.463554	4.082966	48.765291
O	48.674247	3.653668	57.672990	O	46.921239	6.442649	59.123016
C	49.438752	4.671053	57.499041	O	46.574293	4.238581	59.463634
C	46.979125	4.347111	53.321858	C	46.675541	5.443561	59.891199
C	47.812605	3.333334	52.816389	C	16.262162	6.620790	63.347051
C	47.866693	3.067821	51.455712	C	15.179196	6.168795	64.090104
C	47.086138	3.807046	50.574817	C	14.147156	5.478812	63.465153
C	46.222943	4.823018	51.036633	C	12.031150	4.336833	63.582254
C	46.156009	5.087223	52.431013	C	13.063191	5.025817	64.207206
C	45.244318	6.053657	52.899741	O	10.943187	3.908837	64.361307
C	44.457216	6.767547	52.005395	C	31.882275	6.620600	63.346211
C	44.537742	6.545952	50.640437	C	30.799322	6.168606	64.089282
C	45.425734	5.571197	50.130386	C	29.767267	5.478629	63.464346
O	43.738290	7.345044	49.825955	C	27.651260	4.336658	63.581482
O	47.127229	5.793153	55.214286	C	28.683314	5.025635	64.206417
O	46.817689	3.586190	55.567382	O	26.563309	3.908663	64.360554
C	46.974144	4.591655	54.787204	C	47.502389	6.620356	63.345091
C	42.841729	5.603942	56.990439	C	46.419447	6.168363	64.088179
C	42.279461	6.695065	57.679417	C	45.387379	5.478391	63.463260
C	42.529519	3.729185	55.409859	C	43.271369	4.336426	63.580429
O	45.080885	6.396791	57.019707	C	44.303437	5.025398	64.205349
O	44.743667	4.191678	57.352096	O	42.183431	3.908432	64.359519
C	44.308009	5.378598	57.121560	H	12.119205	8.126988	26.935857

H	10.573014	6.786801	25.566394	H	31.124947	7.499541	21.165332
H	13.383961	2.323446	22.982372	H	29.992303	7.518340	27.131902
H	9.847471	3.169800	22.676992	H	43.108940	7.703158	27.043921
H	22.115907	2.811262	28.210858	H	41.666207	6.198635	25.788280
H	24.516878	2.282000	28.271556	H	30.625457	3.573716	24.371174
H	26.008586	3.092164	26.516356	H	44.785192	1.859160	23.217615
H	21.502672	5.272274	24.067504	H	35.854573	6.562982	30.214625
H	23.002617	6.019462	22.328602	H	31.418210	4.719833	29.560085
H	19.531966	2.329427	22.589919	H	29.521658	4.362765	31.027304
H	19.679350	1.794090	20.190510	H	31.292299	6.861162	17.596329
H	18.480529	3.170848	18.536718	H	40.804865	5.755081	21.418952
H	16.651757	6.145567	22.827104	H	41.263098	2.201159	22.965135
H	15.507011	7.501000	21.165373	H	53.552007	3.699075	28.380999
H	14.495478	7.507771	27.088040	H	55.987677	3.325906	28.455657
H	27.582640	7.987286	27.006352	H	57.384066	3.866287	26.497830
H	26.094872	6.500636	25.773113	H	52.703481	5.453594	24.015689
H	14.941550	3.634234	24.311121	H	54.081091	5.976324	22.116963
H	29.117024	2.137933	23.131890	H	50.777400	2.334516	22.589144
H	19.773943	6.912684	30.323860	H	50.920814	1.795206	20.189767
H	15.697537	4.476148	29.299692	H	49.720330	3.170939	18.535923
H	13.824242	3.720207	30.623374	H	47.863783	6.134901	22.823868
H	15.672059	6.861142	17.596378	H	46.741365	7.496848	21.165091
H	25.133343	6.196299	21.521615	H	45.525811	7.295362	27.170680
H	25.596104	2.518567	22.939610	H	46.258380	3.322662	24.472612
H	37.704349	2.874525	28.298929	H	50.938821	7.204431	30.278021
H	40.083450	2.262741	28.385056	H	47.070741	4.429212	29.312580
H	41.591285	2.900955	26.574268	H	45.244091	3.583620	30.646869
H	37.156257	5.120154	24.031005	H	46.913185	6.861825	17.595775
H	38.670796	5.691501	22.234649	H	56.055930	5.976964	21.104253
H	35.148209	2.327828	22.590832	H	10.790574	8.126887	42.500083
H	35.298361	1.793414	20.190369	H	9.244362	6.786854	41.130264
H	34.099912	3.170583	18.536495	H	12.055946	2.325981	38.542911
H	32.265133	6.144043	22.825998	H	8.519335	3.171137	38.239804

H	20.601793	2.644305	43.899591	H	31.586228	8.588638	36.908387
H	22.973277	2.021932	44.083675	H	28.368309	7.400702	43.058505
H	24.563007	2.669773	42.343880	H	41.739115	7.740419	42.609098
H	20.233951	4.858854	39.601283	H	40.377468	6.382075	41.116193
H	21.824612	5.421367	37.867012	H	29.375896	3.462059	40.449210
H	18.009692	2.130417	37.978922	H	43.685465	2.454996	38.154855
H	18.053023	1.670856	35.563948	H	34.138470	7.746994	45.683622
H	16.938252	3.172123	33.998844	H	35.970643	7.091229	32.611598
H	15.253818	6.098494	38.432481	H	34.080112	6.616841	34.077013
H	14.126499	7.546570	36.846533	H	30.632069	4.559908	44.785143
H	13.168791	7.505353	42.651841	H	28.804688	3.591973	46.085771
H	25.876962	7.509003	43.109837	H	28.618256	4.470358	33.125119
H	24.528826	5.930854	41.824367	H	31.228992	8.099431	33.511805
H	13.612691	3.636767	39.860312	H	39.534475	6.525385	36.944325
H	28.037794	1.908370	39.075555	H	40.156812	2.749946	37.831876
H	18.550139	6.721740	45.817353	H	52.223551	3.706439	43.946547
H	19.609438	7.422301	32.723548	H	54.659220	3.327336	44.019582
H	17.719285	6.606600	34.035681	H	56.055380	3.866422	42.061123
H	14.338073	4.502967	44.850402	H	51.374846	5.453435	39.578994
H	12.418447	3.903703	46.189840	H	52.752217	5.975806	37.680124
H	12.824613	3.520610	32.669224	H	49.705592	2.686931	38.001668
H	14.184784	7.182729	33.318450	H	49.802148	2.190062	35.597097
H	23.998355	5.524758	37.163633	H	48.476566	3.482618	34.013254
H	24.624069	2.026456	38.610744	H	46.436849	6.253098	38.398399
H	36.483168	2.514079	43.185370	H	45.108129	7.493157	36.792053
H	38.881108	1.768051	43.077017	H	44.156433	7.344337	42.801298
H	40.405316	2.723548	41.415129	H	45.078144	3.763004	39.658123
H	35.966730	5.519117	39.461054	H	49.628748	7.198589	45.846365
H	37.441370	6.359933	37.692797	H	50.711795	7.785840	32.657063
H	32.464820	2.023826	38.435169	H	48.866130	6.888786	33.979775
H	32.401501	1.461955	35.991025	H	45.685948	4.544833	44.842744
H	32.085532	3.217953	34.329960	H	43.835759	3.732837	46.167840
H	32.040632	6.858510	38.590501	H	44.245148	3.373798	32.693354

H	45.200089	7.067974	33.271952	H	34.494841	5.402884	55.129927
H	54.726267	5.972412	36.666013	H	35.966272	5.962942	53.293667
H	9.463364	8.127032	58.062952	H	32.765261	2.667219	53.523921
H	7.916948	6.786729	56.693489	H	33.014535	2.265403	51.113272
H	10.728378	2.325485	54.106719	H	31.821112	3.645135	49.497424
H	7.191738	3.170762	53.803455	H	29.595489	6.328227	53.849362
H	19.526294	2.925147	59.275929	H	28.389860	7.648691	52.204110
H	21.923998	2.376501	59.291817	H	27.324106	7.512218	58.194203
H	23.384169	3.154004	57.495496	H	40.503841	7.805673	58.151424
H	18.850449	5.382236	55.142586	H	39.042125	6.389470	56.820440
H	20.317864	6.092751	53.359512	H	27.978218	3.670829	55.295072
H	16.900288	2.460439	53.496427	H	42.095143	2.126302	54.053345
H	16.923941	1.976273	51.088167	H	32.786868	6.742113	61.409353
H	15.706676	3.397111	49.529821	H	33.835650	8.364644	48.099025
H	13.996788	6.325104	53.953984	H	32.093517	7.295759	49.446023
H	12.787844	7.707072	52.369837	H	28.750448	4.373617	60.400116
H	11.840495	7.509098	58.212507	H	26.897913	3.574282	61.718423
H	24.915432	7.977114	58.079968	H	27.880314	3.348664	48.093037
H	23.435518	6.528606	56.796471	H	28.644407	7.290771	48.678864
H	12.285103	3.636245	55.427459	H	38.076340	5.993787	52.412680
H	26.472560	2.263843	54.017086	H	38.576261	2.512644	53.839142
H	17.168420	6.739348	61.410757	H	50.895005	3.699945	59.506371
H	18.410847	7.316946	48.197662	H	53.331570	3.325521	59.581294
H	16.465265	6.673776	49.521811	H	54.727853	3.865742	57.623117
H	13.129709	4.375523	60.400584	H	50.047660	5.459524	55.145398
H	11.277919	3.574374	61.719226	H	51.424840	5.977028	53.243047
H	11.416374	3.805119	48.241905	H	48.426849	2.747893	53.491083
H	12.815554	7.313201	48.845541	H	48.515630	2.282679	51.080596
H	22.432631	6.241707	52.504102	H	47.150285	3.564741	49.523737
H	22.946073	2.615494	53.868864	H	45.115427	6.265791	53.955153
H	35.130249	3.125063	59.367629	H	43.763195	7.511472	52.373250
H	37.513921	2.522291	59.406091	H	42.909693	7.344110	58.276747
H	38.976598	3.143148	57.553653	H	43.590485	3.511360	55.368614

H	48.405699	6.744563	61.407905	C	33.643098	11.016967	40.536480
H	49.413502	7.760642	48.229547	C	32.284543	10.437054	40.127226
H	47.543683	6.899892	49.539298	O	32.723163	8.151801	40.679708
H	44.381327	4.364309	60.399408	C	29.822089	9.846274	43.768176
H	42.519349	3.571688	61.717655	C	28.503176	10.351936	43.697878
H	42.840093	3.511447	48.214860	C	27.504740	9.875308	44.547821
H	43.821351	7.119712	48.849569	C	27.777846	8.872051	45.487261
H	53.398480	5.970742	52.227811	C	29.081265	8.368742	45.568077
H	17.068262	7.157999	63.836018	C	30.093598	8.847790	44.734603
H	15.148095	6.357251	65.155563	N	30.806491	10.338192	42.924594
H	10.263264	3.421880	63.796859	H	33.283062	10.441692	43.965672
H	32.687882	7.158644	63.835004	H	31.883197	8.583405	43.019719
H	30.767901	6.357388	65.154653	H	30.837607	8.950576	40.763439
H	25.881770	3.424643	63.795430	H	34.627642	11.812507	42.319165
H	48.307521	7.159120	63.833761	H	32.898828	12.192786	42.205652
H	46.387751	6.357306	65.153494	H	33.888814	11.894385	39.910094
H	41.501425	3.425105	63.794253	H	34.424329	10.257189	40.349071
H	54.922558	4.682783	55.325804	H	31.499501	11.215202	40.226875
H	56.250092	4.683140	39.763727	H	32.285465	10.123825	39.067756
H	57.578893	4.683406	24.200677	H	34.088426	9.406941	42.766784
H	32.654296	5.043307	18.026535	H	28.265609	11.121494	42.954557
H	17.034876	5.043568	18.026682	H	26.493137	10.286964	44.463441
H	10.176553	4.915350	24.089676	H	26.988886	8.491312	46.142250
H	8.847986	4.915601	39.653361	H	29.331871	7.582348	46.286687
H	7.520590	4.915659	55.216399	H	31.103010	8.450277	44.849244
H	12.998983	5.199026	65.269027	H	31.313866	6.459376	40.754934
H	28.618792	5.199034	65.268152	H	30.492757	11.044407	42.267047
H	44.238656	5.198873	65.267032				
H	48.273988	5.043114	18.026066	(R,R)-2-TS3			
C	31.891378	9.217877	40.988577	C	12.487000	7.261000	26.395000
C	31.956023	9.547884	42.511205	C	11.616000	6.503000	25.622000
C	33.305287	10.178036	42.893581	C	12.086000	5.395000	24.927000
C	33.647291	11.394718	42.025720	C	13.428000	5.043000	25.007000

C	13.027000	3.179000	23.539000	C	18.266838	4.337436	23.747107
C	11.685000	3.529000	23.460000	C	14.301000	5.801000	25.782000
C	11.215000	4.638000	24.154000	C	13.829000	6.909000	26.476000
O	10.782000	2.793000	22.654000	C	28.026948	7.145762	26.533147
Cu	18.543745	6.084628	26.025203	C	27.180609	6.295099	25.830245
Cu	17.955154	3.694834	26.529620	C	27.679885	5.166472	25.149126
C	22.226423	3.962421	26.387934	C	29.074044	4.893815	25.199790
C	22.759067	3.167184	27.419209	C	13.900000	3.935000	24.313000
C	24.114818	2.865077	27.460077	C	28.724496	2.985350	23.738363
C	24.963950	3.344431	26.468350	C	27.360070	3.218514	23.711011
C	24.471319	4.116310	25.399536	C	26.812214	4.312639	24.417658
C	23.083082	4.414799	25.343066	O	26.583595	2.322781	22.978987
C	22.584778	5.122671	24.228122	O	16.596689	6.401801	25.859048
C	23.446196	5.563145	23.228238	O	16.057099	4.260822	26.320553
C	24.813124	5.310017	23.303514	C	15.736473	5.459892	25.988374
C	25.337343	4.576323	24.376333	C	17.921302	5.795579	30.246473
O	25.660918	5.752711	22.294037	C	18.913201	6.557058	30.891507
O	20.436502	5.523343	26.199554	C	16.779324	5.369772	30.982870
O	19.921840	3.373913	26.649572	C	15.704860	4.696775	30.363093
C	20.775898	4.306267	26.421165	C	14.605134	4.284601	31.109846
C	18.226927	4.022014	22.293999	O	18.430608	6.394897	27.990603
C	18.992915	2.941012	21.873981	O	17.902604	4.247107	28.434779
C	19.081890	2.638017	20.519979	C	18.100407	5.459457	28.806085
C	18.404876	3.417023	19.587993	Cu	34.196480	6.078976	26.036156
C	17.639888	4.497024	20.008011	Cu	33.622835	3.692529	26.568353
C	17.550913	4.800019	21.362013	C	37.879145	3.921306	26.343956
C	16.783924	5.881020	21.784030	C	38.410104	3.189947	27.422751
C	16.107910	6.659026	20.850045	C	39.754285	2.842498	27.457563
C	16.197885	6.355031	19.497042	C	40.593076	3.211965	26.412618
C	16.963875	5.274030	19.076025	C	40.101349	3.921958	25.300831
O	15.523872	7.185037	18.539057	C	38.723582	4.266205	25.252073
O	18.565471	5.530824	24.116544	C	38.222545	4.913178	24.103276
O	18.026509	3.388288	24.574537	C	39.073491	5.241540	23.051978

C	40.433955	4.948756	23.118172	C	31.378888	5.449226	26.132342
C	40.960825	4.283707	24.234091	C	33.879229	5.799555	30.286144
O	41.273324	5.292967	22.064416	C	35.033473	6.358673	30.864230
O	36.099288	5.500449	26.125423	C	32.722801	5.601601	31.088846
O	35.582304	3.364663	26.636466	C	31.520722	5.110801	30.541178
C	36.435603	4.285819	26.373665	C	30.394669	4.955576	31.345963
C	33.846854	4.021972	22.293718	O	34.191609	6.388090	28.001376
C	34.612831	2.940969	21.873683	O	33.635586	4.254218	28.481732
C	34.701781	2.637978	20.519678	C	33.904798	5.458705	28.837724
C	34.024753	3.416989	19.587708	Cu	49.694961	6.208051	25.983486
C	33.259776	4.496991	20.007741	Cu	49.343813	3.790887	26.565516
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.146693	5.534177	24.124971	C	53.770890	5.287813	24.113936
O	33.647075	3.386634	24.594708	C	54.557834	5.591815	23.007897
C	33.871502	4.335427	23.757424	C	55.929834	5.377800	23.052821
C	29.927424	5.740576	25.962458	C	56.515889	4.858782	24.200784
C	29.387397	6.873722	26.597258	O	56.643771	5.617805	21.841785
C	43.530883	6.874652	26.489569	O	51.637566	5.839302	26.123955
C	42.726876	6.018173	25.748400	O	51.334307	3.663575	26.640401
C	43.269488	4.904908	25.073591	C	52.092902	4.668399	26.382631
C	44.667060	4.658940	25.163916	C	49.466779	4.021876	22.293156
C	29.581495	3.805382	24.461356	C	50.232745	2.940872	21.873104
C	44.396782	2.750174	23.688063	C	50.321669	2.637885	20.519096
C	43.029819	2.963981	23.611864	C	49.644627	3.416901	19.587140
C	42.440245	4.044153	24.306486	C	48.879661	4.496905	20.007192
O	42.292515	2.057328	22.853725	C	48.790737	4.799893	21.361200
O	32.226982	6.400781	25.972316	C	48.023772	5.880897	21.783251
O	31.725216	4.251074	26.432050	C	47.347731	6.658913	20.849295

C	47.437655	6.354926	19.496287	C	23.539640	2.881590	42.202355
C	48.203620	5.273922	19.075235	C	23.137291	3.655614	41.099122
O	46.763613	7.184943	18.538331	C	21.766442	4.006332	40.960960
O	49.731827	5.592331	24.089762	C	21.354373	4.699818	39.804779
O	49.388174	3.426874	24.609531	C	22.284615	5.069726	38.837947
C	49.526603	4.369432	23.750063	C	23.637256	4.786072	39.004605
C	45.480562	5.528008	25.942645	C	24.077374	4.086148	40.134172
C	44.894251	6.635973	26.581984	O	24.554151	5.176370	38.037200
C	45.216554	3.579624	24.444325	O	19.128530	5.272502	41.695008
O	47.715241	6.340048	25.881976	O	18.509323	3.152874	42.154793
O	47.394062	4.171938	26.414236	C	19.408472	4.042571	41.939585
C	46.949235	5.331476	26.085776	C	16.819145	3.949858	37.784119
C	49.186785	5.999087	30.218599	C	17.460800	2.808271	37.271143
C	50.123912	6.849756	30.833115	C	17.471200	2.550404	35.906657
C	48.075512	5.524605	30.971057	C	16.837466	3.424317	35.030091
C	47.052779	4.754305	30.377764	C	16.151872	4.562823	35.500959
C	45.981030	4.298224	31.139076	C	16.125259	4.820221	36.898075
O	49.603283	6.569851	27.939115	C	15.381864	5.919033	37.374313
O	49.291502	4.396169	28.457135	C	14.721391	6.758624	36.486021
C	49.379621	5.633393	28.788025	C	14.770570	6.540348	35.119296
C	11.158286	7.260970	41.959133	C	15.494215	5.442783	34.601354
C	10.287269	6.502976	41.186145	O	14.103159	7.457929	34.311095
C	10.757253	5.394976	40.491133	O	17.240389	5.397025	39.627972
C	12.099253	5.042971	40.571108	O	16.624286	3.271952	40.065856
C	11.698221	3.178978	39.103109	C	16.901252	4.220004	39.245484
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.256355	6.494513	43.000095
Cu	17.253807	5.931767	41.539125	C	25.579180	5.690791	42.106818
Cu	16.566515	3.568420	42.036519	C	26.243431	4.726694	41.280744
C	20.841009	3.625980	41.973308	C	27.678271	4.614970	41.412665
C	21.286309	2.831790	43.046733	C	12.571237	3.934972	39.877096
C	22.621315	2.463021	43.158656	C	27.666520	2.901525	39.685516

C	26.255720	2.995921	39.554773	O	35.155960	5.405242	41.895967
C	25.537152	3.901355	40.330862	O	34.347139	3.307847	41.916711
O	25.742741	2.136488	38.629731	C	35.285830	4.151485	41.812788
O	15.305397	6.339832	41.402521	C	32.461700	4.190176	37.950604
O	14.695189	4.218409	41.858939	C	32.621298	2.890582	37.499993
C	14.409507	5.430632	41.544770	C	32.515414	2.608991	36.122518
C	16.663876	5.669070	45.759444	C	32.223571	3.615818	35.225777
C	17.697885	6.391747	46.383330	C	31.996473	4.966877	35.645886
C	18.819190	6.851028	32.245973	C	32.121670	5.253055	37.052038
C	17.730059	6.396273	32.981045	C	31.859216	6.579112	37.509024
C	16.697664	5.658269	32.371549	C	31.503006	7.563211	36.622190
C	15.503186	5.324490	46.508224	C	31.402371	7.299673	35.228971
C	14.395787	4.686590	45.910240	C	31.650853	6.024034	34.731607
C	13.278110	4.354281	46.669851	O	31.061114	8.399793	34.492502
C	14.543817	4.525849	32.480055	O	33.403649	5.433743	39.730524
C	15.578589	5.219543	33.121797	O	32.153896	3.632742	40.219140
O	13.438728	4.108101	33.213329	C	32.688107	4.452442	39.402213
O	17.176871	6.236566	43.502607	C	28.357061	5.488072	42.335198
O	16.550386	4.115798	43.948037	C	27.653731	6.409059	43.105094
C	16.809942	5.317367	44.319361	C	42.198388	6.939114	42.113898
Cu	33.543014	6.427878	41.519696	C	41.419768	6.158786	41.267193
Cu	32.492640	3.946990	42.099887	C	41.996899	5.159893	40.457568
C	36.673833	3.647046	41.587373	C	43.398983	4.939200	40.530454
C	37.172790	2.660473	42.415937	C	28.359510	3.685290	40.572403
C	38.534853	2.292767	42.326467	C	43.185886	3.227801	38.821536
C	39.369979	2.911511	41.420460	C	41.815238	3.419382	38.757504
C	38.888044	3.907193	40.508419	C	41.201564	4.385134	39.578474
C	37.493398	4.252413	40.578052	O	41.101114	2.607988	37.880385
C	36.967230	5.163695	39.617468	O	30.301291	6.658154	42.900097
C	37.781185	5.731648	38.667095	O	30.553819	4.535914	42.216365
C	39.176114	5.460123	38.641349	C	29.829536	5.509369	42.467782
C	39.733010	4.559659	39.547219	C	32.616778	5.989047	45.745105
O	39.970409	6.081272	37.725589	C	33.485559	6.891484	46.331146

C	35.072933	6.675458	32.216170	C	47.477160	5.121920	36.897824
C	33.954229	6.458247	33.012529	C	46.606222	6.131638	37.354233
C	32.765551	5.935643	32.469869	C	45.859482	6.876910	36.450150
C	31.498157	5.460931	46.473780	C	45.939375	6.644259	35.087130
C	30.523549	4.611422	45.876690	C	46.787688	5.629866	34.588606
C	29.435191	4.167934	46.588306	O	45.175571	7.467337	34.262587
C	30.438648	5.267107	32.703769	O	48.454566	5.827249	39.659799
C	31.618752	5.753904	33.275434	O	48.119921	3.635220	40.071554
O	29.306768	5.106810	33.492759	C	48.278921	4.619334	39.262908
O	33.089446	6.573919	43.508534	C	44.184728	5.719036	41.423509
O	32.733000	4.410376	43.982157	C	43.568289	6.726456	42.187384
C	32.844817	5.623460	44.316204	C	43.980463	3.970296	39.689092
Cu	48.411324	6.335883	41.580153	O	46.431333	6.514312	41.465222
Cu	48.006528	3.899828	42.041708	O	46.070373	4.319934	41.844819
C	52.242278	4.464620	41.931334	C	45.648421	5.504484	41.585168
C	52.828353	3.947597	43.079285	C	47.851063	5.958187	45.789994
C	54.201353	3.732577	43.123183	C	48.811542	6.763797	46.429715
C	54.987278	4.036581	42.018131	C	50.006244	7.189639	32.175110
C	54.401203	4.554604	40.869180	C	48.947331	6.692402	32.926982
C	53.028203	4.768624	40.826281	C	47.970031	5.861390	32.347108
C	52.442128	5.287648	39.677330	C	46.716720	5.508959	46.522477
C	53.229054	5.591652	38.571278	C	45.677560	4.778986	45.907932
C	54.601054	5.377632	38.616177	C	44.582533	4.349038	46.651475
C	55.187129	4.858609	39.764128	C	45.899920	4.586854	32.498977
O	55.314970	5.617639	37.405129	C	46.883066	5.373840	33.114369
O	50.346982	5.902366	41.722175	O	44.825683	4.120439	33.248260
O	49.985782	3.720651	42.173043	O	48.308400	6.603180	43.545492
C	50.770712	4.711690	41.952046	O	47.906688	4.422037	43.960161
C	48.259825	4.348090	37.799499	C	48.037926	5.639670	44.347794
C	49.046013	3.292587	37.303019	C	9.830848	7.260896	57.522290
C	49.100539	3.023490	35.942460	C	8.959816	6.502907	56.749315
C	48.366571	3.798559	35.052251	C	9.429783	5.394908	56.054291
C	47.544183	4.851247	35.504162	C	10.771783	5.042898	56.134241

C	10.370718	3.178911	54.666243	C	15.671986	4.444651	54.791855
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.305808	7.080196	57.511011
Cu	15.897896	6.120821	57.131618	C	24.473453	6.237417	56.784377
Cu	15.336931	3.711069	57.558430	C	24.986657	5.121937	56.091473
C	19.596053	4.011068	57.433823	C	26.382516	4.858330	56.148824
C	20.148698	3.246022	58.477005	C	11.243751	3.934900	55.440217
C	21.501318	2.928426	58.488988	C	26.057438	2.973778	54.651592
C	22.325305	3.359982	57.455016	C	24.690876	3.196467	54.619054
C	21.810422	4.103286	56.375947	C	24.129730	4.273186	55.341805
C	20.425939	4.420789	56.352318	O	23.925683	2.304279	53.871185
C	19.902729	5.105607	55.234947	O	13.942982	6.423541	56.972252
C	20.737057	5.494726	54.191588	O	13.431126	4.265426	57.376645
C	22.102032	5.221604	54.231619	C	13.091584	5.470735	57.087776
C	22.650951	4.519579	55.313577	C	15.283046	5.695821	61.352095
O	22.923607	5.618083	53.182259	C	16.314087	6.385804	61.978046
O	17.799158	5.570627	57.294952	C	17.620819	6.733487	47.727042
O	17.301333	3.402809	57.674399	C	16.506742	6.366970	48.472752
C	18.146843	4.348981	57.480294	C	15.437433	5.663102	47.886671
C	15.635734	4.186980	53.326604	C	14.198081	5.242825	62.095148
C	16.331252	3.071318	52.825960	C	13.166040	4.552842	61.469196
C	16.347120	2.792238	51.466684	C	12.083075	4.099846	62.213249
C	15.663671	3.617424	50.581785	C	13.231259	4.641660	48.031731
C	14.935356	4.735838	51.037450	C	14.298994	5.305730	48.651155
C	14.907335	5.017497	52.430305	O	12.108925	4.300121	48.778124
C	14.124641	6.094727	52.891743	O	15.767132	6.369002	59.105877
C	13.428672	6.893125	51.992552	O	15.278838	4.200034	59.482510
C	13.476222	6.651253	50.629567	C	15.449810	5.404643	59.893142
C	14.233507	5.569125	50.126274	Cu	31.471283	6.151134	57.128789
O	12.776332	7.534106	49.810157	Cu	30.968047	3.726701	57.544005
O	15.943900	5.630140	55.204111	C	35.213133	4.096769	57.450120
O	15.427075	3.468235	55.587291	C	35.756124	3.370492	58.526006

C	37.101379	3.025898	58.548157	C	41.679479	2.888664	54.667172
C	37.927736	3.389053	57.490981	C	40.314075	3.119407	54.619003
C	37.424444	4.098089	56.383583	C	39.748653	4.190745	55.347030
C	36.047474	4.448351	56.352825	O	39.553673	2.236007	53.856174
C	35.535620	5.104967	55.214439	O	29.500645	6.410340	56.999849
C	36.373794	5.429271	54.151794	O	29.054299	4.230742	57.366361
C	37.732044	5.122147	54.195792	C	28.678025	5.430217	57.106834
C	38.270581	4.450871	55.302691	C	30.903120	5.695641	61.351269
O	38.557446	5.456828	53.128357	C	31.934175	6.385618	61.977205
O	33.391231	5.633829	57.269226	C	33.317831	7.258489	47.683387
O	32.932133	3.460186	57.664984	C	32.273567	6.745523	48.422030
C	33.760390	4.419647	57.470142	C	31.316539	5.844507	47.850973
C	31.317174	4.225324	53.308070	C	29.818167	5.242646	62.094340
C	32.069849	3.132759	52.839124	C	28.786113	4.552669	61.468405
C	32.176407	2.868610	51.480713	C	27.703159	4.099675	62.212476
C	31.524855	3.683071	50.562683	C	29.268595	4.508530	47.957057
C	30.734157	4.770723	50.983452	C	30.198314	5.330623	48.591538
C	30.620455	5.043747	52.374332	O	28.200667	4.027260	48.650299
C	29.789413	6.101882	52.792827	O	31.360699	6.384435	59.105364
C	29.126617	6.886733	51.854582	O	30.900210	4.207725	59.472521
C	29.251662	6.646306	50.496364	C	31.061877	5.412149	59.889410
C	30.054526	5.582132	50.042344	Cu	47.046876	6.244771	57.146035
O	28.573770	7.504456	49.634878	Cu	46.685888	3.789404	57.533326
O	31.510837	5.678489	55.195010	C	50.914829	4.464394	57.493750
O	31.070768	3.498349	55.567364	C	51.500923	3.947364	58.641689
C	31.292033	4.484778	54.775933	C	52.873923	3.732339	58.685563
C	27.222289	5.698734	56.933131	C	53.659830	4.036343	57.580498
C	26.666341	6.815642	57.583803	C	53.073736	4.554373	56.431559
C	40.906433	6.953486	57.579390	C	51.700736	4.768398	56.388685
C	40.082855	6.128407	56.825685	C	51.114643	5.287428	55.239746
C	40.601415	5.023249	56.119726	C	51.901549	5.591433	54.133681
C	41.997267	4.756158	56.185628	C	53.273549	5.377407	54.178555
C	26.903589	3.787248	55.395413	C	53.859642	4.858378	55.326493

O	53.987445	5.617415	52.967495	C	45.494098	5.372795	48.650430
O	48.988758	5.856156	57.297108	O	43.396636	4.183833	48.744765
O	48.672692	3.652270	57.668144	O	46.917259	6.441458	59.120646
C	49.437046	4.670276	57.496493	O	46.573581	4.237225	59.462108
C	46.948042	4.351163	53.311961	C	46.674407	5.442568	59.890041
C	47.754511	3.318855	52.798914	C	16.262162	6.620790	63.347051
C	47.791581	3.052822	51.437660	C	15.179196	6.168795	64.090104
C	47.020324	3.808276	50.562995	C	14.147156	5.478812	63.465153
C	46.184083	4.843434	51.030717	C	12.031150	4.336833	63.582254
C	46.134902	5.110430	52.425791	C	13.063191	5.025817	64.207206
C	45.250489	6.099922	52.899251	O	10.943187	3.908837	64.361307
C	44.473138	6.830818	52.009314	C	31.882275	6.620600	63.346211
C	44.536298	6.604093	50.644245	C	30.799322	6.168606	64.089282
C	45.397754	5.608818	50.128823	C	29.767267	5.478629	63.464346
O	43.748424	7.419503	49.835034	C	27.651260	4.336658	63.581482
O	47.117584	5.792499	55.209342	C	28.683314	5.025635	64.206417
O	46.809183	3.585788	55.560877	O	26.563309	3.908663	64.360554
C	46.958748	4.592479	54.780019	C	47.502389	6.620356	63.345091
C	42.831914	5.591567	56.980083	C	46.419447	6.168363	64.088179
C	42.265892	6.690511	57.654119	C	45.387379	5.478391	63.463260
C	42.522028	3.691581	55.427095	C	43.271369	4.336426	63.580429
O	45.071845	6.390901	57.016861	C	44.303437	5.025398	64.205349
O	44.739126	4.185892	57.350780	O	42.183431	3.908432	64.359519
C	44.300179	5.371003	57.117171	H	12.119148	8.126810	26.936120
C	46.523195	5.695406	61.350162	H	10.573014	6.786735	25.566630
C	47.554262	6.385378	61.976082	H	13.382386	2.322459	22.982829
C	48.688708	7.091127	47.773434	H	9.847434	3.169537	22.676425
C	47.601258	6.626197	48.503116	H	22.112669	2.794756	28.206186
C	46.604856	5.833881	47.901067	H	24.512619	2.260096	28.268547
C	45.438253	5.242413	62.093251	H	26.014507	3.094851	26.534698
C	44.406185	4.552442	61.467332	H	21.528494	5.332980	24.100960
C	43.323243	4.099449	62.211421	H	23.039831	6.107683	22.386783
C	44.494387	4.623994	48.014044	H	19.532688	2.330022	22.589848

H	19.679862	1.794462	20.190459	H	31.289170	6.859474	17.596510
H	18.480883	3.171000	18.536739	H	40.790283	5.802907	21.339817
H	16.654327	6.146537	22.827181	H	41.311314	2.276284	22.825106
H	15.507586	7.501999	21.163878	H	53.552185	3.700598	28.381532
H	14.495376	7.507694	27.088221	H	55.987764	3.326392	28.455845
H	27.623029	8.018080	27.036642	H	57.384054	3.866433	26.497976
H	26.127484	6.537312	25.807224	H	52.703572	5.453970	24.015745
H	14.941235	3.633099	24.313726	H	54.081390	5.976929	22.117007
H	29.121591	2.148191	23.179833	H	50.777472	2.335022	22.589426
H	19.774588	6.909420	30.334938	H	50.920784	1.795168	20.189799
H	15.688550	4.492904	29.297734	H	49.720299	3.170770	18.535993
H	13.795482	3.768545	30.612046	H	47.864487	6.135485	22.823793
H	15.672671	6.862191	17.596195	H	46.741365	7.497413	21.163709
H	25.174866	6.290762	21.592224	H	45.507942	7.318149	27.159853
H	25.604408	2.552462	22.985858	H	46.279163	3.364643	24.443962
H	37.770052	2.897221	28.247785	H	50.958929	7.239961	30.261924
H	40.150357	2.285358	28.300562	H	47.056327	4.504734	29.322111
H	41.634369	2.925395	26.472890	H	45.210319	3.708350	30.661812
H	37.172333	5.163482	23.994539	H	46.907005	6.857885	17.596269
H	38.666053	5.738526	22.182129	H	56.056812	5.973990	21.102092
H	35.150024	2.329229	22.590660	H	10.790573	8.126876	42.500115
H	35.298906	1.793801	20.190345	H	9.244397	6.786902	41.130389
H	34.100153	3.170629	18.536537	H	12.054461	2.325295	38.542955
H	32.266462	6.144150	22.826192	H	8.520484	3.174008	38.235158
H	31.125227	7.500300	21.163927	H	20.586915	2.511043	43.811131
H	30.031340	7.539574	27.160797	H	22.949460	1.857157	43.997401
H	43.093417	7.731549	26.991680	H	24.573217	2.582379	42.323570
H	41.671742	6.244629	25.693948	H	20.313603	4.949387	39.622706
H	30.640272	3.577838	24.415624	H	21.944030	5.596452	37.956464
H	44.825122	1.919425	23.143311	H	17.969364	2.123521	37.940457
H	35.913928	6.535862	30.256458	H	17.978216	1.670758	35.523557
H	31.433810	4.851015	29.489928	H	16.870109	3.191490	33.975123
H	29.480851	4.582583	30.903252	H	15.285783	6.139667	38.431386

H	14.155709	7.601935	36.859275	H	30.639446	4.299316	44.840280
H	13.169196	7.504876	42.651706	H	28.690840	3.527912	46.099669
H	25.706982	7.214910	43.613331	H	28.532273	4.710177	32.981133
H	24.495015	5.820363	42.040430	H	30.948219	8.196461	33.550775
H	13.612388	3.636253	39.860700	H	39.440743	6.699713	37.196741
H	28.189878	2.194104	39.036935	H	40.113913	2.815201	37.862054
H	18.574995	6.683674	45.816416	H	52.223565	3.706557	43.946538
H	19.597845	7.430159	32.731888	H	54.659244	3.327408	44.019610
H	17.691827	6.639685	34.034354	H	56.055342	3.866410	42.061235
H	14.368535	4.447009	44.852694	H	51.374936	5.456069	39.580968
H	12.443505	3.862370	46.189099	H	52.752597	5.977092	37.680422
H	12.777716	3.592267	32.651764	H	49.630126	2.682863	37.983403
H	14.148626	7.226855	33.333251	H	49.717187	2.210332	35.573573
H	24.132107	5.725123	37.301756	H	48.433867	3.555859	34.001356
H	24.785676	2.238248	38.511163	H	46.476677	6.353947	38.407253
H	36.517035	2.198772	43.159196	H	45.196485	7.653286	36.808239
H	38.933300	1.523611	42.995672	H	44.160587	7.341512	42.855782
H	40.424337	2.618844	41.393514	H	45.048539	3.779335	39.680014
H	35.902588	5.403836	39.613636	H	49.665043	7.135792	45.873805
H	37.354543	6.417538	37.925235	H	50.741712	7.839740	32.637864
H	32.852312	2.099435	38.217737	H	48.887584	6.975437	33.969358
H	32.669451	1.586808	35.762584	H	45.686905	4.540355	44.849829
H	32.154927	3.355111	34.164754	H	43.799161	3.789692	46.158278
H	31.931686	6.818024	38.572670	H	44.200952	3.541023	32.707483
H	31.292982	8.580347	36.963538	H	45.248414	7.225068	33.289290
H	28.194789	7.069056	43.785160	H	54.726624	5.966808	36.663025
H	41.734775	7.712703	42.717775	H	9.463430	8.127146	58.062832
H	40.356362	6.356361	41.238202	H	7.917028	6.786919	56.693476
H	29.443685	3.596821	40.616960	H	10.726918	2.324704	54.106920
H	43.638737	2.485022	38.177777	H	7.193561	3.175391	53.796565
H	34.301657	7.312311	45.738759	H	19.519776	2.905246	59.291912
H	35.975935	7.091801	32.651271	H	21.915643	2.345634	59.305282
H	34.021901	6.713766	34.062547	H	23.373357	3.095361	57.496749

H	18.847362	5.339128	55.143088	H	39.031308	6.373372	56.786219
H	20.312178	6.019277	53.346564	H	27.964527	3.569263	55.353486
H	16.869715	2.417440	53.502930	H	42.089367	2.068501	54.092927
H	16.891664	1.930301	51.094878	H	32.787645	6.739954	61.409294
H	15.695838	3.362756	49.532116	H	34.016516	7.963509	48.143334
H	14.027098	6.331786	53.945021	H	32.167982	7.056639	49.465933
H	12.836224	7.722995	52.354142	H	28.750397	4.373292	60.400134
H	11.840698	7.508839	58.212464	H	26.898021	3.573739	61.718725
H	24.891129	7.940673	58.025977	H	27.668963	3.449399	48.079090
H	23.419896	6.476120	56.753681	H	28.698385	7.273425	48.660920
H	12.284878	3.635448	55.428946	H	38.068398	5.966847	52.407695
H	26.464785	2.149694	54.081142	H	38.578021	2.478136	53.831569
H	17.168871	6.738413	61.410907	H	50.894859	3.699634	59.506114
H	18.429783	7.285091	48.195205	H	53.331526	3.325361	59.581251
H	16.480301	6.650686	49.516152	H	54.727797	3.865607	57.623223
H	13.129502	4.375128	60.400691	H	50.047792	5.460857	55.146018
H	11.278001	3.573873	61.719528	H	51.425188	5.977967	53.243217
H	11.425342	3.794407	48.234630	H	48.361298	2.719102	53.468201
H	12.839278	7.298966	48.834481	H	48.419886	2.254363	51.056550
H	22.423952	6.142317	52.479444	H	47.070539	3.563759	49.511705
H	22.946687	2.534525	53.865697	H	45.135423	6.318110	53.954915
H	35.122568	3.072275	59.353933	H	43.800769	7.593009	52.380214
H	37.506612	2.469657	59.387168	H	42.893347	7.347267	58.246495
H	38.968539	3.098472	57.537998	H	43.582318	3.469295	55.395381
H	34.487008	5.368622	55.124054	H	48.405526	6.744636	61.407777
H	35.958367	5.932646	53.289353	H	49.439708	7.710099	48.253534
H	32.590180	2.489813	53.540584	H	47.535761	6.903879	49.546396
H	32.769928	2.028127	51.135132	H	44.382319	4.362982	60.399598
H	31.633062	3.443195	49.513250	H	42.519568	3.570976	61.717959
H	29.629228	6.332517	53.840615	H	42.760416	3.631048	48.189458
H	28.495486	7.702184	52.183157	H	43.807092	7.180239	48.860236
H	27.299034	7.476246	58.166180	H	53.398691	5.964446	52.224631
H	40.487098	7.804222	58.106645	H	17.068467	7.157627	63.836112

H	15.148261	6.357127	65.155563	N	32.623980	10.707553	42.892537
H	10.261794	3.422546	63.798060	H	35.046498	10.324248	41.864554
H	32.688187	7.158113	63.835107	H	33.387424	8.796402	42.940795
H	30.768112	6.357258	65.154654	H	31.002439	8.877650	42.050086
H	25.879138	3.427455	63.796198	H	34.797693	10.738113	39.379195
H	48.307476	7.159243	63.833715	H	33.583587	11.638469	40.295080
H	46.387827	6.357481	65.153435	H	32.497801	10.513984	38.345153
H	41.497996	3.429485	63.794642	H	33.133205	8.941650	38.870671
H	54.922501	4.682764	55.325505	H	31.144117	10.676378	40.461097
H	56.250043	4.683192	39.763403	H	30.745899	9.184487	39.579092
H	57.578861	4.683541	24.200338	H	34.696118	8.842466	40.951858
H	32.654191	5.043642	18.026515	H	31.312466	12.774337	43.917031
H	17.034722	5.043892	18.026656	H	29.911547	12.762744	45.954201
H	10.176539	4.915037	24.089471	H	29.580329	10.647972	47.262872
H	8.847951	4.915251	39.653274	H	30.690170	8.540965	46.458790
H	7.520537	4.915276	55.216414	H	32.054821	8.537322	44.434014
H	12.998675	5.198814	65.268994	H	31.272204	6.747687	42.736572
H	28.618505	5.198903	65.268105	H	32.536076	11.549316	42.333664
H	44.238351	5.198855	65.266963				
H	48.273823	5.043387	18.026057				
C	31.886569	8.858477	41.380104	(<i>R,R</i>)-2-PC			
C	33.059683	9.517926	42.180381	C	12.487000	7.261000	26.395000
C	34.266924	9.812256	41.272571	C	11.616000	6.503000	25.622000
C	33.901929	10.613068	40.014822	C	12.086000	5.395000	24.927000
C	32.775104	9.920674	39.236218	C	13.428000	5.043000	25.007000
C	31.551051	9.699182	40.132034	C	13.027000	3.179000	23.539000
O	32.155237	7.548263	40.982897	C	11.685000	3.529000	23.460000
C	31.805657	10.661831	44.014857	C	11.215000	4.638000	24.154000
C	31.173366	11.840573	44.474566	O	10.782000	2.793000	22.654000
C	30.384948	11.831032	45.625102	Cu	18.545211	6.099706	26.004396
C	30.195417	10.651423	46.357851	Cu	17.957621	3.712909	26.529586
C	30.811954	9.479505	45.906767	C	22.221207	3.972023	26.370636
C	31.600828	9.474083	44.754241	C	22.764886	3.214615	27.423776
				C	24.118096	2.901312	27.452650

C	24.952702	3.333636	26.427392	C	27.336646	3.163299	23.592046
C	24.446952	4.068344	25.337960	C	26.775183	4.235322	24.322233
C	23.060449	4.373771	25.293200	O	26.571630	2.272218	22.842322
C	22.545304	5.036966	24.158835	O	16.595625	6.409533	25.840243
C	23.390644	5.428201	23.125328	O	16.060871	4.270955	26.319640
C	24.758122	5.174392	23.189753	C	15.737715	5.466436	25.980565
C	25.297986	4.485402	24.284302	C	17.917761	5.856229	30.218759
O	25.590849	5.570430	22.148912	C	18.909843	6.621169	30.858682
O	20.438399	5.538538	26.177222	C	16.766136	5.452020	30.950082
O	19.921198	3.393754	26.650254	C	15.689591	4.782581	30.329903
C	20.774832	4.322449	26.409936	C	14.582923	4.385399	31.074233
C	18.226927	4.022014	22.293999	O	18.434937	6.427667	27.962775
C	18.992915	2.941012	21.873981	O	17.905256	4.284243	28.428683
C	19.081890	2.638017	20.519979	C	18.102646	5.501028	28.786111
C	18.404876	3.417023	19.587993	Cu	34.126310	5.987200	26.089034
C	17.639888	4.497024	20.008011	Cu	33.551789	3.584558	26.543220
C	17.550913	4.800019	21.362013	C	37.810428	3.836259	26.412284
C	16.783924	5.881020	21.784030	C	38.326233	3.092758	27.489711
C	16.107910	6.659026	20.850045	C	39.671868	2.753213	27.544445
C	16.197885	6.355031	19.497042	C	40.526980	3.141906	26.519435
C	16.963875	5.274030	19.076025	C	40.050108	3.862470	25.408047
O	15.523872	7.185037	18.539057	C	38.671631	4.201388	25.340775
O	18.566589	5.534636	24.104811	C	38.186422	4.862058	24.193079
O	18.028183	3.394469	24.576217	C	39.052885	5.208143	23.160384
C	18.267660	4.339912	23.743957	C	40.412770	4.916459	23.243236
C	14.301000	5.801000	25.782000	C	40.923900	4.237242	24.357851
C	13.829000	6.909000	26.476000	O	41.267492	5.275409	22.206798
C	27.956207	7.032197	26.505965	O	36.028958	5.413074	26.202683
C	27.120978	6.194168	25.775136	O	35.510847	3.260445	26.637283
C	27.631757	5.081004	25.076105	C	36.365085	4.192834	26.421274
C	29.026575	4.816167	25.131071	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.703912	2.946048	23.616103	C	34.701781	2.637978	20.519678

C	34.024753	3.416989	19.587708	Cu	49.687381	6.194920	25.986368
C	33.259776	4.496991	20.007741	Cu	49.348200	3.774899	26.563795
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.116988	5.496104	24.161846	C	53.770890	5.287813	24.113936
O	33.609987	3.336919	24.568199	C	54.557834	5.591815	23.007897
C	33.846807	4.307023	23.760581	C	55.929834	5.377800	23.052821
C	29.866107	5.644536	25.926558	C	56.515889	4.858782	24.200784
C	29.315867	6.761068	26.581023	O	56.643771	5.617805	21.841785
C	43.530396	6.838114	26.562617	O	51.632356	5.833805	26.124940
C	42.711717	5.967643	25.854309	O	51.338020	3.655033	26.633752
C	43.243398	4.851571	25.175566	C	52.092332	4.663762	26.380332
C	44.644427	4.613480	25.232646	C	49.466779	4.021876	22.293156
C	29.549001	3.754989	24.364516	C	50.232745	2.940872	21.873104
C	44.345413	2.683258	23.790816	C	50.321669	2.637885	20.519096
C	42.976220	2.891150	23.744994	C	49.644627	3.416901	19.587140
C	42.400202	3.981432	24.434854	C	48.879661	4.496905	20.007192
O	42.223734	1.973309	23.015316	C	48.790737	4.799893	21.361200
O	32.160923	6.305968	25.990791	C	48.023772	5.880897	21.783251
O	31.655912	4.144013	26.387837	C	47.347731	6.658913	20.849295
C	31.313109	5.349246	26.112288	C	47.437655	6.354926	19.496287
C	33.679966	5.584291	30.321158	C	48.203620	5.273922	19.075235
C	34.757805	6.253428	30.928931	O	46.763613	7.184943	18.538331
C	32.543840	5.236848	31.104830	O	49.726340	5.586859	24.092610
C	31.404135	4.637213	30.530862	O	49.389029	3.418936	24.606680
C	30.302143	4.321856	31.321453	C	49.524183	4.364848	23.750152
O	34.070108	6.238227	28.063068	C	45.473344	5.496586	25.978679
O	33.526563	4.086122	28.468262	C	44.897351	6.609138	26.619150
C	33.764130	5.283785	28.864875	C	45.180618	3.528702	24.511449

O	47.705792	6.316031	25.888199	O	18.653556	3.450163	42.089667
O	47.397066	4.146344	26.421180	C	19.499042	4.392228	41.873887
C	46.945049	5.304226	26.098019	C	16.899511	4.145258	37.734453
C	49.185355	5.978101	30.217883	C	17.601230	3.040879	37.219520
C	50.110001	6.846905	30.825531	C	17.613679	2.778225	35.856494
C	48.082109	5.491956	30.973995	C	16.923257	3.611817	34.983605
C	47.068066	4.705994	30.386182	C	16.180920	4.713804	35.457279
C	46.006871	4.234803	31.152881	C	16.149545	4.971859	36.853511
O	49.595835	6.551878	27.940744	C	15.345288	6.024759	37.334322
O	49.299014	4.375419	28.456572	C	14.634411	6.826093	36.450112
C	49.379189	5.612948	28.788233	C	14.690586	6.612802	35.082957
C	11.158286	7.260970	41.959133	C	15.470091	5.555605	34.561398
C	10.287269	6.502976	41.186145	O	13.974650	7.496688	34.278418
C	10.757253	5.394976	40.491133	O	17.247008	5.613406	39.576156
C	12.099253	5.042971	40.571108	O	16.752861	3.455855	40.012386
C	11.698221	3.178978	39.103109	C	16.972908	4.419386	39.193754
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.791182	6.874167	42.538323
Cu	17.238250	6.144506	41.487977	C	25.952682	6.135142	41.728368
Cu	16.685958	3.745008	41.980649	C	26.431519	5.043529	40.931598
C	20.953443	4.060853	41.900959	C	27.834802	4.730012	41.021433
C	21.445223	3.295529	42.974305	C	12.571237	3.934972	39.877096
C	22.793830	2.977610	43.068240	C	27.541034	2.966359	39.378079
C	23.678262	3.406879	42.085480	C	26.152450	3.256672	39.287845
C	23.231855	4.154137	40.980045	C	25.585970	4.272205	40.055579
C	21.849956	4.476505	40.874940	O	25.494399	2.439809	38.411226
C	21.397685	5.166159	39.731351	O	15.273255	6.435570	41.361506
C	22.296788	5.556192	38.743161	O	14.774818	4.283092	41.808690
C	23.655036	5.272662	38.861409	C	14.425755	5.481886	41.506768
C	24.133517	4.564973	39.969602	C	16.702715	5.831146	45.712463
O	24.534096	5.652970	37.855413	C	17.713110	6.591735	46.329516
O	19.147040	5.603527	41.634548	C	18.806701	6.939091	32.206607

C	17.708858	6.502278	32.939587	C	31.384488	6.155821	37.491871
C	16.677423	5.759050	32.333572	C	30.991933	7.082484	36.560973
C	15.568748	5.429531	46.472817	C	30.990384	6.776517	35.174232
C	14.483839	4.746711	45.883478	C	31.364258	5.510845	34.732415
C	13.390784	4.361319	46.653677	O	30.602108	7.827733	34.389990
C	14.518274	4.636774	32.442379	O	32.846551	5.307348	39.782158
C	15.553570	5.331175	33.082485	O	32.142968	3.247195	40.336703
O	13.408543	4.230460	33.174940	C	32.401064	4.158957	39.492371
O	17.153237	6.438814	43.452917	C	28.672783	5.519319	41.869946
O	16.646014	4.285245	43.893553	C	28.169512	6.578987	42.601170
C	16.846064	5.496846	44.268428	C	42.282457	7.206410	42.068224
Cu	32.932179	6.127311	41.585165	C	41.465250	6.409624	41.275173
Cu	32.420283	3.665814	42.252521	C	41.996081	5.350121	40.512769
C	36.607821	4.013075	41.741041	C	43.392410	5.089460	40.573136
C	37.128529	3.170998	42.706856	C	28.358074	3.673303	40.221409
C	38.507970	2.870573	42.714338	C	43.097067	3.304451	38.955828
C	39.342550	3.393840	41.750374	C	41.730132	3.526159	38.914782
C	38.848170	4.238928	40.703609	C	41.160287	4.554246	39.691961
C	37.439724	4.545786	40.701694	O	40.975892	2.680463	38.106088
C	36.918297	5.333091	39.634973	O	30.921104	6.174521	41.639619
C	37.741271	5.809345	38.642332	O	30.496317	4.088854	42.358931
C	39.138687	5.551206	38.660834	C	30.136787	5.237077	41.961033
C	39.695579	4.771510	39.672750	C	32.422747	5.983127	45.791183
O	39.935305	6.063311	37.681396	C	33.293383	6.877113	46.387198
O	34.830659	5.571220	41.687303	C	34.749556	6.534389	32.288800
O	34.359537	3.402079	42.083045	C	33.655463	6.170745	33.065534
C	35.153774	4.356823	41.836129	C	32.537031	5.534830	32.495232
C	32.197823	3.843975	38.044160	C	31.291940	5.466349	46.505328
C	32.476637	2.550289	37.633444	C	30.306620	4.648065	45.881421
C	32.429067	2.217844	36.264357	C	29.215901	4.199286	46.584961
C	32.092602	3.171787	35.326630	C	30.300812	4.596505	32.687368
C	31.745770	4.511190	35.696415	C	31.408050	5.209656	33.282074
C	31.788746	4.845624	37.098335	O	29.189964	4.283820	33.460069

O	32.934268	6.511297	43.549245	C	44.216457	5.884090	41.416608
O	32.615657	4.350620	44.095330	C	43.644709	6.949596	42.135216
C	32.678328	5.582609	44.371730	C	43.929984	4.068068	39.765945
Cu	48.451353	6.404301	41.573756	O	46.479669	6.622603	41.444818
Cu	47.998449	3.978766	42.047612	O	46.070998	4.439867	41.841807
C	52.242278	4.464620	41.931334	C	45.675008	5.631729	41.572621
C	52.828353	3.947597	43.079285	C	47.843729	6.057421	45.781282
C	54.201353	3.732577	43.123183	C	48.785679	6.887232	46.417225
C	54.987278	4.036581	42.018131	C	49.988532	7.195259	32.164653
C	54.401203	4.554604	40.869180	C	48.938669	6.686084	32.921068
C	53.028203	4.768624	40.826281	C	47.974479	5.834587	32.348227
C	52.442128	5.287648	39.677330	C	46.720928	5.584278	46.517299
C	53.229054	5.591652	38.571278	C	45.690402	4.839643	45.905090
C	54.601054	5.377632	38.616177	C	44.612674	4.377822	46.654628
C	55.187129	4.858609	39.764128	C	45.926480	4.526204	32.512090
O	55.314970	5.617639	37.405129	C	46.897354	5.333352	33.120374
O	50.375134	5.934729	41.729163	O	44.863598	4.043889	33.267506
O	49.973361	3.761190	42.185667	O	48.337104	6.684857	43.537426
C	50.776091	4.736728	41.959867	O	47.900298	4.512357	43.960543
C	48.304136	4.389376	37.810888	C	48.042940	5.730098	44.342372
C	49.127935	3.358473	37.325349	C	9.830848	7.260896	57.522290
C	49.194193	3.080256	35.967218	C	8.959816	6.502907	56.749315
C	48.434881	3.822889	35.070004	C	9.429783	5.394908	56.054291
C	47.577413	4.851848	35.512945	C	10.771783	5.042898	56.134241
C	47.498951	5.129879	36.903846	C	10.370718	3.178911	54.666243
C	46.595417	6.112902	37.353867	C	9.028718	3.528920	54.587293
C	45.823951	6.825744	36.444946	C	8.558750	4.637919	55.281317
C	45.914786	6.588728	35.083146	O	8.125684	2.792932	53.781319
C	46.797132	5.599655	34.591980	Cu	15.891522	6.155334	57.135290
O	45.128147	7.383745	34.252268	Cu	15.352118	3.737379	57.544434
O	48.497783	5.881555	39.657128	C	19.606139	4.079052	57.412957
O	48.118689	3.698481	40.082379	C	20.169417	3.302784	58.441645
C	48.307345	4.672820	39.269370	C	21.524003	2.994493	58.442266

C	22.339706	3.448919	57.411476	C	24.689444	3.367450	54.526486
C	21.814518	4.206837	56.347207	C	24.127015	4.407257	55.301345
C	20.427205	4.511822	56.333763	O	23.924685	2.507377	53.741167
C	19.892913	5.206384	55.227518	O	13.936013	6.439336	56.974158
C	20.720276	5.624407	54.189930	O	13.441968	4.274243	57.363446
C	22.088438	5.367379	54.222861	C	13.093013	5.478540	57.082763
C	22.647293	4.649394	55.289004	C	15.283046	5.695821	61.352095
O	22.903312	5.792369	53.179590	C	16.314087	6.385804	61.978046
O	17.796353	5.623539	57.297908	C	17.640265	6.917722	47.677373
O	17.318956	3.448123	57.660625	C	16.552075	6.498336	48.433801
C	18.155017	4.403510	57.470893	C	15.505535	5.755631	47.854498
C	15.687578	4.242123	53.318160	C	14.198081	5.242825	62.095148
C	16.418874	3.147111	52.823636	C	13.166040	4.552842	61.469196
C	16.471812	2.881015	51.462663	C	12.083075	4.099846	62.213249
C	15.788830	3.698571	50.569936	C	13.345678	4.642201	48.017051
C	15.023693	4.794753	51.019639	C	14.390423	5.348848	48.628158
C	14.960636	5.063985	52.413830	O	12.246050	4.252167	48.773486
C	14.145010	6.119266	52.868151	O	15.754589	6.387479	59.110258
C	13.451891	6.911347	51.961506	O	15.284268	4.211934	59.472401
C	13.530613	6.680860	50.597910	C	15.446195	5.415018	59.890971
C	14.317809	5.616956	50.101782	Cu	31.463903	6.174286	57.130653
O	12.825683	7.552960	49.770980	Cu	30.949634	3.749534	57.533970
O	15.948098	5.679682	55.205198	C	35.196960	4.101980	57.427724
O	15.451326	3.509931	55.571706	C	35.734129	3.349155	58.488031
C	15.694991	4.493172	54.784355	C	37.080459	3.009437	58.512937
C	11.644816	5.800887	56.909216	C	37.914730	3.406396	57.474164
C	11.172849	6.908886	57.603240	C	37.417613	4.142454	56.381571
C	25.305491	7.115481	57.593251	C	36.038544	4.484353	56.346321
C	24.472279	6.308731	56.827083	C	35.532607	5.163004	55.218113
C	24.983977	5.222865	56.086761	C	36.379735	5.525216	54.175141
C	26.378961	4.955324	56.132828	C	37.740100	5.229636	54.226568
C	11.243751	3.934900	55.440217	C	38.271473	4.529373	55.318590
C	26.056834	3.146973	54.545614	O	38.575038	5.603265	53.179625

O	33.380608	5.645637	57.257414	C	33.115304	7.239235	47.740611
O	32.913254	3.472765	57.647288	C	32.066876	6.721432	48.471264
C	33.745062	4.429187	57.451881	C	31.109922	5.828549	47.887734
C	31.277411	4.265404	53.305162	C	29.818167	5.242646	62.094340
C	32.080221	3.217713	52.819404	C	28.786113	4.552669	61.468405
C	32.163922	2.954074	51.459439	C	27.703159	4.099675	62.212476
C	31.439582	3.725071	50.558135	C	29.056891	4.503162	47.963631
C	30.599642	4.767712	50.998096	C	29.987639	5.307894	48.618504
C	30.508812	5.037919	52.391012	O	27.987963	4.007364	48.646322
C	29.628915	6.044961	52.833033	O	31.364873	6.394423	59.109265
C	28.885628	6.778530	51.914183	O	30.889773	4.218924	59.464405
C	28.983003	6.539973	50.552581	C	31.059477	5.419578	59.887835
C	29.846230	5.534117	50.075022	Cu	47.055651	6.260771	57.153125
O	28.219999	7.345509	49.711536	Cu	46.686572	3.803902	57.527529
O	31.485947	5.712570	55.192979	C	50.914829	4.464394	57.493750
O	31.045828	3.530435	55.558667	C	51.500923	3.947364	58.641689
C	31.264397	4.519981	54.771534	C	52.873923	3.732339	58.685563
C	27.217349	5.754617	56.957700	C	53.659830	4.036343	57.580498
C	26.664535	6.841917	57.658102	C	53.073736	4.554373	56.431559
C	40.919690	6.964412	57.659376	C	51.700736	4.768398	56.388685
C	40.090252	6.158056	56.891158	C	51.114643	5.287428	55.239746
C	40.604860	5.074970	56.148496	C	51.901549	5.591433	54.133681
C	42.001769	4.810587	56.192851	C	53.273549	5.377407	54.178555
C	26.901752	3.922815	55.329273	C	53.859642	4.858378	55.326493
C	41.677328	2.989238	54.621977	O	53.987445	5.617415	52.967495
C	40.310435	3.214753	54.595073	O	48.995154	5.863872	57.303430
C	39.748177	4.262802	55.358949	O	48.671314	3.659467	57.665666
O	39.545715	2.350364	53.814639	C	49.438696	4.675517	57.498128
O	29.497139	6.448322	57.017112	C	46.976219	4.387862	53.312763
O	29.037956	4.267274	57.363193	C	47.814338	3.383025	52.797313
C	28.669601	5.472829	57.119907	C	47.871936	3.133393	51.433674
C	30.903120	5.695641	61.351269	C	47.089466	3.878803	50.559757
C	31.934175	6.385618	61.977205	C	46.220531	4.885378	51.031219

C	46.151263	5.134491	52.428401	C	13.063191	5.025817	64.207206
C	45.235352	6.092407	52.906168	O	10.943187	3.908837	64.361307
C	44.444823	6.811264	52.018520	C	31.882275	6.620600	63.346211
C	44.526305	6.603282	50.651372	C	30.799322	6.168606	64.089282
C	45.419405	5.638222	50.131841	C	29.767267	5.478629	63.464346
O	43.722357	7.405826	49.844686	C	27.651260	4.336658	63.581482
O	47.127066	5.819006	55.215411	C	28.683314	5.025635	64.206417
O	46.816133	3.610217	55.554876	O	26.563309	3.908663	64.360554
C	46.972439	4.620725	54.780567	C	47.502389	6.620356	63.345091
C	42.840918	5.624034	57.003065	C	46.419447	6.168363	64.088179
C	42.280310	6.702261	57.713121	C	45.387379	5.478391	63.463260
C	42.523728	3.772130	55.397558	C	43.271369	4.336426	63.580429
O	45.082212	6.414828	57.026493	C	44.303437	5.025398	64.205349
O	44.742469	4.207977	57.344661	O	42.183431	3.908432	64.359519
C	44.307878	5.397128	57.124541	H	12.119292	8.127223	26.935541
C	46.523195	5.695406	61.350162	H	10.573036	6.786857	25.566326
C	47.554262	6.385378	61.976082	H	13.383710	2.323187	22.982608
C	48.661418	7.210315	47.761676	H	9.847384	3.169534	22.677183
C	47.591475	6.714339	48.496981	H	22.128855	2.878336	28.234723
C	46.611011	5.899901	47.898233	H	24.524568	2.323825	28.277132
C	45.438253	5.242413	62.093251	H	26.001623	3.075333	26.483803
C	44.406185	4.552442	61.467332	H	21.487785	5.249430	24.044641
C	43.323243	4.099449	62.211421	H	22.971879	5.937283	22.267790
C	44.531205	4.638665	48.020107	H	19.532717	2.330044	22.589896
C	45.517142	5.408043	48.652918	H	19.679477	1.794178	20.190515
O	43.451858	4.165480	48.757601	H	18.480499	3.170813	18.536728
O	46.924761	6.447470	59.126507	H	16.649980	6.144787	22.827018
O	46.571188	4.243086	59.457644	H	15.506631	7.500795	21.165206
C	46.675333	5.446344	59.890404	H	14.495691	7.508802	27.086848
C	16.262162	6.620790	63.347051	H	27.544390	7.892515	27.024129
C	15.179196	6.168795	64.090104	H	26.067709	6.434857	25.745019
C	14.147156	5.478812	63.465153	H	14.941446	3.633620	24.312812
C	12.031150	4.336833	63.582254	H	29.112826	2.128754	23.037196

H	19.776906	6.959637	30.302797	H	50.920785	1.795180	20.189773
H	15.678100	4.569578	29.266264	H	49.720358	3.170933	18.535926
H	13.771745	3.871103	30.576881	H	47.862763	6.134480	22.823774
H	15.671866	6.861099	17.596378	H	46.741177	7.496787	21.164899
H	25.094740	6.080172	21.433310	H	45.521778	7.300979	27.173038
H	25.588912	2.485300	22.858991	H	46.244308	3.321880	24.481606
H	37.673078	2.784603	28.298330	H	50.937041	7.247183	30.250249
H	40.055700	2.186978	28.387465	H	47.070039	4.455635	29.330869
H	41.569179	2.861991	26.594490	H	45.243476	3.631840	30.680101
H	37.136923	5.109780	24.071672	H	46.913204	6.861936	17.595746
H	38.657766	5.715916	22.290953	H	56.056144	5.976916	21.104057
H	35.146104	2.325240	22.590313	H	10.790976	8.128083	42.498432
H	35.297709	1.792927	20.190421	H	9.244443	6.787065	41.130005
H	34.099756	3.170442	18.536518	H	12.055519	2.325066	38.544075
H	32.269117	6.145226	22.826304	H	8.519278	3.170935	38.240000
H	31.125577	7.500075	21.165083	H	20.770376	2.953700	43.751062
H	29.951149	7.414422	27.168037	H	23.157589	2.394848	43.908935
H	43.101768	7.697636	27.068403	H	24.721539	3.137374	42.190245
H	41.653339	6.184394	25.829323	H	20.349332	5.398995	39.575118
H	30.610683	3.541548	24.316365	H	21.924656	6.082910	37.874542
H	44.764150	1.847360	23.246573	H	18.152750	2.388272	37.886631
H	35.618886	6.544135	30.337422	H	18.165768	1.926271	35.472286
H	31.343147	4.414637	29.469908	H	16.958184	3.375320	33.929601
H	29.439700	3.860781	30.858716	H	15.240148	6.237771	38.392000
H	31.291693	6.860811	17.596363	H	14.023748	7.635428	36.827431
H	40.793345	5.790108	21.479982	H	13.169313	7.511492	42.645374
H	41.239475	2.180964	23.018429	H	26.396714	7.704135	43.132981
H	53.552011	3.699701	28.381160	H	24.892876	6.408004	41.696563
H	55.987694	3.325991	28.455688	H	13.612084	3.634289	39.867747
H	57.384069	3.866316	26.497848	H	27.933432	2.162732	38.749412
H	52.703450	5.452774	24.015157	H	18.569613	6.924724	45.754180
H	54.081129	5.976133	22.116856	H	19.585040	7.522457	32.688588
H	50.777290	2.334582	22.589267	H	17.663033	6.764077	33.988093

H	14.456045	4.511393	44.824975	H	51.374685	5.452690	39.579208
H	12.573515	3.834708	46.179744	H	52.752229	5.975719	37.680067
H	12.749227	3.710299	32.615608	H	49.730733	2.775141	38.012136
H	14.034985	7.274631	33.299417	H	49.839076	2.285199	35.606290
H	24.084777	6.200632	37.136190	H	48.511046	3.573621	34.021224
H	24.560908	2.677904	38.303713	H	46.461430	6.338365	38.405927
H	36.463121	2.757711	43.469068	H	45.134243	7.580601	36.798354
H	38.916422	2.218605	43.492934	H	44.266979	7.578081	42.762289
H	40.406936	3.141905	41.786961	H	44.992662	3.850969	39.738280
H	35.850234	5.552248	39.594788	H	49.627670	7.279455	45.858211
H	37.318859	6.403114	37.822523	H	50.713735	7.861854	32.620936
H	32.758413	1.805389	38.381304	H	48.875268	6.976365	33.961186
H	32.673317	1.200342	35.943357	H	45.691475	4.615231	44.844110
H	32.084660	2.878167	34.272063	H	43.837034	3.805848	46.163547
H	31.384089	6.424628	38.546901	H	44.248710	3.450076	32.731348
H	30.670725	8.084076	36.860271	H	45.224024	7.150726	33.278671
H	28.832680	7.176160	43.229277	H	54.726531	5.972693	36.665929
H	41.855562	8.027251	42.635993	H	9.463399	8.127109	58.062853
H	40.408878	6.641785	41.248934	H	7.916946	6.786720	56.693530
H	29.419300	3.420240	40.275445	H	10.728169	2.325384	54.106726
H	43.516743	2.517995	38.342242	H	7.191740	3.170751	53.803257
H	34.124896	7.284059	45.805712	H	19.546867	2.944509	59.253514
H	35.597364	7.035897	32.745155	H	21.945941	2.401007	59.247280
H	33.686526	6.399718	34.123299	H	23.389597	3.190561	57.443891
H	30.403710	4.375521	44.830303	H	18.834307	5.425560	55.139833
H	28.459762	3.586512	46.080007	H	20.287161	6.157377	53.354275
H	28.473481	3.807963	32.931790	H	16.958459	2.500826	53.506541
H	30.549859	7.595362	33.449733	H	17.045805	2.035745	51.096013
H	39.400334	6.584743	37.061327	H	15.851557	3.455999	49.518668
H	39.988635	2.885986	38.125797	H	14.019583	6.342893	53.921468
H	52.223991	3.710387	43.947918	H	12.834374	7.724776	52.318247
H	54.659345	3.328203	44.019913	H	11.840450	7.509607	58.212083
H	56.055412	3.866650	42.061230	H	24.893213	7.954395	58.144987

H	23.419820	6.553045	56.802796	H	28.292391	7.085807	48.739468
H	12.285038	3.636243	55.427117	H	38.089230	6.128903	52.468364
H	26.465838	2.353649	53.934267	H	38.565764	2.575991	53.822527
H	17.168075	6.740032	61.410658	H	50.894922	3.700529	59.506444
H	18.432707	7.498032	48.139878	H	53.331584	3.325647	59.581346
H	16.527597	6.770590	49.480349	H	54.727848	3.865728	57.623137
H	13.130836	4.374522	60.400654	H	50.047651	5.459410	55.145286
H	11.278104	3.573997	61.719325	H	51.424893	5.977051	53.243021
H	11.577010	3.724193	48.233474	H	48.430558	2.793083	53.466230
H	12.919154	7.331415	48.794389	H	48.525350	2.355945	51.050520
H	22.396462	6.323929	52.487671	H	47.156979	3.648561	49.506201
H	22.944468	2.731769	53.751071	H	45.105638	6.293333	53.963699
H	35.095294	3.027806	59.302801	H	43.746553	7.547705	52.393414
H	37.480289	2.432389	59.340859	H	42.912671	7.342219	58.318057
H	38.956913	3.121122	57.523539	H	43.584912	3.556439	55.349055
H	34.481833	5.414363	55.119876	H	48.405614	6.744907	61.407981
H	35.969074	6.047131	53.321417	H	49.399651	7.847671	48.238216
H	32.652952	2.607315	53.508492	H	47.526217	6.985589	49.541973
H	32.793476	2.145999	51.099975	H	44.381439	4.364306	60.399424
H	31.527592	3.483826	49.507089	H	42.519341	3.571630	61.717714
H	29.492057	6.271848	53.885316	H	42.826712	3.598181	48.204694
H	28.211233	7.550381	52.261461	H	43.806724	7.190193	48.866223
H	27.298698	7.472282	58.271042	H	53.398692	5.970814	52.227674
H	40.504528	7.799350	58.215008	H	17.068201	7.158110	63.835991
H	39.037476	6.400209	56.869686	H	15.148083	6.357292	65.155550
H	27.963229	3.707903	55.279749	H	10.263157	3.421775	63.797076
H	42.085653	2.189801	54.018283	H	32.688068	7.158307	63.835060
H	32.787217	6.740914	61.409196	H	30.767941	6.357329	65.154661
H	33.817424	7.933123	48.213317	H	25.881862	3.424130	63.795740
H	31.960153	7.020767	49.518578	H	48.307513	7.159135	63.833759
H	28.748062	4.375542	60.400007	H	46.387765	6.357309	65.153493
H	26.897525	3.574889	61.718378	H	41.501220	3.425122	63.794463
H	27.451200	3.451790	48.057936	H	54.922556	4.682785	55.325779

H	56.250097	4.683171	39.763700	H	32.099433	9.941567	39.089462
H	57.578892	4.683412	24.200625	H	33.579480	9.850563	42.998684
H	32.654232	5.043308	18.026530	H	27.803644	10.664901	43.302432
H	17.034810	5.043582	18.026682	H	26.632672	10.509360	45.476593
H	10.176547	4.915299	24.089643	H	27.688335	9.310627	47.409065
H	8.847999	4.915598	39.653310	H	29.948162	8.252587	47.088630
H	7.520561	4.915556	55.216444	H	31.108925	8.392313	44.948320
H	12.998950	5.198991	65.269024	H	33.766798	8.698218	41.139702
H	28.618759	5.198985	65.268152	H	29.758177	10.302918	42.065783
H	44.238629	5.198825	65.267036				
H	48.273990	5.043163	18.026055				
C	31.784209	8.965730	40.986375	(S,S)-1-RC			
C	31.549297	9.257704	42.482529	C	12.487000	7.261000	26.395000
C	32.565751	10.299555	43.005129	C	11.616000	6.503000	25.622000
C	32.556105	11.579479	42.156702	C	12.086000	5.395000	24.927000
C	32.834566	11.270500	40.676436	C	13.428000	5.043000	25.007000
C	31.845086	10.230306	40.124822	C	13.027000	3.179000	23.539000
O	32.995076	8.190427	40.836636	C	11.685000	3.529000	23.460000
C	29.553236	9.558112	43.952943	C	11.215000	4.638000	24.154000
C	28.277752	10.139703	44.139612	O	10.782000	2.793000	22.654000
C	27.618403	10.044646	45.364646	Cu	18.542489	6.090441	26.011393
C	28.203052	9.370033	46.445213	Cu	17.948983	3.703203	26.529401
C	29.460960	8.786187	46.266366	C	22.209936	3.953991	26.377926
C	30.133145	8.871427	45.043599	C	22.754241	3.198747	27.432181
N	30.167670	9.637581	42.711270	C	24.107176	2.884661	27.459556
H	32.340305	10.520713	44.062654	C	24.939881	3.313469	26.431258
H	31.717145	8.304799	42.998534	C	24.432304	4.045895	25.340796
H	30.993409	8.290254	40.636370	C	23.046791	4.353227	25.298408
H	33.293131	12.305449	42.544441	C	22.530200	5.017414	24.164986
H	31.564508	12.064499	42.247204	C	23.374096	5.409069	23.130651
H	32.789126	12.191874	40.068750	C	24.740966	5.152367	23.192214
H	33.872044	10.892442	40.570247	C	25.280915	4.460414	24.284741
H	30.831301	10.674254	40.085680	O	25.573181	5.550254	22.151717
				O	20.432553	5.524159	26.187839

O	19.910158	3.378551	26.652619	C	15.671708	4.769608	30.319163
C	20.765467	4.306683	26.417606	C	14.560078	4.373702	31.056635
C	18.226927	4.022014	22.293999	O	18.429051	6.413199	27.970193
C	18.992915	2.941012	21.873981	O	17.895752	4.269125	28.429535
C	19.081890	2.638017	20.519979	C	18.093675	5.484798	28.790219
C	18.404876	3.417023	19.587993	Cu	34.101812	5.994956	26.096746
C	17.639888	4.497024	20.008011	Cu	33.544049	3.588365	26.547293
C	17.550913	4.800019	21.362013	C	37.803430	3.879693	26.437862
C	16.783924	5.881020	21.784030	C	38.326396	3.143586	27.516755
C	16.107910	6.659026	20.850045	C	39.675336	2.816896	27.571862
C	16.197885	6.355031	19.497042	C	40.526631	3.210161	26.545234
C	16.963875	5.274030	19.076025	C	40.043089	3.923390	25.432042
O	15.523872	7.185037	18.539057	C	38.661664	4.251247	25.365627
O	18.565909	5.530300	24.109626	C	38.170426	4.906199	24.217186
O	18.021477	3.390330	24.574839	C	39.033058	5.256828	23.182824
C	18.264822	4.337135	23.745116	C	40.394803	4.973480	23.263329
C	14.301000	5.801000	25.782000	C	40.912459	4.299301	24.378048
C	13.829000	6.909000	26.476000	O	41.244417	5.332073	22.222570
C	27.940031	7.023154	26.480546	O	36.008162	5.439401	26.226182
C	27.104388	6.180132	25.756631	O	35.506912	3.282115	26.656703
C	27.614102	5.059718	25.068104	C	36.354217	4.222259	26.444855
C	29.007940	4.792152	25.126713	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.681694	2.907221	23.630635	C	34.701781	2.637978	20.519678
C	27.315263	3.128421	23.602675	C	34.024753	3.416989	19.587708
C	26.756805	4.209193	24.321587	C	33.259776	4.496991	20.007741
O	26.547769	2.232703	22.861077	C	33.170826	4.799983	21.361747
O	16.595289	6.405520	25.844525	C	32.403848	5.880986	21.783781
O	16.055322	4.267063	26.319455	C	31.727821	6.658997	20.849810
C	15.735694	5.463901	25.982301	C	31.817771	6.355005	19.496805
C	17.903687	5.836764	30.222573	C	32.583748	5.274002	19.075771
C	18.895309	6.596463	30.869353	O	31.143743	7.185016	18.538835
C	16.746559	5.435277	30.946448	O	34.110742	5.499733	24.166543

O	33.617778	3.337709	24.571828	C	54.557834	5.591815	23.007897
C	33.848146	4.308740	23.763354	C	55.929834	5.377800	23.052821
C	29.847843	5.626960	25.914436	C	56.515889	4.858782	24.200784
C	29.298765	6.750167	26.558825	O	56.643771	5.617805	21.841785
C	43.546871	6.897441	26.555740	O	51.637873	5.838601	26.120489
C	42.719596	6.030196	25.853344	O	51.334198	3.662864	26.636587
C	43.240871	4.906511	25.179385	C	52.092875	4.667858	26.380321
C	44.640424	4.657970	25.234092	C	49.466779	4.021876	22.293156
C	29.528387	3.721925	24.371182	C	50.232745	2.940872	21.873104
C	44.324096	2.728177	23.795854	C	50.321669	2.637885	20.519096
C	42.956171	2.945146	23.753777	C	49.644627	3.416901	19.587140
C	42.388937	4.039265	24.445210	C	48.879661	4.496905	20.007192
O	42.196081	2.032442	23.025524	C	48.790737	4.799893	21.361200
O	32.137056	6.298259	25.982336	C	48.023772	5.880897	21.783251
O	31.644393	4.133224	26.377521	C	47.347731	6.658913	20.849295
C	31.295180	5.336538	26.100748	C	47.437655	6.354926	19.496287
C	33.565027	5.597002	30.325498	C	48.203620	5.273922	19.075235
C	34.604210	6.293020	30.969366	O	46.763613	7.184943	18.538331
C	32.409482	5.226695	31.071371	O	49.732220	5.591592	24.087884
C	31.298531	4.613828	30.456743	O	49.385118	3.426875	24.608984
C	30.175429	4.278084	31.207597	C	49.525607	4.368998	23.749368
O	34.020514	6.247716	28.073548	C	45.477844	5.536449	25.975946
O	33.493269	4.090868	28.472536	C	44.911858	6.656628	26.612241
C	33.704409	5.292709	28.871732	C	45.166997	3.567899	24.514081
Cu	49.695914	6.207882	25.979662	O	47.715487	6.339909	25.881134
Cu	49.344038	3.791403	26.564608	O	47.393981	4.173323	26.418891
C	53.571003	4.464792	26.367939	C	46.948655	5.333487	26.093602
C	54.157058	3.947774	27.515902	C	49.212283	6.003903	30.214069
C	55.530059	3.732759	27.559826	C	50.162866	6.845375	30.819863
C	56.316002	4.036762	26.454787	C	48.102101	5.542001	30.974387
C	55.729946	4.554780	25.305823	C	47.067414	4.781737	30.389069
C	54.356947	4.768795	25.262899	C	45.997191	4.336608	31.158800
C	53.770890	5.287813	24.113936	O	49.608597	6.571690	27.933050

O	49.297558	4.398529	28.455261	C	14.585642	6.801769	36.438090
C	49.390593	5.635982	28.783666	C	14.640524	6.585855	35.071283
C	11.158286	7.260970	41.959133	C	15.431604	5.536966	34.550129
C	10.287269	6.502976	41.186145	O	13.913205	7.460290	34.266653
C	10.757253	5.394976	40.491133	O	17.237310	5.643124	39.551841
C	12.099253	5.042971	40.571108	O	16.775746	3.481073	40.001595
C	11.698221	3.178978	39.103109	C	16.976813	4.443460	39.177198
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.889203	7.471702	41.839265
Cu	17.234486	6.183516	41.461713	C	26.022869	6.574174	41.248669
Cu	16.711703	3.780013	41.967112	C	26.477207	5.338387	40.684423
C	20.977846	4.154223	41.878940	C	27.884084	5.043046	40.786531
C	21.486363	3.428541	42.971886	C	12.571237	3.934972	39.877096
C	22.843318	3.150814	43.077915	C	27.527149	2.985562	39.541087
C	23.719493	3.580437	42.087623	C	26.133521	3.250849	39.461532
C	23.254768	4.279809	40.959055	C	25.600210	4.407367	40.024109
C	21.865641	4.563867	40.843079	O	25.438977	2.276206	38.802658
C	21.398766	5.211088	39.680586	O	15.266926	6.452940	41.345636
C	22.290170	5.591841	38.680877	O	14.792070	4.296265	41.797791
C	23.654436	5.340566	38.806724	C	14.429415	5.491693	41.496921
C	24.146129	4.679707	39.936654	C	16.715184	5.876816	45.691500
O	24.528480	5.715929	37.794586	C	17.716010	6.652515	46.305067
O	19.150183	5.666212	41.598392	C	18.785205	6.913336	32.216895
O	18.685388	3.510400	42.072389	C	17.680910	6.480523	32.942396
C	19.518258	4.462012	41.847875	C	16.650627	5.741014	32.329501
C	16.896518	4.159821	37.720520	C	15.593573	5.452168	46.458109
C	17.608147	3.061033	37.207177	C	14.513927	4.758156	45.872068
C	17.612724	2.789326	35.845981	C	13.434050	4.348429	46.648325
C	16.906106	3.609447	34.973399	C	14.488448	4.623043	32.424710
C	16.154803	4.705951	35.446009	C	15.521340	5.314994	33.071390
C	16.128290	4.970377	36.840883	O	13.373938	4.217789	33.150524
C	15.311481	6.013465	37.321865	O	17.156121	6.484008	43.427603

O	16.670476	4.327372	43.876805	C	28.268125	7.185038	41.922324
C	16.859092	5.541902	44.247238	C	42.280844	7.191460	42.230225
Cu	32.993527	6.313271	41.497810	C	41.441089	6.394531	41.460450
Cu	32.367934	3.867838	42.153405	C	41.950639	5.341658	40.677076
C	36.531303	3.892434	41.899917	C	43.350019	5.087124	40.690011
C	37.066875	3.090784	42.888937	C	28.375682	3.846416	40.187162
C	38.459277	2.859699	42.931537	C	43.008733	3.310470	39.073237
C	39.289552	3.406207	41.976927	C	41.640070	3.524848	39.079890
C	38.780967	4.213224	40.907179	C	41.090768	4.547273	39.879629
C	37.361263	4.457548	40.874505	O	40.864387	2.682039	38.288349
C	36.830823	5.230811	39.801624	O	31.024890	6.605324	41.323049
C	37.654876	5.758187	38.835245	O	30.516761	4.549232	42.081732
C	39.059900	5.544568	38.872871	C	30.204313	5.689086	41.621997
C	39.625706	4.771812	39.886371	C	32.359015	6.200094	45.684619
O	39.853569	6.087869	37.908033	C	33.223212	7.108005	46.269677
O	34.764309	5.431799	41.821541	C	34.537734	6.583045	32.326419
O	34.250895	3.277443	42.172869	C	33.426750	6.193783	33.066622
C	35.073698	4.214431	41.965621	C	32.350073	5.518642	32.462671
C	32.491805	3.998790	37.925216	C	31.289995	5.608313	46.437991
C	33.160053	2.870156	37.487096	C	30.312368	4.763540	45.838279
C	33.201305	2.575806	36.106877	C	29.290839	4.226650	46.583927
C	32.564685	3.393362	35.195494	C	30.128896	4.532602	32.575969
C	31.824199	4.551486	35.600887	C	31.207733	5.153905	33.214484
C	31.785404	4.844708	37.010665	O	28.990745	4.212131	33.304709
C	30.998470	5.944254	37.458054	O	32.842135	6.749015	43.430813
C	30.303614	6.718940	36.566256	O	32.526040	4.586364	43.976596
C	30.368253	6.466134	35.169388	C	32.587723	5.820894	44.254726
C	31.123379	5.404972	34.674740	Cu	48.443031	6.400560	41.595456
O	29.646199	7.361256	34.432171	Cu	47.995076	3.973161	42.062418
O	32.974124	5.506529	39.667444	C	52.242278	4.464620	41.931334
O	32.256156	3.444773	40.216254	C	52.828353	3.947597	43.079285
C	32.570005	4.340736	39.380041	C	54.201353	3.732577	43.123183
C	28.750404	5.981905	41.435654	C	54.987278	4.036581	42.018131

C	54.401203	4.554604	40.869180	C	49.000726	6.703642	32.922094
C	53.028203	4.768624	40.826281	C	48.010014	5.882485	32.350216
C	52.442128	5.287648	39.677330	C	46.742147	5.603403	46.532109
C	53.229054	5.591652	38.571278	C	45.684412	4.908925	45.907868
C	54.601054	5.377632	38.616177	C	44.581134	4.492842	46.646504
C	55.187129	4.858609	39.764128	C	45.928081	4.629411	32.518494
O	55.314970	5.617639	37.405129	C	46.922077	5.409646	33.124808
O	50.369997	5.931371	41.729629	O	44.855009	4.174380	33.276551
O	49.972762	3.756529	42.182641	O	48.353896	6.672377	43.560980
C	50.774090	4.733795	41.958234	O	47.916331	4.498409	43.978493
C	48.264578	4.402013	37.822443	C	48.069327	5.713674	44.364155
C	49.047844	3.339242	37.337588	C	9.830848	7.260896	57.522290
C	49.113117	3.063828	35.978961	C	8.959816	6.502907	56.749315
C	48.392874	3.840981	35.079198	C	9.429783	5.394908	56.054291
C	47.573717	4.901254	35.520098	C	10.771783	5.042898	56.134241
C	47.495661	5.177319	36.911832	C	10.370718	3.178911	54.666243
C	46.626504	6.192863	37.357810	C	9.028718	3.528920	54.587293
C	45.893626	6.940820	36.444984	C	8.558750	4.637919	55.281317
C	45.986449	6.705323	35.083235	O	8.125684	2.792932	53.781319
C	46.829954	5.681500	34.595847	Cu	15.894838	6.137623	57.134966
O	45.239001	7.533723	34.248724	Cu	15.340878	3.724064	57.551119
O	48.469703	5.887107	39.675845	C	19.594526	4.036739	57.442878
O	48.095190	3.702423	40.094143	C	20.144684	3.274484	58.489010
C	48.275461	4.680521	39.283358	C	21.496818	2.956371	58.504619
C	44.199287	5.881042	41.509580	C	22.322430	3.385823	57.471041
C	43.645966	6.940503	42.251381	C	21.809225	4.127019	56.389205
C	43.864896	4.073499	39.859401	C	20.424967	4.443380	56.361707
O	46.466730	6.618204	41.491902	C	19.902572	5.122952	55.240682
O	46.064041	4.433028	41.879608	C	20.738705	5.511987	54.198889
C	45.662962	5.626854	41.627437	C	22.104116	5.242156	54.243627
C	47.886806	6.033299	45.805300	C	22.651024	4.541891	55.327615
C	48.864386	6.811793	46.451673	O	22.928289	5.638701	53.196429
C	50.059567	7.188420	32.161939	O	17.796575	5.593068	57.302024

O	17.303516	3.422037	57.671567	C	16.575750	6.521375	48.419241
C	18.146143	4.371580	57.484561	C	15.536484	5.766577	47.842843
C	15.684590	4.216711	53.321974	C	14.198081	5.242825	62.095148
C	16.402237	3.110261	52.832899	C	13.166040	4.552842	61.469196
C	16.463731	2.844646	51.472079	C	12.083075	4.099846	62.213249
C	15.802164	3.673700	50.573645	C	13.395778	4.617848	48.014204
C	15.047551	4.779159	51.017682	C	14.433262	5.338045	48.621761
C	14.977145	5.049328	52.411576	O	12.308763	4.204486	48.776526
C	14.173156	6.116495	52.859086	O	15.759213	6.378082	59.108506
C	13.497573	6.917330	51.946809	O	15.277744	4.206113	59.477145
C	13.581823	6.683748	50.584180	C	15.446347	5.409689	59.892097
C	14.358654	5.609528	50.094476	Cu	31.469262	6.139595	57.128713
O	12.889993	7.560938	49.751502	Cu	30.966457	3.715605	57.549419
O	15.949942	5.656286	55.206680	C	35.210087	4.086115	57.448602
O	15.438962	3.490811	55.578075	C	35.752493	3.357802	58.523215
C	15.689571	4.470684	54.788237	C	37.099567	3.021262	58.550200
C	11.644816	5.800887	56.909216	C	37.928719	3.396574	57.499307
C	11.172849	6.908886	57.603240	C	37.425587	4.107201	56.392518
C	25.309153	7.062557	57.569391	C	36.046016	4.445894	56.355750
C	24.474865	6.232212	56.830398	C	35.533376	5.098183	55.215157
C	24.986609	5.129018	56.116118	C	36.374154	5.434689	54.158642
C	26.382494	4.866310	56.163064	C	37.735236	5.142136	54.210020
C	11.243751	3.934900	55.440217	C	38.273849	4.471292	55.317126
C	26.055761	3.008228	54.634461	O	38.563445	5.488283	53.148457
C	24.688485	3.227550	54.612726	O	33.388382	5.621135	57.263899
C	24.128606	4.291801	55.355039	O	32.930146	3.448618	57.667470
O	23.921255	2.343640	53.856810	C	33.757608	4.407598	57.468119
O	13.939637	6.431860	56.972364	C	31.301231	4.209927	53.312050
O	13.434970	4.270491	57.369038	C	32.088663	3.148401	52.830796
C	13.091945	5.475275	57.084445	C	32.197704	2.900113	51.468972
C	15.283046	5.695821	61.352095	C	31.515271	3.701350	50.560425
C	16.314087	6.385804	61.978046	C	30.686800	4.754475	50.995023
C	17.648832	6.967274	47.656058	C	30.568157	5.007455	52.389679

C	29.695376	6.023569	52.824967	O	31.365290	6.377315	59.104495
C	28.995125	6.789610	51.899675	O	30.901996	4.202080	59.476863
C	29.126182	6.572930	50.537767	C	31.064223	5.407574	59.890558
C	29.972391	5.550007	50.065760	Cu	47.052121	6.254635	57.152195
O	28.404944	7.410739	49.691352	Cu	46.686257	3.798129	57.530836
O	31.499085	5.663056	55.195826	C	50.914829	4.464394	57.493750
O	31.065312	3.482003	55.572756	C	51.500923	3.947364	58.641689
C	31.282208	4.467930	54.779609	C	52.873923	3.732339	58.685563
C	27.223215	5.692949	56.958832	C	53.659830	4.036343	57.580498
C	26.669796	6.797120	57.632137	C	53.073736	4.554373	56.431559
C	40.911594	6.955273	57.617810	C	51.700736	4.768398	56.388685
C	40.086238	6.134608	56.860580	C	51.114643	5.287428	55.239746
C	40.605253	5.040672	56.137200	C	51.901549	5.591433	54.133681
C	42.002802	4.780653	56.189193	C	53.273549	5.377407	54.178555
C	26.903080	3.810651	55.388160	C	53.859642	4.858378	55.326493
C	41.686055	2.933631	54.646474	O	53.987445	5.617415	52.967495
C	40.318478	3.153974	54.614383	O	48.992602	5.861248	57.303070
C	39.752000	4.212821	55.359929	O	48.671867	3.656496	57.665545
O	39.557389	2.272907	53.849142	C	49.437991	4.673548	57.497670
O	29.500177	6.400982	57.009195	C	46.949082	4.379053	53.314108
O	29.053210	4.221076	57.376045	C	47.753858	3.349559	52.794140
C	28.677851	5.421773	57.121266	C	47.797427	3.098852	51.430299
C	30.903120	5.695641	61.351269	C	47.035689	3.869547	50.560084
C	31.934175	6.385618	61.977205	C	46.201077	4.902938	51.035594
C	33.105392	7.407231	47.645601	C	46.141816	5.149995	52.433593
C	32.119149	6.820111	48.409660	C	45.252764	6.131213	52.915345
C	31.165564	5.913144	47.841626	C	44.485935	6.878797	52.030813
C	29.818167	5.242646	62.094340	C	44.563501	6.676716	50.662792
C	28.786113	4.552669	61.468405	C	45.425212	5.685650	50.139244
C	27.703159	4.099675	62.212476	O	43.789442	7.511680	49.859823
C	29.187833	4.480966	47.977573	O	47.123027	5.809564	55.215922
C	30.106396	5.318318	48.609067	O	46.809322	3.601841	55.558258
O	28.179319	3.911965	48.695117	C	46.960933	4.611902	54.782272

C	42.837880	5.608288	56.990013	C	46.419447	6.168363	64.088179
C	42.272515	6.696847	57.680285	C	45.387379	5.478391	63.463260
C	42.528996	3.731714	55.410448	C	43.271369	4.336426	63.580429
O	45.077976	6.404714	57.023445	C	44.303437	5.025398	64.205349
O	44.741487	4.198733	57.349791	O	42.183431	3.908432	64.359519
C	44.305120	5.385652	57.121738	H	12.119263	8.127158	26.935633
C	46.523195	5.695406	61.350162	H	10.573035	6.786858	25.566322
C	47.554262	6.385378	61.976082	H	13.383772	2.323346	22.982395
C	48.749426	7.127563	47.798885	H	9.847425	3.169682	22.676989
C	47.653422	6.675918	48.524874	H	22.119084	2.865283	28.244982
C	46.639535	5.911942	47.914646	H	24.514796	2.309379	28.285019
C	45.438253	5.242413	62.093251	H	25.988723	3.054757	26.486491
C	44.406185	4.552442	61.467332	H	21.472888	5.231817	24.052698
C	43.323243	4.099449	62.211421	H	22.954725	5.920898	22.275035
C	44.502917	4.746809	48.013534	H	19.532193	2.329631	22.589927
C	45.520323	5.463435	48.659085	H	19.679319	1.794064	20.190516
O	43.396929	4.320511	48.739998	H	18.480437	3.170779	18.536730
O	46.921441	6.445032	59.125165	H	16.650954	6.145170	22.827088
O	46.574134	4.240231	59.460379	H	15.506794	7.500910	21.165223
C	46.675449	5.444536	59.890888	H	14.495595	7.508486	27.087266
C	16.262162	6.620790	63.347051	H	27.529555	7.889405	26.989929
C	15.179196	6.168795	64.090104	H	26.051743	6.422994	25.723097
C	14.147156	5.478812	63.465153	H	14.941489	3.633928	24.311564
C	12.031150	4.336833	63.582254	H	29.088616	2.082604	23.060788
C	13.063191	5.025817	64.207206	H	19.766899	6.932289	30.319048
O	10.943187	3.908837	64.361307	H	15.665521	4.558172	29.255200
C	31.882275	6.620600	63.346211	H	13.750584	3.861985	30.553899
C	30.799322	6.168606	64.089282	H	15.671792	6.861068	17.596366
C	29.767267	5.478629	63.464346	H	25.077397	6.065255	21.439635
C	27.651260	4.336658	63.581482	H	25.566274	2.452096	22.871032
C	28.683314	5.025635	64.206417	H	37.676270	2.831166	28.326089
O	26.563309	3.908663	64.360554	H	40.064675	2.256271	28.416096
C	47.502389	6.620356	63.345091	H	41.571213	2.939372	26.620442

H 37.118971 5.145534 24.096092	H 46.913326 6.862029 17.595724
H 38.632926 5.759662 22.312799	H 56.056181 5.977208 21.104174
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H 53.552009 3.700243 28.381296	H 24.959876 6.832776 41.206568
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H 47.061323 4.531556 29.333522	H 38.881744 2.251634 43.737271
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H 40.383508 6.616678 41.470207	H 7.916936 6.786691 56.693580
H 29.439589 3.611160 40.233232	H 10.728195 2.325373 54.106753
H 43.411555 2.530874 38.439947	H 7.191544 3.170264 53.803920
H 34.012807 7.566198 45.670243	H 19.513734 2.934921 59.302452
H 35.352809 7.113520 32.808943	H 21.908865 2.374545 59.323209
H 33.407791 6.440151 34.120618	H 23.370290 3.120993 57.515234
H 30.360644 4.543863 44.771208	H 18.846664 5.352422 55.145330
H 28.542424 3.588006 46.099580	H 20.314888 6.033047 53.351070
H 28.301962 3.723833 32.750913	H 16.925978 2.455460 53.520025
H 29.621850 7.139693 33.488605	H 17.028227 1.991010 51.110107
H 39.308046 6.561518 37.259477	H 15.872059 3.432733 49.522413
H 39.875773 2.870099 38.353497	H 14.042212 6.342322 53.911232
H 52.223825 3.709908 43.947655	H 12.888082 7.739013 52.298411
H 54.659329 3.328124 44.019887	H 11.840582 7.509217 58.212297
H 56.055402 3.866610 42.061214	H 24.896517 7.913942 58.101486
H 51.374594 5.452980 39.579559	H 23.421145 6.471024 56.807470
H 52.752248 5.975798 37.680105	H 12.285080 3.636295 55.426823
H 49.621251 2.728581 38.025791	H 26.463185 2.195876 54.047563
H 49.727528 2.244244 35.619652	H 17.168330 6.739337 61.410643
H 48.468487 3.594119 34.029802	H 18.434824 7.558233 48.116095
H 46.488270 6.417340 38.409363	H 16.556683 6.782938 49.468666
H 45.232564 7.722153 36.795505	H 13.128714 4.376221 60.400558
H 44.284826 7.566899 42.863696	H 11.277802 3.574511 61.719255
H 44.927465 3.863505 39.794318	H 11.644107 3.669477 48.238040

H	12.983948	7.334869	48.775932	H	48.424677	2.301621	51.044067
H	22.429696	6.160578	52.491325	H	47.091842	3.638149	49.506145
H	22.940033	2.563766	53.869352	H	45.125134	6.329409	53.973449
H	35.117096	3.052308	59.346676	H	43.810554	7.634747	52.408756
H	37.503815	2.462889	59.388747	H	42.901395	7.348135	58.276636
H	38.971463	3.113815	57.550375	H	43.590834	3.519011	55.365641
H	34.481970	5.347700	55.117842	H	48.405637	6.744723	61.407917
H	35.958029	5.934574	53.294375	H	49.514269	7.725447	48.284619
H	32.634846	2.519212	53.524434	H	47.595156	6.941754	49.571641
H	32.818312	2.083333	51.113582	H	44.381542	4.364289	60.399376
H	31.627238	3.477925	49.507578	H	42.519347	3.571640	61.717684
H	29.529791	6.232456	53.876693	H	42.744987	3.795251	48.176363
H	28.328061	7.569975	52.241874	H	43.867964	7.300086	48.880049
H	27.304770	7.447059	58.223420	H	53.398569	5.970644	52.227698
H	40.492863	7.798336	58.158316	H	17.068275	7.157983	63.836017
H	39.033101	6.374347	56.832026	H	15.148112	6.357241	65.155560
H	27.964461	3.596492	55.337621	H	10.263231	3.421680	63.797075
H	42.097577	2.125655	54.056462	H	32.688251	7.157999	63.835100
H	32.787981	6.739251	61.409320	H	30.768036	6.357172	65.154686
H	33.812253	8.104139	48.106727	H	25.881905	3.424183	63.795656
H	32.063202	7.066703	49.474619	H	48.307499	7.159164	63.833743
H	28.749233	4.375167	60.399856	H	46.387743	6.357335	65.153480
H	26.897727	3.574577	61.718385	H	41.501056	3.425548	63.794300
H	27.640314	3.350759	48.114412	H	54.922543	4.682786	55.325780
H	28.539331	7.201502	48.713741	H	56.250089	4.683169	39.763722
H	38.072710	5.994148	52.426111	H	57.578894	4.683426	24.200638
H	38.577046	2.496935	53.849799	H	32.654267	5.043331	18.026521
H	50.894863	3.700241	59.506315	H	17.034799	5.043580	18.026681
H	53.331562	3.325559	59.581312	H	10.176552	4.915318	24.089626
H	54.727844	3.865747	57.623131	H	8.847996	4.915605	39.653311
H	50.047590	5.459409	55.145353	H	7.520558	4.915552	55.216477
H	51.424876	5.977080	53.243044	H	12.998962	5.198993	65.269023
H	48.355033	2.740815	53.459902	H	28.618792	5.198981	65.268146

H	44.238616	5.198867	65.267017				
H	48.274026	5.043188	18.026053	(S,S)-1-TS1			
C	34.329541	9.363119	40.775252	C	35.450154	8.360430	42.171931
C	34.506673	8.580803	39.527143	C	35.059571	8.300237	40.755465
C	33.427980	8.522027	38.470415	C	35.660053	9.336453	39.817147
C	32.054559	8.950796	39.009650	C	35.839394	10.702414	40.493575
C	32.150291	10.259707	39.802378	C	36.627657	10.563595	41.804654
C	33.037485	10.111892	41.051537	C	35.909730	9.639559	42.798898
O	34.214195	7.928242	40.769298	O	33.817037	8.686376	41.312952
C	37.326828	7.272706	43.440611	C	37.896830	7.066970	43.436333
C	38.635820	7.541192	43.891086	C	38.992795	7.874251	43.786364
C	39.014899	7.254883	45.204199	C	39.509464	7.837031	45.083810
C	38.100599	6.703190	46.109617	C	38.930711	7.011163	46.054281
C	36.793995	6.445762	45.673562	C	37.823633	6.224459	45.711593
C	36.407664	6.722554	44.360821	C	37.304881	6.247032	44.415391
N	36.933192	7.577784	42.140036	N	37.330983	7.143922	42.155753
H	33.379003	7.494766	38.069967	H	35.007653	9.409680	38.928803
H	35.533663	8.380962	39.185903	H	35.038669	7.296181	40.308466
H	35.231936	9.680915	41.314632	H	35.100814	7.552608	42.811391
H	31.642283	8.158909	39.657865	H	34.842988	11.130415	40.707523
H	31.355428	9.059019	38.163137	H	36.353673	11.399317	39.807862
H	32.569253	11.050612	39.148070	H	37.630779	10.146234	41.584126
H	31.144161	10.599763	40.104880	H	36.793766	11.551350	42.269804
H	32.499108	9.551104	41.839458	H	35.011423	10.133393	43.211859
H	33.277357	11.102834	41.475658	H	36.551878	9.395862	43.664013
H	33.737521	9.188757	37.641611	H	36.640152	8.951105	39.470456
H	39.353636	7.994013	43.199471	H	39.433441	8.534585	43.031078
H	40.040292	7.471377	45.523882	H	40.370159	8.464280	45.338908
H	38.400024	6.481634	47.138787	H	39.336680	6.984509	47.070043
H	36.058768	6.018407	46.364230	H	37.356283	5.578105	46.461428
H	35.389932	6.514058	44.022773	H	36.443631	5.628385	44.147824
H	37.675375	7.528451	41.446223	H	37.967525	7.409873	41.406589
H	36.095016	7.086098	41.824986	H	36.737447	6.347100	41.893737

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C	12.487000	7.261000	26.395000	C	16.107910	6.659026	20.850045
C	11.616000	6.503000	25.622000	C	16.197885	6.355031	19.497042
C	12.086000	5.395000	24.927000	C	16.963875	5.274030	19.076025
C	13.428000	5.043000	25.007000	O	15.523872	7.185037	18.539057
C	13.027000	3.179000	23.539000	O	18.565010	5.528780	24.114193
C	11.685000	3.529000	23.460000	O	18.021544	3.387367	24.573223
C	11.215000	4.638000	24.154000	C	18.264490	4.336136	23.746029
O	10.782000	2.793000	22.654000	C	14.301000	5.801000	25.782000
Cu	18.543313	6.082753	26.020038	C	13.829000	6.909000	26.476000
Cu	17.949293	3.694182	26.528077	C	27.971081	7.113769	26.432185
C	22.215572	3.949606	26.388564	C	27.132807	6.244118	25.743107
C	22.754763	3.192570	27.444176	C	27.641942	5.105818	25.084885
C	24.109764	2.887700	27.483839	C	29.037988	4.846027	25.141157
C	24.950478	3.327116	26.466322	C	13.900000	3.935000	24.313000
C	24.449044	4.059435	25.373423	C	28.708047	2.914495	23.706465
C	23.061371	4.358361	25.318882	C	27.340790	3.131533	23.678676
C	22.551814	5.023172	24.182974	C	26.782350	4.230544	24.369436
C	23.402830	5.419502	23.156052	O	26.572808	2.215923	22.962241
C	24.770481	5.168377	23.228230	O	16.596575	6.401564	25.853857
C	25.305335	4.479947	24.325463	O	16.054431	4.261740	26.318817
O	25.608623	5.567350	22.192828	C	15.735717	5.460517	25.985840
O	20.434337	5.516178	26.192926	C	17.910659	5.803242	30.236513
O	19.912714	3.369151	26.650443	C	18.900797	6.565457	30.882665
C	20.768572	4.298707	26.420434	C	16.764509	5.382425	30.968168
C	18.226927	4.022014	22.293999	C	15.688894	4.715119	30.344085
C	18.992915	2.941012	21.873981	C	14.586716	4.303745	31.087448
C	19.081890	2.638017	20.519979	O	18.429524	6.395612	27.983170
C	18.404876	3.417023	19.587993	O	17.895618	4.249654	28.430929
C	17.639888	4.497024	20.008011	C	18.094717	5.462657	28.799152
C	17.550913	4.800019	21.362013	Cu	34.142416	6.085712	26.031431
C	16.783924	5.881020	21.784030	Cu	33.584258	3.695575	26.562080
				C	37.837286	3.965240	26.416361
				C	38.357809	3.252534	27.512150

C	39.701712	2.907204	27.566479	C	44.350460	2.716261	23.768637
C	40.549807	3.258264	26.522411	C	42.983097	2.933405	23.714220
C	40.067895	3.948973	25.393953	C	42.410279	4.027568	24.400895
C	38.691476	4.295131	25.328326	O	42.229015	2.019014	22.981932
C	38.200905	4.926701	24.166477	O	32.174120	6.385791	25.918424
C	39.060516	5.236732	23.116878	O	31.684061	4.237110	26.396932
C	40.418656	4.937040	23.196157	C	31.332233	5.429413	26.079731
C	40.934852	4.287023	24.325730	C	33.678999	5.840046	30.271596
O	41.266210	5.256868	22.141237	C	34.700549	6.629899	30.831710
O	36.048771	5.528692	26.168620	C	32.569836	5.461697	31.081208
O	35.543361	3.385103	26.659960	C	31.480873	4.736490	30.555269
C	36.391549	4.316457	26.419272	C	30.408458	4.387009	31.370592
C	33.846854	4.021972	22.293718	O	34.077613	6.404508	27.992525
C	34.612831	2.940969	21.873683	O	33.564602	4.261409	28.472985
C	34.701781	2.637978	20.519678	C	33.779762	5.477119	28.827977
C	34.024753	3.416989	19.587708	Cu	49.694256	6.200379	25.985316
C	33.259776	4.496991	20.007741	Cu	49.347196	3.781058	26.562257
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.142354	5.532485	24.124086	C	53.770890	5.287813	24.113936
O	33.636235	3.385675	24.591319	C	54.557834	5.591815	23.007897
C	33.867798	4.334089	23.756040	C	55.929834	5.377800	23.052821
C	29.881702	5.710021	25.893817	C	56.515889	4.858782	24.200784
C	29.332429	6.850872	26.505954	O	56.643771	5.617805	21.841785
C	43.547593	6.881546	26.528832	O	51.636349	5.835600	26.125881
C	42.727855	6.017862	25.813864	O	51.337030	3.657236	26.634134
C	43.254998	4.893785	25.144241	C	52.093309	4.664771	26.380821
C	44.653022	4.643761	25.213170	C	49.466779	4.021876	22.293156
C	29.556697	3.753468	24.417181	C	50.232745	2.940872	21.873104

C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.247793	6.039840	41.498162
C	48.879661	4.496905	20.007192	Cu	16.630034	3.661040	42.014927
C	48.790737	4.799893	21.361200	C	20.902283	3.861799	41.978767
C	48.023772	5.880897	21.783251	C	21.372656	3.163944	43.106302
C	47.347731	6.658913	20.849295	C	22.720855	2.858794	43.247262
C	47.437655	6.354926	19.496287	C	23.625613	3.239842	42.262312
C	48.203620	5.273922	19.075235	C	23.197307	3.910304	41.102285
O	46.763613	7.184943	18.538331	C	21.815372	4.206311	40.943554
O	49.732436	5.589549	24.090983	C	21.379950	4.808375	39.745879
O	49.389005	3.422900	24.606685	C	22.296058	5.131739	38.748901
C	49.526635	4.367440	23.749514	C	23.656483	4.887192	38.923114
C	45.482288	5.519969	25.965987	C	24.119541	4.281961	40.096774
C	44.911063	6.638541	26.600162	O	24.556743	5.217984	37.918508
C	45.186462	3.554769	24.496162	O	19.140846	5.440629	41.649650
O	47.715858	6.328514	25.884275	O	18.586337	3.309058	42.138628
O	47.397513	4.159869	26.416564	C	19.457757	4.225208	41.917877
C	46.951327	5.319788	26.091800	C	16.856633	4.018464	37.763002
C	49.185038	5.978034	30.217959	C	17.540822	2.901440	37.252131
C	50.114979	6.835874	30.832656	C	17.555746	2.638543	35.888855
C	48.080255	5.490273	30.970964	C	16.885758	3.484944	35.011845
C	47.060614	4.716835	30.376299	C	16.159584	4.598982	35.481773
C	45.997605	4.244000	31.139522	C	16.124399	4.856646	36.878077
O	49.600784	6.556612	27.941212	C	15.335069	5.922380	37.355231
O	49.296703	4.380423	28.454219	C	14.640516	6.734354	36.467856
C	49.379885	5.617097	28.787332	C	14.701375	6.521338	35.100840
C	11.158286	7.260970	41.959133	C	15.468968	5.453806	34.582419
C	10.287269	6.502976	41.186145	O	14.000181	7.414293	34.293285
C	10.757253	5.394976	40.491133	O	17.238994	5.491009	39.592176
C	12.099253	5.042971	40.571108	O	16.693977	3.349947	40.048148
C	11.698221	3.178978	39.103109	C	16.936779	4.300737	39.220581
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108

C	26.417872	7.057925	42.510142	C	37.353577	4.115799	40.853414
C	25.691432	6.136049	41.785749	C	36.847890	4.915911	39.787410
C	26.317812	5.053334	41.086717	C	37.688145	5.460685	38.844667
C	27.752091	4.937642	41.197015	C	39.090763	5.238343	38.903136
C	12.571237	3.934972	39.877096	C	39.630472	4.424087	39.899630
C	27.684349	2.981213	39.754036	O	39.906358	5.812387	37.978271
C	26.273716	3.096578	39.622994	O	34.906462	5.314898	41.873850
C	25.582699	4.111506	40.278585	O	34.160691	3.288968	42.337418
O	25.727603	2.133591	38.821802	C	35.093187	4.070409	42.026893
O	15.289708	6.388459	41.370650	C	32.684315	4.856234	38.076561
O	14.737340	4.252603	41.833928	C	33.462008	3.762095	37.734678
C	14.418649	5.457248	41.522039	C	33.603322	3.391119	36.381164
C	16.691202	5.784177	45.723199	C	32.931893	4.082323	35.393822
C	17.714283	6.530553	46.336531	C	32.086980	5.200409	35.691690
C	18.802073	6.863834	32.235578	C	31.983230	5.602145	37.073568
C	17.710150	6.410686	32.967776	C	31.139316	6.704167	37.399393
C	16.679445	5.671326	32.356182	C	30.438299	7.364877	36.424936
C	15.548386	5.409484	46.483898	C	30.531408	6.976828	35.061939
C	14.448891	4.748929	45.895848	C	31.346445	5.913263	34.682064
C	13.348901	4.386385	46.667075	O	29.767480	7.751312	34.233677
C	14.524308	4.540505	32.458272	O	32.694136	6.413478	39.870164
C	15.558348	5.232075	33.103225	O	32.451563	4.218562	40.321587
O	13.416496	4.124824	33.188562	C	32.592052	5.205773	39.535098
O	17.171417	6.355346	43.460116	C	28.478367	5.928623	41.934715
O	16.599759	4.222188	43.920837	C	27.823490	6.973852	42.563767
C	16.832919	5.431463	44.283733	C	42.237296	7.054609	42.055943
Cu	32.409605	7.542349	41.547181	C	41.412021	6.182474	41.355689
Cu	32.510394	4.476018	42.254568	C	41.940626	5.078630	40.658780
C	36.500856	3.571809	41.874238	C	43.343542	4.847598	40.693537
C	37.003144	2.696877	42.817128	C	28.403438	3.871817	40.508953
C	38.383183	2.386550	42.829790	C	43.029410	2.937268	39.228579
C	39.240859	2.953294	41.911443	C	41.658707	3.133029	39.214865
C	38.765857	3.832912	40.883304	C	41.095094	4.210924	39.925213

O	40.895894	2.222575	38.488948	C	50.771052	4.711570	41.952610
O	30.536030	7.035300	41.746755	C	48.272578	4.321862	37.809817
O	30.575304	4.864496	42.312709	C	49.083001	3.282280	37.320342
C	29.976587	5.935184	41.997189	C	49.155352	3.015813	35.960135
C	32.452064	6.703599	45.812734	C	48.413429	3.777291	35.064168
C	33.291884	7.590044	46.459634	C	47.564331	4.811398	35.510429
C	34.658043	7.017834	32.164064	C	47.480933	5.079184	36.903398
C	33.586855	6.636919	32.963102	C	46.585547	6.069064	37.355196
C	32.531581	5.863004	32.446097	C	45.827773	6.797829	36.447312
C	31.385700	6.052630	46.516835	C	45.923113	6.569551	35.084452
C	30.453053	5.199965	45.857881	C	46.796604	5.574087	34.590720
C	29.418915	4.616915	46.548990	O	45.146965	7.377126	34.255817
C	30.382281	4.755414	32.713129	O	48.458242	5.811615	39.658813
C	31.429871	5.505407	33.258130	O	48.115037	3.623029	40.084238
O	29.292256	4.418375	33.505156	C	48.282028	4.601279	39.270266
O	32.776505	7.395443	43.568454	C	44.178728	5.719059	41.448290
O	32.767334	5.189467	44.052964	C	43.605873	6.827811	42.098813
C	32.676309	6.417839	44.354545	C	43.873796	3.778401	39.944891
Cu	48.410673	6.332330	41.574258	O	46.430581	6.507071	41.453536
Cu	48.009064	3.899165	42.052742	O	46.071319	4.319803	41.867524
C	52.242278	4.464620	41.931334	C	45.646951	5.499702	41.591274
C	52.828353	3.947597	43.079285	C	47.841777	5.977950	45.784806
C	54.201353	3.732577	43.123183	C	48.779103	6.814194	46.419087
C	54.987278	4.036581	42.018131	C	49.998943	7.168733	32.176288
C	54.401203	4.554604	40.869180	C	48.948534	6.656013	32.929765
C	53.028203	4.768624	40.826281	C	47.977315	5.817922	32.349201
C	52.442128	5.287648	39.677330	C	46.720729	5.501196	46.520341
C	53.229054	5.591652	38.571278	C	45.697293	4.746022	45.909174
C	54.601054	5.377632	38.616177	C	44.620095	4.281737	46.657743
C	55.187129	4.858609	39.764128	C	45.920782	4.521385	32.501923
O	55.314970	5.617639	37.405129	C	46.897820	5.315700	33.117612
O	50.346311	5.901869	41.722307	O	44.854615	4.039129	33.253055
O	49.987315	3.720402	42.175800	O	48.301844	6.612958	43.537585

O	47.918210	4.431446	43.966666	C	13.460260	6.927339	51.975551
C	48.038337	5.652459	44.345868	C	13.532522	6.696888	50.611730
C	9.830848	7.260896	57.522290	C	14.305332	5.623802	50.112996
C	8.959816	6.502907	56.749315	O	12.835967	7.577962	49.787199
C	9.429783	5.394908	56.054291	O	15.947200	5.669129	55.208249
C	10.771783	5.042898	56.134241	O	15.443338	3.501516	55.577895
C	10.370718	3.178911	54.666243	C	15.687421	4.483548	54.789220
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.312619	7.132058	57.579832
Cu	15.891856	6.148340	57.136744	C	24.477483	6.309376	56.832945
Cu	15.347389	3.731930	57.549592	C	24.989202	5.216538	56.103050
C	19.601796	4.066243	57.426699	C	26.385630	4.955749	56.143204
C	20.160064	3.292182	58.459788	C	11.243751	3.934900	55.440217
C	21.514922	2.985253	58.468411	C	26.059142	3.119230	54.588797
C	22.335648	3.438438	57.441076	C	24.691159	3.334872	54.574920
C	21.814940	4.192520	56.371903	C	24.130801	4.387111	55.333933
C	20.427751	4.496858	56.350740	O	23.923962	2.459510	53.809109
C	19.898476	5.188657	55.240300	O	13.936931	6.435871	56.974496
C	20.730502	5.603367	54.205144	O	13.438558	4.272548	57.368627
C	22.098287	5.345662	54.244802	C	13.092169	5.476825	57.084755
C	22.652072	4.631548	55.316136	C	15.283046	5.695821	61.352095
O	22.918020	5.766502	53.203606	C	16.314087	6.385804	61.978046
O	17.795118	5.612858	57.301856	C	17.646845	6.863940	47.682817
O	17.313209	3.438603	57.666116	C	16.552011	6.465659	48.441202
C	18.151157	4.392564	57.477866	C	15.491822	5.740343	47.864445
C	15.670539	4.232127	53.323559	C	14.198081	5.242825	62.095148
C	16.383992	3.126544	52.826708	C	13.166040	4.552842	61.469196
C	16.426846	2.858652	51.465904	C	12.083075	4.099846	62.213249
C	15.751854	3.685487	50.575745	C	13.311193	4.668292	48.030292
C	15.003723	4.792355	51.028139	C	14.370079	5.355252	48.639510
C	14.949456	5.062551	52.422309	O	12.205238	4.299852	48.788343
C	14.147199	6.127002	52.879602	O	15.755322	6.384240	59.110422

O	15.282758	4.209586	59.475875	C	26.673622	6.866823	57.637532
C	15.446265	5.413116	59.892235	C	40.917790	6.942527	57.671533
Cu	31.474477	6.196029	57.141919	C	40.089213	6.143638	56.894832
Cu	30.957745	3.768106	57.523219	C	40.603648	5.063983	56.146894
C	35.203303	4.116834	57.431134	C	41.999636	4.795708	56.194242
C	35.740446	3.363025	58.490666	C	26.906678	3.913087	55.351229
C	37.084951	3.016134	58.510665	C	41.675746	2.984714	54.611338
C	37.916895	3.406774	57.467664	C	40.309411	3.213878	54.581388
C	37.419323	4.144534	56.376253	C	39.747507	4.258899	55.349539
C	36.042212	4.493635	56.346183	O	39.544636	2.355414	53.794410
C	35.535034	5.174148	55.219718	O	29.506716	6.469000	57.020881
C	36.379643	5.530984	54.172969	O	29.048141	4.286024	57.353831
C	37.738897	5.229342	54.219577	C	28.679340	5.492008	57.115163
C	38.271157	4.527167	55.310112	C	30.903120	5.695641	61.351269
O	38.571568	5.600640	53.169895	C	31.934175	6.385618	61.977205
O	33.390608	5.665640	57.273225	C	33.140830	7.821283	47.846331
O	32.919884	3.489117	57.639449	C	32.142328	7.190935	48.558633
C	33.752779	4.446683	57.456630	C	31.217838	6.295775	47.926934
C	31.281377	4.340895	53.296866	C	29.818167	5.242646	62.094340
C	32.049633	3.280831	52.783120	C	28.786113	4.552669	61.468405
C	32.153138	3.073193	51.414155	C	27.703159	4.099675	62.212476
C	31.486606	3.916412	50.532005	C	29.262448	4.825149	47.945482
C	30.676128	4.969481	51.000359	C	30.147417	5.651232	48.636355
C	30.558945	5.177440	52.401633	O	28.241230	4.214756	48.609032
C	29.701861	6.192980	52.869774	O	31.367184	6.403527	59.117480
C	29.019530	7.004002	51.970155	O	30.892672	4.225283	59.457952
C	29.154365	6.834454	50.602083	C	31.060072	5.424172	59.888446
C	29.983606	5.813164	50.098086	Cu	47.050342	6.246866	57.149750
O	28.458093	7.718937	49.782965	Cu	46.687901	3.790654	57.535721
O	31.506761	5.750740	55.205323	C	50.914829	4.464394	57.493750
O	31.057018	3.566356	55.543348	C	51.500923	3.947364	58.641689
C	31.277433	4.565803	54.768452	C	52.873923	3.732339	58.685563
C	27.226437	5.770964	56.950562	C	53.659830	4.036343	57.580498

C	53.073736	4.554373	56.431559	C	47.579351	6.646794	48.496130
C	51.700736	4.768398	56.388685	C	46.605282	5.823403	47.898986
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.533238	4.549326	48.021624
O	53.987445	5.617415	52.967495	C	45.511967	5.329326	48.652760
O	48.990789	5.856815	57.297841	O	43.455100	4.072191	48.758212
O	48.673629	3.653369	57.671429	O	46.922579	6.441515	59.123191
C	49.437999	4.670857	57.497717	O	46.573857	4.237700	59.463220
C	46.974073	4.350968	53.319548	C	46.676038	5.442656	59.891221
C	47.817693	3.346721	52.811905	C	16.262162	6.620790	63.347051
C	47.875890	3.085944	51.450485	C	15.179196	6.168795	64.090104
C	47.088802	3.819776	50.570969	C	14.147156	5.478812	63.465153
C	46.214332	4.825193	51.034872	C	12.031150	4.336833	63.582254
C	46.143788	5.084933	52.429926	C	13.063191	5.025817	64.207206
C	45.221744	6.040531	52.900517	O	10.943187	3.908837	64.361307
C	44.426572	6.747561	52.007260	C	31.882275	6.620600	63.346211
C	44.511407	6.531423	50.641643	C	30.799322	6.168606	64.089282
C	45.409669	5.567216	50.129830	C	29.767267	5.478629	63.464346
O	43.706335	7.325726	49.827663	C	27.651260	4.336658	63.581482
O	47.118938	5.795327	55.213328	C	28.683314	5.025635	64.206417
O	46.815630	3.587267	55.565028	O	26.563309	3.908663	64.360554
C	46.968671	4.593813	54.785420	C	47.502389	6.620356	63.345091
C	42.837972	5.602703	57.011468	C	46.419447	6.168363	64.088179
C	42.277578	6.677161	57.727315	C	45.387379	5.478391	63.463260
C	42.521580	3.760065	55.395368	C	43.271369	4.336426	63.580429
O	45.077098	6.395714	57.026417	C	44.303437	5.025398	64.205349
O	44.741945	4.189234	57.352919	O	42.183431	3.908432	64.359519
C	44.304987	5.377088	57.130154	H	12.119255	8.127032	26.935827
C	46.523195	5.695406	61.350162	H	10.573025	6.786807	25.566429
C	47.554262	6.385378	61.976082	H	13.383809	2.323431	22.982298
C	48.649701	7.143285	47.761677	H	9.847419	3.169622	22.677189

H	22.114244	2.852353	28.249961	H	41.672614	6.247162	25.775772
H	24.512925	2.312189	28.311370	H	30.618050	3.538003	24.372540
H	26.000865	3.076813	26.531688	H	44.766881	1.877499	23.227048
H	21.494398	5.233085	24.062702	H	35.539348	6.944764	30.220981
H	22.988285	5.929893	22.297265	H	31.432599	4.440895	29.512545
H	19.532135	2.329568	22.589926	H	29.586292	3.827918	30.944204
H	19.679382	1.794107	20.190539	H	31.291768	6.860917	17.596353
H	18.480517	3.170833	18.536734	H	40.788656	5.750904	21.402367
H	16.651707	6.145323	22.827180	H	41.246845	2.235868	22.974599
H	15.506988	7.501042	21.165230	H	53.552068	3.699828	28.381225
H	14.495549	7.507996	27.087791	H	55.987722	3.325996	28.455671
H	27.560505	7.992844	26.918991	H	57.384067	3.866269	26.497799
H	26.078336	6.479576	25.712413	H	52.703430	5.452518	24.014951
H	14.941568	3.634326	24.310813	H	54.081133	5.976057	22.116810
H	29.114392	2.074846	23.158599	H	50.777677	2.334931	22.589244
H	19.763983	6.915804	30.328100	H	50.920884	1.795262	20.189740
H	15.673913	4.515713	29.277927	H	49.720339	3.170940	18.535919
H	13.776108	3.791969	30.586635	H	47.863628	6.134706	22.823907
H	15.672182	6.861297	17.596367	H	46.741250	7.496845	21.164903
H	25.115402	6.075975	21.474510	H	45.537068	7.326063	27.157638
H	25.590912	2.433848	22.969496	H	46.248605	3.339254	24.474659
H	37.708869	2.970647	28.333671	H	50.943444	7.237121	30.260109
H	40.089095	2.363910	28.422830	H	47.059724	4.478270	29.318106
H	41.590305	2.972216	26.596572	H	45.229476	3.651530	30.661045
H	37.152452	5.179568	24.046982	H	46.912980	6.861830	17.595738
H	38.661340	5.722886	22.237014	H	56.056137	5.976855	21.104022
H	35.149474	2.328864	22.590764	H	10.790867	8.127624	42.499081
H	35.298599	1.793594	20.190364	H	9.244460	6.787081	41.129974
H	34.099872	3.170561	18.536508	H	12.055728	2.325676	38.543251
H	32.263438	6.143040	22.826036	H	8.519547	3.171612	38.239185
H	31.124610	7.499363	21.165214	H	20.683190	2.873055	43.890899
H	29.969941	7.530003	27.060432	H	23.069469	2.331373	44.129849
H	43.122797	7.747337	27.027151	H	24.669987	2.992785	42.406918

H	20.331737	5.020814	39.557518	H	40.351742	6.387514	41.343430
H	21.937959	5.586484	37.834922	H	29.487167	3.766663	40.576844
H	18.079036	2.240772	37.922071	H	43.444265	2.114195	38.661295
H	18.095710	1.777582	35.507490	H	34.079048	8.096437	45.893564
H	16.923338	3.249571	33.957624	H	35.457499	7.623528	32.579708
H	15.229143	6.137235	38.412527	H	33.582909	6.964567	33.994919
H	14.039716	7.552284	36.842499	H	30.549662	5.001254	44.790113
H	13.169626	7.508505	42.647833	H	28.706142	3.974752	46.017969
H	25.901218	7.871714	43.029000	H	28.629848	3.830100	33.021382
H	24.604522	6.259101	41.747216	H	29.792427	7.455079	33.310950
H	13.612370	3.635639	39.863472	H	39.378914	6.315916	37.336639
H	28.178019	2.168133	39.215265	H	39.906635	2.418162	38.512500
H	18.576864	6.845202	45.759893	H	52.223721	3.706426	43.946616
H	19.579648	7.444565	32.722155	H	54.659293	3.327298	44.019547
H	17.668292	6.656968	34.020255	H	56.055398	3.866383	42.061114
H	14.414460	4.514819	44.837298	H	51.374759	5.453828	39.579944
H	12.520474	3.876682	46.194060	H	52.752401	5.975875	37.680057
H	12.755564	3.612069	32.624426	H	49.673609	2.684833	38.005584
H	14.062356	7.192055	33.314441	H	49.792898	2.216075	35.596487
H	24.117543	5.702670	37.149656	H	48.496416	3.538765	34.013385
H	24.773900	2.252382	38.693300	H	46.445959	6.287285	38.407808
H	36.328708	2.284948	43.572566	H	45.145674	7.558843	36.802194
H	38.776969	1.706696	43.591879	H	44.234201	7.514429	42.655437
H	40.307312	2.713973	41.968987	H	44.939125	3.583028	39.886466
H	35.775557	5.096487	39.702344	H	49.620731	7.207748	45.860358
H	37.269679	6.062127	38.029124	H	50.729770	7.824795	32.638728
H	33.957168	3.192168	38.525168	H	48.890772	6.932638	33.973877
H	34.237485	2.539308	36.114459	H	45.704964	4.513403	44.849977
H	33.050383	3.748240	34.357956	H	43.850277	3.701284	46.167514
H	31.049354	7.023613	38.437123	H	44.235628	3.455522	32.710278
H	29.781927	8.204158	36.669555	H	45.249551	7.154529	33.280311
H	28.407562	7.730078	43.094162	H	54.726637	5.972242	36.665649
H	41.814698	7.911751	42.569885	H	9.463400	8.127107	58.062853

H 7.916962 6.786754 56.693476	H 32.758675 2.257062 51.032589
H 10.728214 2.325424 54.106692	H 31.595211 3.725819 49.472396
H 7.191743 3.170763 53.803272	H 29.535480 6.368435 53.927383
H 19.533510 2.935333 59.269191	H 28.366910 7.785249 52.337373
H 21.933154 2.394147 59.277111	H 27.309000 7.509047 58.236740
H 23.385828 3.182133 57.480004	H 40.502705 7.774616 58.231583
H 18.840299 5.407964 55.147380	H 39.037183 6.388785 56.871806
H 20.301357 6.134020 53.365982	H 27.968647 3.703520 55.293630
H 16.917063 2.472913 53.507738	H 42.083757 2.186760 54.005507
H 16.986790 2.004805 51.097428	H 32.787144 6.741567 61.409457
H 15.806807 3.441370 49.524456	H 33.821643 8.508644 48.358891
H 14.026786 6.351679 53.933198	H 32.052852 7.394601 49.630506
H 12.853113 7.747560 52.334496	H 28.749448 4.374923 60.399964
H 11.840431 7.509402 58.212300	H 26.897644 3.574679 61.718402
H 24.900196 7.976325 58.123234	H 27.728435 3.670523 47.989367
H 23.423170 6.546145 56.815898	H 28.592572 7.540247 48.799133
H 12.285124 3.636330 55.427420	H 38.086349 6.137767 52.466982
H 26.466767 2.316852 53.988420	H 38.563499 2.575621 53.811411
H 17.168197 6.739776 61.410674	H 50.894959 3.699877 59.506310
H 18.449368 7.432327 48.142773	H 53.331575 3.325519 59.581308
H 16.532970 6.741423 49.486911	H 54.727861 3.865760 57.623184
H 13.130053 4.375193 60.400593	H 50.047679 5.459194 55.145126
H 11.277943 3.574286 61.719272	H 51.424943 5.976993 53.243003
H 11.525707 3.784232 48.249503	H 48.437453 2.765669 53.485425
H 12.926222 7.357419 48.810076	H 48.533580 2.308918 51.073673
H 22.414144 6.294342 52.506679	H 47.157649 3.581503 49.519324
H 22.942998 2.680805 53.821857	H 45.091702 6.249060 53.956675
H 35.102821 3.045610 59.307924	H 43.724371 7.483036 52.376567
H 37.484970 2.437945 59.337722	H 42.909653 7.312421 58.337509
H 38.957515 3.115432 57.513190	H 43.582194 3.540196 55.351911
H 34.485137 5.431604 55.126351	H 48.405837 6.744378 61.408016
H 35.967616 6.054004 53.320537	H 49.383642 7.786440 48.237303
H 32.586447 2.622464 53.456679	H 47.509615 6.923858 49.539368

H	44.381332	4.364330	60.399443	C	37.341498	6.828482	43.550381
H	42.519320	3.571612	61.717769	C	38.657543	7.226913	43.784853
H	42.850939	3.475365	48.213299	C	39.254221	6.934663	45.015378
H	43.813200	7.120246	48.849483	C	38.527328	6.261701	46.002860
H	53.399033	5.972106	52.228095	C	37.202400	5.879070	45.758933
H	17.068204	7.158116	63.835978	C	36.600932	6.156579	44.528848
H	15.148079	6.357296	65.155545	N	36.698985	7.122398	42.275095
H	10.263108	3.421930	63.796999	H	35.178034	9.194506	38.972689
H	32.687947	7.158499	63.835039	H	34.903962	7.253571	40.496257
H	30.767919	6.357336	65.154658	H	34.887150	7.837082	42.993730
H	25.881420	3.424972	63.795537	H	35.313533	11.075876	40.608096
H	48.307563	7.159028	63.833811	H	36.824065	11.005984	39.669567
H	46.387788	6.357258	65.153514	H	37.944639	9.757107	41.537506
H	41.501188	3.425031	63.794599	H	37.306662	11.297562	42.128860
H	54.922581	4.682826	55.325855	H	35.250007	10.165937	42.991236
H	56.250120	4.683133	39.763657	H	36.698407	9.464639	43.738147
H	57.578891	4.683400	24.200591	H	36.693803	8.513735	39.604545
H	32.654245	5.043349	18.026539	H	39.211173	7.771216	43.013696
H	17.034856	5.043609	18.026692	H	40.289052	7.237997	45.201346
H	10.176559	4.915318	24.089682	H	38.993934	6.036832	46.966884
H	8.848023	4.915616	39.653303	H	36.627078	5.356116	46.528476
H	7.520585	4.915609	55.216383	H	35.570832	5.848299	44.328093
H	12.998946	5.199012	65.269013	H	37.396744	7.295152	41.543082
H	28.618717	5.199023	65.268139	H	36.095575	6.257526	41.984238
H	44.238629	5.198818	65.267053				
H	48.273941	5.043153	18.026052				
C	35.643123	8.221280	42.296787	(S,S)-1-Int3			
C	34.962314	8.284446	40.899974	C	12.487000	7.261000	26.395000
C	35.790821	9.099264	39.885375	C	11.616000	6.503000	25.622000
C	36.217822	10.468350	40.421568	C	12.086000	5.395000	24.927000
C	37.001563	10.312306	41.732883	C	13.428000	5.043000	25.007000
C	36.157509	9.573145	42.780442	C	13.027000	3.179000	23.539000
O	33.701715	8.809728	41.078780	C	11.685000	3.529000	23.460000
				C	11.215000	4.638000	24.154000

O	10.782000	2.793000	22.654000	C	28.045295	7.154748	26.538707
Cu	18.543832	6.107254	26.003160	C	27.196540	6.298931	25.844884
Cu	17.963211	3.719571	26.530347	C	27.693550	5.164615	25.171012
C	22.230158	3.999870	26.401639	C	29.087553	4.891783	25.219624
C	22.756089	3.223695	27.450424	C	13.900000	3.935000	24.313000
C	24.111060	2.921917	27.505489	C	28.734676	2.974896	23.770736
C	24.965917	3.382891	26.509999	C	27.369873	3.206464	23.747283
C	24.479561	4.135477	25.424290	C	26.824254	4.306317	24.446862
C	23.091978	4.433062	25.354004	O	26.591116	2.304817	23.024671
C	22.599535	5.119203	24.223127	O	16.594332	6.411827	25.835894
C	23.466744	5.541731	23.220487	O	16.064162	4.272994	26.319211
C	24.833317	5.290342	23.308735	C	15.738349	5.467653	25.978873
C	25.351010	4.575842	24.397413	C	17.918160	5.864046	30.218689
O	25.687179	5.712815	22.295723	C	18.907664	6.634046	30.856547
O	20.438353	5.554200	26.182809	C	16.770835	5.452701	30.952923
O	19.928752	3.407512	26.653444	C	15.697441	4.775541	30.335688
C	20.779970	4.340515	26.419553	C	14.595419	4.370914	31.082820
C	18.226927	4.022014	22.293999	O	18.429665	6.437275	27.961350
C	18.992915	2.941012	21.873981	O	17.909183	4.292021	28.428836
C	19.081890	2.638017	20.519979	C	18.102103	5.509640	28.785589
C	18.404876	3.417023	19.587993	Cu	34.206789	6.089923	26.026947
C	17.639888	4.497024	20.008011	Cu	33.644395	3.704432	26.571102
C	17.550913	4.800019	21.362013	C	37.894340	3.943109	26.329528
C	16.783924	5.881020	21.784030	C	38.427051	3.215967	27.409992
C	16.107910	6.659026	20.850045	C	39.770665	2.867834	27.443588
C	16.197885	6.355031	19.497042	C	40.606948	3.233776	26.395475
C	16.963875	5.274030	19.076025	C	40.113024	3.941397	25.282584
O	15.523872	7.185037	18.539057	C	38.735331	4.284461	25.234852
O	18.568766	5.538205	24.103524	C	38.231026	4.925985	24.084422
O	18.034150	3.397805	24.577775	C	39.080197	5.254192	23.031677
C	18.270931	4.342461	23.744010	C	40.441456	4.965106	23.097829
C	14.301000	5.801000	25.782000	C	40.970293	4.302200	24.213976
C	13.829000	6.909000	26.476000	O	41.279435	5.307991	22.042601

O	36.111483	5.518180	26.115718	C	32.906490	5.422101	31.187000
O	35.602314	3.379040	26.621690	C	31.785072	4.689572	30.747588
C	36.451391	4.303823	26.360141	C	30.794139	4.311363	31.649558
C	33.846854	4.021972	22.293718	O	34.199981	6.406443	27.990651
C	34.612831	2.940969	21.873683	O	33.681415	4.268575	28.485318
C	34.701781	2.637978	20.519678	C	33.931978	5.479015	28.836444
C	34.024753	3.416989	19.587708	Cu	49.694738	6.196303	25.988585
C	33.259776	4.496991	20.007741	Cu	49.348636	3.774568	26.557756
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.156754	5.538126	24.118672	C	53.770890	5.287813	24.113936
O	33.650368	3.394197	24.597538	C	54.557834	5.591815	23.007897
C	33.875797	4.339365	23.756318	C	55.929834	5.377800	23.052821
C	29.942449	5.742645	25.974801	C	56.515889	4.858782	24.200784
C	29.405360	6.881532	26.601188	O	56.643771	5.617805	21.841785
C	43.539060	6.853924	26.516962	O	51.635987	5.832761	26.127420
C	42.735389	6.011977	25.758814	O	51.338483	3.652630	26.629830
C	43.277805	4.909363	25.065627	C	52.093639	4.661972	26.379911
C	44.674746	4.661141	25.152500	C	49.466779	4.021876	22.293156
C	29.593510	3.800507	24.484681	C	50.232745	2.940872	21.873104
C	44.406906	2.781784	23.639764	C	50.321669	2.637885	20.519096
C	43.039503	2.994705	23.568839	C	49.644627	3.416901	19.587140
C	42.449330	4.061848	24.283183	C	48.879661	4.496905	20.007192
O	42.302619	2.100036	22.795890	C	48.790737	4.799893	21.361200
O	32.238651	6.405278	25.963487	C	48.023772	5.880897	21.783251
O	31.744353	4.259482	26.450665	C	47.347731	6.658913	20.849295
C	31.394073	5.454053	26.140094	C	47.437655	6.354926	19.496287
C	33.933299	5.832641	30.288487	C	48.203620	5.273922	19.075235
C	34.986004	6.633164	30.772327	O	46.763613	7.184943	18.538331

O	49.731681	5.588834	24.092371	C	21.459249	5.229755	39.803160
O	49.390682	3.420596	24.603621	C	22.379077	5.614014	38.831163
C	49.527027	4.366865	23.748841	C	23.736671	5.341585	38.984058
C	45.486524	5.513839	25.949113	C	24.194622	4.661514	40.117348
C	44.901359	6.610523	26.607826	O	24.638785	5.723196	37.999120
C	45.225705	3.597406	24.411485	O	19.150598	5.662880	41.655697
O	47.717546	6.325333	25.887791	O	18.677141	3.505684	42.113849
O	47.398532	4.153843	26.409767	C	19.514179	4.457930	41.908930
C	46.953516	5.315231	26.087879	C	16.936010	4.177753	37.741799
C	49.190369	5.953923	30.221084	C	17.654137	3.082818	37.229365
C	50.119048	6.810164	30.839813	C	17.667918	2.815298	35.867352
C	48.091187	5.453412	30.973733	C	16.962420	3.634489	34.992966
C	47.073143	4.679740	30.376066	C	16.204624	4.727048	35.464022
C	46.016160	4.193478	31.139025	C	16.171963	4.989753	36.859407
O	49.602349	6.545628	27.946180	C	15.352356	6.031757	37.338004
O	49.299183	4.367135	28.449996	C	14.627618	6.818846	36.452232
C	49.383085	5.602039	28.788394	C	14.684970	6.601863	35.085682
C	11.158286	7.260970	41.959133	C	15.479479	5.554678	34.566388
C	10.287269	6.502976	41.186145	O	13.954911	7.472556	34.279426
C	10.757253	5.394976	40.491133	O	17.260357	5.651067	39.584362
C	12.099253	5.042971	40.571108	O	16.791511	3.487486	40.018776
C	11.698221	3.178978	39.103109	C	17.002387	4.453698	39.201005
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	27.069919	7.640118	41.440063
Cu	17.235782	6.181895	41.496568	C	26.165117	6.678518	41.042730
Cu	16.705723	3.776811	41.985644	C	26.575021	5.356923	40.676361
C	20.972776	4.148727	41.975817	C	27.981947	5.044884	40.772059
C	21.448829	3.411973	43.076111	C	12.571237	3.934972	39.877096
C	22.801424	3.130759	43.218945	C	27.506224	2.806255	39.939928
C	23.705815	3.563066	42.255830	C	26.118401	3.097183	39.865717
C	23.274431	4.267231	41.117087	C	25.642519	4.355126	40.225588
C	21.890513	4.563738	40.968424	O	25.371729	2.043210	39.416265

O	15.268481	6.451471	41.360130	C	33.437252	4.552112	38.179032
O	14.788595	4.293252	41.798994	C	34.164186	3.448571	37.767860
C	14.428875	5.490100	41.501280	C	34.247559	3.137783	36.393831
C	16.680842	5.857334	45.720121	C	33.564861	3.893730	35.462685
C	17.678692	6.631358	46.340826	C	32.766265	5.021830	35.838565
C	18.805586	6.951828	32.204568	C	32.730696	5.369527	37.238168
C	17.711352	6.509914	32.939794	C	31.940363	6.484337	37.645408
C	16.683073	5.760190	32.336412	C	31.232200	7.213573	36.725931
C	15.557021	5.428047	46.480684	C	31.255000	6.876917	35.345486
C	14.479790	4.736454	45.887550	C	32.004025	5.793696	34.891760
C	13.397179	4.322914	46.658106	O	30.490278	7.710249	34.579742
C	14.531802	4.623308	32.450780	O	33.647339	5.987827	40.061852
C	15.563283	5.326090	33.088006	O	32.978094	3.868814	40.380550
O	13.426124	4.210461	33.185839	C	33.348375	4.832718	39.647309
O	17.135892	6.474127	43.462239	C	28.897888	6.059618	41.219995
O	16.644368	4.316011	43.897599	C	28.443077	7.335702	41.518814
C	16.831714	5.528662	44.275177	C	42.253148	7.092710	41.874487
Cu	33.051786	6.866102	41.763118	C	41.387164	6.104502	41.428454
Cu	32.559668	4.124089	42.260416	C	41.873277	4.880253	40.931649
C	36.825203	4.075357	43.246915	C	43.278647	4.657167	40.898636
C	37.524223	3.647819	44.358895	C	28.407490	3.742898	40.376405
C	38.876461	3.260360	44.223661	C	42.872876	2.521812	39.814019
C	39.520349	3.371209	43.010289	C	41.502468	2.700430	39.901876
C	38.852372	3.864706	41.842474	C	40.982556	3.884655	40.458993
C	37.455665	4.187935	41.965607	O	40.697668	1.663063	39.439172
C	36.765281	4.679477	40.823020	O	31.147182	6.792341	41.315199
C	37.409719	4.837093	39.621164	O	30.715416	4.646530	41.809235
C	38.793573	4.539751	39.492024	C	30.359210	5.809547	41.448941
C	39.517878	4.064298	40.585284	C	31.646626	5.625582	45.959524
O	39.415435	4.733049	38.297726	C	32.278653	6.701784	46.566037
O	35.183367	5.436440	44.238504	C	35.057306	6.995671	32.110554
O	34.527620	3.934939	42.688654	C	34.070909	6.578353	32.995128
C	35.398512	4.476852	43.381475	C	32.985693	5.797807	32.558290

C	30.670632	4.851901	46.677269	C	45.964928	6.533618	35.081099
C	29.909232	3.812300	46.071010	C	46.811562	5.512878	34.593300
C	28.993771	3.088529	46.797981	O	45.218060	7.363059	34.247115
C	30.883663	4.656264	32.995924	O	48.450393	5.739102	39.647172
C	31.967830	5.408754	33.459295	O	48.108638	3.557048	40.105281
O	29.875726	4.287768	33.877532	C	48.268845	4.524268	39.276444
O	32.673773	6.204710	43.897412	C	44.158025	5.641668	41.439137
O	32.004430	4.107931	44.142994	C	43.620158	6.861502	41.891195
C	32.102068	5.295028	44.578719	C	43.760523	3.478393	40.295582
Cu	48.393094	6.289984	41.551877	O	46.411522	6.440339	41.417463
Cu	48.011187	3.863327	42.071096	O	46.069533	4.264795	41.890738
C	52.242278	4.464620	41.931334	C	45.632828	5.431676	41.580171
C	52.828353	3.947597	43.079285	C	47.850552	5.993762	45.772442
C	54.201353	3.732577	43.123183	C	48.818273	6.797543	46.402331
C	54.987278	4.036581	42.018131	C	50.007176	7.129323	32.187159
C	54.401203	4.554604	40.869180	C	48.962164	6.604389	32.939925
C	53.028203	4.768624	40.826281	C	47.992110	5.767873	32.354993
C	52.442128	5.287648	39.677330	C	46.718192	5.553951	46.512189
C	53.229054	5.591652	38.571278	C	45.669055	4.834196	45.902909
C	54.601054	5.377632	38.616177	C	44.575594	4.411860	46.653059
C	55.187129	4.858609	39.764128	C	45.941810	4.460558	32.503499
O	55.314970	5.617639	37.405129	C	46.916458	5.255605	33.121452
O	50.332893	5.883223	41.709790	O	44.880688	3.966885	33.254384
O	49.993100	3.703691	42.186220	O	48.280982	6.602172	43.511454
C	50.768336	4.699201	41.950806	O	47.923407	4.423373	43.977433
C	48.243719	4.228489	37.818919	C	48.034169	5.651388	44.336412
C	49.024245	3.163815	37.334431	C	9.830848	7.260896	57.522290
C	49.088405	2.888511	35.975300	C	8.959816	6.502907	56.749315
C	48.371259	3.668875	35.075142	C	9.429783	5.394908	56.054291
C	47.551722	4.728359	35.516711	C	10.771783	5.042898	56.134241
C	47.470968	5.001097	36.908586	C	10.370718	3.178911	54.666243
C	46.597045	6.012833	37.355197	C	9.028718	3.528920	54.587293
C	45.865746	6.762849	36.443034	C	8.558750	4.637919	55.281317

O	8.125684	2.792932	53.781319	C	25.312347	6.837903	57.620845
Cu	15.901671	6.097073	57.131764	C	24.477954	6.012051	56.877780
Cu	15.318919	3.693576	57.566475	C	24.984906	4.896179	56.179486
C	19.574270	3.945545	57.472043	C	26.376541	4.615342	56.247672
C	20.102233	3.194377	58.537643	C	11.243751	3.934900	55.440217
C	21.446277	2.845472	58.567280	C	26.044502	2.743763	54.737599
C	22.285887	3.232104	57.528462	C	24.681552	2.986437	54.688162
C	21.795239	3.962506	56.428899	C	24.126103	4.065195	55.412832
C	20.419044	4.311513	56.387897	O	23.912730	2.106936	53.928898
C	19.918520	4.982461	55.252094	O	13.947332	6.413812	56.971324
C	20.768951	5.329849	54.206804	O	13.420225	4.260869	57.384303
C	22.127428	5.028032	54.264126	C	13.089561	5.466655	57.090486
C	22.652324	4.336740	55.364587	C	15.283046	5.695821	61.352095
O	22.966818	5.385726	53.215261	C	16.314087	6.385804	61.978046
O	17.798593	5.527548	57.299284	C	17.606631	6.939713	47.692948
O	17.275444	3.366726	57.687420	C	16.531763	6.488584	48.450337
C	18.131132	4.303077	57.496143	C	15.495283	5.735340	47.866786
C	15.645817	4.156844	53.332735	C	14.198081	5.242825	62.095148
C	16.350395	3.044012	52.839526	C	13.166040	4.552842	61.469196
C	16.400791	2.778056	51.478161	C	12.083075	4.099846	62.213249
C	15.741814	3.613821	50.583781	C	13.354322	4.585406	48.025294
C	14.998725	4.725061	51.032801	C	14.390190	5.301677	48.639986
C	14.937622	4.994024	52.427162	O	12.264462	4.168989	48.781818
C	14.142964	6.065837	52.880343	O	15.773643	6.355930	59.103746
C	13.467738	6.872275	51.972767	O	15.268194	4.192394	59.488220
C	13.545214	6.641348	50.609288	C	15.449350	5.397276	59.894425
C	14.313356	5.563400	50.114190	Cu	31.455851	5.935919	57.114712
O	12.856616	7.525439	49.781259	Cu	30.991576	3.529066	57.667761
O	15.944709	5.600887	55.207478	C	35.229880	3.954895	57.488199
O	15.408430	3.444236	55.594606	C	35.790785	3.263533	58.577666
C	15.666688	4.416414	54.797659	C	37.144292	2.954821	58.607697
C	11.644816	5.800887	56.909216	C	37.962501	3.322196	57.545667
C	11.172849	6.908886	57.603240	C	37.442017	3.996482	56.424360

C	36.055245	4.304593	56.383225	O	39.587698	2.147575	53.905680
C	35.526689	4.916723	55.227430	O	29.485350	6.167926	57.015967
C	36.358926	5.250376	54.163241	O	29.066884	4.002076	57.486237
C	37.726329	4.990780	54.219503	C	28.675595	5.187802	57.186655
C	38.280247	4.353752	55.338757	C	30.903120	5.695641	61.351269
O	38.545666	5.333070	53.149831	C	31.934175	6.385618	61.977205
O	33.382211	5.450038	57.246476	C	32.015448	7.019292	47.913400
O	32.961337	3.297536	57.777020	C	31.129018	6.259198	48.644532
C	33.772226	4.255150	57.511314	C	30.423665	5.153867	48.064886
C	31.247121	3.795210	53.424231	C	29.818167	5.242646	62.094340
C	32.238383	2.935454	52.920956	C	28.786113	4.552669	61.468405
C	32.287886	2.623689	51.568821	C	27.703159	4.099675	62.212476
C	31.344079	3.159550	50.698773	C	28.797547	3.330828	48.183881
C	30.316644	4.004612	51.165712	C	29.496710	4.354397	48.817950
C	30.260849	4.319308	52.548866	O	27.921924	2.565211	48.892138
C	29.213422	5.130976	53.024512	O	31.376023	6.278290	59.076796
C	28.254039	5.620679	52.145280	O	30.938278	4.118862	59.559909
C	28.313635	5.346050	50.788158	C	31.085298	5.345546	59.909850
C	29.353978	4.543601	50.278261	Cu	47.047282	6.247519	57.148601
O	27.343186	5.930782	49.979521	Cu	46.689161	3.790943	57.532298
O	31.457210	5.352525	55.210031	C	50.914829	4.464394	57.493750
O	31.075442	3.185216	55.713335	C	51.500923	3.947364	58.641689
C	31.263785	4.130179	54.868113	C	52.873923	3.732339	58.685563
C	27.218301	5.445780	57.037355	C	53.659830	4.036343	57.580498
C	26.669298	6.560123	57.697387	C	53.073736	4.554373	56.431559
C	40.894612	6.918087	57.579974	C	51.700736	4.768398	56.388685
C	40.077101	6.073553	56.840356	C	51.114643	5.287428	55.239746
C	40.607356	4.972327	56.136632	C	51.901549	5.591433	54.133681
C	42.008093	4.730771	56.188935	C	53.273549	5.377407	54.178555
C	26.892051	3.539498	55.498065	C	53.859642	4.858378	55.326493
C	41.710412	2.853869	54.678456	O	53.987445	5.617415	52.967495
C	40.339878	3.053674	54.650385	O	48.989549	5.858457	57.300477
C	39.762156	4.118194	55.379122	O	48.674071	3.653577	57.666541

C	49.437762	4.671873	57.497094	O	46.577029	4.236740	59.461941
C	46.950742	4.365259	53.311295	C	46.675228	5.442228	59.890434
C	47.756532	3.334426	52.795362	C	16.262162	6.620790	63.347051
C	47.802681	3.079702	51.432221	C	15.179196	6.168795	64.090104
C	47.041531	3.846603	50.558087	C	14.147156	5.478812	63.465153
C	46.204246	4.879748	51.028788	C	12.031150	4.336833	63.582254
C	46.144472	5.133003	52.426228	C	13.063191	5.025817	64.207206
C	45.254984	6.116136	52.902854	O	10.943187	3.908837	64.361307
C	44.486126	6.857362	52.014493	C	31.882275	6.620600	63.346211
C	44.561509	6.646654	50.647469	C	30.799322	6.168606	64.089282
C	45.424530	5.654552	50.128439	C	29.767267	5.478629	63.464346
O	43.781950	7.472785	49.840777	C	27.651260	4.336658	63.581482
O	47.119094	5.799881	55.212126	C	28.683314	5.025635	64.206417
O	46.811460	3.592167	55.558503	O	26.563309	3.908663	64.360554
C	46.960260	4.601156	54.780109	C	47.502389	6.620356	63.345091
C	42.834847	5.580404	56.975653	C	46.419447	6.168363	64.088179
C	42.258448	6.675478	57.646167	C	45.387379	5.478391	63.463260
C	42.545334	3.676688	55.424472	C	43.271369	4.336426	63.580429
O	45.071621	6.391005	57.018243	C	44.303437	5.025398	64.205349
O	44.744327	4.184878	57.351520	O	42.183431	3.908432	64.359519
C	44.303090	5.368479	57.116955	H	12.119316	8.127274	26.935477
C	46.523195	5.695406	61.350162	H	10.573047	6.786884	25.566300
C	47.554262	6.385378	61.976082	H	13.383696	2.323147	22.982663
C	48.707010	7.127322	47.746696	H	9.847477	3.169785	22.676871
C	47.624464	6.664722	48.486190	H	22.104642	2.865308	28.239429
C	46.619348	5.877300	47.891870	H	24.503121	2.331578	28.327878
C	45.438253	5.242413	62.093251	H	26.015905	3.134251	26.587213
C	44.406185	4.552442	61.467332	H	21.543605	5.325826	24.086694
C	43.323243	4.099449	62.211421	H	23.065217	6.070065	22.366376
C	44.501457	4.681714	48.017669	H	19.533147	2.330445	22.589885
C	45.512634	5.419470	48.649185	H	19.679655	1.794319	20.190489
O	43.406315	4.247424	48.755776	H	18.480617	3.170906	18.536719
O	46.916702	6.441901	59.122108	H	16.649873	6.144613	22.827052

H	15.506636	7.500796	21.165209	H	53.552057	3.699481	28.381141
H	14.495768	7.508982	27.086590	H	55.987706	3.326019	28.455696
H	27.644139	8.032017	27.036405	H	57.384070	3.866316	26.497846
H	26.143497	6.541792	25.823007	H	52.703456	5.452905	24.015179
H	14.941437	3.633499	24.313293	H	54.081142	5.976177	22.116864
H	29.131049	2.135340	23.215446	H	50.777803	2.334880	22.589129
H	19.772114	6.976531	30.299050	H	50.920908	1.795281	20.189747
H	15.684766	4.561906	29.272221	H	49.720335	3.170945	18.535924
H	13.786869	3.850429	30.587642	H	47.863651	6.134680	22.823918
H	15.672237	6.861349	17.596353	H	46.741104	7.496731	21.164914
H	25.204900	6.236948	21.581129	H	45.515552	7.281409	27.197766
H	25.611111	2.531018	23.037315	H	46.288772	3.384601	24.406445
H	37.788288	2.925944	28.236611	H	50.944079	7.219490	30.267992
H	40.167662	2.312881	28.287960	H	47.068421	4.451157	29.315795
H	41.648030	2.946447	26.454458	H	45.250093	3.600070	30.658501
H	37.179755	5.172272	23.976292	H	46.912570	6.861458	17.595824
H	38.670716	5.747647	22.160650	H	56.056199	5.977167	21.104133
H	35.150567	2.329693	22.590650	H	10.791020	8.128292	42.498137
H	35.298849	1.793779	20.190328	H	9.244473	6.787163	41.129873
H	34.100000	3.170646	18.536493	H	12.055444	2.324899	38.544297
H	32.264756	6.142957	22.826385	H	8.519486	3.171522	38.239226
H	31.124763	7.499457	21.165216	H	20.758773	3.070894	43.839864
H	30.051710	7.551606	27.156384	H	23.152846	2.577761	44.084688
H	43.102849	7.703430	27.033150	H	24.753715	3.335223	42.405538
H	41.680978	6.242029	25.705679	H	20.412445	5.450602	39.619657
H	30.652517	3.575323	24.434438	H	22.023958	6.126098	37.946813
H	44.836620	1.962681	23.078815	H	18.216155	2.440741	37.897803
H	35.764112	6.972264	30.097390	H	18.232274	1.970527	35.485109
H	31.647797	4.412460	29.707649	H	16.998366	3.394197	33.939863
H	29.944146	3.747743	31.288601	H	15.246188	6.247223	38.395084
H	31.292311	6.861285	17.596307	H	14.005339	7.620193	36.827668
H	40.794664	5.815948	21.317941	H	13.169261	7.512551	42.644414
H	41.321203	2.318448	22.770628	H	26.720175	8.643271	41.703405

H	25.105491	6.950992	41.006562	H	30.501596	7.476204	33.638638
H	13.612010	3.634023	39.869049	H	38.788294	5.105172	37.656027
H	27.831856	1.810038	39.628732	H	39.711285	1.852576	39.529639
H	18.526456	6.986327	45.765669	H	52.223451	3.704667	43.946005
H	19.581991	7.539144	32.684909	H	54.659153	3.326950	44.019442
H	17.666269	6.772291	33.988163	H	56.055360	3.866336	42.061110
H	14.449266	4.517422	44.825578	H	51.374706	5.453233	39.579257
H	12.585380	3.790709	46.181069	H	52.752281	5.975808	37.680109
H	12.768692	3.686229	32.628065	H	49.599576	2.554878	38.022497
H	14.018198	7.249372	33.300885	H	49.702398	2.068856	35.615610
H	24.197622	6.230749	37.246476	H	48.448821	3.425318	34.025005
H	24.426696	2.250628	39.348611	H	46.452402	6.232036	38.406976
H	37.027526	3.597867	45.331783	H	45.202107	7.541766	36.794174
H	39.420249	2.884691	45.095809	H	44.272559	7.635775	42.278563
H	40.573704	3.081528	42.948999	H	44.818644	3.285062	40.162247
H	35.715433	4.959134	40.892803	H	49.669798	7.162560	45.839464
H	36.852744	5.218169	38.757201	H	50.737294	7.783703	32.653129
H	34.668812	2.827354	38.512748	H	48.907754	6.869975	33.987181
H	34.842945	2.279288	36.066765	H	45.670436	4.600204	44.843372
H	33.637926	3.605711	34.409050	H	43.782777	3.862728	46.163426
H	31.888097	6.761010	38.699556	H	44.261682	3.386437	32.708496
H	30.617960	8.065091	37.030348	H	45.322056	7.139141	33.272096
H	29.162034	8.092695	41.838907	H	54.726409	5.972193	36.665806
H	41.859151	8.040808	42.222007	H	9.463327	8.126887	58.063159
H	40.326871	6.319923	41.457607	H	7.916923	6.786658	56.693615
H	29.465431	3.490556	40.418141	H	10.728208	2.325481	54.106594
H	43.252530	1.615083	39.361507	H	7.191662	3.170551	53.803528
H	32.998608	7.285384	45.988677	H	19.459574	2.885610	59.354216
H	35.881669	7.607066	32.464936	H	21.840746	2.271728	59.400070
H	34.156662	6.883015	34.030594	H	23.326627	2.942412	57.582898
H	30.050194	3.593625	45.013608	H	18.869136	5.237920	55.149179
H	28.412462	2.299171	46.306480	H	20.362529	5.845352	53.347169
H	29.167966	3.716315	33.439800	H	16.873557	2.385382	53.523422

H	16.955627	1.919729	51.112477	H	32.792227	6.730120	61.410245
H	15.803877	3.373408	49.531899	H	32.528455	7.863843	48.383441
H	14.019214	6.290991	53.933529	H	30.960147	6.523609	49.693038
H	12.865228	7.697246	52.328671	H	28.748177	4.377653	60.399269
H	11.840772	7.508165	58.213059	H	26.897474	3.575017	61.718287
H	24.903533	7.698757	58.140506	H	27.540504	1.883015	48.315809
H	23.427989	6.264689	56.839216	H	27.431465	5.679583	49.006815
H	12.285203	3.636477	55.426628	H	38.045603	5.821582	52.421986
H	26.448257	1.918735	54.166063	H	38.603399	2.352775	53.914015
H	17.169098	6.737551	61.410741	H	50.894850	3.699973	59.506230
H	18.390274	7.529558	48.158404	H	53.331562	3.325509	59.581291
H	16.508930	6.745363	49.500884	H	54.727846	3.865736	57.623128
H	13.125092	4.379529	60.400334	H	50.047610	5.459328	55.145250
H	11.277308	3.575366	61.719136	H	51.424903	5.977059	53.243022
H	11.600526	3.638495	48.238019	H	48.356900	2.727798	53.463804
H	12.943138	7.299348	48.804998	H	48.431203	2.281761	51.049588
H	22.485387	5.903858	52.495608	H	47.099937	3.612234	49.504883
H	22.937476	2.351653	53.911522	H	45.128190	6.320296	53.959914
H	35.164969	2.966885	59.411723	H	43.809783	7.614348	52.388646
H	37.562468	2.425777	59.458312	H	42.880542	7.343285	58.231290
H	39.011103	3.062845	57.600654	H	43.609794	3.478792	55.376185
H	34.469651	5.137049	55.123359	H	48.405659	6.744429	61.407797
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H	32.982168	2.513420	53.587123	H	47.568936	6.940942	49.530473
H	33.062698	1.963734	51.191133	H	44.381842	4.364054	60.399390
H	31.414026	2.891649	49.652858	H	42.519409	3.571537	61.717717
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H	27.446571	6.237414	52.518508	H	43.859408	7.256183	48.861881
H	27.306184	7.213028	58.283414	H	53.398672	5.970785	52.227670
H	40.467234	7.766340	58.105355	H	17.068482	7.157600	63.836089
H	39.021085	6.300110	56.809549	H	15.148154	6.357150	65.155579
H	27.949369	3.302507	55.474229	H	10.263266	3.421560	63.797132
H	42.130642	2.041702	54.100473	H	32.689381	7.155911	63.835532

H	30.768303	6.356652	65.154796	H	36.133156	8.530436	44.151304
H	25.882086	3.423707	63.795816	H	33.964805	9.488662	40.759877
H	48.307538	7.159099	63.833755	H	35.070392	10.136187	39.534083
H	46.387772	6.357310	65.153489	H	36.502333	11.147908	41.291768
H	41.501260	3.425111	63.794454	H	34.836434	11.693840	41.522646
H	54.922551	4.682795	55.325765	H	34.457686	9.994435	43.296950
H	56.250084	4.683152	39.763698	H	35.856194	11.009557	43.725430
H	57.578895	4.683436	24.200629	H	36.919033	8.666389	40.421594
H	32.654269	5.043360	18.026533	H	40.127920	10.251687	43.603599
H	17.034874	5.043623	18.026683	H	41.907602	9.169406	44.937546
H	10.176555	4.915318	24.089629	H	41.557076	6.882079	45.905397
H	8.848002	4.915621	39.653285	H	39.373742	5.718965	45.501364
H	7.520559	4.915550	55.216452	H	37.600945	6.775778	44.182925
H	12.998944	5.198984	65.269024	H	37.993153	10.165507	42.705539
H	28.618796	5.198898	65.268170	H	34.270501	5.861736	44.102766
H	44.238635	5.198851	65.267027				
H	48.273907	5.043129	18.026067				
C	36.327567	8.965065	43.155176	(S,S)-1-Int3-2			
C	35.821930	7.903105	42.116146	C	12.487000	7.261000	26.395000
C	35.864277	8.460688	40.685057	C	11.616000	6.503000	25.622000
C	35.024921	9.738965	40.564357	C	12.086000	5.395000	24.927000
C	35.486843	10.801373	41.573034	C	13.428000	5.043000	25.007000
C	35.491790	10.249052	43.009341	C	13.027000	3.179000	23.539000
O	34.550472	7.563508	42.532201	C	11.685000	3.529000	23.460000
C	38.725736	8.603639	43.785087	C	11.215000	4.638000	24.154000
C	39.963723	9.248747	44.015206	O	10.782000	2.793000	22.654000
C	40.963576	8.638365	44.772051	Cu	18.540281	6.076179	26.028925
C	40.769418	7.363243	45.317562	Cu	17.945814	3.686048	26.527192
C	39.548907	6.718848	45.093418	C	22.213190	3.945125	26.392919
C	38.534732	7.318887	44.342618	C	22.745410	3.159120	27.430902
N	37.746717	9.240066	43.037660	C	24.101197	2.858556	27.475102
H	35.490809	7.683928	39.995471	C	24.950198	3.332168	26.480126
H	36.503510	7.029490	42.184066	C	24.456353	4.094202	25.404303
				C	23.067923	4.388199	25.343836

C	22.567174	5.081875	24.221028	O	16.595917	6.397963	25.859921
C	23.427373	5.514684	23.216852	O	16.051330	4.257737	26.320266
C	24.795135	5.268042	23.296489	C	15.734294	5.457694	25.988815
C	25.320890	4.548016	24.377552	C	17.914041	5.774339	30.248862
O	25.642599	5.701587	22.282751	C	18.896404	6.551155	30.889907
O	20.429964	5.509839	26.204740	C	16.785500	5.324879	30.991699
O	19.909578	3.359643	26.647139	C	15.714481	4.642907	30.375601
C	20.765119	4.291331	26.423821	C	14.630502	4.203196	31.129394
C	18.226927	4.022014	22.293999	O	18.423149	6.381477	27.994685
C	18.992915	2.941012	21.873981	O	17.894520	4.232548	28.432493
C	19.081890	2.638017	20.519979	C	18.091643	5.443788	28.807116
C	18.404876	3.417023	19.587993	Cu	34.177000	6.091014	26.027421
C	17.639888	4.497024	20.008011	Cu	33.596631	3.707613	26.567866
C	17.550913	4.800019	21.362013	C	37.851829	3.930117	26.376498
C	16.783924	5.881020	21.784030	C	38.374657	3.205792	27.463655
C	16.107910	6.659026	20.850045	C	39.716239	2.850040	27.506164
C	16.197885	6.355031	19.497042	C	40.560567	3.205759	26.460780
C	16.963875	5.274030	19.076025	C	40.076726	3.909450	25.341240
O	15.523872	7.185037	18.539057	C	38.701113	4.260434	25.284437
O	18.564576	5.526605	24.119459	C	38.206723	4.897694	24.127296
O	18.017064	3.384943	24.571889	C	39.063025	5.213443	23.076605
C	18.262863	4.334964	23.747257	C	40.421922	4.915550	23.150858
C	14.301000	5.801000	25.782000	C	40.941434	4.257054	24.274067
C	13.829000	6.909000	26.476000	O	41.266663	5.244546	22.096571
C	28.007340	7.156775	26.492035	O	36.077860	5.512013	26.140301
C	27.160782	6.291736	25.806687	O	35.553895	3.378775	26.655895
C	27.662243	5.158135	25.134642	C	36.409904	4.297764	26.395382
C	29.058123	4.896036	25.176217	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.712138	2.971775	23.735315	C	34.701781	2.637978	20.519678
C	27.345474	3.191906	23.720227	C	34.024753	3.416989	19.587708
C	26.795627	4.289521	24.419865	C	33.259776	4.496991	20.007741
O	26.569463	2.282754	23.004161	C	33.170826	4.799983	21.361747

C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.147995	5.536204	24.120586	C	53.770890	5.287813	24.113936
O	33.638412	3.392171	24.595813	C	54.557834	5.591815	23.007897
C	33.870122	4.337381	23.756430	C	55.929834	5.377800	23.052821
C	29.910329	5.753889	25.926108	C	56.515889	4.858782	24.200784
C	29.369298	6.891945	26.550507	O	56.643771	5.617805	21.841785
C	43.533786	6.819243	26.538781	O	51.626947	5.823624	26.134005
C	42.721726	5.969037	25.799365	O	51.342478	3.638565	26.622030
C	43.255849	4.857109	25.115009	C	52.091907	4.653930	26.378695
C	44.653477	4.606626	25.192884	C	49.466779	4.021876	22.293156
C	29.568503	3.806923	24.440892	C	50.232745	2.940872	21.873104
C	44.366400	2.707296	23.708619	C	50.321669	2.637885	20.519096
C	42.999431	2.924943	23.644255	C	49.644627	3.416901	19.587140
C	42.418489	4.003931	24.348112	C	48.879661	4.496905	20.007192
O	42.253770	2.024832	22.886115	C	48.790737	4.799893	21.361200
O	32.209287	6.412823	25.940459	C	48.023772	5.880897	21.783251
O	31.702515	4.266515	26.411548	C	47.347731	6.658913	20.849295
C	31.359809	5.462980	26.101869	C	47.437655	6.354926	19.496287
C	33.783705	5.849859	30.270491	C	48.203620	5.273922	19.075235
C	34.918316	6.432713	30.863124	O	46.763613	7.184943	18.538331
C	32.604466	5.673818	31.045504	O	49.721937	5.581260	24.099945
C	31.423395	5.150399	30.482628	O	49.392743	3.408133	24.598363
C	30.274635	5.018224	31.258713	C	49.523446	4.360405	23.749565
O	34.146748	6.411468	27.989118	C	45.474952	5.469663	25.969199
O	33.588639	4.280169	28.478857	C	44.896535	6.575402	26.619103
C	33.845332	5.489372	28.828072	C	45.194597	3.531343	24.461416
Cu	49.681887	6.175059	25.999661	O	47.703179	6.290627	25.900474
Cu	49.351264	3.747786	26.553457	O	47.397625	4.114888	26.411326
C	53.571003	4.464792	26.367939	C	46.944723	5.275300	26.096899

C	49.164171	5.899654	30.228635	C	17.505942	2.773549	37.314371
C	50.076752	6.763975	30.859646	C	17.536897	2.513090	35.950439
C	48.066877	5.378440	30.970196	C	16.897214	3.374041	35.064409
C	47.061748	4.598023	30.359336	C	16.182949	4.499069	35.525559
C	46.007936	4.089277	31.111742	C	16.133342	4.755979	36.921834
O	49.586017	6.510395	27.959982	C	15.358802	5.836753	37.389225
O	49.299473	4.326264	28.448773	C	14.693199	6.663404	36.493422
C	49.370740	5.559526	28.795176	C	14.766993	6.449282	35.127338
C	11.158286	7.260970	41.959133	C	15.518409	5.366020	34.618087
C	10.287269	6.502976	41.186145	O	14.092066	7.354717	34.311252
C	10.757253	5.394976	40.491133	O	17.237922	5.375158	39.640584
C	12.099253	5.042971	40.571108	O	16.635283	3.251944	40.106712
C	11.698221	3.178978	39.103109	C	16.909201	4.190521	39.274379
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.045799	7.053880	42.292029
Cu	17.244066	5.938651	41.541562	C	25.401828	6.016097	41.651709
Cu	16.558366	3.580342	42.072831	C	26.115899	4.917635	41.068986
C	20.822450	3.665470	42.073018	C	27.549873	4.913365	41.214230
C	21.302206	3.064363	43.250395	C	12.571237	3.934972	39.877096
C	22.649769	2.757673	43.395270	C	27.654421	2.831544	39.962552
C	23.541047	3.046888	42.367078	C	26.243235	2.836884	39.790139
C	23.097168	3.618387	41.160341	C	25.470411	3.856371	40.335916
C	21.716181	3.902938	40.995635	O	25.781777	1.771917	39.070489
C	21.261911	4.399851	39.757368	O	15.299633	6.341250	41.393015
C	22.162501	4.629509	38.721292	O	14.690166	4.222985	41.868506
C	23.526526	4.410294	38.901725	C	14.405983	5.432298	41.543965
C	24.005785	3.918845	40.121325	C	16.634062	5.738188	45.759813
O	24.415939	4.668928	37.866743	C	17.664002	6.473063	46.375522
O	19.114391	5.284345	41.716106	C	18.808735	6.835864	32.246666
O	18.497789	3.172913	42.223562	C	17.735835	6.354216	32.988711
C	19.393030	4.064213	42.003841	C	16.712146	5.600545	32.383458
C	16.836462	3.903277	37.816704	C	15.477610	5.390953	46.512489

C	14.370009	4.748838	45.919179	C	31.382272	6.338385	34.609686
C	13.260369	4.405079	46.685209	O	31.031434	8.719486	34.093138
C	14.579630	4.429260	32.502474	O	32.442120	6.241824	39.866020
C	15.607607	5.136495	33.140055	O	31.829684	4.173572	40.343803
O	13.487851	3.988665	33.242317	C	31.995115	5.098748	39.493757
O	17.157697	6.273064	43.498676	C	28.186844	6.024827	41.853309
O	16.523528	4.160383	43.972580	C	27.452143	7.079565	42.366467
C	16.784211	5.366742	44.326477	C	42.167377	6.789359	41.528857
Cu	31.969176	7.862518	41.384085	C	41.424027	5.855063	40.818789
Cu	32.300143	4.935391	42.108927	C	42.019540	4.691886	40.293593
C	36.474829	4.128723	41.103525	C	43.412827	4.481741	40.491049
C	36.824666	3.563090	42.321207	C	28.290698	3.835222	40.646843
C	38.137514	3.111513	42.553707	C	43.250039	2.437819	39.187742
C	39.101523	3.255865	41.581264	C	41.886568	2.610895	39.026004
C	38.804497	3.818182	40.297869	C	41.254193	3.752146	39.557338
C	37.442278	4.217719	40.034373	O	41.198799	1.613498	38.339935
C	37.129897	4.658146	38.716937	O	30.139438	7.225323	41.403092
C	38.099941	4.770021	37.749536	O	30.363009	5.214816	42.384555
C	39.456858	4.476831	38.033442	C	29.675155	6.158550	41.884056
C	39.815340	3.989381	39.290421	C	32.142587	7.099272	45.655852
O	40.405582	4.660783	37.074914	C	32.833111	8.129223	46.266188
O	34.904684	5.568428	40.072655	C	34.916216	6.798996	32.202690
O	34.239962	4.414871	41.874042	C	33.772447	6.612604	32.970734
C	35.112348	4.707643	41.034389	C	32.600543	6.069665	32.411365
C	31.790751	4.779042	38.055274	C	31.272542	6.245135	46.411889
C	31.867691	3.431179	37.721462	C	30.481365	5.235829	45.794152
C	31.815437	3.023927	36.376841	C	29.617485	4.464951	46.534590
C	31.676578	3.961156	35.374995	C	30.268987	5.401485	32.598694
C	31.553060	5.359984	35.651839	C	31.423607	5.932546	33.183563
C	31.607653	5.776369	37.034134	O	29.113168	5.268065	33.357232
C	31.450129	7.163161	37.323807	O	32.100065	7.843565	43.404858
C	31.253290	8.075095	36.318366	O	32.698732	5.718918	43.830751
C	31.220119	7.677259	34.955485	C	32.317881	6.881350	44.182001

Cu	48.363003	6.210281	41.517833	O	46.381014	6.312426	41.357308
Cu	48.029932	3.777239	42.046052	O	46.083862	4.130221	41.837053
C	52.242278	4.464620	41.931334	C	45.629196	5.280392	41.493930
C	52.828353	3.947597	43.079285	C	47.816302	5.925350	45.737060
C	54.201353	3.732577	43.123183	C	48.761539	6.769105	46.349055
C	54.987278	4.036581	42.018131	C	49.952134	7.070475	32.208819
C	54.401203	4.554604	40.869180	C	48.910633	6.523812	32.951168
C	53.028203	4.768624	40.826281	C	47.956060	5.678201	32.353694
C	52.442128	5.287648	39.677330	C	46.706718	5.455241	46.492360
C	53.229054	5.591652	38.571278	C	45.680213	4.687697	45.903186
C	54.601054	5.377632	38.616177	C	44.608559	4.237978	46.668849
C	55.187129	4.858609	39.764128	C	45.924102	4.339779	32.478601
O	55.314970	5.617639	37.405129	C	46.884255	5.142084	33.109748
O	50.308892	5.847734	41.696179	O	44.865422	3.824809	33.218432
O	50.010706	3.663436	42.179924	O	48.226448	6.529713	43.472854
C	50.766121	4.673447	41.943803	O	47.913733	4.346228	43.948712
C	48.269442	4.134440	37.794110	C	47.999492	5.577990	44.302125
C	49.084103	3.099959	37.301291	C	9.830848	7.260896	57.522290
C	49.145401	2.829297	35.940902	C	8.959816	6.502907	56.749315
C	48.393394	3.585919	35.048510	C	9.429783	5.394908	56.054291
C	47.541585	4.615752	35.499398	C	10.771783	5.042898	56.134241
C	47.460819	4.879766	36.892571	C	10.370718	3.178911	54.666243
C	46.553097	5.856428	37.349894	C	9.028718	3.528920	54.587293
C	45.787679	6.582363	36.446610	C	8.558750	4.637919	55.281317
C	45.887645	6.364812	35.082873	O	8.125684	2.792932	53.781319
C	46.770268	5.380013	34.584225	Cu	15.891831	6.147556	57.137137
O	45.105897	7.171305	34.258233	Cu	15.346574	3.731335	57.550947
O	48.449644	5.651222	39.617451	C	19.601582	4.063134	57.422580
O	48.151341	3.463879	40.082034	C	20.159655	3.288656	58.455418
C	48.294405	4.431653	39.250635	C	21.514059	2.979615	58.463049
C	44.166299	5.432513	41.240612	C	22.334716	3.430975	57.434770
C	43.523179	6.582043	41.735610	C	21.814304	4.185169	56.365648
C	44.017907	3.358193	39.891686	C	20.427419	4.491780	56.345586

C	19.898357	5.183893	55.235331	O	13.936840	6.435490	56.976582
C	20.730125	5.596003	54.198850	O	13.437784	4.272344	57.370930
C	22.097600	5.336063	54.237395	C	13.091848	5.476552	57.086293
C	22.651419	4.622270	55.308924	C	15.283046	5.695821	61.352095
O	22.917197	5.756051	53.195706	C	16.314087	6.385804	61.978046
O	17.795448	5.611276	57.299226	C	17.589030	6.821806	47.717335
O	17.312628	3.437504	57.665040	C	16.482121	6.446302	48.469535
C	18.151035	4.390806	57.475095	C	15.416842	5.730068	47.890414
C	15.647263	4.234495	53.326158	C	14.198081	5.242825	62.095148
C	16.358489	3.131969	52.819917	C	13.166040	4.552842	61.469196
C	16.380124	2.861768	51.459234	C	12.083075	4.099846	62.213249
C	15.686595	3.683947	50.579062	C	13.222012	4.686220	48.048523
C	14.942203	4.789478	51.041628	C	14.287510	5.359575	48.661393
C	14.908257	5.060732	52.435856	O	12.109545	4.330435	48.802982
C	14.108519	6.122266	52.904577	O	15.757154	6.383341	59.110777
C	13.403556	6.918326	52.010712	O	15.283514	4.208989	59.476845
C	13.456896	6.687907	50.646093	C	15.447086	5.412609	59.892689
C	14.228473	5.618997	50.136462	Cu	31.473522	6.227338	57.141409
O	12.746106	7.567003	49.831704	Cu	30.968252	3.794601	57.505230
O	15.943226	5.668673	55.209028	C	35.209716	4.162779	57.441903
O	15.439045	3.501148	55.579959	C	35.746535	3.421402	58.510229
C	15.679103	4.483776	54.791068	C	37.090301	3.072189	58.532895
C	11.644816	5.800887	56.909216	C	37.921013	3.446465	57.482975
C	11.172849	6.908886	57.603240	C	37.422903	4.170081	56.382212
C	25.308839	7.136958	57.559264	C	36.047236	4.524123	56.351040
C	24.474978	6.308827	56.817300	C	35.539714	5.193041	55.217778
C	24.988616	5.214601	56.091049	C	36.382033	5.528726	54.162072
C	26.386303	4.958812	56.128612	C	37.739591	5.219175	54.207498
C	11.243751	3.934900	55.440217	C	38.272531	4.532611	55.307575
C	26.061498	3.115901	54.581213	O	38.569882	5.565422	53.147569
C	24.692642	3.326523	54.570650	O	33.392142	5.705458	57.278742
C	24.130742	4.379598	55.327248	O	32.929572	3.525439	57.635203
O	23.926339	2.446257	53.809553	C	33.758686	4.487527	57.460695

C	31.366325	4.387547	53.284065	C	29.818167	5.242646	62.094340
C	32.196851	3.366188	52.789347	C	28.786113	4.552669	61.468405
C	32.350246	3.170353	51.423056	C	27.703159	4.099675	62.212476
C	31.667209	3.982466	50.524020	C	29.493490	4.644773	47.938026
C	30.790332	4.989942	50.971863	C	30.246353	5.619983	48.591814
C	30.632976	5.193991	52.370623	O	28.626439	3.867253	48.644511
C	29.727140	6.174906	52.818665	O	31.357342	6.420632	59.119403
C	29.022860	6.948107	51.903031	O	30.887903	4.239154	59.444201
C	29.182940	6.773365	50.538384	C	31.054470	5.434937	59.884298
C	30.071674	5.793208	50.052529	Cu	47.054976	6.254820	57.148490
O	28.440208	7.603990	49.703637	Cu	46.686404	3.799208	57.530240
O	31.520910	5.795699	55.200866	C	50.914829	4.464394	57.493750
O	31.089168	3.605290	55.523420	C	51.500923	3.947364	58.641689
C	31.316343	4.609315	54.755916	C	52.873923	3.732339	58.685563
C	27.226615	5.780264	56.930816	C	53.659830	4.036343	57.580498
C	26.670784	6.876390	57.615298	C	53.073736	4.554373	56.431559
C	40.926398	6.979329	57.625347	C	51.700736	4.768398	56.388685
C	40.095896	6.171024	56.860914	C	51.114643	5.287428	55.239746
C	40.606872	5.076488	56.132446	C	51.901549	5.591433	54.133681
C	42.001589	4.802982	56.186426	C	53.273549	5.377407	54.178555
C	26.908553	3.915244	55.338637	C	53.859642	4.858378	55.326493
C	41.671169	2.966181	54.634403	O	53.987445	5.617415	52.967495
C	40.306054	3.201228	54.598376	O	48.994042	5.860820	57.300858
C	39.748116	4.261408	55.348313	O	48.671848	3.657049	57.668273
O	39.538327	2.332930	53.825219	C	49.438464	4.673446	57.497957
O	29.504023	6.489830	57.012374	C	46.981538	4.362580	53.313838
O	29.056578	4.301841	57.325317	C	47.811285	3.343509	52.812530
C	28.681498	5.507517	57.095241	C	47.867135	3.073515	51.452876
C	30.903120	5.695641	61.351269	C	47.090473	3.811898	50.568121
C	31.934175	6.385618	61.977205	C	46.229671	4.832168	51.024674
C	32.735083	8.310013	47.665017	C	46.163895	5.104126	52.418139
C	31.925835	7.492641	48.425359	C	45.257297	6.078033	52.880829
C	31.145270	6.446112	47.833682	C	44.473281	6.790273	51.981879

C	44.550376	6.558320	50.618290	C	30.799322	6.168606	64.089282
C	45.432197	5.575295	50.114092	C	29.767267	5.478629	63.464346
O	43.753376	7.354839	49.798969	C	27.651260	4.336658	63.581482
O	47.127653	5.806508	55.210578	C	28.683314	5.025635	64.206417
O	46.815749	3.599413	55.559210	O	26.563309	3.908663	64.360554
C	46.973045	4.606203	54.780452	C	47.502389	6.620356	63.345091
C	42.842026	5.619897	56.992048	C	46.419447	6.168363	64.088179
C	42.284660	6.708769	57.688461	C	45.387379	5.478391	63.463260
C	42.519735	3.751987	55.405067	C	43.271369	4.336426	63.580429
O	45.082862	6.407783	57.019128	C	44.303437	5.025398	64.205349
O	44.741768	4.202351	57.345331	O	42.183431	3.908432	64.359519
C	44.308098	5.390746	57.118775	H	12.119193	8.126959	26.935907
C	46.523195	5.695406	61.350162	H	10.573009	6.786780	25.566456
C	47.554262	6.385378	61.976082	H	13.383801	2.323529	22.982139
C	48.650630	7.112104	47.689817	H	9.847454	3.169754	22.676953
C	47.589543	6.624522	48.443612	H	22.098576	2.792914	28.220108
C	46.606782	5.796256	47.867786	H	24.498460	2.259883	28.288940
C	45.438253	5.242413	62.093251	H	26.001087	3.084842	26.548844
C	44.406185	4.552442	61.467332	H	21.509859	5.286234	24.091925
C	43.323243	4.099449	62.211421	H	23.019568	6.048001	22.368831
C	44.532595	4.530633	48.028671	H	19.531773	2.329351	22.589970
C	45.520577	5.315220	48.639581	H	19.679290	1.794053	20.190507
O	43.458504	4.071154	48.782267	H	18.480471	3.170812	18.536728
O	46.922941	6.445694	59.123314	H	16.652494	6.145579	22.827240
O	46.571234	4.241837	59.459065	H	15.507065	7.501117	21.165185
C	46.674885	5.445686	59.889737	H	14.495422	7.507674	27.088211
C	16.262162	6.620790	63.347051	H	27.602743	8.033605	26.987832
C	15.179196	6.168795	64.090104	H	26.105921	6.526997	25.789361
C	14.147156	5.478812	63.465153	H	14.941619	3.634586	24.310199
C	12.031150	4.336833	63.582254	H	29.112028	2.134260	23.179464
C	13.063191	5.025817	64.207206	H	19.746049	6.922807	30.328377
O	10.943187	3.908837	64.361307	H	15.687819	4.454478	29.307743
C	31.882275	6.620600	63.346211	H	13.823569	3.680139	30.634325

H	15.671940	6.861193	17.596352	H	46.741435	7.496983	21.164875
H	25.154448	6.226893	21.573023	H	45.516957	7.253832	27.193757
H	25.588187	2.503321	23.019240	H	46.256986	3.316014	24.448204
H	37.729573	2.923017	28.287806	H	50.899304	7.189444	30.296076
H	40.105276	2.296133	28.354902	H	47.064183	4.381611	29.296585
H	41.599653	2.912541	26.526342	H	45.251742	3.491693	30.620892
H	37.157656	5.149807	24.011833	H	46.913432	6.862109	17.595714
H	38.660913	5.703683	22.200319	H	56.056195	5.977057	21.104086
H	35.149746	2.329217	22.590824	H	10.790632	8.127009	42.499923
H	35.298682	1.793659	20.190313	H	9.244380	6.786878	41.130268
H	34.100002	3.170666	18.536477	H	12.055777	2.325928	38.542885
H	32.263784	6.143240	22.826019	H	8.519401	3.171276	38.239590
H	31.124626	7.499402	21.165138	H	20.623084	2.856202	44.069436
H	30.013394	7.566618	27.102752	H	23.009223	2.307558	44.315550
H	43.103971	7.676266	27.047870	H	24.586658	2.808285	42.516192
H	41.667252	6.200184	25.753309	H	20.210880	4.603118	39.571827
H	30.629165	3.591344	24.383162	H	21.790968	5.002146	37.776001
H	44.788725	1.879374	23.155029	H	18.021859	2.102151	37.991103
H	35.813999	6.596638	30.274488	H	18.066417	1.642863	35.575529
H	31.370486	4.844197	29.441648	H	16.948096	3.141913	34.009951
H	29.379786	4.613144	30.805235	H	15.242452	6.052451	38.445256
H	31.292131	6.861252	17.596267	H	14.103617	7.492764	36.860726
H	40.787738	5.746847	21.364101	H	13.169172	7.505300	42.651423
H	41.273254	2.247643	22.863581	H	25.462141	7.874854	42.720454
H	53.551989	3.698260	28.380741	H	24.310465	6.061938	41.587200
H	55.987670	3.325668	28.455557	H	13.612657	3.636577	39.860755
H	57.384070	3.866306	26.497837	H	28.216697	2.008692	39.513177
H	52.703453	5.454609	24.016838	H	18.537279	6.767242	45.804229
H	54.081216	5.976740	22.117071	H	19.580619	7.427872	32.728688
H	50.777334	2.334081	22.588860	H	17.702707	6.589646	34.044028
H	50.920764	1.795168	20.189752	H	14.336793	4.515175	44.860472
H	49.720416	3.170987	18.535916	H	12.425896	3.908791	46.208619
H	47.863901	6.134892	22.823855	H	12.826932	3.472824	32.680995

H	14.166070	7.134696	33.332637	H	49.784762	2.032522	35.573989
H	23.965200	5.091873	37.068454	H	48.469609	3.346803	33.997281
H	24.824411	1.812551	38.920762	H	46.408760	6.066264	38.403483
H	36.079108	3.517404	43.115415	H	45.097545	7.333863	36.806245
H	38.397850	2.687047	43.526468	H	44.087793	7.325903	42.286705
H	40.122701	2.931103	41.803621	H	45.084499	3.174223	39.940056
H	36.105162	4.906558	38.456578	H	49.595498	7.156092	45.774554
H	37.824263	5.107896	36.743235	H	50.669987	7.731505	32.684416
H	31.996563	2.696200	38.518074	H	48.846592	6.779690	34.000231
H	31.895785	1.961836	36.125638	H	45.682392	4.435447	44.848010
H	31.654397	3.604206	34.340636	H	43.834146	3.649765	46.195527
H	31.490760	7.505077	38.355817	H	44.264395	3.231483	32.666414
H	31.121536	9.137658	36.539153	H	45.212837	6.957070	33.281466
H	27.971311	7.929562	42.816933	H	54.726588	5.972575	36.665863
H	41.690171	7.684006	41.916647	H	9.463387	8.127081	58.062891
H	40.374121	6.059996	40.666789	H	7.916952	6.786724	56.693525
H	29.376782	3.808657	40.747702	H	10.728205	2.325409	54.106721
H	43.721546	1.570173	38.744950	H	7.191724	3.170711	53.803441
H	33.468301	8.784102	45.665307	H	19.533167	2.933042	59.265431
H	35.804536	7.236495	32.648072	H	21.931879	2.388170	59.271734
H	33.808443	6.908543	34.011528	H	23.384562	3.173117	57.472776
H	30.537522	5.077012	44.716970	H	18.840510	5.405475	55.143713
H	29.007029	3.703103	46.035339	H	20.301123	6.126899	53.359773
H	28.357284	4.845867	32.838100	H	16.904503	2.481506	53.493713
H	30.964118	8.436359	33.167746	H	16.937138	2.009271	51.083265
H	40.000961	5.031554	36.274095	H	15.723997	3.436829	49.527779
H	40.204290	1.774214	38.294245	H	14.004389	6.348451	53.959528
H	52.223254	3.700825	43.944821	H	12.798631	7.736406	52.378284
H	54.659053	3.326100	44.019118	H	11.840315	7.509332	58.212507
H	56.055350	3.866218	42.061077	H	24.894599	7.981786	58.100432
H	51.375026	5.454186	39.578959	H	23.419955	6.542454	56.801314
H	52.752312	5.975849	37.680109	H	12.285157	3.636351	55.427731
H	49.687660	2.511833	37.983184	H	26.470316	2.313096	53.982256

H	17.168272	6.739750	61.410763	H	50.894910	3.700260	59.506365
H	18.395550	7.383039	48.179043	H	53.331583	3.325667	59.581355
H	16.457966	6.732738	49.512230	H	54.727850	3.865772	57.623149
H	13.130146	4.375178	60.400585	H	50.047656	5.459292	55.145088
H	11.277957	3.574249	61.719288	H	51.424886	5.977024	53.243008
H	11.428219	3.818089	48.263196	H	48.420912	2.756581	53.490137
H	12.818151	7.343202	48.853898	H	48.513498	2.284436	51.081685
H	22.413837	6.286441	52.500382	H	47.155808	3.565310	49.518140
H	22.943912	2.660514	53.829720	H	45.130150	6.297301	53.934969
H	35.108793	3.113718	59.331062	H	43.783008	7.540045	52.344924
H	37.490291	2.503409	59.366450	H	42.918208	7.351888	58.288753
H	38.960859	3.152616	57.530073	H	43.579440	3.528085	55.363949
H	34.491456	5.457735	55.126372	H	48.405507	6.744903	61.407849
H	35.970167	6.041997	53.303596	H	49.391567	7.759244	48.148741
H	32.746110	2.732233	53.476170	H	47.533110	6.912869	49.484554
H	33.007720	2.387898	51.057080	H	44.381244	4.364549	60.399383
H	31.817910	3.804369	49.467570	H	42.519286	3.571724	61.717700
H	29.538991	6.349796	53.872972	H	42.827685	3.496648	48.243704
H	28.326923	7.698463	52.254920	H	43.836747	7.124644	48.823663
H	27.304708	7.522628	58.211737	H	53.398784	5.971494	52.227924
H	40.514046	7.822937	58.169903	H	17.068217	7.158091	63.835995
H	39.045217	6.421052	56.831034	H	15.148116	6.357243	65.155558
H	27.971066	3.709289	55.278258	H	10.263079	3.421937	63.797036
H	42.076273	2.156505	54.042280	H	32.687728	7.158939	63.834930
H	32.786132	6.743319	61.409029	H	30.767907	6.357413	65.154640
H	33.307805	9.108019	48.147756	H	25.881464	3.424920	63.795559
H	31.874742	7.661545	49.505603	H	48.307483	7.159191	63.833745
H	28.750249	4.373400	60.400225	H	46.387708	6.357409	65.153469
H	26.897922	3.574187	61.718490	H	41.500989	3.425592	63.794352
H	28.172421	3.254041	48.043832	H	54.922555	4.682833	55.325794
H	28.572442	7.407657	48.722924	H	56.250099	4.683168	39.763715
H	38.084611	6.086848	52.432575	H	57.578898	4.683439	24.200629
H	38.561066	2.570087	53.821063	H	32.654297	5.043409	18.026509

H	17.034831	5.043615	18.026680	H	40.270886	6.090198	43.992394
H	10.176551	4.915316	24.089663	H	38.992725	4.980974	45.848182
H	8.848005	4.915598	39.653323	H	36.492047	5.150674	45.867197
H	7.520594	4.915631	55.216384	H	35.295597	6.357993	44.099507
H	12.998948	5.199014	65.269016	H	37.085463	8.148999	41.382075
H	28.618753	5.199038	65.268137	H	33.961202	5.941906	40.056400
H	44.238607	5.198880	65.267019				
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C	35.119988	8.201373	42.128675	(S,S)-1-TS3			
C	34.627035	8.747348	40.754098	C	12.487000	7.261000	26.395000
C	35.368574	10.047229	40.373512	C	11.616000	6.503000	25.622000
C	35.261342	11.112646	41.470719	C	12.086000	5.395000	24.927000
C	35.751413	10.569302	42.820815	C	13.428000	5.043000	25.007000
C	34.990419	9.295101	43.207720	C	13.027000	3.179000	23.539000
O	33.268413	9.016597	40.824209	C	11.685000	3.529000	23.460000
C	37.098617	6.971102	43.035132	C	11.215000	4.638000	24.154000
C	38.508224	6.869764	43.038206	O	10.782000	2.793000	22.654000
C	39.178123	6.155851	44.028999	Cu	18.543745	6.084628	26.025203
C	38.467110	5.532492	45.062825	Cu	17.955154	3.694834	26.529620
C	37.071589	5.633353	45.072734	C	22.226423	3.962421	26.387934
C	36.386586	6.334711	44.077501	C	22.759067	3.167184	27.419209
N	36.463038	7.652068	42.009161	C	24.114818	2.865077	27.460077
H	34.939955	10.413693	39.424289	C	24.963950	3.344431	26.468350
H	34.853932	7.981567	39.984913	C	24.471319	4.116310	25.399536
H	34.448206	7.364783	42.385427	C	23.083082	4.414799	25.343066
H	34.202174	11.411137	41.563981	C	22.584778	5.122671	24.228122
H	35.832681	12.014826	41.182737	C	23.446196	5.563145	23.228238
H	36.836340	10.349277	42.763264	C	24.813124	5.310017	23.303514
H	35.630568	11.333178	43.610627	C	25.337343	4.576323	24.376333
H	33.918153	9.520631	43.326046	O	25.660918	5.752711	22.294037
H	35.356986	8.902070	44.172295	O	20.436502	5.523343	26.199554
H	36.433833	9.815546	40.168258	O	19.921840	3.373913	26.649572
H	39.073020	7.369521	42.244032	C	20.775898	4.306267	26.421165
				C	18.226927	4.022014	22.293999

C	18.992915	2.941012	21.873981	O	17.902604	4.247107	28.434779
C	19.081890	2.638017	20.519979	C	18.100407	5.459457	28.806085
C	18.404876	3.417023	19.587993	Cu	34.196480	6.078976	26.036156
C	17.639888	4.497024	20.008011	Cu	33.622835	3.692529	26.568353
C	17.550913	4.800019	21.362013	C	37.879145	3.921306	26.343956
C	16.783924	5.881020	21.784030	C	38.410104	3.189947	27.422751
C	16.107910	6.659026	20.850045	C	39.754285	2.842498	27.457563
C	16.197885	6.355031	19.497042	C	40.593076	3.211965	26.412618
C	16.963875	5.274030	19.076025	C	40.101349	3.921958	25.300831
O	15.523872	7.185037	18.539057	C	38.723582	4.266205	25.252073
O	18.565471	5.530824	24.116544	C	38.222545	4.913178	24.103276
O	18.026509	3.388288	24.574537	C	39.073491	5.241540	23.051978
C	18.266838	4.337436	23.747107	C	40.433955	4.948756	23.118172
C	14.301000	5.801000	25.782000	C	40.960825	4.283707	24.234091
C	13.829000	6.909000	26.476000	O	41.273324	5.292967	22.064416
C	28.026948	7.145762	26.533147	O	36.099288	5.500449	26.125423
C	27.180609	6.295099	25.830245	O	35.582304	3.364663	26.636466
C	27.679885	5.166472	25.149126	C	36.435603	4.285819	26.373665
C	29.074044	4.893815	25.199790	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.724496	2.985350	23.738363	C	34.701781	2.637978	20.519678
C	27.360070	3.218514	23.711011	C	34.024753	3.416989	19.587708
C	26.812214	4.312639	24.417658	C	33.259776	4.496991	20.007741
O	26.583595	2.322781	22.978987	C	33.170826	4.799983	21.361747
O	16.596689	6.401801	25.859048	C	32.403848	5.880986	21.783781
O	16.057099	4.260822	26.320553	C	31.727821	6.658997	20.849810
C	15.736473	5.459892	25.988374	C	31.817771	6.355005	19.496805
C	17.921302	5.795579	30.246473	C	32.583748	5.274002	19.075771
C	18.913201	6.557058	30.891507	O	31.143743	7.185016	18.538835
C	16.779324	5.369772	30.982870	O	34.146693	5.534177	24.124971
C	15.704860	4.696775	30.363093	O	33.647075	3.386634	24.594708
C	14.605134	4.284601	31.109846	C	33.871502	4.335427	23.757424
O	18.430608	6.394897	27.990603	C	29.927424	5.740576	25.962458

C	29.387397	6.873722	26.597258	O	56.643771	5.617805	21.841785
C	43.530883	6.874652	26.489569	O	51.637566	5.839302	26.123955
C	42.726876	6.018173	25.748400	O	51.334307	3.663575	26.640401
C	43.269488	4.904908	25.073591	C	52.092902	4.668399	26.382631
C	44.667060	4.658940	25.163916	C	49.466779	4.021876	22.293156
C	29.581495	3.805382	24.461356	C	50.232745	2.940872	21.873104
C	44.396782	2.750174	23.688063	C	50.321669	2.637885	20.519096
C	43.029819	2.963981	23.611864	C	49.644627	3.416901	19.587140
C	42.440245	4.044153	24.306486	C	48.879661	4.496905	20.007192
O	42.292515	2.057328	22.853725	C	48.790737	4.799893	21.361200
O	32.226982	6.400781	25.972316	C	48.023772	5.880897	21.783251
O	31.725216	4.251074	26.432050	C	47.347731	6.658913	20.849295
C	31.378888	5.449226	26.132342	C	47.437655	6.354926	19.496287
C	33.879229	5.799555	30.286144	C	48.203620	5.273922	19.075235
C	35.033473	6.358673	30.864230	O	46.763613	7.184943	18.538331
C	32.722801	5.601601	31.088846	O	49.731827	5.592331	24.089762
C	31.520722	5.110801	30.541178	O	49.388174	3.426874	24.609531
C	30.394669	4.955576	31.345963	C	49.526603	4.369432	23.750063
O	34.191609	6.388090	28.001376	C	45.480562	5.528008	25.942645
O	33.635586	4.254218	28.481732	C	44.894251	6.635973	26.581984
C	33.904798	5.458705	28.837724	C	45.216554	3.579624	24.444325
Cu	49.694961	6.208051	25.983486	O	47.715241	6.340048	25.881976
Cu	49.343813	3.790887	26.565516	O	47.394062	4.171938	26.414236
C	53.571003	4.464792	26.367939	C	46.949235	5.331476	26.085776
C	54.157058	3.947774	27.515902	C	49.186785	5.999087	30.218599
C	55.530059	3.732759	27.559826	C	50.123912	6.849756	30.833115
C	56.316002	4.036762	26.454787	C	48.075512	5.524605	30.971057
C	55.729946	4.554780	25.305823	C	47.052779	4.754305	30.377764
C	54.356947	4.768795	25.262899	C	45.981030	4.298224	31.139076
C	53.770890	5.287813	24.113936	O	49.603283	6.569851	27.939115
C	54.557834	5.591815	23.007897	O	49.291502	4.396169	28.457135
C	55.929834	5.377800	23.052821	C	49.379621	5.633393	28.788025
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133

C	10.287269	6.502976	41.186145	O	14.103159	7.457929	34.311095
C	10.757253	5.394976	40.491133	O	17.240389	5.397025	39.627972
C	12.099253	5.042971	40.571108	O	16.624286	3.271952	40.065856
C	11.698221	3.178978	39.103109	C	16.901252	4.220004	39.245484
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.256355	6.494513	43.000095
Cu	17.253807	5.931767	41.539125	C	25.579180	5.690791	42.106818
Cu	16.566515	3.568420	42.036519	C	26.243431	4.726694	41.280744
C	20.841009	3.625980	41.973308	C	27.678271	4.614970	41.412665
C	21.286309	2.831790	43.046733	C	12.571237	3.934972	39.877096
C	22.621315	2.463021	43.158656	C	27.666520	2.901525	39.685516
C	23.539640	2.881590	42.202355	C	26.255720	2.995921	39.554773
C	23.137291	3.655614	41.099122	C	25.537152	3.901355	40.330862
C	21.766442	4.006332	40.960960	O	25.742741	2.136488	38.629731
C	21.354373	4.699818	39.804779	O	15.305397	6.339832	41.402521
C	22.284615	5.069726	38.837947	O	14.695189	4.218409	41.858939
C	23.637256	4.786072	39.004605	C	14.409507	5.430632	41.544770
C	24.077374	4.086148	40.134172	C	16.663876	5.669070	45.759444
O	24.554151	5.176370	38.037200	C	17.697885	6.391747	46.383330
O	19.128530	5.272502	41.695008	C	18.819190	6.851028	32.245973
O	18.509323	3.152874	42.154793	C	17.730059	6.396273	32.981045
C	19.408472	4.042571	41.939585	C	16.697664	5.658269	32.371549
C	16.819145	3.949858	37.784119	C	15.503186	5.324490	46.508224
C	17.460800	2.808271	37.271143	C	14.395787	4.686590	45.910240
C	17.471200	2.550404	35.906657	C	13.278110	4.354281	46.669851
C	16.837466	3.424317	35.030091	C	14.543817	4.525849	32.480055
C	16.151872	4.562823	35.500959	C	15.578589	5.219543	33.121797
C	16.125259	4.820221	36.898075	O	13.438728	4.108101	33.213329
C	15.381864	5.919033	37.374313	O	17.176871	6.236566	43.502607
C	14.721391	6.758624	36.486021	O	16.550386	4.115798	43.948037
C	14.770570	6.540348	35.119296	C	16.809942	5.317367	44.319361
C	15.494215	5.442783	34.601354	Cu	33.543014	6.427878	41.519696

Cu	32.492640	3.946990	42.099887	C	41.996899	5.159893	40.457568
C	36.673833	3.647046	41.587373	C	43.398983	4.939200	40.530454
C	37.172790	2.660473	42.415937	C	28.359510	3.685290	40.572403
C	38.534853	2.292767	42.326467	C	43.185886	3.227801	38.821536
C	39.369979	2.911511	41.420460	C	41.815238	3.419382	38.757504
C	38.888044	3.907193	40.508419	C	41.201564	4.385134	39.578474
C	37.493398	4.252413	40.578052	O	41.101114	2.607988	37.880385
C	36.967230	5.163695	39.617468	O	30.301291	6.658154	42.900097
C	37.781185	5.731648	38.667095	O	30.553819	4.535914	42.216365
C	39.176114	5.460123	38.641349	C	29.829536	5.509369	42.467782
C	39.733010	4.559659	39.547219	C	32.616778	5.989047	45.745105
O	39.970409	6.081272	37.725589	C	33.485559	6.891484	46.331146
O	35.155960	5.405242	41.895967	C	35.072933	6.675458	32.216170
O	34.347139	3.307847	41.916711	C	33.954229	6.458247	33.012529
C	35.285830	4.151485	41.812788	C	32.765551	5.935643	32.469869
C	32.461700	4.190176	37.950604	C	31.498157	5.460931	46.473780
C	32.621298	2.890582	37.499993	C	30.523549	4.611422	45.876690
C	32.515414	2.608991	36.122518	C	29.435191	4.167934	46.588306
C	32.223571	3.615818	35.225777	C	30.438648	5.267107	32.703769
C	31.996473	4.966877	35.645886	C	31.618752	5.753904	33.275434
C	32.121670	5.253055	37.052038	O	29.306768	5.106810	33.492759
C	31.859216	6.579112	37.509024	O	33.089446	6.573919	43.508534
C	31.503006	7.563211	36.622190	O	32.733000	4.410376	43.982157
C	31.402371	7.299673	35.228971	C	32.844817	5.623460	44.316204
C	31.650853	6.024034	34.731607	Cu	48.411324	6.335883	41.580153
O	31.061114	8.399793	34.492502	Cu	48.006528	3.899828	42.041708
O	33.403649	5.433743	39.730524	C	52.242278	4.464620	41.931334
O	32.153896	3.632742	40.219140	C	52.828353	3.947597	43.079285
C	32.688107	4.452442	39.402213	C	54.201353	3.732577	43.123183
C	28.357061	5.488072	42.335198	C	54.987278	4.036581	42.018131
C	27.653731	6.409059	43.105094	C	54.401203	4.554604	40.869180
C	42.198388	6.939114	42.113898	C	53.028203	4.768624	40.826281
C	41.419768	6.158786	41.267193	C	52.442128	5.287648	39.677330

C	53.229054	5.591652	38.571278	C	45.677560	4.778986	45.907932
C	54.601054	5.377632	38.616177	C	44.582533	4.349038	46.651475
C	55.187129	4.858609	39.764128	C	45.899920	4.586854	32.498977
O	55.314970	5.617639	37.405129	C	46.883066	5.373840	33.114369
O	50.346982	5.902366	41.722175	O	44.825683	4.120439	33.248260
O	49.985782	3.720651	42.173043	O	48.308400	6.603180	43.545492
C	50.770712	4.711690	41.952046	O	47.906688	4.422037	43.960161
C	48.259825	4.348090	37.799499	C	48.037926	5.639670	44.347794
C	49.046013	3.292587	37.303019	C	9.830848	7.260896	57.522290
C	49.100539	3.023490	35.942460	C	8.959816	6.502907	56.749315
C	48.366571	3.798559	35.052251	C	9.429783	5.394908	56.054291
C	47.544183	4.851247	35.504162	C	10.771783	5.042898	56.134241
C	47.477160	5.121920	36.897824	C	10.370718	3.178911	54.666243
C	46.606222	6.131638	37.354233	C	9.028718	3.528920	54.587293
C	45.859482	6.876910	36.450150	C	8.558750	4.637919	55.281317
C	45.939375	6.644259	35.087130	O	8.125684	2.792932	53.781319
C	46.787688	5.629866	34.588606	Cu	15.897896	6.120821	57.131618
O	45.175571	7.467337	34.262587	Cu	15.336931	3.711069	57.558430
O	48.454566	5.827249	39.659799	C	19.596053	4.011068	57.433823
O	48.119921	3.635220	40.071554	C	20.148698	3.246022	58.477005
C	48.278921	4.619334	39.262908	C	21.501318	2.928426	58.488988
C	44.184728	5.719036	41.423509	C	22.325305	3.359982	57.455016
C	43.568289	6.726456	42.187384	C	21.810422	4.103286	56.375947
C	43.980463	3.970296	39.689092	C	20.425939	4.420789	56.352318
O	46.431333	6.514312	41.465222	C	19.902729	5.105607	55.234947
O	46.070373	4.319934	41.844819	C	20.737057	5.494726	54.191588
C	45.648421	5.504484	41.585168	C	22.102032	5.221604	54.231619
C	47.851063	5.958187	45.789994	C	22.650951	4.519579	55.313577
C	48.811542	6.763797	46.429715	O	22.923607	5.618083	53.182259
C	50.006244	7.189639	32.175110	O	17.799158	5.570627	57.294952
C	48.947331	6.692402	32.926982	O	17.301333	3.402809	57.674399
C	47.970031	5.861390	32.347108	C	18.146843	4.348981	57.480294
C	46.716720	5.508959	46.522477	C	15.635734	4.186980	53.326604

C	16.331252	3.071318	52.825960	C	13.166040	4.552842	61.469196
C	16.347120	2.792238	51.466684	C	12.083075	4.099846	62.213249
C	15.663671	3.617424	50.581785	C	13.231259	4.641660	48.031731
C	14.935356	4.735838	51.037450	C	14.298994	5.305730	48.651155
C	14.907335	5.017497	52.430305	O	12.108925	4.300121	48.778124
C	14.124641	6.094727	52.891743	O	15.767132	6.369002	59.105877
C	13.428672	6.893125	51.992552	O	15.278838	4.200034	59.482510
C	13.476222	6.651253	50.629567	C	15.449810	5.404643	59.893142
C	14.233507	5.569125	50.126274	Cu	31.471283	6.151134	57.128789
O	12.776332	7.534106	49.810157	Cu	30.968047	3.726701	57.544005
O	15.943900	5.630140	55.204111	C	35.213133	4.096769	57.450120
O	15.427075	3.468235	55.587291	C	35.756124	3.370492	58.526006
C	15.671986	4.444651	54.791855	C	37.101379	3.025898	58.548157
C	11.644816	5.800887	56.909216	C	37.927736	3.389053	57.490981
C	11.172849	6.908886	57.603240	C	37.424444	4.098089	56.383583
C	25.305808	7.080196	57.511011	C	36.047474	4.448351	56.352825
C	24.473453	6.237417	56.784377	C	35.535620	5.104967	55.214439
C	24.986657	5.121937	56.091473	C	36.373794	5.429271	54.151794
C	26.382516	4.858330	56.148824	C	37.732044	5.122147	54.195792
C	11.243751	3.934900	55.440217	C	38.270581	4.450871	55.302691
C	26.057438	2.973778	54.651592	O	38.557446	5.456828	53.128357
C	24.690876	3.196467	54.619054	O	33.391231	5.633829	57.269226
C	24.129730	4.273186	55.341805	O	32.932133	3.460186	57.664984
O	23.925683	2.304279	53.871185	C	33.760390	4.419647	57.470142
O	13.942982	6.423541	56.972252	C	31.317174	4.225324	53.308070
O	13.431126	4.265426	57.376645	C	32.069849	3.132759	52.839124
C	13.091584	5.470735	57.087776	C	32.176407	2.868610	51.480713
C	15.283046	5.695821	61.352095	C	31.524855	3.683071	50.562683
C	16.314087	6.385804	61.978046	C	30.734157	4.770723	50.983452
C	17.620819	6.733487	47.727042	C	30.620455	5.043747	52.374332
C	16.506742	6.366970	48.472752	C	29.789413	6.101882	52.792827
C	15.437433	5.663102	47.886671	C	29.126617	6.886733	51.854582
C	14.198081	5.242825	62.095148	C	29.251662	6.646306	50.496364

C	30.054526	5.582132	50.042344	Cu	47.046876	6.244771	57.146035
O	28.573770	7.504456	49.634878	Cu	46.685888	3.789404	57.533326
O	31.510837	5.678489	55.195010	C	50.914829	4.464394	57.493750
O	31.070768	3.498349	55.567364	C	51.500923	3.947364	58.641689
C	31.292033	4.484778	54.775933	C	52.873923	3.732339	58.685563
C	27.222289	5.698734	56.933131	C	53.659830	4.036343	57.580498
C	26.666341	6.815642	57.583803	C	53.073736	4.554373	56.431559
C	40.906433	6.953486	57.579390	C	51.700736	4.768398	56.388685
C	40.082855	6.128407	56.825685	C	51.114643	5.287428	55.239746
C	40.601415	5.023249	56.119726	C	51.901549	5.591433	54.133681
C	41.997267	4.756158	56.185628	C	53.273549	5.377407	54.178555
C	26.903589	3.787248	55.395413	C	53.859642	4.858378	55.326493
C	41.679479	2.888664	54.667172	O	53.987445	5.617415	52.967495
C	40.314075	3.119407	54.619003	O	48.988758	5.856156	57.297108
C	39.748653	4.190745	55.347030	O	48.672692	3.652270	57.668144
O	39.553673	2.236007	53.856174	C	49.437046	4.670276	57.496493
O	29.500645	6.410340	56.999849	C	46.948042	4.351163	53.311961
O	29.054299	4.230742	57.366361	C	47.754511	3.318855	52.798914
C	28.678025	5.430217	57.106834	C	47.791581	3.052822	51.437660
C	30.903120	5.695641	61.351269	C	47.020324	3.808276	50.562995
C	31.934175	6.385618	61.977205	C	46.184083	4.843434	51.030717
C	33.317831	7.258489	47.683387	C	46.134902	5.110430	52.425791
C	32.273567	6.745523	48.422030	C	45.250489	6.099922	52.899251
C	31.316539	5.844507	47.850973	C	44.473138	6.830818	52.009314
C	29.818167	5.242646	62.094340	C	44.536298	6.604093	50.644245
C	28.786113	4.552669	61.468405	C	45.397754	5.608818	50.128823
C	27.703159	4.099675	62.212476	O	43.748424	7.419503	49.835034
C	29.268595	4.508530	47.957057	O	47.117584	5.792499	55.209342
C	30.198314	5.330623	48.591538	O	46.809183	3.585788	55.560877
O	28.200667	4.027260	48.650299	C	46.958748	4.592479	54.780019
O	31.360699	6.384435	59.105364	C	42.831914	5.591567	56.980083
O	30.900210	4.207725	59.472521	C	42.265892	6.690511	57.654119
C	31.061877	5.412149	59.889410	C	42.522028	3.691581	55.427095

O	45.071845	6.390901	57.016861	C	44.303437	5.025398	64.205349
O	44.739126	4.185892	57.350780	O	42.183431	3.908432	64.359519
C	44.300179	5.371003	57.117171	H	12.119148	8.126810	26.936120
C	46.523195	5.695406	61.350162	H	10.573014	6.786735	25.566630
C	47.554262	6.385378	61.976082	H	13.382386	2.322459	22.982829
C	48.688708	7.091127	47.773434	H	9.847434	3.169537	22.676425
C	47.601258	6.626197	48.503116	H	22.112669	2.794756	28.206186
C	46.604856	5.833881	47.901067	H	24.512619	2.260096	28.268547
C	45.438253	5.242413	62.093251	H	26.014507	3.094851	26.534698
C	44.406185	4.552442	61.467332	H	21.528494	5.332980	24.100960
C	43.323243	4.099449	62.211421	H	23.039831	6.107683	22.386783
C	44.494387	4.623994	48.014044	H	19.532688	2.330022	22.589848
C	45.494098	5.372795	48.650430	H	19.679862	1.794462	20.190459
O	43.396636	4.183833	48.744765	H	18.480883	3.171000	18.536739
O	46.917259	6.441458	59.120646	H	16.654327	6.146537	22.827181
O	46.573581	4.237225	59.462108	H	15.507586	7.501999	21.163878
C	46.674407	5.442568	59.890041	H	14.495376	7.507694	27.088221
C	16.262162	6.620790	63.347051	H	27.623029	8.018080	27.036642
C	15.179196	6.168795	64.090104	H	26.127484	6.537312	25.807224
C	14.147156	5.478812	63.465153	H	14.941235	3.633099	24.313726
C	12.031150	4.336833	63.582254	H	29.121591	2.148191	23.179833
C	13.063191	5.025817	64.207206	H	19.774588	6.909420	30.334938
O	10.943187	3.908837	64.361307	H	15.688550	4.492904	29.297734
C	31.882275	6.620600	63.346211	H	13.795482	3.768545	30.612046
C	30.799322	6.168606	64.089282	H	15.672671	6.862191	17.596195
C	29.767267	5.478629	63.464346	H	25.174866	6.290762	21.592224
C	27.651260	4.336658	63.581482	H	25.604408	2.552462	22.985858
C	28.683314	5.025635	64.206417	H	37.770052	2.897221	28.247785
O	26.563309	3.908663	64.360554	H	40.150357	2.285358	28.300562
C	47.502389	6.620356	63.345091	H	41.634369	2.925395	26.472890
C	46.419447	6.168363	64.088179	H	37.172333	5.163482	23.994539
C	45.387379	5.478391	63.463260	H	38.666053	5.738526	22.182129
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H 35.298906 1.793801 20.190345	H 9.244397 6.786902 41.130389
H 34.100153 3.170629 18.536537	H 12.054461 2.325295 38.542955
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H 31.125227 7.500300 21.163927	H 20.586915 2.511043 43.811131
H 30.031340 7.539574 27.160797	H 22.949460 1.857157 43.997401
H 43.093417 7.731549 26.991680	H 24.573217 2.582379 42.323570
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H 30.640272 3.577838 24.415624	H 21.944030 5.596452 37.956464
H 44.825122 1.919425 23.143311	H 17.969364 2.123521 37.940457
H 35.913928 6.535862 30.256458	H 17.978216 1.670758 35.523557
H 31.433810 4.851015 29.489928	H 16.870109 3.191490 33.975123
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H 31.289170 6.859474 17.596510	H 14.155709 7.601935 36.859275
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H 50.777472 2.335022 22.589426	H 17.691827 6.639685 34.034354
H 50.920784 1.795168 20.189799	H 14.368535 4.447009 44.852694
H 49.720299 3.170770 18.535993	H 12.443505 3.862370 46.189099
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H 46.741365 7.497413 21.163709	H 14.148626 7.226855 33.333251
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H 46.279163 3.364643 24.443962	H 24.785676 2.238248 38.511163
H 50.958929 7.239961 30.261924	H 36.517035 2.198772 43.159196
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H 45.210319 3.708350 30.661812	H 40.424337 2.618844 41.393514
H 46.907005 6.857885 17.596269	H 35.902588 5.403836 39.613636
H 56.056812 5.973990 21.102092	H 37.354543 6.417538 37.925235
H 10.790573 8.126876 42.500115	H 32.852312 2.099435 38.217737

H	32.669451	1.586808	35.762584	H	45.686905	4.540355	44.849829
H	32.154927	3.355111	34.164754	H	43.799161	3.789692	46.158278
H	31.931686	6.818024	38.572670	H	44.200952	3.541023	32.707483
H	31.292982	8.580347	36.963538	H	45.248414	7.225068	33.289290
H	28.194789	7.069056	43.785160	H	54.726624	5.966808	36.663025
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H	40.356362	6.356361	41.238202	H	7.917028	6.786919	56.693476
H	29.443685	3.596821	40.616960	H	10.726918	2.324704	54.106920
H	43.638737	2.485022	38.177777	H	7.193561	3.175391	53.796565
H	34.301657	7.312311	45.738759	H	19.519776	2.905246	59.291912
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H	30.948219	8.196461	33.550775	H	16.891664	1.930301	51.094878
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H	40.113913	2.815201	37.862054	H	14.027098	6.331786	53.945021
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H	54.659244	3.327408	44.019610	H	11.840698	7.508839	58.212464
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H	51.374936	5.456069	39.580968	H	23.419896	6.476120	56.753681
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H	49.630126	2.682863	37.983403	H	26.464785	2.149694	54.081142
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H	48.433867	3.555859	34.001356	H	18.429783	7.285091	48.195205
H	46.476677	6.353947	38.407253	H	16.480301	6.650686	49.516152
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H	45.048539	3.779335	39.680014	H	11.425342	3.794407	48.234630
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H	50.741712	7.839740	32.637864	H	22.423952	6.142317	52.479444
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H	35.122568	3.072275	59.353933	H	43.800769	7.593009	52.380214
H	37.506612	2.469657	59.387168	H	42.893347	7.347267	58.246495
H	38.968539	3.098472	57.537998	H	43.582318	3.469295	55.395381
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H	35.958367	5.932646	53.289353	H	49.439708	7.710099	48.253534
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H	32.769928	2.028127	51.135132	H	44.382319	4.362982	60.399598
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H	29.629228	6.332517	53.840615	H	42.760416	3.631048	48.189458
H	28.495486	7.702184	52.183157	H	43.807092	7.180239	48.860236
H	27.299034	7.476246	58.166180	H	53.398691	5.964446	52.224631
H	40.487098	7.804222	58.106645	H	17.068467	7.157627	63.836112
H	39.031308	6.373372	56.786219	H	15.148261	6.357127	65.155563
H	27.964527	3.569263	55.353486	H	10.261794	3.422546	63.798060
H	42.089367	2.068501	54.092927	H	32.688187	7.158113	63.835107
H	32.787645	6.739954	61.409294	H	30.768112	6.357258	65.154654
H	34.016516	7.963509	48.143334	H	25.879138	3.427455	63.796198
H	32.167982	7.056639	49.465933	H	48.307476	7.159243	63.833715
H	28.750397	4.373292	60.400134	H	46.387827	6.357481	65.153435
H	26.898021	3.573739	61.718725	H	41.497996	3.429485	63.794642
H	27.668963	3.449399	48.079090	H	54.922501	4.682764	55.325505
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H	38.068398	5.966847	52.407695	H	57.578861	4.683541	24.200338
H	38.578021	2.478136	53.831569	H	32.654191	5.043642	18.026515
H	50.894859	3.699634	59.506114	H	17.034722	5.043892	18.026656
H	53.331526	3.325361	59.581251	H	10.176539	4.915037	24.089471
H	54.727797	3.865607	57.623223	H	8.847951	4.915251	39.653274
H	50.047792	5.460857	55.146018	H	7.520537	4.915276	55.216414
H	51.425188	5.977967	53.243217	H	12.998675	5.198814	65.268994
H	48.361298	2.719102	53.468201	H	28.618505	5.198903	65.268105
H	48.419886	2.254363	51.056550	H	44.238351	5.198855	65.266963
H	47.070539	3.563759	49.511705	H	48.273823	5.043387	18.026057
H	45.135423	6.318110	53.954915	C	31.886569	8.858477	41.380104

C	33.059683	9.517926	42.180381	C	11.616000	6.503000	25.622000
C	34.266924	9.812256	41.272571	C	12.086000	5.395000	24.927000
C	33.901929	10.613068	40.014822	C	13.428000	5.043000	25.007000
C	32.775104	9.920674	39.236218	C	13.027000	3.179000	23.539000
C	31.551051	9.699182	40.132034	C	11.685000	3.529000	23.460000
O	32.155237	7.548263	40.982897	C	11.215000	4.638000	24.154000
C	31.805657	10.661831	44.014857	O	10.782000	2.793000	22.654000
C	31.173366	11.840573	44.474566	Cu	18.544657	6.086847	26.011838
C	30.384948	11.831032	45.625102	Cu	17.950219	3.699582	26.527281
C	30.195417	10.651423	46.357851	C	22.213101	3.946373	26.371435
C	30.811954	9.479505	45.906767	C	22.754432	3.183026	27.421450
C	31.600828	9.474083	44.754241	C	24.106613	2.865353	27.448754
N	32.623980	10.707553	42.892537	C	24.942321	3.299538	26.425153
H	35.046498	10.324248	41.864554	C	24.438481	4.040247	25.338854
H	33.387424	8.796402	42.940795	C	23.053088	4.350069	25.295549
H	31.002439	8.877650	42.050086	C	22.539841	5.020365	24.164413
H	34.797693	10.738113	39.379195	C	23.386322	5.414177	23.132859
H	33.583587	11.638469	40.295080	C	24.752966	5.155545	23.195958
H	32.497801	10.513984	38.345153	C	25.290459	4.459686	24.287199
H	33.133205	8.941650	38.870671	O	25.587320	5.555548	22.157981
H	31.144117	10.676378	40.461097	O	20.435583	5.519026	26.184977
H	30.745899	9.184487	39.579092	O	19.911961	3.373179	26.646393
H	34.696118	8.842466	40.951858	C	20.768189	4.300789	26.411849
H	31.312466	12.774337	43.917031	C	18.226927	4.022014	22.293999
H	29.911547	12.762744	45.954201	C	18.992915	2.941012	21.873981
H	29.580329	10.647972	47.262872	C	19.081890	2.638017	20.519979
H	30.690170	8.540965	46.458790	C	18.404876	3.417023	19.587993
H	32.054821	8.537322	44.434014	C	17.639888	4.497024	20.008011
H	31.272204	6.747687	42.736572	C	17.550913	4.800019	21.362013
H	32.536076	11.549316	42.333664	C	16.783924	5.881020	21.784030
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(S,S)-1-PC				C	16.197885	6.355031	19.497042
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O	15.523872	7.185037	18.539057	C	38.674796	4.256217	25.353390
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C	13.829000	6.909000	26.476000	O	41.263732	5.298871	22.203316
C	27.948477	7.043110	26.461752	O	36.023353	5.460258	26.200392
C	27.113367	6.192079	25.746505	O	35.519212	3.307500	26.650730
C	27.624136	5.066713	25.067337	C	36.367357	4.244384	26.430372
C	29.018834	4.801668	25.127821	C	33.846854	4.021972	22.293718
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C	27.327226	3.124608	23.615977	C	34.024753	3.416989	19.587708
C	26.767237	4.209626	24.327221	C	33.259776	4.496991	20.007741
O	26.561293	2.225234	22.877138	C	33.170826	4.799983	21.361747
O	16.596783	6.403796	25.846423	C	32.403848	5.880986	21.783781
O	16.055675	4.265545	26.320299	C	31.727821	6.658997	20.849810
C	15.736287	5.462774	25.983508	C	31.817771	6.355005	19.496805
C	17.914128	5.826234	30.224939	C	32.583748	5.274002	19.075771
C	18.899791	6.600533	30.863600	O	31.143743	7.185016	18.538835
C	16.768491	5.408757	30.958589	O	34.118269	5.507784	24.152021
C	15.698490	4.725991	30.341237	O	33.621417	3.349625	24.575160
C	14.599493	4.313681	31.088519	C	33.852430	4.314726	23.759724
O	18.432698	6.406603	27.971453	C	29.858817	5.645596	25.906942
O	17.901209	4.261797	28.428299	C	29.307972	6.773552	26.541203
C	18.099155	5.476826	28.790849	C	43.544936	6.889820	26.556471
Cu	34.117229	6.018443	26.073685	C	42.721937	6.019457	25.852836
Cu	33.558217	3.616324	26.548595	C	43.248724	4.899277	25.176927
C	37.814939	3.897963	26.428169	C	44.649094	4.657770	25.230971
C	38.333690	3.168585	27.513757	C	29.539849	3.724863	24.382177
C	39.680878	2.835973	27.572566	C	44.343092	2.728090	23.790308
C	40.534321	3.216510	26.543009	C	42.974028	2.937305	23.749819
C	40.054396	3.922633	25.423592	C	42.401691	4.028788	24.441171

O	42.218084	2.019875	23.023204	C	48.790737	4.799893	21.361200
O	32.149680	6.320601	25.965074	C	48.023772	5.880897	21.783251
O	31.658216	4.159785	26.383766	C	47.347731	6.658913	20.849295
C	31.307752	5.359658	26.094971	C	47.437655	6.354926	19.496287
C	33.658391	5.655617	30.307586	C	48.203620	5.273922	19.075235
C	34.722508	6.348606	30.913348	O	46.763613	7.184943	18.538331
C	32.525544	5.296422	31.090187	O	49.734421	5.592870	24.087003
C	31.393200	4.683819	30.515168	O	49.385505	3.428955	24.610047
C	30.292652	4.359450	31.303890	C	49.526582	4.370138	23.749425
O	34.052561	6.290199	28.044388	C	45.481739	5.538830	25.974493
O	33.525649	4.137728	28.468786	C	44.911096	6.655648	26.612325
C	33.751965	5.341345	28.854574	C	45.181533	3.571996	24.508544
Cu	49.698256	6.211339	25.978573	O	47.718272	6.344711	25.879681
Cu	49.345783	3.795419	26.565743	O	47.397080	4.178879	26.421239
C	53.571003	4.464792	26.367939	C	46.951935	5.338453	26.094163
C	54.157058	3.947774	27.515902	C	49.207051	6.011871	30.212739
C	55.530059	3.732759	27.559826	C	50.146400	6.867050	30.817072
C	56.316002	4.036762	26.454787	C	48.102856	5.537099	30.974181
C	55.729946	4.554780	25.305823	C	47.075993	4.765249	30.390016
C	54.356947	4.768795	25.262899	C	46.013858	4.304521	31.161665
C	53.770890	5.287813	24.113936	O	49.609673	6.577494	27.931690
C	54.557834	5.591815	23.007897	O	49.300532	4.404606	28.455659
C	55.929834	5.377800	23.052821	C	49.390605	5.642581	28.782990
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.639683	5.840398	26.120564	C	10.757253	5.394976	40.491133
O	51.334761	3.664827	26.637093	C	12.099253	5.042971	40.571108
C	52.093707	4.669286	26.380635	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.233239	6.185329	41.491023
C	48.879661	4.496905	20.007192	Cu	16.704833	3.783237	41.996855

C	20.971566	4.151137	41.947704	C	27.939837	5.064404	40.842659
C	21.455626	3.375544	43.017671	C	12.571237	3.934972	39.877096
C	22.807891	3.081963	43.135815	C	27.509081	2.911225	39.797109
C	23.704803	3.544847	42.180101	C	26.121451	3.205238	39.712483
C	23.265789	4.292460	41.072322	C	25.626985	4.421635	40.175530
C	21.881329	4.595417	40.944692	O	25.391741	2.195779	39.149365
C	21.442361	5.296163	39.802197	O	15.266704	6.452168	41.352712
C	22.356031	5.715303	38.838808	O	14.787738	4.296762	41.807406
C	23.714928	5.443034	38.976510	C	14.427995	5.491306	41.501233
C	24.178915	4.723805	40.082051	C	16.673562	5.896706	45.714752
O	24.611914	5.861842	38.002205	C	17.671113	6.673943	46.331965
O	19.147302	5.668923	41.652850	C	18.795520	6.917772	32.211435
O	18.676352	3.513700	42.121099	C	17.702738	6.471112	32.945789
C	19.512484	4.463952	41.903406	C	16.678596	5.715992	32.341950
C	16.938426	4.155210	37.751091	C	15.543366	5.481831	46.473718
C	17.667403	3.065237	37.243622	C	14.465770	4.789791	45.882089
C	17.685590	2.793474	35.882416	C	13.376578	4.390886	46.651124
C	16.973542	3.603266	35.004435	C	14.534255	4.565940	32.456257
C	16.204709	4.690049	35.471132	C	15.560661	5.276345	33.093024
C	16.167988	4.956907	36.865398	O	13.431292	4.146142	33.191446
C	15.338679	5.992984	37.340080	O	17.132952	6.493214	43.453364
C	14.607158	6.770184	36.451382	O	16.643675	4.337986	43.905708
C	14.667928	6.549489	35.085622	C	16.828838	5.554219	44.273495
C	15.473022	5.508319	34.570387	Cu	33.082910	6.277405	41.485003
O	13.930524	7.410879	34.276021	Cu	32.407003	3.875876	42.196286
O	17.258986	5.640445	39.583251	C	36.585070	3.868641	41.905810
O	16.789668	3.479741	40.032135	C	37.123588	3.105352	42.922620
C	17.002383	4.440168	39.208168	C	38.515688	2.872624	42.966985
C	12.972270	5.800966	41.346096	C	39.341356	3.379290	41.987435
C	12.500286	6.908965	42.040108	C	38.826231	4.135486	40.883951
C	27.017909	7.600305	41.690763	C	37.407663	4.377845	40.847807
C	26.121792	6.675893	41.194398	C	36.865504	5.077669	39.732383
C	26.538696	5.385137	40.734688	C	37.679211	5.541589	38.725483

C	39.085255	5.342371	38.771405	C	30.288011	5.728417	41.597176
C	39.660585	4.640155	39.828996	C	32.435542	6.226112	45.706568
O	39.872075	5.829887	37.770317	C	33.355196	7.074603	46.295279
O	34.857373	5.450782	41.833583	C	34.704223	6.641649	32.270825
O	34.295780	3.305798	42.194460	C	33.615924	6.261286	33.047852
C	35.136473	4.224691	41.977170	C	32.512749	5.597534	32.479655
C	32.480700	3.940365	37.976569	C	31.318086	5.720694	46.450066
C	32.946490	2.710973	37.544358	C	30.293867	4.938944	45.842333
C	32.936373	2.404928	36.166672	C	29.224567	4.486763	46.577052
C	32.444145	3.313255	35.251772	C	30.289344	4.629331	32.670497
C	31.904913	4.578878	35.652286	C	31.390943	5.250706	33.266650
C	31.922474	4.889232	37.058273	O	29.178484	4.310951	33.440944
C	31.339641	6.115853	37.494090	O	32.898828	6.728880	43.438304
C	30.792142	6.991648	36.592614	O	32.570871	4.580208	44.028164
C	30.803387	6.713331	35.199448	C	32.646431	5.817917	44.280987
C	31.352346	5.527320	34.720961	Cu	48.447525	6.405307	41.581496
O	30.244081	7.707823	34.446465	Cu	47.996185	3.981643	42.063505
O	33.122032	5.405129	39.701820	C	52.242278	4.464620	41.931334
O	32.245587	3.413321	40.275583	C	52.828353	3.947597	43.079285
C	32.618862	4.276193	39.425833	C	54.201353	3.732577	43.123183
C	28.839101	6.036144	41.393441	C	54.987278	4.036581	42.018131
C	28.390621	7.288297	41.778401	C	54.401203	4.554604	40.869180
C	42.281066	7.244593	42.005461	C	53.028203	4.768624	40.826281
C	41.451873	6.392618	41.285045	C	52.442128	5.287648	39.677330
C	41.973060	5.283739	40.589957	C	53.229054	5.591652	38.571278
C	43.371728	5.031132	40.642877	C	54.601054	5.377632	38.616177
C	28.390598	3.805065	40.347784	C	55.187129	4.858609	39.764128
C	43.053832	3.144479	39.149067	O	55.314970	5.617639	37.405129
C	41.685129	3.353664	39.125978	O	50.373272	5.935993	41.731917
C	41.125878	4.431087	39.841157	O	49.972410	3.763135	42.191325
O	40.919462	2.449650	38.394451	C	50.775179	4.737888	41.961794
O	31.128822	6.607959	41.249741	C	48.282112	4.387251	37.822235
O	30.574947	4.611711	42.128315	C	49.078278	3.334551	37.337279

C	49.149862	3.063856	35.977852	C	8.959816	6.502907	56.749315
C	48.422259	3.835101	35.078426	C	9.429783	5.394908	56.054291
C	47.588223	4.883285	35.520585	C	10.771783	5.042898	56.134241
C	47.504790	5.154747	36.912578	C	10.370718	3.178911	54.666243
C	46.622963	6.158501	37.360444	C	9.028718	3.528920	54.587293
C	45.881796	6.899792	36.449060	C	8.558750	4.637919	55.281317
C	45.978925	6.668827	35.086867	O	8.125684	2.792932	53.781319
C	46.835483	5.656624	34.597793	Cu	15.889468	6.156466	57.135009
O	45.222242	7.490173	34.253715	Cu	15.348554	3.738428	57.542485
O	48.489257	5.878561	39.667227	C	19.601151	4.076287	57.420329
O	48.104289	3.697680	40.096946	C	20.158966	3.302875	58.454108
C	48.291776	4.670609	39.281412	C	21.513159	2.993468	58.461908
C	44.207621	5.877739	41.423501	C	22.333500	3.443345	57.432852
C	43.643789	6.990628	42.073997	C	21.812930	4.196452	56.362837
C	43.898597	3.964710	39.888059	C	20.426432	4.503599	56.342760
O	46.473154	6.621615	41.454227	C	19.897062	5.194497	55.231833
O	46.067753	4.442134	41.867373	C	20.728380	5.604314	54.194148
C	45.668886	5.630271	41.586444	C	22.095654	5.343377	54.232338
C	47.857289	6.069620	45.792131	C	22.649492	4.631560	55.305106
C	48.814973	6.878092	46.431947	O	22.914650	5.759145	53.188521
C	50.038758	7.210980	32.158641	O	17.793816	5.622542	57.296248
C	48.987683	6.711929	32.920317	O	17.313928	3.447378	57.658071
C	48.008312	5.876181	32.350196	C	18.150814	4.402284	57.471174
C	46.722677	5.619346	46.523562	C	15.669246	4.252112	53.314298
C	45.680643	4.895155	45.906633	C	16.392877	3.154626	52.814319
C	44.591660	4.453151	46.651793	C	16.442065	2.893325	51.452276
C	45.944734	4.593553	32.522046	C	15.761815	3.717591	50.563583
C	46.928984	5.387197	33.126655	C	15.000859	4.814279	51.018685
O	44.880776	4.121555	33.282535	C	14.942762	5.079714	52.414090
O	48.339733	6.692052	43.544872	C	14.132469	6.136985	52.873337
O	47.908028	4.519927	43.976101	C	13.437286	6.932174	51.970656
C	48.051766	5.738926	44.353770	C	13.509281	6.703514	50.606290
C	9.830848	7.260896	57.522290	C	14.294056	5.640453	50.104871

O	12.799637	7.576104	49.783887	Cu	30.951733	3.770066	57.520498
O	15.941978	5.684220	55.204024	C	35.198708	4.119403	57.428663
O	15.444155	3.514401	55.568263	C	35.733794	3.374329	58.495377
C	15.684598	4.499356	54.781577	C	37.079874	3.033916	58.524553
C	11.644816	5.800887	56.909216	C	37.915469	3.421679	57.483295
C	11.172849	6.908886	57.603240	C	37.419437	4.147200	56.383130
C	25.306115	7.136479	57.567251	C	36.040894	4.490632	56.344328
C	24.472739	6.314288	56.817957	C	35.535417	5.158540	55.209703
C	24.985250	5.218107	56.093588	C	36.381712	5.503186	54.159988
C	26.381005	4.955073	56.139564	C	37.741460	5.204410	54.213240
C	11.243751	3.934900	55.440217	C	38.273416	4.520659	55.315540
C	26.056771	3.114308	54.589503	O	38.574961	5.556970	53.157882
C	24.689252	3.332285	54.570133	O	33.384925	5.666473	57.262577
C	24.128163	4.387550	55.324269	O	32.914494	3.490546	57.632056
O	23.923183	2.456283	53.803893	C	33.747529	4.448006	57.448418
O	13.934516	6.440591	56.975741	C	31.266566	4.330388	53.289469
O	13.440007	4.275189	57.363794	C	32.004865	3.241979	52.790462
C	13.091854	5.479387	57.083308	C	32.093663	3.004031	51.425779
C	15.283046	5.695821	61.352095	C	31.438873	3.842469	50.531322
C	16.314087	6.385804	61.978046	C	30.659729	4.925826	50.982675
C	17.592339	6.999230	47.679738	C	30.561611	5.169248	52.380695
C	16.511749	6.560900	48.436407	C	29.735121	6.217374	52.831342
C	15.475997	5.804120	47.856195	C	29.065446	7.024342	51.918000
C	14.198081	5.242825	62.095148	C	29.178994	6.816439	50.553129
C	13.166040	4.552842	61.469196	C	29.973967	5.760328	50.065869
C	12.083075	4.099846	62.213249	O	28.496374	7.698039	49.719382
C	13.329595	4.664918	48.016037	O	31.495894	5.750817	55.195890
C	14.367062	5.380195	48.629550	O	31.044081	3.568347	55.540171
O	12.234592	4.260175	48.771430	C	31.263525	4.565298	54.761435
O	15.754795	6.387229	59.110229	C	27.220213	5.771352	56.947630
O	15.282947	4.211895	59.471414	C	26.666340	6.868829	57.631182
C	15.445946	5.414784	59.890665	C	40.919424	6.977837	57.636570
Cu	31.468161	6.196866	57.135104	C	40.090738	6.163774	56.875677

C	40.606437	5.075235	56.141863	C	51.901549	5.591433	54.133681
C	42.003841	4.813295	56.187751	C	53.273549	5.377407	54.178555
C	26.902971	3.908898	55.352697	C	53.859642	4.858378	55.326493
C	41.681045	2.978572	54.631937	O	53.987445	5.617415	52.967495
C	40.313684	3.200920	54.605013	O	48.997262	5.867465	57.306580
C	39.750354	4.255079	55.359607	O	48.669863	3.662465	57.661823
O	39.549600	2.327124	53.834442	C	49.438919	4.677826	57.498207
O	29.500170	6.470113	57.017037	C	46.967503	4.406111	53.308640
O	29.041863	4.287985	57.355958	C	47.788866	3.390353	52.787595
C	28.672975	5.493271	57.114138	C	47.836505	3.141953	51.423340
C	30.903120	5.695641	61.351269	C	47.061013	3.899972	50.554036
C	31.934175	6.385618	61.977205	C	46.209515	4.918918	51.030698
C	33.239194	7.398844	47.665740	C	46.149703	5.166424	52.428741
C	32.202712	6.892797	48.420946	C	45.249681	6.136877	52.911548
C	31.196237	6.048142	47.848363	C	44.466647	6.869115	52.028335
C	29.818167	5.242646	62.094340	C	44.539264	6.662379	50.660585
C	28.786113	4.552669	61.468405	C	45.416414	5.685732	50.135611
C	27.703159	4.099675	62.212476	O	43.743698	7.478125	49.858976
C	29.121128	4.761158	47.967366	O	47.131693	5.830376	55.215865
C	30.089188	5.534744	48.606389	O	46.813953	3.621848	55.549613
O	28.066094	4.270566	48.675115	C	46.971160	4.634162	54.777625
O	31.363954	6.404450	59.113765	C	42.842250	5.633998	56.991920
O	30.891535	4.226324	59.455962	C	42.280391	6.717812	57.692394
C	31.058939	5.425144	59.886494	C	42.526842	3.769813	55.399674
Cu	47.058278	6.267612	57.154248	O	45.084687	6.424156	57.024047
Cu	46.685394	3.810683	57.523270	O	44.742252	4.217590	57.340388
C	50.914829	4.464394	57.493750	C	44.309074	5.406870	57.118925
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.691200	7.204820	47.775809
C	53.073736	4.554373	56.431559	C	47.607315	6.732279	48.506431
C	51.700736	4.768398	56.388685	C	46.613989	5.936078	47.904158
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251

C	44.406185	4.552442	61.467332	H	21.483054	5.237075	24.051419
C	43.323243	4.099449	62.211421	H	22.969200	5.929476	22.278236
C	44.512078	4.711213	48.018062	H	19.532181	2.329570	22.589908
C	45.510007	5.461609	48.655311	H	19.679345	1.794079	20.190531
O	43.423980	4.253131	48.752115	H	18.480463	3.170787	18.536731
O	46.924974	6.450669	59.127746	H	16.651238	6.145298	22.827100
O	46.570133	4.245914	59.454721	H	15.506902	7.500972	21.165240
C	46.674786	5.448355	59.889815	H	14.495649	7.508305	27.087374
C	16.262162	6.620790	63.347051	H	27.536900	7.913089	26.963697
C	15.179196	6.168795	64.090104	H	26.060167	6.432519	25.712055
C	14.147156	5.478812	63.465153	H	14.941497	3.633966	24.311708
C	12.031150	4.336833	63.582254	H	29.101561	2.075233	23.084032
C	13.063191	5.025817	64.207206	H	19.762740	6.947516	30.306558
O	10.943187	3.908837	64.361307	H	15.685640	4.513286	29.277716
C	31.882275	6.620600	63.346211	H	13.794356	3.787752	30.593530
C	30.799322	6.168606	64.089282	H	15.671936	6.861120	17.596382
C	29.767267	5.478629	63.464346	H	25.093233	6.073070	21.446581
C	27.651260	4.336658	63.581482	H	25.580472	2.447964	22.879456
C	28.683314	5.025635	64.206417	H	37.681425	2.865490	28.325028
O	26.563309	3.908663	64.360554	H	40.066951	2.280631	28.421793
C	47.502389	6.620356	63.345091	H	41.577583	2.941448	26.620968
C	46.419447	6.168363	64.088179	H	37.136736	5.147561	24.075981
C	45.387379	5.478391	63.463260	H	38.654006	5.738231	22.287726
C	43.271369	4.336426	63.580429	H	35.147020	2.326247	22.590457
C	44.303437	5.025398	64.205349	H	35.297891	1.793062	20.190414
O	42.183431	3.908432	64.359519	H	34.099774	3.170458	18.536516
H	12.119263	8.127111	26.935698	H	32.266279	6.144216	22.826081
H	10.573018	6.786804	25.566404	H	31.125069	7.499683	21.165168
H	13.383790	2.323326	22.982449	H	29.943115	7.438148	27.115624
H	9.847415	3.169617	22.677134	H	43.120294	7.752991	27.059454
H	22.117458	2.845585	28.231190	H	41.664303	6.239886	25.828461
H	24.511394	2.283109	28.270726	H	30.601022	3.508339	24.339123
H	25.990486	3.037837	26.480226	H	44.759152	1.892325	23.243850

H	35.579758	6.650684	30.322141	H	18.258871	1.953176	35.503545
H	31.335227	4.461606	29.454055	H	17.013473	3.360332	33.952062
H	29.433743	3.893584	30.839554	H	15.230492	6.211323	38.396394
H	31.291769	6.860842	17.596364	H	13.976956	7.566638	36.823894
H	40.786826	5.800519	21.469260	H	13.169224	7.512677	42.644361
H	41.233931	2.227666	23.030653	H	26.661390	8.581009	42.021238
H	53.552041	3.700519	28.381408	H	25.064378	6.955683	41.145974
H	55.987727	3.326213	28.455772	H	13.612048	3.633604	39.871027
H	57.384069	3.866297	26.497838	H	27.849846	1.950431	39.402436
H	52.703467	5.451521	24.013878	H	18.523076	7.019417	45.757260
H	54.081090	5.975815	22.116738	H	19.568975	7.508645	32.692177
H	50.777680	2.335244	22.589490	H	17.655769	6.733594	33.994022
H	50.920943	1.795299	20.189760	H	14.440425	4.559181	44.822354
H	49.720376	3.170955	18.535920	H	12.563942	3.859018	46.175097
H	47.862951	6.134620	22.823813	H	12.777882	3.616422	32.634164
H	46.741183	7.496776	21.164945	H	13.997299	7.185799	33.298161
H	45.538954	7.346628	27.163395	H	24.167002	6.396933	37.271237
H	46.244904	3.363911	24.475087	H	24.449688	2.411626	39.067127
H	50.975201	7.258031	30.237917	H	36.470343	2.724024	43.710958
H	47.069244	4.517900	29.333898	H	38.942297	2.301337	43.796745
H	45.240565	3.711982	30.691772	H	40.416818	3.190878	42.060716
H	46.913058	6.861821	17.595763	H	35.788291	5.238198	39.658455
H	56.056122	5.977048	21.104138	H	37.240195	6.070720	37.870955
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H	9.244465	6.787141	41.129873	H	33.326661	1.442421	35.820973
H	12.055473	2.324760	38.544531	H	32.461543	3.040179	34.191462
H	8.519520	3.171586	38.239143	H	31.316887	6.363710	38.556128
H	20.771732	3.010097	43.775773	H	30.331646	7.927119	36.920946
H	23.164847	2.494648	43.976310	H	29.106497	8.016290	42.168580
H	24.752678	3.304131	42.309063	H	41.865044	8.106077	42.517245
H	20.394536	5.517774	39.627895	H	40.393781	6.617557	41.259812
H	21.995025	6.255183	37.973626	H	29.449284	3.548316	40.396623
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H 34.186960 7.467003 45.705259	H 19.532367 2.947787 59.264290
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H 33.636268 6.503746 34.102976	H 23.383170 3.184795 57.470964
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H 28.439276 3.897717 46.088233	H 20.299132 6.133900 53.354374
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H 30.214279 7.491091 33.501590	H 17.011176 2.046528 51.081704
H 39.318561 6.258156 37.097374	H 15.822206 3.479254 49.511193
H 39.929622 2.639366 38.436182	H 14.012053 6.359277 53.927530
H 52.224044 3.710566 43.948013	H 12.822804 7.746247 52.331209
H 54.659370 3.328338 44.019961	H 11.840285 7.509666 58.212242
H 56.055399 3.866546 42.061188	H 24.892935 7.982479 58.107354
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H 49.657975 2.729818 38.025465	H 26.465112 2.308844 53.993800
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H 46.481539 6.378375 38.412586	H 16.483412 6.831094 49.483430
H 45.210331 7.671585 36.800955	H 13.130650 4.374639 60.400668
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H 50.776342 7.865194 32.612967	H 22.410799 6.286913 52.491585
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H 45.683221 4.670518 44.845513	H 35.093493 3.059360 59.311458
H 43.806917 3.896816 46.157170	H 37.478296 2.463064 59.357432
H 44.256687 3.535541 32.748480	H 38.957476 3.136362 57.536114
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H 54.726363 5.972120 36.665797	H 35.971149 6.014027 53.299517
H 9.463376 8.127065 58.062910	H 32.527528 2.581390 53.472965
H 7.916939 6.786710 56.693542	H 32.676107 2.165389 51.057100
H 10.728195 2.325371 54.106771	H 31.533065 3.624090 49.475795
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H	28.436938	7.830992	52.272200	H	43.812531	7.256522	48.880687
H	27.300356	7.510895	58.231997	H	53.398610	5.970725	52.227702
H	40.503248	7.816794	58.185344	H	17.068202	7.158106	63.835995
H	39.037609	6.404214	56.852831	H	15.148087	6.357279	65.155556
H	27.964651	3.696619	55.300000	H	10.263186	3.421785	63.797033
H	42.090235	2.174894	54.034496	H	32.687973	7.158489	63.835018
H	32.786990	6.741602	61.409245	H	30.767925	6.357365	65.154655
H	33.985256	8.050571	48.131011	H	25.881860	3.424237	63.795659
H	32.148006	7.156712	49.481845	H	48.307453	7.159242	63.833736
H	28.749597	4.374351	60.400091	H	46.387747	6.357331	65.153488
H	26.897771	3.574486	61.718429	H	41.501217	3.425243	63.794365
H	27.503025	3.733137	48.094602	H	54.922554	4.682770	55.325783
H	28.621331	7.496543	48.738896	H	56.250091	4.683121	39.763695
H	38.087821	6.065619	52.435143	H	57.578893	4.683400	24.200631
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H	50.894908	3.700893	59.506527	H	17.034829	5.043579	18.026681
H	53.331588	3.325694	59.581363	H	10.176549	4.915316	24.089656
H	54.727853	3.865757	57.623141	H	8.848000	4.915616	39.653278
H	50.047658	5.459674	55.145455	H	7.520561	4.915577	55.216441
H	51.424872	5.977068	53.243046	H	12.998956	5.198997	65.269029
H	48.399288	2.790213	53.452754	H	28.618781	5.198983	65.268157
H	48.476489	2.355356	51.036179	H	44.238628	5.198846	65.267033
H	47.119766	3.669713	49.499940	H	48.273986	5.043155	18.026053
H	45.126124	6.337951	53.969660	C	35.709088	8.269142	42.621860
H	43.781076	7.615307	52.407344	C	35.348513	8.338489	41.123026
H	42.911875	7.363438	58.292192	C	35.881537	9.596468	40.434579
H	43.588384	3.556404	55.350429	C	35.495303	10.881874	41.184190
H	48.405484	6.745194	61.407959	C	35.924215	10.816365	42.659015
H	49.440701	7.826315	48.255774	C	35.333955	9.578766	43.350439
H	47.542096	7.006541	49.550702	O	33.915167	8.232468	40.958297
H	44.381550	4.364233	60.399431	C	37.552246	7.058501	43.810914
H	42.519372	3.571605	61.717700	C	38.934525	7.006793	44.100112
H	42.794680	3.691550	48.198020	C	39.434575	6.163177	45.090458

C	38.574210	5.351401	45.840278	C	22.206542	3.934966	26.365674
C	37.203600	5.401014	45.567633	C	22.752841	3.166855	27.409571
C	36.693349	6.232757	44.569499	C	24.105404	2.850215	27.429273
N	37.097496	7.884803	42.791227	C	24.936125	3.290609	26.404221
H	35.516302	9.614686	39.392778	C	24.426601	4.036383	25.323887
H	35.739216	7.435685	40.639113	C	23.040950	4.344212	25.287822
H	35.098257	7.462110	43.030217	C	22.521905	5.019354	24.162018
H	34.397589	11.029610	41.128537	C	23.363821	5.423346	23.130892
H	35.942624	11.759665	40.684608	C	24.731266	5.168922	23.188428
H	37.030432	10.775183	42.713928	C	25.273589	4.464749	24.271948
H	35.623450	11.736377	43.191520	O	25.561800	5.581670	22.152390
H	34.228745	9.663135	43.385308	O	20.431612	5.510011	26.191187
H	35.664230	9.508331	44.401797	O	19.905977	3.363359	26.646902
H	36.984945	9.517651	40.383012	C	20.762736	4.290717	26.413706
H	39.619776	7.643540	43.530531	C	18.226927	4.022014	22.293999
H	40.513529	6.145804	45.279071	C	18.992915	2.941012	21.873981
H	38.964533	4.693934	46.622796	C	19.081890	2.638017	20.519979
H	36.505405	4.775579	46.134518	C	18.404876	3.417024	19.587993
H	35.623942	6.211645	44.360050	C	17.639888	4.497025	20.008011
H	37.791627	8.521230	42.415214	C	17.550913	4.800019	21.362013
H	33.461246	8.944518	41.441203	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355032	19.497042
(S,S)-2-RC				C	16.963876	5.274031	19.076025
C	12.487000	7.261000	26.395000	O	15.523872	7.185038	18.539057
C	11.616000	6.503000	25.622000	O	18.564689	5.526651	24.113591
C	12.086000	5.395000	24.927000	O	18.015305	3.386616	24.572694
C	13.428000	5.043000	25.007000	C	18.262064	4.334813	23.745719
C	13.027000	3.179000	23.539000	C	14.301000	5.801000	25.782000
C	11.685000	3.529000	23.460000	C	13.829000	6.909000	26.476000
C	11.215000	4.638000	24.154000	C	27.921596	7.012383	26.498605
O	10.782000	2.793000	22.654000	C	27.089388	6.172775	25.766734
Cu	18.542604	6.080804	26.017860	C	27.604741	5.066077	25.060449
Cu	17.945156	3.693243	26.528115				

C	29.000675	4.807811	25.111005	C	33.846855	4.021974	22.293721
C	13.900000	3.935000	24.313000	C	34.612832	2.940971	21.873686
C	28.681304	2.933069	23.600660	C	34.701783	2.637980	20.519681
C	27.313722	3.148515	23.575408	C	34.024755	3.416991	19.587710
C	26.750707	4.219167	24.305905	C	33.259777	4.496993	20.007743
O	26.549847	2.257745	22.824105	C	33.170827	4.799985	21.361749
O	16.596355	6.401188	25.851453	C	32.403849	5.880988	21.783783
O	16.052131	4.262729	26.321216	C	31.727822	6.658998	20.849812
C	15.734914	5.460913	25.985814	C	31.817772	6.355006	19.496807
C	17.918646	5.810661	30.232743	C	32.583750	5.274004	19.075773
C	18.906546	6.585253	30.867895	O	31.143744	7.185017	18.538837
C	16.778716	5.388236	30.972679	O	34.106947	5.506772	24.155837
C	15.706645	4.703946	30.360688	O	33.614634	3.346379	24.572605
C	14.614481	4.285070	31.114523	C	33.847209	4.313167	23.760142
O	18.430310	6.396302	27.978444	C	29.838027	5.640797	25.903407
O	17.896422	4.251250	28.430781	C	29.283302	6.751013	26.564837
C	18.097165	5.464991	28.796416	C	43.546493	6.890997	26.604256
Cu	34.094490	6.015711	26.078803	C	42.717645	6.032277	25.893320
Cu	33.535742	3.611502	26.544630	C	43.237932	4.918631	25.202100
C	37.792657	3.899126	26.434972	C	44.637898	4.671947	25.246830
C	38.308307	3.149412	27.508012	C	29.525347	3.746717	24.345715
C	39.654543	2.812836	27.562968	C	44.318150	2.757949	23.788491
C	40.511271	3.213016	26.543626	C	42.949634	2.972672	23.756274
C	40.035174	3.941726	25.437156	C	42.384628	4.059558	24.460521
C	38.655606	4.276063	25.368602	O	42.186552	2.065472	23.024203
C	38.171156	4.941773	24.223177	O	32.127683	6.316502	25.962676
C	39.039745	5.301987	23.197272	O	31.636646	4.152644	26.367225
C	40.400364	5.015558	23.282316	C	31.286479	5.354458	26.086205
C	40.910062	4.326174	24.391248	C	33.590807	5.642979	30.305854
O	41.257031	5.386686	22.251785	C	34.660806	6.300433	30.939331
O	35.999972	5.460752	26.212832	C	32.431419	5.310016	31.060423
O	35.496995	3.306952	26.659065	C	31.295546	4.733883	30.455542
C	36.344730	4.244759	26.439946	C	30.168374	4.435775	31.217139

O	34.017741	6.282866	28.050095	C	45.477259	5.542688	25.994839
O	33.484195	4.129753	28.464636	C	44.912396	6.652308	26.650458
C	33.706735	5.332529	28.854586	C	45.163102	3.591641	24.511292
Cu	49.696061	6.210735	25.980132	O	47.715105	6.344562	25.885713
Cu	49.343764	3.794733	26.566442	O	47.393958	4.177754	26.423292
C	53.571004	4.464799	26.367945	C	46.948360	5.338905	26.102242
C	54.157059	3.947781	27.515908	C	49.204368	6.011091	30.213421
C	55.530060	3.732767	27.559832	C	50.150565	6.854156	30.823842
C	56.316003	4.036770	26.454793	C	48.090875	5.548018	30.968222
C	55.729947	4.554788	25.305829	C	47.059172	4.788171	30.377231
C	54.356948	4.768802	25.262905	C	45.986270	4.340719	31.141610
C	53.770890	5.287820	24.113942	O	49.610217	6.576767	27.933224
C	54.557834	5.591822	23.007903	O	49.298221	4.404046	28.456609
C	55.929834	5.377808	23.052827	C	49.389849	5.641895	28.784119
C	56.515890	4.858790	24.200790	C	11.158284	7.260965	41.959133
O	56.643771	5.617813	21.841791	C	10.287267	6.502972	41.186144
O	51.638259	5.839775	26.119443	C	10.757252	5.394972	40.491132
O	51.333691	3.664694	26.637563	C	12.099252	5.042967	40.571107
C	52.092830	4.668980	26.380336	C	11.698220	3.178974	39.103108
C	49.466780	4.021882	22.293161	C	10.356220	3.528979	39.024133
C	50.232747	2.940878	21.873109	C	9.886236	4.637978	39.718145
C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.236845	6.153087	41.521484
C	48.879663	4.496911	20.007197	Cu	16.684702	3.753959	42.019410
C	48.790739	4.799899	21.361205	C	20.946793	4.097845	42.060436
C	48.023773	5.880903	21.783256	C	21.424340	3.484982	43.233180
C	47.347732	6.658919	20.849300	C	22.769747	3.173342	43.380492
C	47.437657	6.354932	19.496292	C	23.661428	3.445696	42.349235
C	48.203622	5.273928	19.075240	C	23.224070	4.026902	41.144849
O	46.763615	7.184949	18.538336	C	21.851428	4.366649	40.995906
O	49.730625	5.592594	24.088213	C	21.415723	4.927689	39.777667
O	49.383905	3.428232	24.610412	C	22.319294	5.137712	38.738011
C	49.524724	4.369678	23.750007	C	23.662167	4.796908	38.879810

C	24.125568	4.250636	40.080400	C	16.641140	5.852035	45.741256
O	24.538930	4.947093	37.814958	C	17.633816	6.629839	46.365382
O	19.146506	5.620477	41.694397	C	18.810011	6.898559	32.217248
O	18.650596	3.471728	42.173902	C	17.722586	6.448026	32.956900
C	19.495529	4.416551	41.970219	C	16.696531	5.692263	32.357373
C	16.953164	4.132024	37.776379	C	15.513627	5.422721	46.496256
C	17.679470	3.039131	37.271506	C	14.438887	4.731276	45.898104
C	17.700679	2.766696	35.910560	C	13.355433	4.312652	46.664561
C	16.992478	3.577384	35.030317	C	14.557124	4.534403	32.483229
C	16.227109	4.667776	35.494108	C	15.584032	5.249068	33.114255
C	16.189850	4.937658	36.887833	O	13.461302	4.107531	33.225053
C	15.368181	5.981711	37.358676	O	17.126213	6.454118	43.485497
C	14.645031	6.763362	36.466982	O	16.607284	4.303481	43.926341
C	14.703916	6.537082	35.102131	C	16.803265	5.515827	44.299624
C	15.500035	5.487207	34.590761	Cu	33.052600	6.010739	41.498439
O	13.973038	7.400980	34.289218	Cu	32.427671	3.558407	42.047074
O	17.269442	5.612456	39.613045	C	36.600010	3.692059	41.750843
O	16.789694	3.452766	40.055222	C	37.122979	2.737583	42.603479
C	17.010563	4.414061	39.234226	C	38.502521	2.437875	42.564266
C	12.972269	5.800962	41.346096	C	39.333030	3.078611	41.669511
C	12.500284	6.908961	42.040108	C	38.833220	4.044171	40.735523
C	26.938699	7.124340	41.712151	C	37.424571	4.343651	40.774779
C	26.045786	6.183824	41.238924	C	36.893953	5.246654	39.808646
C	26.473686	4.902396	40.760038	C	37.711203	5.842814	38.878639
C	27.882449	4.602843	40.839204	C	39.110410	5.597223	38.866590
C	12.571236	3.934968	39.877095	C	39.673519	4.704463	39.776051
C	27.454955	2.436277	39.820202	O	39.902209	6.233340	37.958456
C	26.063843	2.717612	39.746773	O	34.853507	5.270106	41.878971
C	25.566826	3.934607	40.203650	O	34.330602	3.083054	41.987693
O	25.335810	1.700210	39.204451	C	35.152349	4.041868	41.880834
O	15.272366	6.437050	41.372772	C	32.616438	3.914344	37.835221
O	14.774421	4.282632	41.811000	C	33.189128	2.755263	37.344866
C	14.425435	5.481663	41.509807	C	33.166336	2.497531	35.957550

C	32.546316	3.375908	35.093374	C	30.144724	4.690061	32.586418
C	31.904200	4.570878	35.556090	C	31.253009	5.268048	33.213932
C	31.953182	4.841620	36.969039	O	29.004444	4.409272	33.328334
C	31.298763	6.007138	37.465838	O	32.733775	6.306693	43.439944
C	30.623528	6.848282	36.617719	O	32.561253	4.115161	43.929637
C	30.564693	6.586302	35.222178	C	32.559155	5.342291	44.240655
C	31.215230	5.483288	34.679335	Cu	48.436743	6.379610	41.586319
O	29.835880	7.515726	34.532141	Cu	48.002556	3.947540	42.043806
O	33.190287	5.302908	39.649722	C	52.242277	4.464616	41.931345
O	32.305762	3.278099	40.087956	C	52.828352	3.947593	43.079296
C	32.709666	4.184985	39.302063	C	54.201352	3.732573	43.123194
C	28.779744	5.591451	41.363538	C	54.987277	4.036578	42.018142
C	28.319415	6.837137	41.758034	C	54.401202	4.554601	40.869191
C	42.258542	7.080916	42.229427	C	53.028202	4.768621	40.826292
C	41.439740	6.298579	41.423303	C	52.442128	5.287645	39.677341
C	41.975328	5.283697	40.605140	C	53.229054	5.591649	38.571289
C	43.376734	5.048327	40.626964	C	54.601054	5.377629	38.616189
C	28.337832	3.345583	40.342879	C	55.187129	4.858606	39.764139
C	43.080372	3.310358	38.959114	O	55.314970	5.617636	37.405141
C	41.710115	3.513933	38.947086	O	50.364749	5.921698	41.727808
C	41.139184	4.504893	39.769492	O	49.978815	3.742855	42.172756
O	40.954127	2.692217	38.115532	C	50.774325	4.725828	41.954697
O	31.056278	6.216128	41.197375	C	48.273063	4.392816	37.803992
O	30.558491	4.191255	42.038541	C	49.062176	3.337762	37.311546
C	30.240584	5.311338	41.536725	C	49.122031	3.066590	35.951601
C	32.345526	5.688884	45.680101	C	48.391390	3.840942	35.057829
C	33.180004	6.638027	46.242282	C	47.565488	4.892717	35.506170
C	34.620856	6.584411	32.298127	C	47.491504	5.162948	36.899488
C	33.505992	6.228410	33.048441	C	46.612868	6.166525	37.353326
C	32.397782	5.597834	32.451912	C	45.866042	6.908438	36.446948
C	31.316571	5.058484	46.455127	C	45.956205	6.680596	35.083587
C	30.388806	4.138130	45.888170	C	46.810361	5.669559	34.587870
C	29.402061	3.567757	46.656171	O	45.196846	7.505193	34.256125

O	48.473197	5.872404	39.663934	C	19.585105	3.974745	57.469344
O	48.112197	3.683999	40.074236	C	20.123355	3.234833	58.537532
C	48.286259	4.666017	39.266652	C	21.472664	2.905746	58.568816
C	44.203269	5.828569	41.480269	C	22.307244	3.299895	57.528360
C	43.627565	6.852842	42.253383	C	21.806126	4.016684	56.424777
C	43.915941	4.062798	39.777164	C	20.425033	4.346940	56.383260
O	46.461497	6.585889	41.475920	C	19.914799	5.005917	55.244953
O	46.072603	4.395932	41.854362	C	20.758955	5.357075	54.196092
C	45.665558	5.587952	41.605306	C	22.120914	5.070685	54.251625
C	47.867935	5.995079	45.794949	C	22.656905	4.393803	55.355946
C	48.835242	6.787715	46.439768	O	22.952469	5.428817	53.196458
C	50.040047	7.196904	32.165529	O	17.799679	5.544357	57.298140
C	48.978914	6.709307	32.920816	O	17.287689	3.381181	57.687555
C	47.992659	5.886117	32.344232	C	18.138823	4.321971	57.495440
C	46.732032	5.546878	46.525428	C	15.653737	4.164450	53.332324
C	45.684591	4.833082	45.905722	C	16.383978	3.071213	52.832615
C	44.591906	4.397169	46.649264	C	16.429380	2.807295	51.470527
C	45.912132	4.629391	32.501949	C	15.741175	3.626282	50.582582
C	46.903619	5.408197	33.114493	C	14.974376	4.718433	51.038940
O	44.836513	4.171569	33.254524	C	14.916728	4.983290	52.433915
O	48.336694	6.643533	43.552968	C	14.097220	6.032307	52.895722
O	47.910849	4.465747	43.961883	C	13.392593	6.821192	51.995310
C	48.054206	5.680709	44.352260	C	13.467597	6.596587	50.630569
C	9.830844	7.260885	57.522289	C	14.262125	5.541629	50.127142
C	8.959813	6.502896	56.749314	O	12.751590	7.465464	49.809771
C	9.429780	5.394897	56.054290	O	15.945429	5.609925	55.206327
C	10.771780	5.042887	56.134240	O	15.422086	3.449794	55.593073
C	10.370715	3.178901	54.666241	C	15.675329	4.423363	54.796721
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.329153	6.954193	57.534585
Cu	15.900747	6.105487	57.131383	C	24.490420	6.108150	56.819242
Cu	15.327798	3.699340	57.564204	C	24.995820	4.981634	56.137934

C	26.390261	4.710361	56.195785	C	37.730748	4.972841	54.217304
C	11.243748	3.934890	55.440215	C	38.281175	4.341981	55.341834
C	26.053730	2.815726	54.715589	O	38.551180	5.297266	53.142885
C	24.687799	3.044371	54.683696	O	33.401518	5.505915	57.274214
C	24.133065	4.131143	55.396864	O	32.953343	3.345663	57.749071
O	23.916606	2.147306	53.947660	C	33.776307	4.301335	57.515777
O	13.946154	6.416953	56.971307	C	31.357784	3.936297	53.381045
O	13.425641	4.261667	57.379293	C	32.184758	2.882297	52.952697
C	13.090920	5.467636	57.088820	C	32.310897	2.576915	51.604464
C	15.283042	5.695809	61.352094	C	31.602676	3.309470	50.658772
C	16.314083	6.385792	61.978046	C	30.735215	4.351379	51.042780
C	17.552948	6.942485	47.715878	C	30.606127	4.668344	52.422397
C	16.476404	6.488166	48.469020	C	29.708695	5.683209	52.807973
C	15.445686	5.729405	47.881978	C	28.989543	6.384123	51.846430
C	14.198077	5.242813	62.095147	C	29.122634	6.098827	50.497526
C	13.166036	4.552830	61.469195	C	29.996216	5.076348	50.077359
C	12.083071	4.099834	62.213248	O	28.378043	6.871268	49.610205
C	13.309308	4.569687	48.032519	O	31.519049	5.464734	55.205780
C	14.340688	5.288769	48.651550	O	31.093032	3.296085	55.659159
O	12.219830	4.146227	48.785582	C	31.314910	4.252743	54.833755
O	15.771247	6.360947	59.104256	C	27.235826	5.554473	56.967878
O	15.271258	4.195680	59.486078	C	26.687963	6.681852	57.606991
C	15.449027	5.400356	59.893758	C	40.898590	6.911579	57.571831
Cu	31.481747	6.011103	57.120208	C	40.080078	6.064437	56.836512
Cu	30.987353	3.600154	57.621228	C	40.608487	4.957378	56.140342
C	35.230379	3.987301	57.497451	C	42.008431	4.712346	56.196341
C	35.785264	3.299507	58.591910	C	26.904937	3.630222	55.452000
C	37.136258	2.979072	58.623262	C	41.708145	2.827581	54.696307
C	37.956769	3.330196	57.557219	C	40.338291	3.031654	54.663733
C	37.441148	4.000143	56.431047	C	39.762212	4.101582	55.385880
C	36.057585	4.321180	56.389515	O	39.585144	2.124541	53.921397
C	35.533001	4.931482	55.231115	O	29.512555	6.262134	56.989475
C	36.365960	5.246407	54.161807	O	29.069860	4.094517	57.426923

C	28.691651	5.286245	57.134177	C	47.806264	3.054751	51.441558
C	30.903116	5.695628	61.351271	C	47.041721	3.817474	50.566805
C	31.934171	6.385605	61.977208	C	46.200813	4.848142	51.036648
C	33.065110	6.957125	47.612795	C	46.140248	5.102971	52.433348
C	32.102105	6.353314	48.392802	C	45.246566	6.082747	52.909302
C	31.182313	5.397734	47.849832	C	44.474474	6.819860	52.020469
C	29.818163	5.242633	62.094342	C	44.552280	6.609309	50.653618
C	28.786109	4.552656	61.468406	C	45.419977	5.620519	50.135746
C	27.703155	4.099663	62.212477	O	43.771824	7.433472	49.845624
C	29.278695	3.873518	48.038013	O	47.118501	5.782472	55.213099
C	30.148435	4.784276	48.634938	O	46.813645	3.575388	55.567225
O	28.300877	3.282354	48.779004	C	46.961434	4.581792	54.785728
O	31.374188	6.316643	59.087073	C	42.836043	5.565222	56.978433
O	30.920266	4.151634	59.526595	C	42.261547	6.666094	57.640995
C	31.076095	5.369964	59.901740	C	42.543983	3.651955	55.439470
Cu	47.045961	6.237451	57.147473	O	45.071126	6.377092	57.016963
Cu	46.692050	3.781257	57.539289	O	44.746545	4.171803	57.358758
C	50.914826	4.464382	57.493755	C	44.304035	5.354083	57.119893
C	51.500920	3.947352	58.641694	C	46.523192	5.695393	61.350166
C	52.873920	3.732327	58.685568	C	47.554258	6.385364	61.976087
C	53.659827	4.036331	57.580503	C	48.718636	7.102466	47.786957
C	53.073733	4.554362	56.431564	C	47.630743	6.636063	48.515318
C	51.700733	4.768387	56.388690	C	46.627725	5.855798	47.908199
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.512630	4.653434	48.015982
O	53.987443	5.617405	52.967501	C	45.517589	5.391421	48.656489
O	48.987924	5.853759	57.299199	O	43.417496	4.207378	48.747060
O	48.676956	3.649145	57.671581	O	46.915472	6.437660	59.120425
C	49.438187	4.668585	57.497746	O	46.580486	4.232682	59.466731
C	46.950973	4.340880	53.318489	C	46.676190	5.439505	59.891480
C	47.760311	3.312025	52.804196	C	16.262158	6.620778	63.347051

C	15.179191	6.168782	64.090104	H	26.034406	6.406427	25.743299
C	14.147152	5.478800	63.465152	H	14.941553	3.634216	24.311118
C	12.031146	4.336820	63.582253	H	29.091273	2.114664	23.024046
C	13.063187	5.025805	64.207205	H	19.765835	6.935191	30.307186
O	10.943183	3.908824	64.361306	H	15.687082	4.494840	29.296566
C	31.882271	6.620587	63.346214	H	13.807980	3.757351	30.623689
C	30.799317	6.168593	64.089284	H	15.672081	6.861159	17.596383
C	29.767262	5.478616	63.464348	H	25.065073	6.108832	21.449927
C	27.651255	4.336645	63.581483	H	25.568548	2.478331	22.829285
C	28.683309	5.025622	64.206418	H	37.653893	2.832460	28.312185
O	26.563304	3.908650	64.360554	H	40.037173	2.239019	28.401431
C	47.502385	6.620342	63.345096	H	41.554058	2.935478	26.619097
C	46.419443	6.168348	64.088184	H	37.120687	5.182362	24.097231
C	45.387375	5.478376	63.463264	H	38.645195	5.814729	22.330451
C	43.271365	4.336411	63.580432	H	35.146557	2.326071	22.590618
C	44.303433	5.025383	64.205353	H	35.298074	1.793203	20.190391
O	42.183428	3.908416	64.359522	H	34.099851	3.170529	18.536505
H	12.119250	8.127011	26.935853	H	32.264686	6.144363	22.825705
H	10.573020	6.786799	25.566434	H	31.124857	7.499511	21.165261
H	13.383931	2.323438	22.982376	H	29.916621	7.406040	27.152061
H	9.847427	3.169674	22.677234	H	43.126468	7.748881	27.120122
H	22.119739	2.825458	28.220650	H	41.660518	6.256185	25.876087
H	24.514489	2.264525	28.246708	H	30.587679	3.536492	24.297229
H	25.984923	3.030430	26.453762	H	44.728506	1.926152	23.231806
H	21.464154	5.233112	24.053066	H	35.538928	6.581727	30.369169
H	22.942488	5.943533	22.281294	H	31.256091	4.523000	29.390993
H	19.531862	2.329397	22.589992	H	29.305648	4.001836	30.729206
H	19.679339	1.794077	20.190537	H	31.291573	6.860683	17.596375
H	18.480480	3.170812	18.536729	H	40.782853	5.904131	21.527010
H	16.651775	6.145500	22.827140	H	41.202676	2.274268	23.042215
H	15.507006	7.501005	21.165356	H	53.551983	3.700495	28.381354
H	14.495545	7.507994	27.087822	H	55.987720	3.326194	28.455768
H	27.505873	7.866170	27.024549	H	57.384079	3.866363	26.497857

H	52.703486	5.451570	24.013810	H	18.484201	6.984614	45.794044
H	54.081054	5.975801	22.116753	H	19.585592	7.489084	32.695372
H	50.777442	2.335151	22.589578	H	17.682122	6.707309	34.006261
H	50.920840	1.795227	20.189777	H	14.410416	4.516792	44.835175
H	49.720360	3.170968	18.535922	H	12.545992	3.780129	46.183763
H	47.862113	6.134484	22.823685	H	12.808077	3.573726	32.671542
H	46.741031	7.496634	21.165065	H	14.039340	7.172571	33.312089
H	45.544514	7.334360	27.207620	H	24.138956	5.490071	37.060593
H	46.225623	3.380004	24.471960	H	24.394496	1.916744	39.112036
H	50.986692	7.236450	30.249518	H	36.462173	2.236637	43.315798
H	47.057307	4.540170	29.321182	H	38.915030	1.694564	43.253783
H	45.209019	3.757841	30.666138	H	40.398382	2.827522	41.671534
H	46.912778	6.861599	17.595787	H	35.825142	5.463271	39.791075
H	56.056012	5.977143	21.104276	H	37.281337	6.525893	38.136189
H	10.790932	8.127996	42.498529	H	33.668664	2.056659	38.035714
H	9.244452	6.787085	41.129922	H	33.639884	1.592027	35.565003
H	12.055774	2.325370	38.543778	H	32.541640	3.131683	34.026296
H	8.519752	3.172219	38.238431	H	31.321427	6.231121	38.533899
H	20.740787	3.258995	44.043826	H	30.101052	7.730601	36.994583
H	23.123593	2.712614	44.297822	H	29.032614	7.579060	42.125034
H	24.701884	3.184089	42.495451	H	41.827241	7.866008	42.842799
H	20.376729	5.193905	39.606655	H	40.377640	6.505138	41.433547
H	21.963721	5.557967	37.806257	H	29.400652	3.104835	40.370892
H	18.243071	2.403565	37.944721	H	43.500939	2.550824	38.313148
H	18.273115	1.924926	35.533691	H	33.938405	7.118209	45.618287
H	17.034134	3.333477	33.978287	H	35.459722	7.082708	32.774397
H	15.260673	6.204407	38.414027	H	33.510081	6.466382	34.104543
H	14.023065	7.567772	36.836329	H	30.451662	3.886561	44.829023
H	13.169082	7.511375	42.645753	H	28.695855	2.863678	46.200037
H	26.573808	8.099136	42.050013	H	28.294298	3.943228	32.781689
H	24.983411	6.445135	41.220286	H	29.683905	7.263386	33.608010
H	13.612312	3.634913	39.867501	H	39.361347	6.823550	37.409264
H	27.797491	1.472661	39.434386	H	39.967367	2.900659	38.140560

H	52.223659	3.708589	43.947188	H	12.769779	7.627965	52.357891
H	54.659291	3.327772	44.019755	H	11.840825	7.508342	58.212794
H	56.055389	3.866474	42.061150	H	24.921466	7.824433	58.039412
H	51.374754	5.453614	39.579386	H	23.438429	6.353670	56.787234
H	52.752234	5.975909	37.680170	H	12.285112	3.636385	55.426345
H	49.643267	2.728867	37.994675	H	26.457138	1.986174	54.150399
H	49.739921	2.252193	35.586357	H	17.168906	6.737997	61.410732
H	48.463209	3.597568	34.007292	H	18.331492	7.537449	48.183441
H	46.477337	6.385546	38.406341	H	16.447492	6.747105	49.518853
H	45.196066	7.679149	36.803956	H	13.126110	4.378524	60.400409
H	44.251201	7.466392	42.893679	H	11.277481	3.575083	61.719142
H	44.981577	3.865299	39.723772	H	11.559380	3.614509	48.238729
H	49.690344	7.157533	45.885563	H	12.838329	7.245177	48.832261
H	50.783026	7.841467	32.624925	H	22.461161	5.934835	52.474849
H	48.924728	6.993692	33.963106	H	22.936458	2.372470	53.954966
H	45.686159	4.611794	44.843825	H	35.157151	3.015170	59.428376
H	43.802818	3.848805	46.152581	H	37.550746	2.453401	59.477795
H	44.205103	3.599262	32.714150	H	39.003014	3.061484	57.612802
H	45.295631	7.282319	33.280419	H	34.478292	5.164746	55.129939
H	54.726284	5.972277	36.665952	H	35.940855	5.714721	53.284347
H	9.463326	8.126925	58.063079	H	32.747474	2.304293	53.677078
H	7.916930	6.786682	56.693519	H	32.963368	1.768542	51.288911
H	10.728371	2.325613	54.106485	H	31.727605	3.042125	49.617739
H	7.191878	3.171162	53.802785	H	29.541437	5.943093	53.848160
H	19.485322	2.921677	59.356012	H	28.305818	7.166206	52.149609
H	21.875408	2.342374	59.404809	H	27.326252	7.346783	58.177540
H	23.352436	3.026916	57.584807	H	40.472828	7.764466	58.091076
H	18.862217	5.248283	55.142576	H	39.024798	6.293788	56.803039
H	20.344220	5.862369	53.334346	H	27.964816	3.406298	55.412289
H	16.929583	2.425935	53.511549	H	42.127295	2.010909	54.123884
H	17.002553	1.963521	51.099040	H	32.790506	6.733697	61.409811
H	15.799214	3.387231	49.530136	H	33.748324	7.686864	48.058519
H	13.977157	6.252437	53.950483	H	32.042158	6.622064	49.452028

H	28.747611	4.377328	60.399438	H	46.387781	6.357228	65.153511
H	26.897523	3.574948	61.718299	H	41.501542	3.424815	63.794355
H	27.792573	2.668780	48.224303	H	54.922551	4.682738	55.325804
H	28.504546	6.603932	48.645816	H	56.250092	4.683133	39.763726
H	38.051541	5.774102	52.407223	H	57.578895	4.683415	24.200667
H	38.601911	2.335083	53.922991	H	32.654287	5.043314	18.026532
H	50.894931	3.699488	59.506195	H	17.034856	5.043564	18.026691
H	53.331549	3.325385	59.581253	H	10.176558	4.915348	24.089714
H	54.727843	3.865682	57.623112	H	8.848023	4.915668	39.653261
H	50.047612	5.459318	55.145312	H	7.520564	4.915582	55.216424
H	51.424855	5.976969	53.243037	H	12.998965	5.198990	65.269028
H	48.363559	2.709146	53.473361	H	28.618816	5.198914	65.268172
H	48.437544	2.258508	51.059758	H	44.238667	5.198818	65.267044
H	47.100342	3.581747	49.513906	H	48.274023	5.043172	18.026058
H	45.119338	6.287604	53.966205	C	32.495388	8.998154	40.585397
H	43.795251	7.574423	52.394259	C	33.073503	9.090201	41.943010
H	42.884712	7.336803	58.221629	C	34.126716	10.122363	42.274229
H	43.607790	3.450028	55.394616	C	34.841035	10.642179	41.016398
H	48.405876	6.743969	61.407856	C	33.821406	11.090588	39.959082
H	49.476096	7.711086	48.270918	C	32.930609	9.931769	39.470687
H	47.570774	6.902219	49.561937	O	33.513346	8.064711	41.028528
H	44.381990	4.363785	60.399418	C	26.536710	7.462566	37.394739
H	42.519464	3.571459	61.717696	C	25.397297	7.976156	38.054306
H	42.778588	3.661366	48.188440	C	24.283679	8.404172	37.328816
H	43.855602	7.218917	48.866892	C	24.270040	8.340794	35.928875
H	53.398488	5.970490	52.227719	C	25.407037	7.853234	35.268485
H	17.068426	7.157672	63.836082	C	26.526793	7.422719	35.981567
H	15.148105	6.357185	65.155574	N	27.647327	7.048368	38.110182
H	10.263336	3.421656	63.796943	H	34.847981	9.676437	42.984250
H	32.688942	7.156688	63.835381	H	32.496622	8.685609	42.784780
H	30.768128	6.356915	65.154746	H	31.517840	8.510962	40.480931
H	25.882227	3.423710	63.795652	H	35.483077	9.842506	40.603439
H	48.307604	7.158945	63.833798	H	35.504978	11.481378	41.289221

C	17.902370	5.826273	30.224022	C	32.583750	5.274004	19.075773
C	18.892569	6.587171	30.871638	O	31.143744	7.185017	18.538837
C	16.745276	5.423000	30.947202	O	34.105851	5.497461	24.167792
C	15.671531	4.756372	30.318989	O	33.615579	3.334160	24.570263
C	14.559860	4.358949	31.055635	C	33.845644	4.306556	23.763183
O	18.430560	6.404675	27.972737	C	29.839610	5.607441	25.916224
O	17.894337	4.260715	28.429047	C	29.287232	6.727756	26.562951
C	18.093432	5.475723	28.791482	C	43.550242	6.896517	26.586851
Cu	34.092647	5.990649	26.097465	C	42.720561	6.039203	25.875160
Cu	33.543828	3.581623	26.545989	C	43.239125	4.923050	25.186704
C	37.800769	3.886617	26.434454	C	44.638099	4.671106	25.236980
C	38.324005	3.139241	27.505570	C	29.525761	3.704696	24.368959
C	39.673266	2.814058	27.558125	C	44.316854	2.758342	23.777356
C	40.524450	3.218971	26.535966	C	42.949514	2.979503	23.737964
C	40.040538	3.943375	25.430141	C	42.385156	4.066562	24.442699
C	38.659096	4.271286	25.366941	O	42.186958	2.077607	22.998893
C	38.167910	4.939387	24.225939	O	32.126760	6.286125	25.981713
C	39.030744	5.303324	23.196481	O	31.641720	4.119822	26.379715
C	40.392212	5.018403	23.273567	C	31.288097	5.321748	26.101938
C	40.909512	4.330399	24.379972	C	33.562592	5.590884	30.325332
O	41.241806	5.388780	22.236988	C	34.586711	6.319267	30.958144
O	36.000554	5.441761	26.228954	C	32.420459	5.197702	31.080474
O	35.506881	3.281226	26.651826	C	31.326147	4.541208	30.480333
C	36.350845	4.224940	26.443287	C	30.218665	4.178931	31.242170
C	33.846855	4.021974	22.293721	O	34.009063	6.242304	28.073035
C	34.612832	2.940971	21.873686	O	33.496891	4.082052	28.472098
C	34.701783	2.637980	20.519681	C	33.700571	5.285260	28.871505
C	34.024755	3.416991	19.587710	Cu	49.695799	6.207192	25.981236
C	33.259777	4.496993	20.007743	Cu	49.343771	3.790198	26.564282
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793

C	55.729947	4.554788	25.305829	C	47.063426	4.772094	30.384021
C	54.356948	4.768802	25.262905	C	45.993269	4.322211	31.151167
C	53.770890	5.287820	24.113942	O	49.608499	6.569443	27.935218
C	54.557834	5.591822	23.007903	O	49.296623	4.395918	28.455219
C	55.929834	5.377808	23.052827	C	49.388611	5.633153	28.784857
C	56.515890	4.858790	24.200790	C	11.158284	7.260965	41.959133
O	56.643771	5.617813	21.841791	C	10.287267	6.502972	41.186144
O	51.637666	5.838004	26.120848	C	10.757252	5.394972	40.491132
O	51.334217	3.662018	26.636232	C	12.099252	5.042967	40.571107
C	52.092878	4.667277	26.380356	C	11.698220	3.178974	39.103108
C	49.466780	4.021882	22.293161	C	10.356220	3.528979	39.024133
C	50.232747	2.940878	21.873109	C	9.886236	4.637978	39.718145
C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.233227	6.153773	41.467008
C	48.879663	4.496911	20.007197	Cu	16.692454	3.752846	41.967564
C	48.790739	4.799899	21.361205	C	20.956442	4.082688	41.826777
C	48.023773	5.880903	21.783256	C	21.479139	3.326365	42.891567
C	47.347732	6.658919	20.849300	C	22.832916	3.022636	42.956275
C	47.437657	6.354932	19.496292	C	23.691344	3.460074	41.953749
C	48.203622	5.273928	19.075240	C	23.211890	4.197236	40.855392
O	46.763615	7.184949	18.538336	C	21.824513	4.500264	40.777485
O	49.731177	5.591623	24.088738	C	21.338654	5.175889	39.638824
O	49.385047	3.426471	24.608753	C	22.211459	5.571636	38.629321
C	49.525263	4.368911	23.749482	C	23.576020	5.311713	38.723422
C	45.477986	5.539920	25.986889	C	24.086735	4.620342	39.827123
C	44.914969	6.653317	26.637707	O	24.431516	5.707180	37.703131
C	45.161998	3.587690	24.505146	O	19.143017	5.618917	41.598675
O	47.715746	6.340174	25.884840	O	18.662258	3.464131	42.061689
O	47.393500	4.172745	26.419200	C	19.501402	4.408603	41.832009
C	46.948527	5.334330	26.098059	C	16.881373	4.138485	37.721846
C	49.205887	5.999688	30.215127	C	17.590406	3.037593	37.209164
C	50.152531	6.843460	30.823939	C	17.596856	2.766983	35.847802
C	48.095327	5.533586	30.972689	C	16.894700	3.590074	34.974398

C	16.146393	4.688898	35.446328	C	15.518690	5.300947	33.071218
C	16.118582	4.952857	36.841259	O	13.372288	4.201736	33.148497
C	15.305862	5.999362	37.321581	O	17.159077	6.450612	43.433280
C	14.583655	6.790299	36.437014	O	16.662326	4.295639	43.878536
C	14.638898	6.573817	35.070271	C	16.857346	5.508522	44.251243
C	15.427398	5.522677	34.549798	Cu	32.877006	6.271477	41.544295
O	13.914384	7.449862	34.264923	Cu	32.328509	3.795989	42.176555
O	17.230061	5.617103	39.555681	C	36.508839	4.025418	41.807666
O	16.748144	3.458575	40.001439	C	37.005148	3.153203	42.759528
C	16.959652	4.420150	39.178845	C	38.382076	2.842252	42.786032
C	12.972269	5.800962	41.346096	C	39.239267	3.382728	41.851907
C	12.500284	6.908961	42.040108	C	38.771970	4.260028	40.819615
C	26.684703	7.068780	42.312800	C	37.366462	4.583437	40.801838
C	25.867311	6.289998	41.519724	C	36.877195	5.416121	39.754541
C	26.375924	5.197403	40.743358	C	37.724546	5.914991	38.794272
C	27.789697	4.934142	40.826095	C	39.116373	5.632113	38.825025
C	12.571236	3.934968	39.877095	C	39.644049	4.810678	39.819541
C	27.535353	3.120249	39.228622	O	39.935673	6.163053	37.875161
C	26.135930	3.357776	39.151605	O	34.730945	5.581181	41.711192
C	25.547315	4.375115	39.899075	O	34.252110	3.419356	42.122474
O	25.493174	2.494899	38.310545	C	35.052694	4.370789	41.879494
O	15.269303	6.440165	41.352733	C	32.362768	3.944899	37.961583
O	14.778880	4.286799	41.805610	C	32.993927	2.789651	37.536565
C	14.425597	5.484537	41.503173	C	33.057005	2.493322	36.158021
C	16.713339	5.841952	45.695726	C	32.478365	3.337524	35.233069
C	17.716091	6.613494	46.311421	C	31.774871	4.523550	35.623284
C	18.781294	6.903260	32.219211	C	31.710875	4.818433	37.031553
C	17.677278	6.468490	32.944089	C	30.956868	5.950691	37.456151
C	16.648213	5.728109	32.330339	C	30.332784	6.762889	36.545081
C	15.588274	5.421783	46.460003	C	30.427512	6.507561	35.150062
C	14.507510	4.731289	45.871756	C	31.136220	5.405061	34.680209
C	13.423973	4.326510	46.645414	O	29.773551	7.434760	34.389123
C	14.486984	4.608090	32.423645	O	32.786371	5.463215	39.711706

O	32.181907	3.364162	40.249501	C	52.828352	3.947593	43.079296
C	32.439331	4.282896	39.417555	C	54.201352	3.732573	43.123194
C	28.606481	5.762574	41.659896	C	54.987277	4.036578	42.018142
C	28.071785	6.815165	42.380817	C	54.401202	4.554601	40.869191
C	42.295338	7.232732	42.158099	C	53.028202	4.768621	40.826292
C	41.455411	6.431102	41.394256	C	52.442128	5.287645	39.677341
C	41.961975	5.356829	40.636652	C	53.229054	5.591649	38.571289
C	43.357033	5.082229	40.675489	C	54.601054	5.377629	38.616189
C	28.337618	3.876784	40.042661	C	55.187129	4.858606	39.764139
C	43.010303	3.266754	39.102314	O	55.314970	5.617636	37.405141
C	41.646369	3.507404	39.077730	O	50.372346	5.931496	41.729053
C	41.103359	4.559748	39.841038	O	49.973772	3.756067	42.179328
O	40.867915	2.659827	38.294305	C	50.775296	4.733627	41.957451
O	30.858488	6.455145	41.474355	C	48.267112	4.395457	37.817907
O	30.433832	4.354644	42.157278	C	49.053336	3.334803	37.333146
C	30.074735	5.502746	41.771729	C	49.116547	3.057492	35.974789
C	32.271806	6.061535	45.738948	C	48.390780	3.829972	35.075307
C	33.137160	6.975461	46.312386	C	47.567722	4.887125	35.516346
C	34.519867	6.619763	32.312833	C	47.492397	5.165566	36.907805
C	33.420848	6.212890	33.061147	C	46.620676	6.178550	37.354430
C	32.357618	5.508346	32.467519	C	45.881213	6.920984	36.442228
C	31.175973	5.513630	46.485168	C	45.970168	6.682381	35.080727
C	30.198456	4.661512	45.894968	C	46.817877	5.662299	34.592629
C	29.152107	4.168742	46.637008	O	45.215104	7.504653	34.247049
C	30.167419	4.458325	32.605359	O	48.478212	5.883234	39.668865
C	31.226114	5.128477	33.226609	O	48.096672	3.700364	40.090796
O	29.050012	4.100124	33.348223	C	48.279974	4.676473	39.278313
O	32.791346	6.588074	43.499862	C	44.206399	5.886210	41.485509
O	32.437071	4.430516	44.035182	C	43.657071	6.967391	42.198787
C	32.516892	5.661632	44.317502	C	43.867369	4.038374	39.879366
Cu	48.447210	6.400728	41.587728	O	46.473350	6.618941	41.476743
Cu	47.997322	3.974305	42.058475	O	46.067130	4.436530	41.875813
C	52.242277	4.464616	41.931345	C	45.668292	5.629160	41.614239

C	47.873827	6.039549	45.796995	C	22.648011	4.560487	55.320787
C	48.830483	6.846395	46.440209	O	22.920674	5.665233	53.193123
C	50.045136	7.184665	32.166122	O	17.795263	5.594825	57.299951
C	48.986543	6.695206	32.923640	O	17.304484	3.423553	57.670945
C	47.999897	5.871224	32.348980	C	18.146191	4.373736	57.482124
C	46.741083	5.582069	46.526548	C	15.685801	4.212338	53.322240
C	45.700309	4.858716	45.906063	C	16.411547	3.110296	52.835013
C	44.612265	4.410933	46.648756	C	16.472484	2.841226	51.474902
C	45.921705	4.611141	32.511595	C	15.802579	3.662343	50.575352
C	46.912594	5.392934	33.121189	C	15.040824	4.763635	51.017514
O	44.848380	4.152077	33.266731	C	14.970616	5.037011	52.410800
O	48.350716	6.676059	43.552874	C	14.159341	6.098997	52.857129
O	47.919477	4.501544	43.972977	C	13.475264	6.891699	51.943935
C	48.065540	5.718106	44.357018	C	13.559533	6.655559	50.581696
C	9.830844	7.260885	57.522289	C	14.344650	5.586731	50.093193
C	8.959813	6.502896	56.749314	O	12.860063	7.525844	49.748152
C	9.429780	5.394897	56.054290	O	15.947543	5.655507	55.205255
C	10.771780	5.042887	56.134240	O	15.439599	3.489633	55.578772
C	10.370715	3.178901	54.666241	C	15.689409	4.468873	54.787949
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.302285	7.076475	57.572712
Cu	15.893522	6.138058	57.133928	C	24.469259	6.248584	56.829423
Cu	15.341314	3.724220	57.551298	C	24.982350	5.147998	56.112073
C	19.594812	4.040704	57.437285	C	26.377977	4.884851	56.161298
C	20.148039	3.277351	58.481000	C	11.243748	3.934890	55.440215
C	21.500998	2.962918	58.494399	C	26.054780	3.033073	54.624203
C	22.324427	3.397221	57.461069	C	24.687559	3.252513	54.600473
C	21.808260	4.139904	56.381729	C	24.125995	4.313429	55.346333
C	20.423146	4.452274	56.356163	O	23.921976	2.371554	53.839484
C	19.897815	5.133211	55.237280	O	13.938902	6.431865	56.972258
C	20.732126	5.528436	54.196296	O	13.435043	4.270256	57.369081
C	22.098401	5.262934	54.239532	C	13.091602	5.475124	57.084524

C	15.283042	5.695809	61.352094	C	31.400451	3.702430	50.564590
C	16.314083	6.385792	61.978046	C	30.578044	4.754431	51.014559
C	17.647075	6.928780	47.662130	C	30.494544	5.015083	52.409695
C	16.569914	6.488294	48.422781	C	29.632476	6.033593	52.861388
C	15.528973	5.737395	47.844356	C	28.905436	6.791621	51.949830
C	14.198077	5.242813	62.095147	C	29.000049	6.565285	50.586319
C	13.166036	4.552830	61.469195	C	29.836783	5.541740	50.099592
C	12.083071	4.099834	62.213248	O	28.259423	7.398822	49.752930
C	13.382962	4.597647	48.010796	O	31.483855	5.671003	55.198647
C	14.421817	5.313994	48.620743	O	31.044452	3.490738	55.575515
O	12.291340	4.190839	48.769984	C	31.256731	4.477705	54.782966
O	15.758676	6.378528	59.108011	C	27.216848	5.707545	56.962964
O	15.278097	4.206406	59.477114	C	26.662674	6.810351	57.637923
C	15.446345	5.410061	59.891979	C	40.912843	6.952096	57.633048
Cu	31.463158	6.145080	57.131261	C	40.085483	6.136843	56.872076
Cu	30.955679	3.721428	57.550802	C	40.602156	5.045978	56.142545
C	35.200809	4.083022	57.439972	C	41.999324	4.783090	56.192446
C	35.740992	3.344914	58.509065	C	26.900445	3.832375	55.383204
C	37.087616	3.006710	58.535220	C	41.678523	2.944679	54.640424
C	37.919108	3.390984	57.489395	C	40.311404	3.168255	54.609627
C	37.418746	4.112385	56.388536	C	39.747142	4.224217	55.360880
C	36.039255	4.451810	56.351760	O	39.548364	2.293484	53.839145
C	35.529207	5.113823	55.215669	O	29.494756	6.411430	57.016989
C	36.372868	5.461267	54.164882	O	29.043285	4.232296	57.383513
C	37.733949	5.168753	54.217209	C	28.670470	5.433997	57.128590
C	38.269627	4.486385	55.318641	C	30.903116	5.695628	61.351271
O	38.565034	5.526460	53.161782	C	31.934171	6.385605	61.977208
O	33.381410	5.621871	57.260097	C	32.987078	7.334596	47.669940
O	32.919395	3.449761	57.661365	C	31.973345	6.790459	48.429662
C	33.748705	4.407288	57.461563	C	31.026066	5.870034	47.874023
C	31.252007	4.222674	53.316455	C	29.818163	5.242633	62.094342
C	32.031594	3.161915	52.821544	C	28.786109	4.552656	61.468406
C	32.109403	2.908817	51.459019	C	27.703155	4.099663	62.212477

C	29.029012	4.466787	48.020757	O	47.121677	5.803492	55.214946
C	29.949715	5.308562	48.641957	O	46.812532	3.595558	55.560909
O	28.005190	3.929728	48.740385	C	46.965272	4.604087	54.783449
O	31.365109	6.379866	59.106653	C	42.836563	5.605491	56.996288
O	30.899374	4.204609	59.477424	C	42.273420	6.691242	57.693016
C	31.063481	5.409435	59.891576	C	42.523316	3.736933	55.408608
Cu	47.050949	6.251411	57.151020	O	45.076836	6.400710	57.023780
Cu	46.686624	3.795035	57.532606	O	44.741066	4.194589	57.349994
C	50.914826	4.464382	57.493755	C	44.304085	5.381792	57.123593
C	51.500920	3.947352	58.641694	C	46.523192	5.695393	61.350166
C	52.873920	3.732327	58.685568	C	47.554258	6.385364	61.976087
C	53.659827	4.036331	57.580503	C	48.707509	7.164403	47.786125
C	53.073733	4.554362	56.431564	C	47.625050	6.685352	48.514832
C	51.700733	4.768387	56.388690	C	46.632288	5.891514	47.908393
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.530519	4.665272	48.015334
O	53.987443	5.617405	52.967501	C	45.527299	5.414250	48.655896
O	48.991626	5.859520	57.301076	O	43.440637	4.206394	48.746205
O	48.672403	3.655289	57.668243	O	46.921201	6.443775	59.124218
C	49.437938	4.672495	57.497826	O	46.573317	4.239329	59.461351
C	46.962167	4.367421	53.316260	C	46.675285	5.443905	59.890997
C	47.784155	3.348705	52.801711	C	16.262158	6.620778	63.347051
C	47.836245	3.095645	51.438582	C	15.179191	6.168782	64.090104
C	47.065794	3.852702	50.563962	C	14.147152	5.478800	63.465152
C	46.213412	4.873776	51.034533	C	12.031146	4.336820	63.582253
C	46.146756	5.124103	52.431464	C	13.063187	5.025805	64.207205
C	45.242785	6.093984	52.908388	O	10.943183	3.908824	64.361306
C	44.465640	6.826216	52.019784	C	31.882271	6.620587	63.346214
C	44.548626	6.619895	50.652693	C	30.799317	6.168593	64.089284
C	45.426920	5.640852	50.134486	C	29.767262	5.478616	63.464348
O	43.762003	7.438211	49.844789	C	27.651255	4.336645	63.581483

C	28.683309	5.025622	64.206418	H	37.673627	2.816627	28.310846
O	26.563304	3.908650	64.360554	H	40.062868	2.245237	28.396619
C	47.502385	6.620342	63.345096	H	41.569263	2.948780	26.609008
C	46.419443	6.168348	64.088184	H	37.116516	5.179393	24.106292
C	45.387375	5.478376	63.463264	H	38.630801	5.817257	22.332949
C	43.271365	4.336411	63.580432	H	35.146057	2.325296	22.590354
C	44.303433	5.025383	64.205353	H	35.297750	1.792954	20.190412
O	42.183428	3.908416	64.359522	H	34.099811	3.170464	18.536523
H	12.119252	8.127130	26.935675	H	32.268041	6.144861	22.826147
H	10.573040	6.786856	25.566344	H	31.125420	7.500027	21.164952
H	13.383653	2.323356	22.982287	H	29.921161	7.385893	27.146227
H	9.847463	3.169689	22.676888	H	43.132118	7.757266	27.099189
H	22.115758	2.849669	28.239806	H	41.664396	6.266815	25.854053
H	24.509734	2.285991	28.275294	H	30.587199	3.489089	24.326096
H	25.983300	3.028167	26.475199	H	44.726102	1.924850	23.222442
H	21.469843	5.218677	24.049341	H	35.450271	6.646252	30.389626
H	22.950498	5.901115	22.267853	H	31.302177	4.310915	29.419901
H	19.532045	2.329470	22.589906	H	29.391704	3.675915	30.758846
H	19.679275	1.794029	20.190518	H	31.291830	6.860993	17.596343
H	18.480501	3.170816	18.536733	H	40.762674	5.904799	21.514328
H	16.651615	6.145317	22.827160	H	41.205536	2.298087	23.000642
H	15.506929	7.501071	21.165073	H	53.552008	3.700205	28.381286
H	14.495589	7.508309	27.087432	H	55.987726	3.326163	28.455758
H	27.515289	7.862421	26.994014	H	57.384066	3.866347	26.497870
H	26.042647	6.398234	25.719261	H	52.703445	5.451806	24.014163
H	14.941533	3.634107	24.311235	H	54.081113	5.975912	22.116748
H	29.090929	2.068976	23.052172	H	50.777523	2.335080	22.589463
H	19.763877	6.924659	30.321697	H	50.920925	1.795285	20.189770
H	15.665825	4.545433	29.254917	H	49.720406	3.170967	18.535936
H	13.751364	3.846382	30.552288	H	47.862680	6.134553	22.823785
H	15.671674	6.861055	17.596390	H	46.741113	7.496804	21.164804
H	25.072117	6.039549	21.428785	H	45.548201	7.335223	27.194038
H	25.569131	2.436723	22.852341	H	46.223685	3.370648	24.471905

H 50.986667 7.227528 30.247695	H 36.322089 2.724205 43.496902
H 47.059019 4.524954 29.327744	H 38.770192 2.168194 43.556121
H 45.215560 3.738462 30.677634	H 40.301145 3.122301 41.902444
H 46.913257 6.862043 17.595758	H 35.815259 5.659203 39.708469
H 56.056327 5.977255 21.104073	H 37.325746 6.552044 37.995920
H 10.790981 8.128149 42.498341	H 33.460673 2.130938 38.273553
H 9.244457 6.787099 41.129974	H 33.575882 1.590562 35.820475
H 12.055348 2.324934 38.544144	H 32.556971 3.074179 34.173320
H 8.519431 3.171288 38.239461	H 30.868106 6.171426 38.520550
H 20.824940 2.982152 43.684910	H 29.741180 7.625228 36.864251
H 23.221208 2.446637 43.790538	H 28.714125 7.430530 43.016453
H 24.740000 3.204296 42.037212	H 41.886653 8.064721 42.723043
H 20.284020 5.393650 39.503158	H 40.400198 6.670157 41.387965
H 21.814298 6.087405 37.765215	H 29.406144 3.657844 40.089453
H 18.151045 2.393411 37.876923	H 43.408882 2.461889 38.498690
H 18.153435 1.917272 35.465248	H 33.941942 7.401899 45.708160
H 16.925082 3.347667 33.921661	H 35.324894 7.172622 32.786960
H 15.203167 6.215007 38.379086	H 33.401725 6.465777 34.113778
H 13.966210 7.594830 36.813473	H 30.269168 4.398529 44.838978
H 13.169369 7.511894 42.644910	H 28.403560 3.524527 46.160197
H 26.259120 7.893094 42.893634	H 28.380916 3.570436 32.808665
H 24.799369 6.528749 41.490403	H 29.794720 7.226189 33.442173
H 13.611962 3.633921 39.868338	H 39.418364 6.716264 37.267797
H 27.948028 2.313952 38.616598	H 39.884348 2.881811 38.323135
H 18.564791 6.961444 45.733263	H 52.223866 3.709908 43.947687
H 19.557609 7.484164 32.707158	H 54.659335 3.328160 44.019913
H 17.625032 6.729698 33.992338	H 56.055397 3.866628 42.061240
H 14.474513 4.505768 44.811276	H 51.374593 5.452743 39.579173
H 12.609949 3.794498 46.172047	H 52.752217 5.975698 37.680067
H 12.716272 3.682429 32.584420	H 49.630574 2.727573 38.021247
H 13.971706 7.223666 33.286718	H 49.733597 2.240058 35.615439
H 23.960342 6.246110 36.991155	H 48.464952 3.581744 34.026171
H 24.547224 2.689065 38.223139	H 46.485715 6.405117 38.406054

H 45.217830 7.700186 36.792990	H 13.128868 4.376102 60.400545
H 44.296946 7.601468 42.802305	H 11.277797 3.574471 61.719260
H 44.926734 3.809013 39.834542	H 11.625083 3.659394 48.229889
H 49.681969 7.224702 45.885871	H 12.954339 7.298489 48.772938
H 50.788296 7.829746 32.624106	H 22.420678 6.189233 52.490512
H 48.934896 6.978704 33.966235	H 22.941284 2.594318 53.847121
H 45.701854 4.639893 44.843845	H 35.104061 3.033423 59.329243
H 43.828938 3.855165 46.151391	H 37.489815 2.440487 59.369304
H 44.218487 3.575579 32.729040	H 38.961478 3.106919 57.539799
H 45.308039 7.270134 33.273469	H 34.477678 5.362515 55.117173
H 54.726628 5.972702 36.665869	H 35.958939 5.969375 53.304444
H 9.463385 8.127045 58.062936	H 32.594026 2.535832 53.505108
H 7.916948 6.786702 56.693570	H 32.724431 2.093085 51.092107
H 10.728082 2.325373 54.106648	H 31.487374 3.473234 49.510834
H 7.191610 3.170328 53.803751	H 29.497103 6.252034 53.915512
H 19.518856 2.934581 59.294582	H 28.247899 7.574732 52.304147
H 21.915560 2.380527 59.311129	H 27.296821 7.458264 58.232369
H 23.373003 3.135230 57.503685	H 40.495993 7.793018 58.178158
H 18.841064 5.359078 55.142699	H 39.032712 6.378313 56.845528
H 20.306193 6.050712 53.350332	H 27.961971 3.618317 55.334538
H 16.941417 2.461464 53.523188	H 42.088157 2.138894 54.046220
H 17.042767 1.990955 51.114327	H 32.787936 6.739527 61.409435
H 15.871824 3.418405 49.524825	H 33.685141 8.045625 48.122649
H 14.029458 6.326831 53.909061	H 31.889819 7.084762 49.480637
H 12.859668 7.709232 52.294369	H 28.748503 4.375636 60.399825
H 11.840560 7.509203 58.212312	H 26.897610 3.574741 61.718347
H 24.888787 7.926288 58.106436	H 27.470624 3.352502 48.171394
H 23.415633 6.487487 56.805207	H 28.374152 7.187963 48.772960
H 12.285097 3.636323 55.426864	H 38.076004 6.039006 52.443091
H 26.463307 2.223041 54.034956	H 38.568160 2.518211 53.843177
H 17.168295 6.739366 61.410626	H 50.894893 3.700082 59.506302
H 18.434468 7.516348 48.123866	H 53.331558 3.325525 59.581313
H 16.549221 6.750979 49.471804	H 54.727835 3.865729 57.623155

H	50.047592	5.459327	55.145343	H	7.520572	4.915535	55.216424
H	51.424877	5.977005	53.243003	H	12.998923	5.198968	65.269007
H	48.392113	2.750733	53.471194	H	28.618738	5.198967	65.268132
H	48.476750	2.307159	51.056385	H	44.238590	5.198830	65.267015
H	47.129231	3.620291	49.510660	H	48.273983	5.043212	18.026066
H	45.111850	6.294622	53.965761	C	32.766115	8.585355	39.331889
H	43.777948	7.572942	52.393660	C	33.208144	9.556251	40.357249
H	42.904001	7.338519	58.292091	C	34.531855	10.289460	40.224328
H	43.584766	3.521984	55.363354	C	35.171633	10.136366	38.831097
H	48.405656	6.744618	61.407916	C	35.064134	8.700631	38.298110
H	49.455887	7.784867	48.268911	C	33.595926	8.292853	38.104910
H	47.560394	6.953118	49.560703	O	33.328983	8.132784	40.573390
H	44.381384	4.364380	60.399375	C	30.038289	9.879688	42.631535
H	42.519297	3.571656	61.717704	C	29.336103	11.054778	42.970930
H	42.806284	3.655721	48.186974	C	29.423620	11.588708	44.259618
H	43.848677	7.225828	48.865785	C	30.203426	10.967010	45.242120
H	53.398795	5.970941	52.227648	C	30.902290	9.799440	44.909789
H	17.068268	7.157984	63.836011	C	30.829088	9.260528	43.623803
H	15.148116	6.357234	65.155551	N	29.997241	9.353227	41.339983
H	10.263094	3.421732	63.797175	H	34.376880	11.357585	40.459469
H	32.688226	7.158026	63.835100	H	32.428280	10.009048	40.982105
H	30.768031	6.357177	65.154678	H	31.688678	8.391985	39.252076
H	25.881682	3.424335	63.795760	H	36.227570	10.458262	38.872854
H	48.307514	7.159119	63.833758	H	34.662318	10.816572	38.119744
H	46.387763	6.357312	65.153484	H	35.601702	8.607337	37.336899
H	41.501068	3.425260	63.794504	H	35.547191	8.006151	39.009031
H	54.922535	4.682790	55.325763	H	33.150215	8.846187	37.255553
H	56.250077	4.683175	39.763689	H	33.503499	7.217690	37.875002
H	57.578883	4.683451	24.200610	H	35.209226	9.890435	41.002440
H	32.654254	5.043359	18.026530	H	28.719965	11.551759	42.212776
H	17.034851	5.043671	18.026678	H	28.869674	12.503755	44.498043
H	10.176557	4.915284	24.089609	H	30.264276	11.384919	46.251803
H	8.848003	4.915575	39.653290	H	31.514074	9.287693	45.660542

H	31.391731	8.355658	43.382301	C	17.639888	4.497025	20.008011
H	30.218434	8.356593	41.272644	C	17.550913	4.800019	21.362013
H	29.180401	9.608501	40.791008	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355032	19.497042
(<i>R,R</i>)-2-RC (open-shell singlet)				C	16.963876	5.274031	19.076025
C	12.487000	7.261000	26.395000	O	15.523872	7.185038	18.539057
C	11.616000	6.503000	25.622000	O	18.564826	5.528450	24.111931
C	12.086000	5.395000	24.927000	O	18.020439	3.387577	24.573172
C	13.428000	5.043000	25.007000	C	18.263945	4.335758	23.745203
C	13.027000	3.179000	23.539000	C	14.301000	5.801000	25.782000
C	11.685000	3.529000	23.460000	C	13.829000	6.909000	26.476000
C	11.215000	4.638000	24.154000	C	27.939965	7.064609	26.445164
O	10.782000	2.793000	22.654000	C	27.106590	6.205754	25.736963
Cu	18.544566	6.083742	26.015556	C	27.621154	5.081391	25.059064
Cu	17.949064	3.696088	26.527824	C	29.017624	4.824774	25.114902
C	22.213397	3.943415	26.372783	C	13.900000	3.935000	24.313000
C	22.757992	3.186169	27.425551	C	28.698126	2.918068	23.645146
C	24.111644	2.874477	27.453900	C	27.330242	3.131362	23.617155
C	24.945637	3.308478	26.428655	C	26.766415	4.216580	24.325246
C	24.438513	4.042117	25.339267	O	26.567004	2.224728	22.884458
C	23.051717	4.345767	25.294950	O	16.597062	6.402542	25.851275
C	22.535193	5.008997	24.161246	O	16.054757	4.263354	26.319282
C	23.379497	5.400902	23.127116	C	15.735970	5.461599	25.984937
C	24.747270	5.148268	23.190800	C	17.910463	5.816822	30.229028
C	25.288474	4.460558	24.285477	C	18.902882	6.575867	30.875514
O	25.579114	5.545574	22.149817	C	16.756480	5.410482	30.955936
O	20.435305	5.514917	26.186742	C	15.680859	4.744451	30.330391
O	19.911531	3.369255	26.648707	C	14.571889	4.345186	31.070310
C	20.768045	4.296764	26.413825	O	18.433555	6.400239	27.976640
C	18.226927	4.022014	22.293999	O	17.897081	4.255826	28.429782
C	18.992915	2.941012	21.873981	C	18.097335	5.469877	28.794498
C	19.081890	2.638017	20.519979	Cu	34.115147	6.055775	26.054497
C	18.404876	3.417024	19.587993				

Cu	33.556545	3.658606	26.554235	C	43.246797	4.907924	25.178439
C	37.812133	3.939132	26.433352	C	44.645582	4.658165	25.235006
C	38.329217	3.210002	27.519946	C	29.542183	3.747515	24.372604
C	39.674217	2.869094	27.576428	C	44.330564	2.729810	23.794257
C	40.527676	3.242494	26.544433	C	42.962925	2.947729	23.750917
C	40.049854	3.949862	25.424926	C	42.396173	4.042885	24.440796
C	38.671978	4.290355	25.355946	O	42.202354	2.034445	23.023916
C	38.185764	4.936996	24.200472	O	32.146986	6.354778	25.936638
C	39.051193	5.270153	23.162651	O	31.656777	4.197892	26.376588
C	40.410407	4.976707	23.246602	C	31.305582	5.394588	26.075985
C	40.921780	4.308247	24.367476	C	33.611588	5.751216	30.286976
O	41.263904	5.320732	22.204146	C	34.667485	6.443625	30.907379
O	36.021156	5.500884	26.193097	C	32.453746	5.421451	31.045883
O	35.516923	3.352994	26.665894	C	31.331533	4.808172	30.452515
C	36.365130	4.287290	26.435136	C	30.207282	4.509779	31.216968
C	33.846855	4.021974	22.293721	O	34.041738	6.352069	28.021172
C	34.612832	2.940971	21.873686	O	33.514011	4.204498	28.468808
C	34.701783	2.637980	20.519681	C	33.733363	5.414019	28.840829
C	34.024755	3.416991	19.587710	Cu	49.697168	6.205848	25.981152
C	33.259777	4.496993	20.007743	Cu	49.346545	3.788002	26.562760
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.123586	5.521645	24.139514	C	53.770890	5.287820	24.113942
O	33.626877	3.367683	24.583222	C	54.557834	5.591822	23.007903
C	33.858111	4.324738	23.758296	C	55.929834	5.377808	23.052827
C	29.856088	5.676605	25.886829	C	56.515890	4.858790	24.200790
C	29.301639	6.804090	26.518789	O	56.643771	5.617813	21.841791
C	43.550983	6.894735	26.561358	O	51.638394	5.837344	26.121878
C	42.724927	6.030474	25.854170	O	51.335951	3.660021	26.633082

C	52.093702	4.666381	26.379749	C	11.698220	3.178974	39.103108
C	49.466780	4.021882	22.293161	C	10.356220	3.528979	39.024133
C	50.232747	2.940878	21.873109	C	9.886236	4.637978	39.718145
C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.237808	6.135646	41.480054
C	48.879663	4.496911	20.007197	Cu	16.684412	3.738845	41.985355
C	48.790739	4.799899	21.361205	C	20.954842	4.056338	41.900202
C	48.023773	5.880903	21.783256	C	21.454455	3.310901	42.984010
C	47.347732	6.658919	20.849300	C	22.808564	3.017888	43.087851
C	47.437657	6.354932	19.496292	C	23.691119	3.454209	42.105810
C	48.203622	5.273928	19.075240	C	23.235106	4.173053	40.986264
O	46.763615	7.184949	18.538336	C	21.848158	4.468278	40.869974
O	49.733195	5.591140	24.088507	C	21.388102	5.128383	39.712077
O	49.385647	3.425870	24.607665	C	22.283821	5.511533	38.717716
C	49.525978	4.368703	23.749005	C	23.646310	5.253033	38.845693
C	45.481723	5.534630	25.980018	C	24.132285	4.581006	39.971930
C	44.915559	6.653086	26.619370	O	24.524198	5.629952	37.837637
C	45.172911	3.568990	24.513839	O	19.146144	5.592303	41.622707
O	47.717957	6.337989	25.883236	O	18.653728	3.442482	42.095423
O	47.397075	4.170940	26.420145	C	19.498926	4.383211	41.871503
C	46.951657	5.331587	26.096531	C	16.886269	4.115503	37.738444
C	49.198164	5.992701	30.212298	C	17.590513	3.011020	37.227143
C	50.141056	6.835013	30.828603	C	17.599833	2.741525	35.865521
C	48.083189	5.523882	30.961457	C	16.904755	3.568972	34.990463
C	47.057438	4.759497	30.365385	C	16.160232	4.670884	35.460868
C	45.984579	4.304189	31.125311	C	16.129935	4.934273	36.855988
O	49.608222	6.566437	27.935081	C	15.321806	5.985276	37.334378
O	49.301423	4.391510	28.452934	C	14.607820	6.781657	36.448037
C	49.388914	5.628686	28.783243	C	14.664590	6.564579	35.081445
C	11.158284	7.260965	41.959133	C	15.447403	5.508349	34.562737
C	10.287267	6.502972	41.186144	O	13.945899	7.443996	34.274501
C	10.757252	5.394972	40.491132	O	17.238362	5.594750	39.570585
C	12.099252	5.042967	40.571107	O	16.749430	3.438610	40.019711

C	16.964635	4.398196	39.195446	C	38.546110	2.988417	42.934285
C	12.972269	5.800962	41.346096	C	39.360660	3.433796	41.912879
C	12.500284	6.908961	42.040108	C	38.836037	4.151246	40.789221
C	26.840309	7.283476	42.044395	C	37.413178	4.377237	40.760731
C	25.984161	6.405655	41.411632	C	36.841024	4.964672	39.600459
C	26.455842	5.215182	40.769998	C	37.630832	5.397324	38.567845
C	27.870447	4.942756	40.839844	C	39.046241	5.313528	38.649823
C	12.571236	3.934968	39.877095	C	39.655709	4.653749	39.718335
C	27.532428	2.949528	39.487381	O	39.794568	5.876196	37.662785
C	26.134069	3.195060	39.433410	O	34.865399	5.562300	41.743651
C	25.587180	4.309901	40.062990	O	34.327779	3.417485	42.158501
O	25.449964	2.247676	38.725435	C	35.157385	4.340078	41.925204
O	15.273980	6.431176	41.358584	C	32.580382	4.276861	37.889215
O	14.773199	4.280387	41.811319	C	33.218538	3.132755	37.443278
C	14.425278	5.479447	41.507302	C	33.242941	2.836970	36.064462
C	16.704248	5.839495	45.706767	C	32.608393	3.664227	35.161538
C	17.713574	6.603134	46.321448	C	31.900969	4.840463	35.573512
C	18.796708	6.887805	32.224540	C	31.895049	5.148310	36.981530
C	17.695473	6.450942	32.952307	C	31.158483	6.284794	37.427373
C	16.664304	5.712263	32.340366	C	30.473093	7.069994	36.536350
C	15.573968	5.432904	46.470112	C	30.491126	6.789491	35.142990
C	14.486997	4.752308	45.881841	C	31.202325	5.698691	34.650509
C	13.398884	4.359393	46.655347	O	29.775700	7.689224	34.405223
C	14.503400	4.592247	32.438968	O	32.979622	5.744289	39.697555
C	15.537051	5.284219	33.084245	O	32.386801	3.619415	40.147150
O	13.390640	4.185588	33.166671	C	32.645363	4.571268	39.353750
O	17.158502	6.438099	43.444577	C	28.728958	5.861280	41.530202
O	16.645369	4.287845	43.894519	C	28.226213	7.022146	42.093253
C	16.847899	5.500516	44.264085	C	42.250192	7.224182	41.986380
Cu	33.006899	6.341943	41.579173	C	41.431585	6.392637	41.229616
Cu	32.414230	3.864922	42.113982	C	41.965323	5.313138	40.499874
C	36.608440	3.968295	41.870959	C	43.367691	5.072704	40.551023
C	37.158012	3.257754	42.921841	C	28.373914	3.790086	40.168710

C	43.077692	3.244283	38.983459	O	55.314970	5.617636	37.405141
C	41.705946	3.436124	38.963899	O	50.368889	5.936445	41.720767
C	41.127987	4.476547	39.719760	O	49.963060	3.764091	42.174383
O	40.956260	2.545593	38.199895	C	50.770443	4.738257	41.954811
O	30.996918	6.541087	41.470341	C	48.282612	4.397755	37.789090
O	30.529294	4.420533	42.052320	C	49.078682	3.346279	37.300537
C	30.194083	5.589087	41.687618	C	49.130582	3.063750	35.942596
C	32.364171	5.966691	45.770634	C	48.385586	3.823352	35.047831
C	33.249450	6.847702	46.365644	C	47.554588	4.872504	35.493295
C	34.613168	6.770701	32.256354	C	47.488553	5.153960	36.884307
C	33.497968	6.423021	33.010168	C	46.606789	6.155753	37.336462
C	32.406083	5.752509	32.428043	C	45.846620	6.883524	36.429689
C	31.261103	5.419766	46.505622	C	45.928103	6.644244	35.067793
C	30.270937	4.594868	45.897572	C	46.788283	5.637145	34.574387
C	29.217991	4.101033	46.628941	O	45.156225	7.455773	34.239135
C	30.171078	4.803344	32.578023	O	48.493250	5.887592	39.638017
C	31.262432	5.426002	33.193781	O	48.107636	3.705904	40.061992
O	29.034754	4.513248	33.321919	C	48.296408	4.680149	39.248806
O	32.901819	6.550063	43.553654	C	44.193699	5.894552	41.368423
O	32.465768	4.390801	44.009439	C	43.616082	6.978820	42.054942
C	32.592355	5.606228	44.336072	C	43.909741	4.042631	39.759405
Cu	48.441492	6.410283	41.555429	O	46.465041	6.633558	41.416382
Cu	47.983589	3.986829	42.027227	O	46.053329	4.452407	41.812406
C	52.242277	4.464616	41.931345	C	45.656818	5.643657	41.537853
C	52.828352	3.947593	43.079296	C	47.841397	6.059776	45.765586
C	54.201352	3.732573	43.123194	C	48.796637	6.875418	46.400278
C	54.987277	4.036578	42.018142	C	50.024141	7.174525	32.170322
C	54.401202	4.554601	40.869191	C	48.959698	6.684641	32.919352
C	53.028202	4.768621	40.826292	C	47.977994	5.859687	32.337149
C	52.442128	5.287645	39.677341	C	46.721866	5.589397	46.507984
C	53.229054	5.591649	38.571289	C	45.679875	4.859026	45.898336
C	54.601054	5.377629	38.616189	C	44.606280	4.397314	46.654077
C	55.187129	4.858606	39.764139	C	45.903673	4.591181	32.485508

C	46.887642	5.376318	33.101937	C	15.024817	4.774001	51.022524
O	44.828638	4.125626	33.233986	C	14.960921	5.042663	52.416847
O	48.322276	6.691552	43.519442	C	14.158569	6.109023	52.869363
O	47.880566	4.519787	43.940463	C	13.479543	6.911573	51.961022
C	48.028912	5.736299	44.324129	C	13.559740	6.681026	50.597615
C	9.830844	7.260885	57.522289	C	14.334198	5.607243	50.103282
C	8.959813	6.502896	56.749314	O	12.867105	7.561255	49.768861
C	9.429780	5.394897	56.054290	O	15.948617	5.648566	55.206299
C	10.771780	5.042887	56.134240	O	15.434913	3.484158	55.580188
C	10.370715	3.178901	54.666241	C	15.685016	4.463099	54.789124
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.311261	7.039098	57.578001
Cu	15.895645	6.132391	57.134124	C	24.476974	6.213052	56.834169
Cu	15.338916	3.719960	57.552937	C	24.987570	5.109013	56.120612
C	19.593741	4.027163	57.441415	C	26.382457	4.841102	56.173241
C	20.142857	3.263206	58.486909	C	11.243748	3.934890	55.440215
C	21.494244	2.942049	58.501710	C	26.056407	2.990375	54.635927
C	22.320469	3.369996	57.467941	C	24.689758	3.214383	54.608860
C	21.808916	4.113833	56.387270	C	24.129593	4.276520	55.354178
C	20.425231	4.433626	56.360647	O	23.923312	2.336376	53.845419
C	19.904368	5.116817	55.241202	O	13.940655	6.429316	56.972026
C	20.741325	5.505655	54.199953	O	13.433461	4.268986	57.371170
C	22.106073	5.231898	54.243579	C	13.091660	5.473969	57.085286
C	22.651839	4.528424	55.326177	C	15.283042	5.695809	61.352094
O	22.930656	5.628281	53.196737	C	16.314083	6.385792	61.978046
O	17.797050	5.585629	57.300597	C	17.645225	6.924145	47.670710
O	17.301622	3.415556	57.672104	C	16.563271	6.495405	48.431241
C	18.145513	4.363826	57.483638	C	15.516445	5.751972	47.853588
C	15.672731	4.209178	53.323015	C	14.198077	5.242813	62.095147
C	16.386229	3.101758	52.829704	C	13.166036	4.552830	61.469195
C	16.439074	2.836118	51.468537	C	12.083071	4.099834	62.213248
C	15.774372	3.666853	50.574100	C	13.360139	4.632120	48.020508

C	14.405651	5.338934	48.630006	O	31.055455	3.425799	55.606046
O	12.265172	4.235497	48.780228	C	31.272352	4.403033	54.803475
O	15.761175	6.375298	59.107652	C	27.223168	5.663262	56.973573
O	15.277540	4.204198	59.478520	C	26.670812	6.768571	57.646289
C	15.447082	5.408104	59.892374	C	40.909118	6.941376	57.615612
Cu	31.471375	6.100115	57.130494	C	40.084629	6.115358	56.863070
Cu	30.964506	3.680786	57.576407	C	40.605708	5.021092	56.141787
C	35.210356	4.044504	57.454435	C	42.004179	4.765710	56.191814
C	35.754718	3.315823	58.527771	C	26.902858	3.785480	55.398495
C	37.102785	2.983307	58.554737	C	41.690858	2.913792	54.654345
C	37.931628	3.363763	57.505410	C	40.322516	3.129433	54.624558
C	37.426851	4.073879	56.399334	C	39.753801	4.188397	55.368277
C	36.045834	4.407209	56.361592	O	39.563021	2.244466	53.862286
C	35.531662	5.057387	55.220480	O	29.502455	6.364669	57.012089
C	36.372552	5.399156	54.165498	O	29.050641	4.189855	57.403000
C	37.735076	5.113496	54.218938	C	28.677574	5.389243	57.136867
C	38.274963	4.442976	55.325477	C	30.903116	5.695628	61.351271
O	38.563625	5.466898	53.160032	C	31.934171	6.385605	61.977208
O	33.389592	5.580204	57.265984	C	33.110934	7.174802	47.732253
O	32.929190	3.411891	57.689080	C	32.084109	6.636853	48.478216
C	33.757852	4.367767	57.477820	C	31.116629	5.750869	47.900836
C	31.274785	4.130979	53.341351	C	29.818163	5.242633	62.094342
C	32.056319	3.064878	52.861120	C	28.786109	4.552656	61.468406
C	32.141577	2.799186	51.501473	C	27.703155	4.099663	62.212477
C	31.440926	3.587605	50.595907	C	29.094658	4.379076	48.016573
C	30.620485	4.647128	51.032097	C	30.024932	5.198816	48.652550
C	30.525940	4.917633	52.423876	O	28.059697	3.848787	48.724685
C	29.664051	5.942532	52.861867	O	31.370698	6.358423	59.101964
C	28.953581	6.702335	51.939441	O	30.907404	4.186411	59.495455
C	29.062611	6.469476	50.578636	C	31.068824	5.395903	59.896207
C	29.894509	5.435150	50.106647	Cu	47.051586	6.250040	57.150987
O	28.342829	7.308749	49.732626	Cu	46.688727	3.793537	57.533597
O	31.496897	5.601595	55.205187	C	50.914826	4.464382	57.493755

C	51.500920	3.947352	58.641694	C	46.523192	5.695393	61.350166
C	52.873920	3.732327	58.685568	C	47.554258	6.385364	61.976087
C	53.659827	4.036331	57.580503	C	48.688304	7.186235	47.749091
C	53.073733	4.554362	56.431564	C	47.620892	6.692848	48.489925
C	51.700733	4.768387	56.388690	C	46.627533	5.893200	47.892736
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.540039	4.645668	48.022819
O	53.987443	5.617405	52.967501	C	45.535750	5.405013	48.652476
O	48.992008	5.859470	57.302818	O	43.465996	4.170756	48.766837
O	48.673727	3.654845	57.669077	O	46.919693	6.443394	59.123893
C	49.438558	4.672408	57.498548	O	46.574958	4.238585	59.462106
C	46.969302	4.364735	53.316790	C	46.675347	5.443513	59.891150
C	47.787874	3.342181	52.804565	C	16.262158	6.620778	63.347051
C	47.843861	3.089791	51.441393	C	15.179191	6.168782	64.090104
C	47.078998	3.849995	50.564346	C	14.147152	5.478800	63.465152
C	46.227749	4.872800	51.032652	C	12.031146	4.336820	63.582253
C	46.159843	5.124982	52.429454	C	13.063187	5.025805	64.207205
C	45.260056	6.099982	52.903780	O	10.943183	3.908824	64.361306
C	44.486972	6.833961	52.013336	C	31.882271	6.620587	63.346214
C	44.568495	6.623172	50.646869	C	30.799317	6.168593	64.089284
C	45.442835	5.639421	50.130762	C	29.767262	5.478616	63.464348
O	43.782698	7.440551	49.837170	C	27.651255	4.336645	63.581483
O	47.125699	5.801179	55.215525	C	28.683309	5.025622	64.206418
O	46.815183	3.593541	55.561816	O	26.563304	3.908650	64.360554
C	46.969647	4.601749	54.784134	C	47.502385	6.620342	63.345096
C	42.838195	5.597870	56.988961	C	46.419443	6.168348	64.088184
C	42.270981	6.687414	57.676311	C	45.387375	5.478376	63.463264
C	42.532522	3.716595	55.414748	C	43.271365	4.336411	63.580432
O	45.077332	6.397597	57.020866	C	44.303433	5.025383	64.205353
O	44.743757	4.191706	57.350772	O	42.183428	3.908416	64.359522
C	44.305767	5.377758	57.120951	H	12.119252	8.127090	26.935733

H	10.573040	6.786843	25.566353	H	31.124714	7.499464	21.165138
H	13.383774	2.323382	22.982327	H	29.935512	7.474321	27.088164
H	9.847486	3.169741	22.676924	H	43.130010	7.759417	27.064750
H	22.122524	2.849730	28.236932	H	41.668792	6.257376	25.827433
H	24.519085	2.297386	28.278066	H	30.604603	3.537057	24.326898
H	25.995015	3.052043	26.484767	H	44.742274	1.890784	23.249610
H	21.477422	5.221199	24.048160	H	35.544522	6.722433	30.334068
H	22.959786	5.909982	22.270101	H	31.299690	4.565577	29.394678
H	19.532097	2.329493	22.589889	H	29.356685	4.043777	30.737576
H	19.679348	1.794080	20.190520	H	31.292289	6.861218	17.596351
H	18.480483	3.170803	18.536736	H	40.789737	5.827744	21.471992
H	16.651495	6.145383	22.827126	H	41.219494	2.248488	23.029848
H	15.506921	7.501017	21.165194	H	53.551978	3.700079	28.381241
H	14.495576	7.508130	27.087612	H	55.987708	3.326145	28.455755
H	27.525279	7.933278	26.946725	H	57.384060	3.866333	26.497859
H	26.051702	6.439018	25.707250	H	52.703461	5.452019	24.014190
H	14.941535	3.634123	24.311218	H	54.081068	5.975951	22.116790
H	29.108653	2.089057	23.084409	H	50.777604	2.335082	22.589415
H	19.772357	6.914830	30.323665	H	50.920920	1.795284	20.189774
H	15.671536	4.535641	29.265929	H	49.720355	3.170948	18.535941
H	13.761618	3.833567	30.568862	H	47.863169	6.134688	22.823873
H	15.672066	6.861242	17.596385	H	46.741200	7.496820	21.164933
H	25.082245	6.055773	21.435046	H	45.546056	7.340322	27.172211
H	25.585185	2.442927	22.887539	H	46.234978	3.353973	24.482981
H	37.676868	2.912531	28.333288	H	50.979512	7.219106	30.258730
H	40.058520	2.312459	28.425488	H	47.060389	4.512697	29.309092
H	41.569253	2.961096	26.620924	H	45.212761	3.716850	30.646544
H	37.136461	5.183844	24.076370	H	46.912914	6.861743	17.595811
H	38.655580	5.768205	22.287918	H	56.056148	5.977148	21.104161
H	35.148141	2.327644	22.590747	H	10.790930	8.128028	42.498493
H	35.298438	1.793462	20.190382	H	9.244464	6.787120	41.129909
H	34.099971	3.170596	18.536513	H	12.055536	2.325174	38.543890
H	32.263757	6.143629	22.825814	H	8.519524	3.171537	38.239162

H	20.782217	2.969571	43.763376	H	29.890012	7.931560	36.872465
H	23.178397	2.452057	43.937308	H	28.907180	7.719167	42.588655
H	24.740155	3.211994	42.221109	H	41.821349	8.061305	42.528286
H	20.336247	5.341268	39.549184	H	40.372712	6.611900	41.202209
H	21.906071	6.014112	37.837351	H	29.442492	3.574205	40.188391
H	18.146402	2.363963	37.896009	H	43.501688	2.450337	38.382861
H	18.153845	1.889683	35.483994	H	34.063229	7.270539	45.770655
H	16.938052	3.327969	33.937487	H	35.440106	7.297791	32.722237
H	15.216573	6.200774	38.391635	H	33.489557	6.697202	34.057451
H	13.995061	7.590421	36.823076	H	30.338966	4.354124	44.836360
H	13.169420	7.511204	42.645486	H	28.462622	3.474984	46.139173
H	26.441480	8.189006	42.512754	H	28.340251	4.013099	32.786040
H	24.915626	6.644360	41.397851	H	29.727509	7.450269	33.466694
H	13.612093	3.634333	39.867546	H	39.222214	6.451749	37.125058
H	27.914902	2.071887	38.959670	H	39.963697	2.719751	38.240064
H	18.566480	6.940683	45.743335	H	52.223438	3.710469	43.947444
H	19.574911	7.467138	32.711428	H	54.659353	3.328256	44.019942
H	17.647180	6.709005	34.001552	H	56.055400	3.866636	42.061220
H	14.453123	4.525700	44.821530	H	51.374751	5.452183	39.578203
H	12.580038	3.834442	46.182435	H	52.752203	5.975600	37.680019
H	12.732622	3.667480	32.603876	H	49.669831	2.748617	37.985061
H	14.000759	7.215023	33.296770	H	49.752621	2.251602	35.579756
H	24.065422	6.134906	37.093671	H	48.450269	3.570554	33.999099
H	24.499282	2.431423	38.669869	H	46.480087	6.384885	38.388419
H	36.517684	2.927095	43.744176	H	45.173958	7.652710	36.784868
H	38.979901	2.430370	43.770206	H	44.236329	7.630248	42.660283
H	40.433479	3.223156	41.966853	H	44.975813	3.846026	39.716233
H	35.761220	5.102847	39.527682	H	49.637952	7.263842	45.837477
H	37.171791	5.863455	37.690771	H	50.764434	7.818395	32.634617
H	33.711370	2.476330	38.164957	H	48.900243	6.967727	33.961580
H	33.765964	1.943489	35.709255	H	45.669634	4.645689	44.834900
H	32.644909	3.392287	34.101774	H	43.821190	3.836766	46.164967
H	31.127296	6.529344	38.490208	H	44.204219	3.547074	32.692046

H	45.237817	7.215666	33.265942	H	34.479040	5.301046	55.121334
H	54.726458	5.972420	36.665853	H	35.955391	5.897587	53.301005
H	9.463360	8.127006	58.062982	H	32.614859	2.445131	53.553613
H	7.916941	6.786689	56.693566	H	32.757117	1.978914	51.145565
H	10.728176	2.325380	54.106699	H	31.533974	3.349525	49.544602
H	7.191621	3.170383	53.803725	H	29.517627	6.166525	53.913280
H	19.511500	2.924663	59.300577	H	28.299367	7.492823	52.283088
H	21.905284	2.358931	59.319744	H	27.305750	7.416137	58.240199
H	23.367526	3.102139	57.511310	H	40.488936	7.784705	58.154427
H	18.849099	5.349710	55.146582	H	39.030539	6.350917	56.836625
H	20.318622	6.029976	53.353632	H	27.963581	3.566193	55.354965
H	16.912771	2.445924	53.513711	H	42.104104	2.105649	54.065855
H	16.999208	1.981229	51.102954	H	32.788964	6.737424	61.409690
H	15.837471	3.425518	49.522577	H	33.826480	7.856815	48.202526
H	14.031272	6.332745	53.922436	H	32.007450	6.908242	49.535806
H	12.871130	7.732381	52.316358	H	28.748371	4.376085	60.399705
H	11.840599	7.509022	58.212429	H	26.897578	3.574785	61.718349
H	24.899359	7.891635	58.108725	H	27.517369	3.288720	48.145926
H	23.424400	6.456389	56.806062	H	28.462973	7.088191	48.755710
H	12.285087	3.636260	55.426932	H	38.072009	5.973122	52.438768
H	26.463921	2.179547	54.047080	H	38.581141	2.461514	53.869338
H	17.168444	6.739050	61.410671	H	50.894970	3.700094	59.506373
H	18.436933	7.506766	48.131301	H	53.331570	3.325517	59.581306
H	16.543343	6.761693	49.479359	H	54.727839	3.865721	57.623142
H	13.128566	4.376335	60.400533	H	50.047618	5.459615	55.145580
H	11.277757	3.574562	61.719224	H	51.424868	5.977059	53.243037
H	11.593312	3.711115	48.240226	H	48.390744	2.741086	53.475892
H	12.958261	7.337255	48.792546	H	48.482924	2.299133	51.061245
H	22.432852	6.152348	52.492650	H	47.145705	3.618819	49.510958
H	22.942636	2.559177	53.855066	H	45.128858	6.303469	53.960548
H	35.120207	3.008213	59.351237	H	43.802783	7.584683	52.385603
H	37.508407	2.425201	59.392639	H	42.899112	7.342283	58.269660
H	38.975533	3.085611	57.557402	H	43.595040	3.507334	55.368340

H	48.405704	6.744514	61.407923	C	31.155787	9.953578	42.094815
H	49.437593	7.810829	48.225131	C	32.209274	9.672947	43.178136
H	47.568867	6.953351	49.538348	O	33.575010	8.413976	41.512198
H	44.381641	4.364054	60.399410	C	36.599684	8.164971	39.474195
H	42.519372	3.571558	61.717697	C	37.727157	8.610236	38.752383
H	42.838418	3.602761	48.217489	C	37.669501	8.761189	37.363445
H	43.870941	7.227318	48.858495	C	36.490968	8.479299	36.658642
H	53.398644	5.970533	52.227582	C	35.360886	8.059194	37.375454
H	17.068304	7.157901	63.836040	C	35.406421	7.912026	38.761762
H	15.148106	6.357215	65.155558	N	36.646419	7.975368	40.850083
H	10.263187	3.421715	63.797072	H	33.424912	11.372976	39.851047
H	32.688463	7.157561	63.835223	H	34.973587	9.886519	40.958247
H	30.768039	6.357124	65.154696	H	34.385151	9.203722	43.298924
H	25.881974	3.423930	63.795755	H	30.872623	11.268178	40.373705
H	48.307538	7.159075	63.833774	H	31.914621	11.927645	41.647797
H	46.387782	6.357268	65.153495	H	30.225140	10.307008	42.574422
H	41.501340	3.424937	63.794467	H	30.912195	9.011103	41.573255
H	54.922538	4.682761	55.325772	H	32.325296	10.556153	43.837136
H	56.250071	4.683131	39.763677	H	31.909748	8.822423	43.813851
H	57.578875	4.683434	24.200636	H	32.627852	9.829813	39.512314
H	32.654315	5.043362	18.026547	H	38.665852	8.801899	39.283567
H	17.034831	5.043603	18.026692	H	38.562150	9.103423	36.826595
H	10.176567	4.915314	24.089625	H	36.450897	8.591910	35.570907
H	8.848003	4.915581	39.653302	H	34.427174	7.824886	36.852376
H	7.520566	4.915543	55.216449	H	34.529103	7.541210	39.295049
H	12.998935	5.198973	65.269012	H	35.979630	7.293304	41.218946
H	28.618777	5.198922	65.268152	H	37.577837	7.836505	41.233798
H	44.238638	5.198805	65.267027				
H	48.273973	5.043176	18.026079	(S,S)-1-RC (open-shell singlet)			
C	33.565426	9.365217	42.584987	C	12.487000	7.261000	26.395000
C	33.910351	9.783152	41.205805	C	11.616000	6.503000	25.622000
C	32.913167	10.518689	40.329034	C	12.086000	5.395000	24.927000
C	31.665641	10.999859	41.094071	C	13.428000	5.043000	25.007000

C	13.027000	3.179000	23.539000	C	18.263945	4.335758	23.745203
C	11.685000	3.529000	23.460000	C	14.301000	5.801000	25.782000
C	11.215000	4.638000	24.154000	C	13.829000	6.909000	26.476000
O	10.782000	2.793000	22.654000	C	27.939965	7.064609	26.445164
Cu	18.544566	6.083742	26.015556	C	27.106590	6.205754	25.736963
Cu	17.949064	3.696088	26.527824	C	27.621154	5.081391	25.059064
C	22.213397	3.943415	26.372783	C	29.017624	4.824774	25.114902
C	22.757992	3.186169	27.425551	C	13.900000	3.935000	24.313000
C	24.111644	2.874477	27.453900	C	28.698126	2.918068	23.645146
C	24.945637	3.308478	26.428655	C	27.330242	3.131362	23.617155
C	24.438513	4.042117	25.339267	C	26.766415	4.216580	24.325246
C	23.051717	4.345767	25.294950	O	26.567004	2.224728	22.884458
C	22.535193	5.008997	24.161246	O	16.597062	6.402542	25.851275
C	23.379497	5.400902	23.127116	O	16.054757	4.263354	26.319282
C	24.747270	5.148268	23.190800	C	15.735970	5.461599	25.984937
C	25.288474	4.460558	24.285477	C	17.910463	5.816822	30.229028
O	25.579114	5.545574	22.149817	C	18.902882	6.575867	30.875514
O	20.435305	5.514917	26.186742	C	16.756480	5.410482	30.955936
O	19.911531	3.369255	26.648707	C	15.680859	4.744451	30.330391
C	20.768045	4.296764	26.413825	C	14.571889	4.345186	31.070310
C	18.226927	4.022014	22.293999	O	18.433555	6.400239	27.976640
C	18.992915	2.941012	21.873981	O	17.897081	4.255826	28.429782
C	19.081890	2.638017	20.519979	C	18.097335	5.469877	28.794498
C	18.404876	3.417024	19.587993	Cu	34.115147	6.055775	26.054497
C	17.639888	4.497025	20.008011	Cu	33.556545	3.658606	26.554235
C	17.550913	4.800019	21.362013	C	37.812133	3.939132	26.433352
C	16.783924	5.881020	21.784030	C	38.329217	3.210002	27.519946
C	16.107910	6.659026	20.850045	C	39.674217	2.869094	27.576428
C	16.197885	6.355032	19.497042	C	40.527676	3.242494	26.544433
C	16.963876	5.274031	19.076025	C	40.049854	3.949862	25.424926
O	15.523872	7.185038	18.539057	C	38.671978	4.290355	25.355946
O	18.564826	5.528450	24.111931	C	38.185764	4.936996	24.200472
O	18.020439	3.387577	24.573172	C	39.051193	5.270153	23.162651

C	40.410407	4.976707	23.246602	C	31.305582	5.394588	26.075985
C	40.921780	4.308247	24.367476	C	33.611588	5.751216	30.286976
O	41.263904	5.320732	22.204146	C	34.667485	6.443625	30.907379
O	36.021156	5.500884	26.193097	C	32.453746	5.421451	31.045883
O	35.516923	3.352994	26.665894	C	31.331533	4.808172	30.452515
C	36.365130	4.287290	26.435136	C	30.207282	4.509779	31.216968
C	33.846855	4.021974	22.293721	O	34.041738	6.352069	28.021172
C	34.612832	2.940971	21.873686	O	33.514011	4.204498	28.468808
C	34.701783	2.637980	20.519681	C	33.733363	5.414019	28.840829
C	34.024755	3.416991	19.587710	Cu	49.697168	6.205848	25.981152
C	33.259777	4.496993	20.007743	Cu	49.346545	3.788002	26.562760
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.123586	5.521645	24.139514	C	53.770890	5.287820	24.113942
O	33.626877	3.367683	24.583222	C	54.557834	5.591822	23.007903
C	33.858111	4.324738	23.758296	C	55.929834	5.377808	23.052827
C	29.856088	5.676605	25.886829	C	56.515890	4.858790	24.200790
C	29.301639	6.804090	26.518789	O	56.643771	5.617813	21.841791
C	43.550983	6.894735	26.561358	O	51.638394	5.837344	26.121878
C	42.724927	6.030474	25.854170	O	51.335951	3.660021	26.633082
C	43.246797	4.907924	25.178439	C	52.093702	4.666381	26.379749
C	44.645582	4.658165	25.235006	C	49.466780	4.021882	22.293161
C	29.542183	3.747515	24.372604	C	50.232747	2.940878	21.873109
C	44.330564	2.729810	23.794257	C	50.321671	2.637891	20.519101
C	42.962925	2.947729	23.750917	C	49.644629	3.416907	19.587145
C	42.396173	4.042885	24.440796	C	48.879663	4.496911	20.007197
O	42.202354	2.034445	23.023916	C	48.790739	4.799899	21.361205
O	32.146986	6.354778	25.936638	C	48.023773	5.880903	21.783256
O	31.656777	4.197892	26.376588	C	47.347732	6.658919	20.849300

C	47.437657	6.354932	19.496292	C	23.691119	3.454209	42.105810
C	48.203622	5.273928	19.075240	C	23.235106	4.173053	40.986264
O	46.763615	7.184949	18.538336	C	21.848158	4.468278	40.869974
O	49.733195	5.591140	24.088507	C	21.388102	5.128383	39.712077
O	49.385647	3.425870	24.607665	C	22.283821	5.511533	38.717716
C	49.525978	4.368703	23.749005	C	23.646310	5.253033	38.845693
C	45.481723	5.534630	25.980018	C	24.132285	4.581006	39.971930
C	44.915559	6.653086	26.619370	O	24.524198	5.629952	37.837637
C	45.172911	3.568990	24.513839	O	19.146144	5.592303	41.622707
O	47.717957	6.337989	25.883236	O	18.653728	3.442482	42.095423
O	47.397075	4.170940	26.420145	C	19.498926	4.383211	41.871503
C	46.951657	5.331587	26.096531	C	16.886269	4.115503	37.738444
C	49.198164	5.992701	30.212298	C	17.590513	3.011020	37.227143
C	50.141056	6.835013	30.828603	C	17.599833	2.741525	35.865521
C	48.083189	5.523882	30.961457	C	16.904755	3.568972	34.990463
C	47.057438	4.759497	30.365385	C	16.160232	4.670884	35.460868
C	45.984579	4.304189	31.125311	C	16.129935	4.934273	36.855988
O	49.608222	6.566437	27.935081	C	15.321806	5.985276	37.334378
O	49.301423	4.391510	28.452934	C	14.607820	6.781657	36.448037
C	49.388914	5.628686	28.783243	C	14.664590	6.564579	35.081445
C	11.158284	7.260965	41.959133	C	15.447403	5.508349	34.562737
C	10.287267	6.502972	41.186144	O	13.945899	7.443996	34.274501
C	10.757252	5.394972	40.491132	O	17.238362	5.594750	39.570585
C	12.099252	5.042967	40.571107	O	16.749430	3.438610	40.019711
C	11.698220	3.178974	39.103108	C	16.964635	4.398196	39.195446
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108
O	9.453203	2.792985	38.218146	C	26.840309	7.283476	42.044395
Cu	17.237808	6.135646	41.480054	C	25.984161	6.405655	41.411632
Cu	16.684412	3.738845	41.985355	C	26.455842	5.215182	40.769998
C	20.954842	4.056338	41.900202	C	27.870447	4.942756	40.839844
C	21.454455	3.310901	42.984010	C	12.571236	3.934968	39.877095
C	22.808564	3.017888	43.087851	C	27.532428	2.949528	39.487381

C	26.134069	3.195060	39.433410	O	34.865399	5.562300	41.743651
C	25.587180	4.309901	40.062990	O	34.327779	3.417485	42.158501
O	25.449964	2.247676	38.725435	C	35.157385	4.340078	41.925204
O	15.273980	6.431176	41.358584	C	32.580382	4.276861	37.889215
O	14.773199	4.280387	41.811319	C	33.218538	3.132755	37.443278
C	14.425278	5.479447	41.507302	C	33.242941	2.836970	36.064462
C	16.704248	5.839495	45.706767	C	32.608393	3.664227	35.161538
C	17.713574	6.603134	46.321448	C	31.900969	4.840463	35.573512
C	18.796708	6.887805	32.224540	C	31.895049	5.148310	36.981530
C	17.695473	6.450942	32.952307	C	31.158483	6.284794	37.427373
C	16.664304	5.712263	32.340366	C	30.473093	7.069994	36.536350
C	15.573968	5.432904	46.470112	C	30.491126	6.789491	35.142990
C	14.486997	4.752308	45.881841	C	31.202325	5.698691	34.650509
C	13.398884	4.359393	46.655347	O	29.775700	7.689224	34.405223
C	14.503400	4.592247	32.438968	O	32.979622	5.744289	39.697555
C	15.537051	5.284219	33.084245	O	32.386801	3.619415	40.147150
O	13.390640	4.185588	33.166671	C	32.645363	4.571268	39.353750
O	17.158502	6.438099	43.444577	C	28.728958	5.861280	41.530202
O	16.645369	4.287845	43.894519	C	28.226213	7.022146	42.093253
C	16.847899	5.500516	44.264085	C	42.250192	7.224182	41.986380
Cu	33.006899	6.341943	41.579173	C	41.431585	6.392637	41.229616
Cu	32.414230	3.864922	42.113982	C	41.965323	5.313138	40.499874
C	36.608440	3.968295	41.870959	C	43.367691	5.072704	40.551023
C	37.158012	3.257754	42.921841	C	28.373914	3.790086	40.168710
C	38.546110	2.988417	42.934285	C	43.077692	3.244283	38.983459
C	39.360660	3.433796	41.912879	C	41.705946	3.436124	38.963899
C	38.836037	4.151246	40.789221	C	41.127987	4.476547	39.719760
C	37.413178	4.377237	40.760731	O	40.956260	2.545593	38.199895
C	36.841024	4.964672	39.600459	O	30.996918	6.541087	41.470341
C	37.630832	5.397324	38.567845	O	30.529294	4.420533	42.052320
C	39.046241	5.313528	38.649823	C	30.194083	5.589087	41.687618
C	39.655709	4.653749	39.718335	C	32.364171	5.966691	45.770634
O	39.794568	5.876196	37.662785	C	33.249450	6.847702	46.365644

C	34.613168	6.770701	32.256354	C	47.488553	5.153960	36.884307
C	33.497968	6.423021	33.010168	C	46.606789	6.155753	37.336462
C	32.406083	5.752509	32.428043	C	45.846620	6.883524	36.429689
C	31.261103	5.419766	46.505622	C	45.928103	6.644244	35.067793
C	30.270937	4.594868	45.897572	C	46.788283	5.637145	34.574387
C	29.217991	4.101033	46.628941	O	45.156225	7.455773	34.239135
C	30.171078	4.803344	32.578023	O	48.493250	5.887592	39.638017
C	31.262432	5.426002	33.193781	O	48.107636	3.705904	40.061992
O	29.034754	4.513248	33.321919	C	48.296408	4.680149	39.248806
O	32.901819	6.550063	43.553654	C	44.193699	5.894552	41.368423
O	32.465768	4.390801	44.009439	C	43.616082	6.978820	42.054942
C	32.592355	5.606228	44.336072	C	43.909741	4.042631	39.759405
Cu	48.441492	6.410283	41.555429	O	46.465041	6.633558	41.416382
Cu	47.983589	3.986829	42.027227	O	46.053329	4.452407	41.812406
C	52.242277	4.464616	41.931345	C	45.656818	5.643657	41.537853
C	52.828352	3.947593	43.079296	C	47.841397	6.059776	45.765586
C	54.201352	3.732573	43.123194	C	48.796637	6.875418	46.400278
C	54.987277	4.036578	42.018142	C	50.024141	7.174525	32.170322
C	54.401202	4.554601	40.869191	C	48.959698	6.684641	32.919352
C	53.028202	4.768621	40.826292	C	47.977994	5.859687	32.337149
C	52.442128	5.287645	39.677341	C	46.721866	5.589397	46.507984
C	53.229054	5.591649	38.571289	C	45.679875	4.859026	45.898336
C	54.601054	5.377629	38.616189	C	44.606280	4.397314	46.654077
C	55.187129	4.858606	39.764139	C	45.903673	4.591181	32.485508
O	55.314970	5.617636	37.405141	C	46.887642	5.376318	33.101937
O	50.368889	5.936445	41.720767	O	44.828638	4.125626	33.233986
O	49.963060	3.764091	42.174383	O	48.322276	6.691552	43.519442
C	50.770443	4.738257	41.954811	O	47.880566	4.519787	43.940463
C	48.282612	4.397755	37.789090	C	48.028912	5.736299	44.324129
C	49.078682	3.346279	37.300537	C	9.830844	7.260885	57.522289
C	49.130582	3.063750	35.942596	C	8.959813	6.502896	56.749314
C	48.385586	3.823352	35.047831	C	9.429780	5.394897	56.054290
C	47.554588	4.872504	35.493295	C	10.771780	5.042887	56.134240

C	10.370715	3.178901	54.666241	C	15.685016	4.463099	54.789124
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.311261	7.039098	57.578001
Cu	15.895645	6.132391	57.134124	C	24.476974	6.213052	56.834169
Cu	15.338916	3.719960	57.552937	C	24.987570	5.109013	56.120612
C	19.593741	4.027163	57.441415	C	26.382457	4.841102	56.173241
C	20.142857	3.263206	58.486909	C	11.243748	3.934890	55.440215
C	21.494244	2.942049	58.501710	C	26.056407	2.990375	54.635927
C	22.320469	3.369996	57.467941	C	24.689758	3.214383	54.608860
C	21.808916	4.113833	56.387270	C	24.129593	4.276520	55.354178
C	20.425231	4.433626	56.360647	O	23.923312	2.336376	53.845419
C	19.904368	5.116817	55.241202	O	13.940655	6.429316	56.972026
C	20.741325	5.505655	54.199953	O	13.433461	4.268986	57.371170
C	22.106073	5.231898	54.243579	C	13.091660	5.473969	57.085286
C	22.651839	4.528424	55.326177	C	15.283042	5.695809	61.352094
O	22.930656	5.628281	53.196737	C	16.314083	6.385792	61.978046
O	17.797050	5.585629	57.300597	C	17.645225	6.924145	47.670710
O	17.301622	3.415556	57.672104	C	16.563271	6.495405	48.431241
C	18.145513	4.363826	57.483638	C	15.516445	5.751972	47.853588
C	15.672731	4.209178	53.323015	C	14.198077	5.242813	62.095147
C	16.386229	3.101758	52.829704	C	13.166036	4.552830	61.469195
C	16.439074	2.836118	51.468537	C	12.083071	4.099834	62.213248
C	15.774372	3.666853	50.574100	C	13.360139	4.632120	48.020508
C	15.024817	4.774001	51.022524	C	14.405651	5.338934	48.630006
C	14.960921	5.042663	52.416847	O	12.265172	4.235497	48.780228
C	14.158569	6.109023	52.869363	O	15.761175	6.375298	59.107652
C	13.479543	6.911573	51.961022	O	15.277540	4.204198	59.478520
C	13.559740	6.681026	50.597615	C	15.447082	5.408104	59.892374
C	14.334198	5.607243	50.103282	Cu	31.471375	6.100115	57.130494
O	12.867105	7.561255	49.768861	Cu	30.964506	3.680786	57.576407
O	15.948617	5.648566	55.206299	C	35.210356	4.044504	57.454435
O	15.434913	3.484158	55.580188	C	35.754718	3.315823	58.527771

C	37.102785	2.983307	58.554737	C	41.690858	2.913792	54.654345
C	37.931628	3.363763	57.505410	C	40.322516	3.129433	54.624558
C	37.426851	4.073879	56.399334	C	39.753801	4.188397	55.368277
C	36.045834	4.407209	56.361592	O	39.563021	2.244466	53.862286
C	35.531662	5.057387	55.220480	O	29.502455	6.364669	57.012089
C	36.372552	5.399156	54.165498	O	29.050641	4.189855	57.403000
C	37.735076	5.113496	54.218938	C	28.677574	5.389243	57.136867
C	38.274963	4.442976	55.325477	C	30.903116	5.695628	61.351271
O	38.563625	5.466898	53.160032	C	31.934171	6.385605	61.977208
O	33.389592	5.580204	57.265984	C	33.110934	7.174802	47.732253
O	32.929190	3.411891	57.689080	C	32.084109	6.636853	48.478216
C	33.757852	4.367767	57.477820	C	31.116629	5.750869	47.900836
C	31.274785	4.130979	53.341351	C	29.818163	5.242633	62.094342
C	32.056319	3.064878	52.861120	C	28.786109	4.552656	61.468406
C	32.141577	2.799186	51.501473	C	27.703155	4.099663	62.212477
C	31.440926	3.587605	50.595907	C	29.094658	4.379076	48.016573
C	30.620485	4.647128	51.032097	C	30.024932	5.198816	48.652550
C	30.525940	4.917633	52.423876	O	28.059697	3.848787	48.724685
C	29.664051	5.942532	52.861867	O	31.370698	6.358423	59.101964
C	28.953581	6.702335	51.939441	O	30.907404	4.186411	59.495455
C	29.062611	6.469476	50.578636	C	31.068824	5.395903	59.896207
C	29.894509	5.435150	50.106647	Cu	47.051586	6.250040	57.150987
O	28.342829	7.308749	49.732626	Cu	46.688727	3.793537	57.533597
O	31.496897	5.601595	55.205187	C	50.914826	4.464382	57.493755
O	31.055455	3.425799	55.606046	C	51.500920	3.947352	58.641694
C	31.272352	4.403033	54.803475	C	52.873920	3.732327	58.685568
C	27.223168	5.663262	56.973573	C	53.659827	4.036331	57.580503
C	26.670812	6.768571	57.646289	C	53.073733	4.554362	56.431564
C	40.909118	6.941376	57.615612	C	51.700733	4.768387	56.388690
C	40.084629	6.115358	56.863070	C	51.114640	5.287417	55.239751
C	40.605708	5.021092	56.141787	C	51.901547	5.591423	54.133687
C	42.004179	4.765710	56.191814	C	53.273547	5.377397	54.178561
C	26.902858	3.785480	55.398495	C	53.859639	4.858367	55.326499

O	53.987443	5.617405	52.967501	C	45.535750	5.405013	48.652476
O	48.992008	5.859470	57.302818	O	43.465996	4.170756	48.766837
O	48.673727	3.654845	57.669077	O	46.919693	6.443394	59.123893
C	49.438558	4.672408	57.498548	O	46.574958	4.238585	59.462106
C	46.969302	4.364735	53.316790	C	46.675347	5.443513	59.891150
C	47.787874	3.342181	52.804565	C	16.262158	6.620778	63.347051
C	47.843861	3.089791	51.441393	C	15.179191	6.168782	64.090104
C	47.078998	3.849995	50.564346	C	14.147152	5.478800	63.465152
C	46.227749	4.872800	51.032652	C	12.031146	4.336820	63.582253
C	46.159843	5.124982	52.429454	C	13.063187	5.025805	64.207205
C	45.260056	6.099982	52.903780	O	10.943183	3.908824	64.361306
C	44.486972	6.833961	52.013336	C	31.882271	6.620587	63.346214
C	44.568495	6.623172	50.646869	C	30.799317	6.168593	64.089284
C	45.442835	5.639421	50.130762	C	29.767262	5.478616	63.464348
O	43.782698	7.440551	49.837170	C	27.651255	4.336645	63.581483
O	47.125699	5.801179	55.215525	C	28.683309	5.025622	64.206418
O	46.815183	3.593541	55.561816	O	26.563304	3.908650	64.360554
C	46.969647	4.601749	54.784134	C	47.502385	6.620342	63.345096
C	42.838195	5.597870	56.988961	C	46.419443	6.168348	64.088184
C	42.270981	6.687414	57.676311	C	45.387375	5.478376	63.463264
C	42.532522	3.716595	55.414748	C	43.271365	4.336411	63.580432
O	45.077332	6.397597	57.020866	C	44.303433	5.025383	64.205353
O	44.743757	4.191706	57.350772	O	42.183428	3.908416	64.359522
C	44.305767	5.377758	57.120951	H	12.119252	8.127090	26.935733
C	46.523192	5.695393	61.350166	H	10.573040	6.786843	25.566353
C	47.554258	6.385364	61.976087	H	13.383774	2.323382	22.982327
C	48.688304	7.186235	47.749091	H	9.847486	3.169741	22.676924
C	47.620892	6.692848	48.489925	H	22.122524	2.849730	28.236932
C	46.627533	5.893200	47.892736	H	24.519085	2.297386	28.278066
C	45.438249	5.242399	62.093255	H	25.995015	3.052043	26.484767
C	44.406182	4.552428	61.467335	H	21.477422	5.221199	24.048160
C	43.323240	4.099435	62.211424	H	22.959786	5.909982	22.270101
C	44.540039	4.645668	48.022819	H	19.532097	2.329493	22.589889

H	19.679348	1.794080	20.190520	H	31.292289	6.861218	17.596351
H	18.480483	3.170803	18.536736	H	40.789737	5.827744	21.471992
H	16.651495	6.145383	22.827126	H	41.219494	2.248488	23.029848
H	15.506921	7.501017	21.165194	H	53.551978	3.700079	28.381241
H	14.495576	7.508130	27.087612	H	55.987708	3.326145	28.455755
H	27.525279	7.933278	26.946725	H	57.384060	3.866333	26.497859
H	26.051702	6.439018	25.707250	H	52.703461	5.452019	24.014190
H	14.941535	3.634123	24.311218	H	54.081068	5.975951	22.116790
H	29.108653	2.089057	23.084409	H	50.777604	2.335082	22.589415
H	19.772357	6.914830	30.323665	H	50.920920	1.795284	20.189774
H	15.671536	4.535641	29.265929	H	49.720355	3.170948	18.535941
H	13.761618	3.833567	30.568862	H	47.863169	6.134688	22.823873
H	15.672066	6.861242	17.596385	H	46.741200	7.496820	21.164933
H	25.082245	6.055773	21.435046	H	45.546056	7.340322	27.172211
H	25.585185	2.442927	22.887539	H	46.234978	3.353973	24.482981
H	37.676868	2.912531	28.333288	H	50.979512	7.219106	30.258730
H	40.058520	2.312459	28.425488	H	47.060389	4.512697	29.309092
H	41.569253	2.961096	26.620924	H	45.212761	3.716850	30.646544
H	37.136461	5.183844	24.076370	H	46.912914	6.861743	17.595811
H	38.655580	5.768205	22.287918	H	56.056148	5.977148	21.104161
H	35.148141	2.327644	22.590747	H	10.790930	8.128028	42.498493
H	35.298438	1.793462	20.190382	H	9.244464	6.787120	41.129909
H	34.099971	3.170596	18.536513	H	12.055536	2.325174	38.543890
H	32.263757	6.143629	22.825814	H	8.519524	3.171537	38.239162
H	31.124714	7.499464	21.165138	H	20.782217	2.969571	43.763376
H	29.935512	7.474321	27.088164	H	23.178397	2.452057	43.937308
H	43.130010	7.759417	27.064750	H	24.740155	3.211994	42.221109
H	41.668792	6.257376	25.827433	H	20.336247	5.341268	39.549184
H	30.604603	3.537057	24.326898	H	21.906071	6.014112	37.837351
H	44.742274	1.890784	23.249610	H	18.146402	2.363963	37.896009
H	35.544522	6.722433	30.334068	H	18.153845	1.889683	35.483994
H	31.299690	4.565577	29.394678	H	16.938052	3.327969	33.937487
H	29.356685	4.043777	30.737576	H	15.216573	6.200774	38.391635

H	13.995061	7.590421	36.823076	H	30.338966	4.354124	44.836360
H	13.169420	7.511204	42.645486	H	28.462622	3.474984	46.139173
H	26.441480	8.189006	42.512754	H	28.340251	4.013099	32.786040
H	24.915626	6.644360	41.397851	H	29.727509	7.450269	33.466694
H	13.612093	3.634333	39.867546	H	39.222214	6.451749	37.125058
H	27.914902	2.071887	38.959670	H	39.963697	2.719751	38.240064
H	18.566480	6.940683	45.743335	H	52.223438	3.710469	43.947444
H	19.574911	7.467138	32.711428	H	54.659353	3.328256	44.019942
H	17.647180	6.709005	34.001552	H	56.055400	3.866636	42.061220
H	14.453123	4.525700	44.821530	H	51.374751	5.452183	39.578203
H	12.580038	3.834442	46.182435	H	52.752203	5.975600	37.680019
H	12.732622	3.667480	32.603876	H	49.669831	2.748617	37.985061
H	14.000759	7.215023	33.296770	H	49.752621	2.251602	35.579756
H	24.065422	6.134906	37.093671	H	48.450269	3.570554	33.999099
H	24.499282	2.431423	38.669869	H	46.480087	6.384885	38.388419
H	36.517684	2.927095	43.744176	H	45.173958	7.652710	36.784868
H	38.979901	2.430370	43.770206	H	44.236329	7.630248	42.660283
H	40.433479	3.223156	41.966853	H	44.975813	3.846026	39.716233
H	35.761220	5.102847	39.527682	H	49.637952	7.263842	45.837477
H	37.171791	5.863455	37.690771	H	50.764434	7.818395	32.634617
H	33.711370	2.476330	38.164957	H	48.900243	6.967727	33.961580
H	33.765964	1.943489	35.709255	H	45.669634	4.645689	44.834900
H	32.644909	3.392287	34.101774	H	43.821190	3.836766	46.164967
H	31.127296	6.529344	38.490208	H	44.204219	3.547074	32.692046
H	29.890012	7.931560	36.872465	H	45.237817	7.215666	33.265942
H	28.907180	7.719167	42.588655	H	54.726458	5.972420	36.665853
H	41.821349	8.061305	42.528286	H	9.463360	8.127006	58.062982
H	40.372712	6.611900	41.202209	H	7.916941	6.786689	56.693566
H	29.442492	3.574205	40.188391	H	10.728176	2.325380	54.106699
H	43.501688	2.450337	38.382861	H	7.191621	3.170383	53.803725
H	34.063229	7.270539	45.770655	H	19.511500	2.924663	59.300577
H	35.440106	7.297791	32.722237	H	21.905284	2.358931	59.319744
H	33.489557	6.697202	34.057451	H	23.367526	3.102139	57.511310

H 18.849099 5.349710 55.146582	H 39.030539 6.350917 56.836625
H 20.318622 6.029976 53.353632	H 27.963581 3.566193 55.354965
H 16.912771 2.445924 53.513711	H 42.104104 2.105649 54.065855
H 16.999208 1.981229 51.102954	H 32.788964 6.737424 61.409690
H 15.837471 3.425518 49.522577	H 33.826480 7.856815 48.202526
H 14.031272 6.332745 53.922436	H 32.007450 6.908242 49.535806
H 12.871130 7.732381 52.316358	H 28.748371 4.376085 60.399705
H 11.840599 7.509022 58.212429	H 26.897578 3.574785 61.718349
H 24.899359 7.891635 58.108725	H 27.517369 3.288720 48.145926
H 23.424400 6.456389 56.806062	H 28.462973 7.088191 48.755710
H 12.285087 3.636260 55.426932	H 38.072009 5.973122 52.438768
H 26.463921 2.179547 54.047080	H 38.581141 2.461514 53.869338
H 17.168444 6.739050 61.410671	H 50.894970 3.700094 59.506373
H 18.436933 7.506766 48.131301	H 53.331570 3.325517 59.581306
H 16.543343 6.761693 49.479359	H 54.727839 3.865721 57.623142
H 13.128566 4.376335 60.400533	H 50.047618 5.459615 55.145580
H 11.277757 3.574562 61.719224	H 51.424868 5.977059 53.243037
H 11.593312 3.711115 48.240226	H 48.390744 2.741086 53.475892
H 12.958261 7.337255 48.792546	H 48.482924 2.299133 51.061245
H 22.432852 6.152348 52.492650	H 47.145705 3.618819 49.510958
H 22.942636 2.559177 53.855066	H 45.128858 6.303469 53.960548
H 35.120207 3.008213 59.351237	H 43.802783 7.584683 52.385603
H 37.508407 2.425201 59.392639	H 42.899112 7.342283 58.269660
H 38.975533 3.085611 57.557402	H 43.595040 3.507334 55.368340
H 34.479040 5.301046 55.121334	H 48.405704 6.744514 61.407923
H 35.955391 5.897587 53.301005	H 49.437593 7.810829 48.225131
H 32.614859 2.445131 53.553613	H 47.568867 6.953351 49.538348
H 32.757117 1.978914 51.145565	H 44.381641 4.364054 60.399410
H 31.533974 3.349525 49.544602	H 42.519372 3.571558 61.717697
H 29.517627 6.166525 53.913280	H 42.838418 3.602761 48.217489
H 28.299367 7.492823 52.283088	H 43.870941 7.227318 48.858495
H 27.305750 7.416137 58.240199	H 53.398644 5.970533 52.227582
H 40.488936 7.784705 58.154427	H 17.068304 7.157901 63.836040

H	15.148106	6.357215	65.155558	N	36.646419	7.975368	40.850083
H	10.263187	3.421715	63.797072	H	33.424912	11.372976	39.851047
H	32.688463	7.157561	63.835223	H	34.973587	9.886519	40.958247
H	30.768039	6.357124	65.154696	H	34.385151	9.203722	43.298924
H	25.881974	3.423930	63.795755	H	30.872623	11.268178	40.373705
H	48.307538	7.159075	63.833774	H	31.914621	11.927645	41.647797
H	46.387782	6.357268	65.153495	H	30.225140	10.307008	42.574422
H	41.501340	3.424937	63.794467	H	30.912195	9.011103	41.573255
H	54.922538	4.682761	55.325772	H	32.325296	10.556153	43.837136
H	56.250071	4.683131	39.763677	H	31.909748	8.822423	43.813851
H	57.578875	4.683434	24.200636	H	32.627852	9.829813	39.512314
H	32.654315	5.043362	18.026547	H	38.665852	8.801899	39.283567
H	17.034831	5.043603	18.026692	H	38.562150	9.103423	36.826595
H	10.176567	4.915314	24.089625	H	36.450897	8.591910	35.570907
H	8.848003	4.915581	39.653302	H	34.427174	7.824886	36.852376
H	7.520566	4.915543	55.216449	H	34.529103	7.541210	39.295049
H	12.998935	5.198973	65.269012	H	35.979630	7.293304	41.218946
H	28.618777	5.198922	65.268152	H	37.577837	7.836505	41.233798
H	44.238638	5.198805	65.267027				
H	48.273973	5.043176	18.026079				
C	33.565426	9.365217	42.584987	(S,S)-2-RC (open-shell singlet)			
C	33.910351	9.783152	41.205805	C	12.487000	7.261000	26.395000
C	32.913167	10.518689	40.329034	C	11.616000	6.503000	25.622000
C	31.665641	10.999859	41.094071	C	12.086000	5.395000	24.927000
C	31.155787	9.953578	42.094815	C	13.428000	5.043000	25.007000
C	32.209274	9.672947	43.178136	C	13.027000	3.179000	23.539000
O	33.575010	8.413976	41.512198	C	11.685000	3.529000	23.460000
C	36.599684	8.164971	39.474195	C	11.215000	4.638000	24.154000
C	37.727157	8.610236	38.752383	O	10.782000	2.793000	22.654000
C	37.669501	8.761189	37.363445	Cu	18.542576	6.080825	26.017802
C	36.490968	8.479299	36.658642	Cu	17.945099	3.693217	26.528078
C	35.360886	8.059194	37.375454	C	22.206563	3.934905	26.365668
C	35.406421	7.912026	38.761762	C	22.752900	3.166800	27.409614
				C	24.105433	2.850222	27.429269

C	24.936180	3.290587	26.404182	C	27.313764	3.148571	23.575410
C	24.426703	4.036360	25.323900	C	26.750671	4.219142	24.305877
C	23.041061	4.344179	25.287802	O	26.549920	2.257772	22.824095
C	22.521900	5.019388	24.162087	O	16.596374	6.401214	25.851491
C	23.363804	5.423351	23.130870	O	16.052124	4.262699	26.321198
C	24.731248	5.168892	23.188417	C	15.734822	5.460957	25.985889
C	25.273616	4.464731	24.271941	C	17.918655	5.810725	30.232771
O	25.561701	5.581686	22.152384	C	18.906584	6.585305	30.867954
O	20.431599	5.510017	26.191201	C	16.778688	5.388255	30.972783
O	19.905956	3.363378	26.646924	C	15.706726	4.703912	30.360690
C	20.762829	4.290664	26.413792	C	14.614465	4.285066	31.114500
C	18.226927	4.022014	22.293999	O	18.430344	6.396284	27.978421
C	18.992915	2.941012	21.873981	O	17.896443	4.251251	28.430776
C	19.081890	2.638017	20.519979	C	18.097238	5.465005	28.796517
C	18.404876	3.417024	19.587993	Cu	34.094490	6.015710	26.078757
C	17.639888	4.497025	20.008011	Cu	33.535723	3.611445	26.544625
C	17.550913	4.800019	21.362013	C	37.792676	3.899047	26.434983
C	16.783924	5.881020	21.784030	C	38.308365	3.149347	27.508045
C	16.107910	6.659026	20.850045	C	39.654595	2.812850	27.562971
C	16.197885	6.355032	19.497042	C	40.511346	3.213009	26.543591
C	16.963876	5.274031	19.076025	C	40.035272	3.941692	25.437182
O	15.523872	7.185038	18.539057	C	38.655711	4.276031	25.368585
O	18.564663	5.526681	24.113588	C	38.171145	4.941804	24.223266
O	18.015335	3.386585	24.572712	C	39.039728	5.301990	23.197262
C	18.262144	4.334762	23.745633	C	40.400328	5.015520	23.282308
C	14.301000	5.801000	25.782000	C	40.910097	4.326155	24.391234
C	13.829000	6.909000	26.476000	O	41.256914	5.386694	22.251760
C	27.921566	7.012391	26.498572	O	35.999960	5.460735	26.212850
C	27.089338	6.172780	25.766690	O	35.496962	3.306939	26.659072
C	27.604650	5.066095	25.060447	C	36.344789	4.244723	26.440009
C	29.000576	4.807784	25.111002	C	33.846855	4.021974	22.293721
C	13.900000	3.935000	24.313000	C	34.612832	2.940971	21.873686
C	28.681315	2.933019	23.600603	C	34.701783	2.637980	20.519681

C	34.024755	3.416991	19.587710	Cu	49.696102	6.210740	25.980077
C	33.259777	4.496993	20.007743	Cu	49.343786	3.794683	26.566409
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.106902	5.506807	24.155838	C	53.770890	5.287820	24.113942
O	33.614619	3.346356	24.572637	C	54.557834	5.591822	23.007903
C	33.847238	4.313122	23.760070	C	55.929834	5.377808	23.052827
C	29.838009	5.640847	25.903405	C	56.515890	4.858790	24.200790
C	29.283253	6.751079	26.564877	O	56.643771	5.617813	21.841791
C	43.546476	6.890983	26.604238	O	51.638280	5.839790	26.119416
C	42.717612	6.032266	25.893306	O	51.333704	3.664668	26.637593
C	43.237834	4.918633	25.202069	C	52.092935	4.668980	26.380430
C	44.637796	4.671944	25.246811	C	49.466780	4.021882	22.293161
C	29.525381	3.746706	24.345791	C	50.232747	2.940878	21.873109
C	44.318159	2.757867	23.788467	C	50.321671	2.637891	20.519101
C	42.949668	2.972703	23.756267	C	49.644629	3.416907	19.587145
C	42.384598	4.059546	24.460482	C	48.879663	4.496911	20.007197
O	42.186625	2.065479	23.024203	C	48.790739	4.799899	21.361205
O	32.127755	6.316508	25.962741	C	48.023773	5.880903	21.783256
O	31.636684	4.152659	26.367243	C	47.347732	6.658919	20.849300
C	31.286423	5.354432	26.086311	C	47.437657	6.354932	19.496292
C	33.590833	5.643056	30.305914	C	48.203622	5.273928	19.075240
C	34.660839	6.300466	30.939372	O	46.763615	7.184949	18.538336
C	32.431391	5.310025	31.060519	O	49.730566	5.592635	24.088214
C	31.295600	4.733869	30.455570	O	49.383898	3.428217	24.610425
C	30.168357	4.435810	31.217135	C	49.524728	4.369645	23.749918
O	34.017729	6.282843	28.050077	C	45.477220	5.542712	25.994793
O	33.484190	4.129740	28.464659	C	44.912359	6.652392	26.650480
C	33.706752	5.332532	28.854674	C	45.163129	3.591612	24.511351

O	47.715142	6.344552	25.885775	O	18.650582	3.471741	42.173896
O	47.393991	4.177747	26.423280	C	19.495624	4.416543	41.970249
C	46.948294	5.338975	26.102311	C	16.953145	4.132003	37.776344
C	49.204379	6.011119	30.213460	C	17.679523	3.039055	37.271457
C	50.150596	6.854204	30.823900	C	17.700655	2.766705	35.910517
C	48.090856	5.548025	30.968341	C	16.992450	3.577380	35.030257
C	47.059231	4.788152	30.377239	C	16.227095	4.667775	35.494013
C	45.986247	4.340720	31.141596	C	16.189858	4.937653	36.887728
O	49.610200	6.576740	27.933208	C	15.368226	5.981724	37.358708
O	49.298178	4.404033	28.456587	C	14.644973	6.763401	36.466980
C	49.389847	5.641934	28.784213	C	14.703910	6.537044	35.102166
C	11.158284	7.260965	41.959133	C	15.500021	5.487224	34.590713
C	10.287267	6.502972	41.186144	O	13.973037	7.400959	34.289282
C	10.757252	5.394972	40.491132	O	17.269456	5.612476	39.613077
C	12.099252	5.042967	40.571107	O	16.789755	3.452793	40.055267
C	11.698220	3.178974	39.103108	C	17.010654	4.413995	39.234204
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108
O	9.453203	2.792985	38.218146	C	26.938689	7.124298	41.712190
Cu	17.236844	6.153136	41.521455	C	26.045798	6.183834	41.238974
Cu	16.684656	3.753955	42.019406	C	26.473659	4.902440	40.760025
C	20.946852	4.097753	42.060476	C	27.882511	4.602859	40.839210
C	21.424389	3.484909	43.233206	C	12.571236	3.934968	39.877095
C	22.769788	3.173305	43.380495	C	27.455003	2.436273	39.820174
C	23.661490	3.445637	42.349183	C	26.063846	2.717646	39.746759
C	23.224164	4.026852	41.144891	C	25.566796	3.934616	40.203648
C	21.851536	4.366626	40.995893	O	25.335882	1.700219	39.204415
C	21.415751	4.927684	39.777727	O	15.272403	6.437077	41.372763
C	22.319278	5.137670	38.737990	O	14.774428	4.282599	41.810941
C	23.662130	4.796913	38.879777	C	14.425359	5.481706	41.509822
C	24.125546	4.250601	40.080404	C	16.641131	5.852114	45.741259
O	24.538837	4.947126	37.814973	C	17.633837	6.629905	46.365437
O	19.146536	5.620474	41.694383	C	18.810009	6.898558	32.217278

C	17.722546	6.448043	32.956951	C	31.298718	6.007157	37.465849
C	16.696548	5.692287	32.357476	C	30.623520	6.848304	36.617744
C	15.513594	5.422755	46.496358	C	30.564717	6.586276	35.222153
C	14.438964	4.731247	45.898102	C	31.215242	5.483320	34.679295
C	13.355420	4.312651	46.664547	O	29.835870	7.515756	34.532174
C	14.557118	4.534438	32.483203	O	33.190141	5.302889	39.649694
C	15.584023	5.249089	33.114279	O	32.305716	3.277991	40.087761
O	13.461304	4.107524	33.224945	C	32.709699	4.184963	39.302657
O	17.126230	6.454128	43.485453	C	28.779623	5.591532	41.363586
O	16.607304	4.303492	43.926319	C	28.319513	6.837132	41.758041
C	16.803319	5.515877	44.299692	C	42.258491	7.080932	42.229410
Cu	33.052714	6.010966	41.498554	C	41.439682	6.298577	41.423250
Cu	32.427714	3.558245	42.047231	C	41.975228	5.283709	40.605124
C	36.600176	3.691933	41.750907	C	43.376619	5.048290	40.626958
C	37.122926	2.737606	42.603440	C	28.337856	3.345589	40.342842
C	38.502590	2.437920	42.564262	C	43.080360	3.310333	38.959048
C	39.333022	3.078612	41.669520	C	41.710146	3.513920	38.947047
C	38.833239	4.044144	40.735534	C	41.139165	4.504894	39.769493
C	37.424483	4.343664	40.774775	O	40.954168	2.692256	38.115536
C	36.893948	5.246673	39.808610	O	31.056181	6.216131	41.197430
C	37.711182	5.842837	38.878624	O	30.558454	4.191150	42.038416
C	39.110420	5.597215	38.866605	C	30.241035	5.311247	41.536860
C	39.673554	4.704503	39.776064	C	32.345579	5.688983	45.680256
O	39.902165	6.233279	37.958395	C	33.179988	6.638008	46.242238
O	34.853564	5.270167	41.878789	C	34.620873	6.584427	32.298160
O	34.330724	3.083065	41.987626	C	33.505933	6.228477	33.048478
C	35.151758	4.041834	41.881005	C	32.397812	5.597876	32.452003
C	32.616422	3.914194	37.835021	C	31.316591	5.058472	46.455052
C	33.188981	2.755243	37.345006	C	30.388777	4.138136	45.888156
C	33.166272	2.497561	35.957530	C	29.402031	3.567774	46.656133
C	32.546379	3.375916	35.093385	C	30.144695	4.690073	32.586386
C	31.904204	4.570834	35.556057	C	31.253023	5.268090	33.213915
C	31.953181	4.841601	36.969117	O	29.004470	4.409277	33.328267

O	32.733805	6.306732	43.440014	C	44.203168	5.828607	41.480268
O	32.561087	4.115174	43.929705	C	43.627502	6.852887	42.253412
C	32.559327	5.342249	44.240140	C	43.915930	4.062772	39.777204
Cu	48.436772	6.379616	41.586312	O	46.461492	6.585860	41.475995
Cu	48.002565	3.947486	42.043827	O	46.072597	4.395907	41.854337
C	52.242277	4.464616	41.931345	C	45.665500	5.587971	41.605367
C	52.828352	3.947593	43.079296	C	47.867969	5.995104	45.794964
C	54.201352	3.732573	43.123194	C	48.835281	6.787778	46.439814
C	54.987277	4.036578	42.018142	C	50.040042	7.196905	32.165558
C	54.401202	4.554601	40.869191	C	48.978872	6.709313	32.920867
C	53.028202	4.768621	40.826292	C	47.992662	5.886133	32.344344
C	52.442128	5.287645	39.677341	C	46.732032	5.546887	46.525538
C	53.229054	5.591649	38.571289	C	45.684670	4.833060	45.905719
C	54.601054	5.377629	38.616189	C	44.591904	4.397171	46.649241
C	55.187129	4.858606	39.764139	C	45.912120	4.629387	32.501948
O	55.314970	5.617636	37.405141	C	46.903626	5.408195	33.114532
O	50.364765	5.921711	41.727740	O	44.836531	4.171542	33.254451
O	49.978815	3.742822	42.172759	O	48.336681	6.643516	43.552933
C	50.774420	4.725814	41.954751	O	47.910813	4.465732	43.961862
C	48.273024	4.392798	37.803977	C	48.054218	5.680737	44.352340
C	49.062221	3.337691	37.311534	C	9.830844	7.260885	57.522289
C	49.122019	3.066612	35.951590	C	8.959813	6.502896	56.749314
C	48.391363	3.840944	35.057798	C	9.429780	5.394897	56.054290
C	47.565458	4.892713	35.506095	C	10.771780	5.042887	56.134240
C	47.491503	5.162944	36.899397	C	10.370715	3.178901	54.666241
C	46.612896	6.166549	37.353363	C	9.028715	3.528910	54.587291
C	45.866018	6.908520	36.446944	C	8.558747	4.637908	55.281315
C	45.956229	6.680615	35.083616	O	8.125681	2.792922	53.781316
C	46.810352	5.669578	34.587838	Cu	15.900714	6.105541	57.131398
O	45.196881	7.505207	34.256177	Cu	15.327741	3.699339	57.564231
O	48.473106	5.872419	39.663992	C	19.585137	3.974703	57.469378
O	48.112185	3.684015	40.074297	C	20.123414	3.234788	58.537565
C	48.286246	4.665946	39.266647	C	21.472693	2.905736	58.568815

C	22.307294	3.299882	57.528311	C	24.687816	3.044362	54.683726
C	21.806234	4.016658	56.424797	C	24.133031	4.131126	55.396853
C	20.425149	4.346936	56.383237	O	23.916650	2.147296	53.947706
C	19.914796	5.005938	55.245021	O	13.946167	6.416967	56.971302
C	20.758935	5.357081	54.196071	O	13.425643	4.261621	57.379225
C	22.120909	5.070689	54.251618	C	13.090834	5.467677	57.088810
C	22.656933	4.393811	55.355948	C	15.283042	5.695809	61.352094
O	22.952385	5.428855	53.196468	C	16.314083	6.385792	61.978046
O	17.799661	5.544342	57.298097	C	17.552936	6.942476	47.715914
O	17.287661	3.381183	57.687540	C	16.476354	6.488183	48.469081
C	18.138932	4.321969	57.495444	C	15.445692	5.729440	47.882074
C	15.653709	4.164402	53.332291	C	14.198077	5.242813	62.095147
C	16.384010	3.071152	52.832567	C	13.166036	4.552830	61.469195
C	16.429373	2.807313	51.470505	C	12.083071	4.099834	62.213248
C	15.741150	3.626300	50.582545	C	13.309296	4.569722	48.032495
C	14.974362	4.718419	51.038833	C	14.340673	5.288789	48.651576
C	14.916699	4.983315	52.433807	O	12.219823	4.146210	48.785473
C	14.097280	6.032331	52.895750	O	15.771279	6.360964	59.104269
C	13.392555	6.821276	51.995312	O	15.271233	4.195655	59.486097
C	13.467597	6.596555	50.630592	C	15.449106	5.400375	59.893866
C	14.262086	5.541656	50.127112	Cu	31.481759	6.011152	57.120216
O	12.751590	7.465466	49.809835	Cu	30.987339	3.600143	57.621253
O	15.945404	5.609909	55.206357	C	35.230398	3.987298	57.497462
O	15.422141	3.449781	55.593129	C	35.785301	3.299452	58.591965
C	15.675418	4.423357	54.796631	C	37.136276	2.979063	58.623254
C	11.644813	5.800876	56.909215	C	37.956819	3.330172	57.557193
C	11.172845	6.908875	57.603239	C	37.441234	4.000127	56.431049
C	25.329135	6.954177	57.534575	C	36.057691	4.321162	56.389537
C	24.490384	6.108147	56.819212	C	35.532988	4.931515	55.231172
C	24.995737	4.981642	56.137905	C	36.365938	5.246406	54.161804
C	26.390162	4.710358	56.195779	C	37.730728	4.972843	54.217286
C	11.243748	3.934890	55.440215	C	38.281197	4.341970	55.341850
C	26.053722	2.815647	54.715571	O	38.551081	5.297296	53.142890

O	33.401495	5.505957	57.274150	C	33.065080	6.957126	47.612856
O	32.953329	3.345712	57.749048	C	32.102094	6.353359	48.392799
C	33.776356	4.301255	57.515811	C	31.182327	5.397778	47.849849
C	31.357795	3.936257	53.380942	C	29.818163	5.242633	62.094342
C	32.184803	2.882240	52.952632	C	28.786109	4.552656	61.468406
C	32.310888	2.576905	51.604400	C	27.703155	4.099663	62.212477
C	31.602631	3.309468	50.658699	C	29.278725	3.873519	48.038020
C	30.735196	4.351353	51.042676	C	30.148453	4.784255	48.634975
C	30.606127	4.668350	52.422281	O	28.300871	3.282348	48.778938
C	29.708734	5.683231	52.807962	O	31.374195	6.316676	59.087074
C	28.989488	6.384156	51.846410	O	30.920207	4.151619	59.526601
C	29.122594	6.098839	50.497554	C	31.076131	5.369980	59.901835
C	29.996218	5.076349	50.077341	Cu	47.045986	6.237482	57.147482
O	28.378052	6.871241	49.610248	Cu	46.692054	3.781235	57.539319
O	31.519018	5.464762	55.205774	C	50.914826	4.464382	57.493755
O	31.093109	3.296113	55.659151	C	51.500920	3.947352	58.641694
C	31.314980	4.252695	54.833708	C	52.873920	3.732327	58.685568
C	27.235807	5.554494	56.967849	C	53.659827	4.036331	57.580503
C	26.687936	6.681922	57.607035	C	53.073733	4.554362	56.431564
C	40.898539	6.911565	57.571806	C	51.700733	4.768387	56.388690
C	40.080025	6.064433	56.836482	C	51.114640	5.287417	55.239751
C	40.608372	4.957375	56.140300	C	51.901547	5.591423	54.133687
C	42.008309	4.712353	56.196347	C	53.273547	5.377397	54.178561
C	26.904961	3.630209	55.452035	C	53.859639	4.858367	55.326499
C	41.708148	2.827518	54.696278	O	53.987443	5.617405	52.967501
C	40.338293	3.031637	54.663756	O	48.987937	5.853770	57.299107
C	39.762177	4.101559	55.385876	O	48.676960	3.649114	57.671554
O	39.585196	2.124527	53.921439	C	49.438289	4.668577	57.497761
O	29.512616	6.262128	56.989470	C	46.950960	4.340859	53.318440
O	29.069920	4.094507	57.426835	C	47.760367	3.311946	52.804138
C	28.691630	5.286286	57.134163	C	47.806249	3.054755	51.441521
C	30.903116	5.695628	61.351271	C	47.041696	3.817473	50.566757
C	31.934171	6.385605	61.977208	C	46.200787	4.848129	51.036540

C	46.140254	5.102965	52.433228	C	13.063187	5.025805	64.207205
C	45.246595	6.082746	52.909323	O	10.943183	3.908824	64.361306
C	44.474441	6.819921	52.020468	C	31.882271	6.620587	63.346214
C	44.552307	6.609321	50.653629	C	30.799317	6.168593	64.089284
C	45.419978	5.620543	50.135711	C	29.767262	5.478616	63.464348
O	43.771859	7.433483	49.845677	C	27.651255	4.336645	63.581483
O	47.118430	5.782482	55.213127	C	28.683309	5.025622	64.206418
O	46.813643	3.575407	55.567254	O	26.563304	3.908650	64.360554
C	46.961443	4.581724	54.785637	C	47.502385	6.620342	63.345096
C	42.835984	5.565223	56.978402	C	46.419443	6.168348	64.088184
C	42.261475	6.666178	57.641043	C	45.387375	5.478376	63.463264
C	42.543994	3.651955	55.439488	C	43.271365	4.336411	63.580432
O	45.071143	6.377064	57.016971	C	44.303433	5.025383	64.205353
O	44.746576	4.171780	57.358699	O	42.183428	3.908416	64.359522
C	44.303943	5.354181	57.119883	H	12.119248	8.127008	26.935861
C	46.523192	5.695393	61.350166	H	10.573030	6.786802	25.566446
C	47.554258	6.385364	61.976087	H	13.383808	2.323397	22.982341
C	48.718636	7.102482	47.786976	H	9.847449	3.169628	22.677206
C	47.630713	6.636077	48.515368	H	22.119693	2.825435	28.220742
C	46.627742	5.855821	47.908290	H	24.514504	2.264603	28.246600
C	45.438249	5.242399	62.093255	H	25.984937	3.030459	26.453718
C	44.406182	4.552428	61.467335	H	21.464136	5.233174	24.053091
C	43.323240	4.099435	62.211424	H	22.942498	5.943527	22.281326
C	44.512630	4.653437	48.015962	H	19.531865	2.329405	22.589989
C	45.517603	5.391427	48.656514	H	19.679348	1.794080	20.190536
O	43.417515	4.207355	48.746960	H	18.480491	3.170810	18.536740
O	46.915441	6.437691	59.120426	H	16.651876	6.145499	22.827168
O	46.580400	4.232667	59.466739	H	15.506984	7.501049	21.165229
C	46.676176	5.439532	59.891582	H	14.495541	7.507987	27.087825
C	16.262158	6.620778	63.347051	H	27.505858	7.866105	27.024430
C	15.179191	6.168782	64.090104	H	26.034404	6.406400	25.743242
C	14.147152	5.478800	63.465152	H	14.941570	3.634219	24.311220
C	12.031146	4.336820	63.582253	H	29.091236	2.114657	23.024008

H	19.765932	6.935226	30.307146	H	50.920842	1.795225	20.189779
H	15.687118	4.494775	29.296548	H	49.720366	3.170956	18.535934
H	13.808015	3.757365	30.623694	H	47.862200	6.134477	22.823712
H	15.672058	6.861205	17.596404	H	46.741005	7.496675	21.164943
H	25.065095	6.108856	21.449826	H	45.544587	7.334431	27.207656
H	25.568591	2.478292	22.829329	H	46.225689	3.379975	24.472082
H	37.653869	2.832410	28.312275	H	50.986788	7.236481	30.249480
H	40.037239	2.239134	28.401334	H	47.057331	4.540114	29.321168
H	41.554085	2.935517	26.619045	H	45.209023	3.757858	30.666166
H	37.120666	5.182449	24.097291	H	46.912720	6.861611	17.595816
H	38.645206	5.814719	22.330497	H	56.056145	5.977135	21.104157
H	35.146553	2.326073	22.590614	H	10.790932	8.127999	42.498529
H	35.298074	1.793200	20.190391	H	9.244464	6.787093	41.129930
H	34.099859	3.170523	18.536517	H	12.055653	2.325328	38.543745
H	32.264795	6.144350	22.825735	H	8.519784	3.172195	38.238379
H	31.124834	7.499554	21.165135	H	20.740734	3.258923	44.043911
H	29.916660	7.406113	27.152137	H	23.123629	2.712663	44.297690
H	43.126474	7.748783	27.120055	H	24.701901	3.184044	42.495399
H	41.660530	6.256131	25.876072	H	20.376766	5.194001	39.606705
H	30.587745	3.536457	24.297365	H	21.963769	5.557931	37.806254
H	44.728457	1.926094	23.231811	H	18.243144	2.403499	37.944757
H	35.539031	6.581755	30.369113	H	18.273021	1.925009	35.533656
H	31.256123	4.522889	29.391020	H	17.034099	3.333526	33.978274
H	29.305660	4.001857	30.729254	H	15.260774	6.204419	38.414094
H	31.291527	6.860709	17.596402	H	14.023024	7.567782	36.836281
H	40.782865	5.904184	21.526913	H	13.169079	7.511376	42.645746
H	41.202727	2.274245	23.042219	H	26.573822	8.099121	42.050060
H	53.551989	3.700496	28.381353	H	24.983418	6.445142	41.220229
H	55.987723	3.326196	28.455771	H	13.612328	3.634923	39.867604
H	57.384069	3.866362	26.497866	H	27.797565	1.472652	39.434270
H	52.703463	5.451610	24.013877	H	18.484283	6.984667	45.794017
H	54.081052	5.975818	22.116742	H	19.585480	7.489018	32.695375
H	50.777435	2.335149	22.589573	H	17.682085	6.707280	34.006273

H	14.410451	4.516712	44.835160	H	51.374731	5.453647	39.579462
H	12.546032	3.780145	46.183778	H	52.752232	5.975923	37.680156
H	12.807984	3.573691	32.671547	H	49.643346	2.728821	37.994757
H	14.039366	7.172601	33.312125	H	49.739865	2.252314	35.586360
H	24.138992	5.490069	37.060477	H	48.463172	3.597598	34.007313
H	24.394563	1.916725	39.111962	H	46.477421	6.385573	38.406410
H	36.462208	2.236638	43.315782	H	45.196076	7.679236	36.803878
H	38.915074	1.694571	43.253809	H	44.251230	7.466472	42.893724
H	40.398389	2.827564	41.671514	H	44.981602	3.865275	39.723898
H	35.825139	5.463297	39.791064	H	49.690445	7.157595	45.885521
H	37.281307	6.525953	38.136171	H	50.782913	7.841387	32.624929
H	33.668587	2.056595	38.035757	H	48.924694	6.993663	33.963117
H	33.639833	1.592006	35.565042	H	45.686201	4.611733	44.843809
H	32.541652	3.131706	34.026298	H	43.802855	3.848822	46.152585
H	31.321409	6.231127	38.533913	H	44.205014	3.599227	32.714185
H	30.101022	7.730656	36.994611	H	45.295597	7.282274	33.280456
H	29.032631	7.579067	42.125137	H	54.726409	5.972256	36.665825
H	41.827224	7.865944	42.842685	H	9.463329	8.126931	58.063076
H	40.377629	6.505114	41.433509	H	7.916942	6.786694	56.693526
H	29.400670	3.104836	40.370902	H	10.728254	2.325576	54.106446
H	43.500853	2.550805	38.313074	H	7.191916	3.171153	53.802722
H	33.938414	7.118207	45.618344	H	19.485280	2.921655	59.356113
H	35.459620	7.082627	32.774400	H	21.875423	2.342438	59.404684
H	33.510042	6.466439	34.104536	H	23.352443	3.026925	57.584758
H	30.451670	3.886572	44.829012	H	18.862196	5.248341	55.142599
H	28.695803	2.863694	46.199962	H	20.344238	5.862361	53.334363
H	28.294202	3.943216	32.781755	H	16.929636	2.425882	53.511618
H	29.683923	7.263439	33.608040	H	17.002488	1.963630	51.099035
H	39.361351	6.823562	37.409233	H	15.799196	3.387284	49.530144
H	39.967369	2.900634	38.140551	H	13.977268	6.252470	53.950557
H	52.223668	3.708590	43.947188	H	12.769780	7.628022	52.357830
H	54.659293	3.327773	44.019757	H	11.840821	7.508344	58.212787
H	56.055379	3.866472	42.061162	H	24.921463	7.824314	58.039365

H	23.438445	6.353637	56.787205	H	28.504561	6.603974	48.645818
H	12.285129	3.636400	55.426434	H	38.051554	5.774133	52.407126
H	26.457054	1.986095	54.150414	H	38.601942	2.335093	53.922979
H	17.168907	6.737994	61.410739	H	50.894940	3.699485	59.506192
H	18.331379	7.537344	48.183479	H	53.331548	3.325382	59.581255
H	16.447433	6.747081	49.518862	H	54.727833	3.865676	57.623126
H	13.126173	4.378487	60.400390	H	50.047590	5.459349	55.145389
H	11.277469	3.575065	61.719148	H	51.424852	5.976983	53.243024
H	11.559287	3.614444	48.238743	H	48.363642	2.709088	53.473408
H	12.838335	7.245204	48.832300	H	48.437469	2.258607	51.059733
H	22.461191	5.934868	52.474762	H	47.100303	3.581776	49.513903
H	22.936489	2.372504	53.954945	H	45.119422	6.287612	53.966264
H	35.157102	3.015134	59.428478	H	43.795241	7.574475	52.394184
H	37.550745	2.453448	59.477676	H	42.884734	7.336869	58.221706
H	39.003015	3.061500	57.612767	H	43.607840	3.450032	55.394689
H	34.478269	5.164802	55.129969	H	48.405872	6.743972	61.407865
H	35.940860	5.714720	53.284378	H	49.475987	7.711030	48.270910
H	32.747541	2.304223	53.677102	H	47.570757	6.902188	49.561940
H	32.963267	1.768621	51.288864	H	44.382059	4.363764	60.399400
H	31.727548	3.042139	49.617710	H	42.519449	3.571445	61.717699
H	29.541551	5.943115	53.848192	H	42.778495	3.661340	48.188443
H	28.305766	7.166234	52.149515	H	43.855580	7.218886	48.866924
H	27.326316	7.346837	58.177630	H	53.398606	5.970464	52.227591
H	40.472789	7.764354	58.091004	H	17.068429	7.157670	63.836085
H	39.024788	6.293747	56.802991	H	15.148116	6.357185	65.155565
H	27.964871	3.406286	55.412375	H	10.263250	3.421641	63.797056
H	42.127223	2.010854	54.123874	H	32.688944	7.156689	63.835383
H	32.790505	6.733697	61.409820	H	30.768141	6.356916	65.154737
H	33.748287	7.686934	48.058561	H	25.882127	3.423710	63.795758
H	32.042093	6.622077	49.452040	H	48.307605	7.158948	63.833797
H	28.747678	4.377301	60.399419	H	46.387794	6.357236	65.153501
H	26.897508	3.574933	61.718304	H	41.501438	3.424823	63.794455
H	27.792544	2.668772	48.224248	H	54.922536	4.682745	55.325778

H	56.250077	4.683142	39.763697	H	32.031440	10.327350	38.965742
H	57.578881	4.683428	24.200634	H	33.628945	10.957993	42.804112
H	32.654265	5.043340	18.026541	H	25.390860	8.017005	39.147257
H	17.034837	5.043596	18.026699	H	23.410992	8.788309	37.868950
H	10.176567	4.915317	24.089695	H	23.396281	8.678547	35.362989
H	8.848034	4.915642	39.653240	H	25.425748	7.812799	34.173428
H	7.520577	4.915561	55.216401	H	27.418040	7.073057	35.450315
H	12.998935	5.198970	65.269014	H	28.260321	6.378630	37.653353
H	28.618788	5.198898	65.268157	H	27.503496	6.846186	39.095424
H	44.238642	5.198806	65.267028				
H	48.273999	5.043194	18.026068	RCext1			
C	32.495385	8.998120	40.585410	C	12.487000	7.261000	26.395000
C	33.073510	9.090174	41.943015	C	11.616000	6.503000	25.622000
C	34.126679	10.122367	42.274216	C	12.086000	5.395000	24.927000
C	34.840985	10.642179	41.016395	C	13.428000	5.043000	25.007000
C	33.821362	11.090568	39.959079	C	13.027000	3.179000	23.539000
C	32.930594	9.931724	39.470700	C	11.685000	3.529000	23.460000
O	33.513327	8.064683	41.028558	C	11.215000	4.638000	24.154000
C	26.536703	7.462564	37.394762	O	10.782000	2.793000	22.654000
C	25.397288	7.976174	38.054337	Cu	18.546181	6.113565	26.005094
C	24.283674	8.404174	37.328823	Cu	17.970658	3.726077	26.534990
C	24.270013	8.340751	35.928876	C	22.241758	4.014458	26.404081
C	25.407045	7.853227	35.268496	C	22.773540	3.244197	27.454792
C	26.526804	7.422716	35.981575	C	24.129589	2.944706	27.505503
N	27.647327	7.048395	38.110196	C	24.980007	3.400435	26.503913
H	34.847939	9.676500	42.984258	C	24.488823	4.146502	25.416355
H	32.496642	8.685582	42.784782	C	23.100479	4.444210	25.351453
H	31.517823	8.510972	40.480965	C	22.603826	5.127310	24.220845
H	35.483024	9.842492	40.603477	C	23.466280	5.541771	23.210680
H	35.504951	11.481363	41.289190	C	24.832910	5.287447	23.291753
H	33.181609	11.879625	40.401921	C	25.356208	4.580061	24.382598
H	34.333890	11.552634	39.096591	O	25.680992	5.702367	22.270838
H	33.464918	9.318455	38.721189	O	20.443729	5.564465	26.184123

O	19.939048	3.418520	26.661380	C	15.693417	4.788318	30.335200
C	20.789081	4.352247	26.424169	C	14.584813	4.391152	31.076784
C	18.226927	4.022014	22.293999	O	18.432828	6.446592	27.965204
C	18.992915	2.941012	21.873981	O	17.912557	4.302104	28.434387
C	19.081890	2.638017	20.519979	C	18.104084	5.520304	28.790969
C	18.404876	3.417024	19.587993	Cu	34.218090	6.109385	26.014950
C	17.639888	4.497025	20.008011	Cu	33.649373	3.728226	26.572888
C	17.550913	4.800019	21.362013	C	37.902795	3.955084	26.337648
C	16.783924	5.881020	21.784030	C	38.437141	3.245841	27.429548
C	16.107910	6.659026	20.850045	C	39.781113	2.898277	27.466729
C	16.197885	6.355032	19.497042	C	40.615795	3.244233	26.410665
C	16.963876	5.274031	19.076025	C	40.119499	3.928747	25.284789
O	15.523872	7.185038	18.539057	C	38.742157	4.274052	25.234547
O	18.569530	5.541877	24.103960	C	38.236266	4.895983	24.074067
O	18.043906	3.400389	24.581528	C	39.081569	5.193484	23.009010
C	18.274776	4.344692	23.745372	C	40.441912	4.899243	23.075106
C	14.301000	5.801000	25.782000	C	40.974117	4.264388	24.205870
C	13.829000	6.909000	26.476000	O	41.276085	5.212741	22.007737
C	28.054213	7.197552	26.471221	O	36.122685	5.532890	26.106870
C	27.205956	6.333128	25.787858	O	35.607726	3.400460	26.634323
C	27.701139	5.182426	25.141835	C	36.459894	4.320247	26.364444
C	29.093947	4.903696	25.205522	C	33.846855	4.021974	22.293721
C	13.900000	3.935000	24.313000	C	34.612832	2.940971	21.873686
C	28.739246	2.960469	23.791914	C	34.701783	2.637980	20.519681
C	27.375965	3.199148	23.754241	C	34.024755	3.416991	19.587710
C	26.831022	4.313686	24.430768	C	33.259777	4.496993	20.007743
O	26.597902	2.288877	23.042191	C	33.170827	4.799985	21.361749
O	16.594846	6.414776	25.838705	C	32.403849	5.880988	21.783783
O	16.068625	4.274714	26.319582	C	31.727822	6.658998	20.849812
C	15.739992	5.469002	25.979699	C	31.817772	6.355006	19.496807
C	17.914797	5.876634	30.224843	C	32.583750	5.274004	19.075773
C	18.901477	6.647486	30.866997	O	31.143744	7.185017	18.538837
C	16.763917	5.466637	30.955754	O	34.164411	5.545420	24.110398

O	33.661131	3.403480	24.601432	C	54.557834	5.591822	23.007903
C	33.882768	4.344909	23.754769	C	55.929834	5.377808	23.052827
C	29.949225	5.765814	25.949290	C	56.515890	4.858790	24.200790
C	29.412364	6.918554	26.550729	O	56.643771	5.617813	21.841791
C	43.532059	6.899085	26.424299	O	51.641268	5.843502	26.122114
C	42.732743	6.031844	25.690569	O	51.332370	3.669567	26.642670
C	43.279345	4.907698	25.037157	C	52.093482	4.671970	26.383321
C	44.676595	4.664415	25.138625	C	49.466780	4.021882	22.293161
C	29.598043	3.794398	24.496448	C	50.232747	2.940878	21.873109
C	44.416395	2.736337	23.686171	C	50.321671	2.637891	20.519101
C	43.048944	2.944059	23.604113	C	49.644629	3.416907	19.587145
C	42.454502	4.032736	24.281151	C	48.879663	4.496911	20.007197
O	42.316334	2.022300	22.859751	C	48.790739	4.799899	21.361205
O	32.248281	6.427586	25.949803	C	48.023773	5.880903	21.783256
O	31.749996	4.284594	26.442814	C	47.347732	6.658919	20.849300
C	31.401338	5.477716	26.125311	C	47.437657	6.354932	19.496292
C	33.911132	5.877682	30.272260	C	48.203622	5.273928	19.075240
C	35.001149	6.595319	30.799410	O	46.763615	7.184949	18.538336
C	32.823272	5.541027	31.125441	O	49.738148	5.595579	24.085198
C	31.666833	4.903056	30.632645	O	49.388689	3.432143	24.609926
C	30.612032	4.600296	31.489361	C	49.529494	4.372311	23.748673
O	34.213344	6.440090	27.976847	C	45.484745	5.542868	25.912744
O	33.676347	4.307926	28.480963	C	44.894368	6.660403	26.531306
C	33.933231	5.518922	28.824898	C	45.231200	3.577683	24.434390
Cu	49.700096	6.216463	25.977100	O	47.720923	6.353131	25.869701
Cu	49.342242	3.801445	26.564130	O	47.393630	4.187358	26.407019
C	53.571004	4.464799	26.367945	C	46.952251	5.346009	26.070894
C	54.157059	3.947781	27.515908	C	49.192106	6.014251	30.212246
C	55.530060	3.732767	27.559832	C	50.139479	6.850651	30.830664
C	56.316003	4.036770	26.454793	C	48.076395	5.547550	30.962234
C	55.729947	4.554788	25.305829	C	47.044802	4.792198	30.364673
C	54.356948	4.768802	25.262905	C	45.968438	4.343519	31.123843
C	53.770890	5.287820	24.113942	O	49.606996	6.583002	27.931878

O	49.289035	4.410896	28.453378	C	14.653457	6.853874	36.457268
C	49.381917	5.648098	28.782151	C	14.694240	6.633285	35.090518
C	11.158284	7.260965	41.959133	C	15.461320	5.568539	34.566209
C	10.287267	6.502972	41.186144	O	13.976809	7.518382	34.288940
C	10.757252	5.394972	40.491132	O	17.259662	5.616893	39.583904
C	12.099252	5.042967	40.571107	O	16.763496	3.458606	40.011898
C	11.698220	3.178974	39.103108	C	16.983334	4.424965	39.196088
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108
O	9.453203	2.792985	38.218146	C	27.061955	7.333472	41.963419
Cu	17.245620	6.140641	41.499176	C	26.159593	6.450505	41.406532
Cu	16.689538	3.741057	41.981810	C	26.568140	5.191965	40.858924
C	20.964484	4.054276	41.954534	C	27.969093	4.857213	40.939389
C	21.425596	3.258993	43.020982	C	12.571236	3.934968	39.877095
C	22.772324	2.944486	43.151740	C	27.516162	2.773487	39.768623
C	23.687458	3.404401	42.212532	C	26.129880	3.080159	39.711053
C	23.273257	4.174521	41.111403	C	25.647218	4.273682	40.241495
C	21.894519	4.500081	40.970473	O	25.390631	2.108146	39.098424
C	21.480949	5.223950	39.833218	O	15.277900	6.434515	41.368476
C	22.413356	5.641024	38.886857	O	14.777437	4.280771	41.804548
C	23.765991	5.345418	39.037455	C	14.428141	5.480968	41.507655
C	24.205535	4.604969	40.138996	C	16.693336	5.816528	45.722474
O	24.680624	5.759428	38.077583	C	17.698535	6.581292	46.343743
O	19.156956	5.596938	41.653061	C	18.793459	6.965294	32.215005
O	18.658641	3.443848	42.099965	C	17.696158	6.524355	32.946185
C	19.507826	4.385623	41.896370	C	16.669464	5.776427	32.338794
C	16.904066	4.155536	37.734567	C	15.558154	5.410200	46.479349
C	17.590252	3.042639	37.216303	C	14.476130	4.725860	45.886151
C	17.586627	2.774904	35.854100	C	13.378758	4.342806	46.651770
C	16.896520	3.611699	34.984393	C	14.513022	4.648664	32.443581
C	16.170975	4.723378	35.460129	C	15.544645	5.346745	33.085971
C	16.155248	4.987451	36.856147	O	13.400826	4.242288	33.172366
C	15.366660	6.051195	37.338984	O	17.155117	6.428682	43.465520

O	16.642495	4.275005	43.897610	C	28.433232	7.009170	42.024693
C	16.842449	5.485294	44.277400	C	42.200892	7.041270	41.833331
Cu	33.171219	6.231492	41.745492	C	41.401873	6.135307	41.145975
Cu	32.516299	3.766207	42.260251	C	41.957591	5.006509	40.512829
C	36.717629	3.867824	42.185098	C	43.364032	4.801133	40.580150
C	37.305571	3.301832	43.299380	C	28.407777	3.629068	40.362212
C	38.691615	3.020610	43.286424	C	43.108983	2.843473	39.166800
C	39.461105	3.311039	42.178245	C	41.733144	2.998189	39.145753
C	38.890563	3.877836	40.992148	C	41.136379	4.085624	39.814952
C	37.472727	4.122172	40.998555	O	40.999390	2.024103	38.473605
C	36.850120	4.577626	39.804032	O	31.163091	6.394674	41.509536
C	37.590922	4.837212	38.680785	O	30.629586	4.301657	42.127127
C	39.007403	4.731013	38.704424	C	30.328915	5.468301	41.730020
C	39.661375	4.223327	39.827357	C	32.336274	5.976874	45.877414
O	39.710251	5.127646	37.609559	C	33.210244	6.827480	46.532589
O	35.011699	5.484207	42.048310	C	35.050616	6.937275	32.144452
O	34.423969	3.335713	42.390147	C	34.006524	6.580231	32.989153
C	35.272245	4.256189	42.215850	C	32.882467	5.889020	32.503064
C	32.819748	4.128611	38.054584	C	31.195864	5.431472	46.552083
C	33.281901	2.908882	37.590560	C	30.208300	4.635955	45.898566
C	33.337255	2.658902	36.203586	C	29.119663	4.155645	46.588971
C	32.894383	3.607278	35.305382	C	30.681081	4.913603	32.844613
C	32.362825	4.867825	35.731156	C	31.810060	5.557653	33.360925
C	32.342954	5.133662	37.146932	O	29.618859	4.608030	33.685753
C	31.805975	6.377134	37.591906	O	32.962199	6.574789	43.683634
C	31.342441	7.308498	36.699585	O	32.508491	4.412430	44.125088
C	31.364132	7.059594	35.301423	C	32.622084	5.628810	44.452198
C	31.856303	5.853408	34.811254	Cu	48.403642	6.328721	41.556798
O	30.860281	8.090381	34.560809	Cu	47.998642	3.896532	42.030553
O	33.265170	5.510995	39.910162	C	52.242277	4.464616	41.931345
O	32.526650	3.425475	40.300443	C	52.828352	3.947593	43.079296
C	32.864247	4.370463	39.528518	C	54.201352	3.732573	43.123194
C	28.877325	5.785657	41.549073	C	54.987277	4.036578	42.018142

C	54.401202	4.554601	40.869191	C	48.962758	6.693417	32.924395
C	53.028202	4.768621	40.826292	C	47.976090	5.876460	32.340183
C	52.442128	5.287645	39.677341	C	46.706662	5.517321	46.511632
C	53.229054	5.591649	38.571289	C	45.664385	4.787475	45.902556
C	54.601054	5.377629	38.616189	C	44.572607	4.358448	46.651902
C	55.187129	4.858606	39.764139	C	45.892265	4.623875	32.485886
O	55.314970	5.617636	37.405141	C	46.885067	5.395492	33.105030
O	50.341230	5.900090	41.718774	O	44.814224	4.164195	33.233716
O	49.981121	3.718333	42.167231	O	48.282541	6.607790	43.521846
C	50.767095	4.709872	41.949689	O	47.893992	4.426510	43.946826
C	48.245024	4.327743	37.785534	C	48.018807	5.646271	44.329392
C	49.002394	3.252588	37.286422	C	9.830844	7.260885	57.522289
C	49.043482	2.981203	35.925690	C	8.959813	6.502896	56.749314
C	48.326194	3.774752	35.037881	C	9.429780	5.394897	56.054290
C	47.531990	4.847412	35.492678	C	10.771780	5.042887	56.134240
C	47.475715	5.118656	36.886462	C	10.370715	3.178901	54.666241
C	46.627686	6.146726	37.345650	C	9.028715	3.528910	54.587291
C	45.897932	6.911655	36.444118	C	8.558747	4.637908	55.281315
C	45.971923	6.680955	35.080615	O	8.125681	2.792922	53.781316
C	46.793433	5.646226	34.579770	Cu	15.899776	6.129092	57.132055
O	45.229728	7.525738	34.258086	Cu	15.342929	3.717548	57.552012
O	48.464480	5.809291	39.640896	C	19.602987	4.022957	57.426205
O	48.113636	3.621681	40.061337	C	20.158762	3.257294	58.467457
C	48.277230	4.601663	39.248510	C	21.510880	2.937069	58.474133
C	44.171131	5.702132	41.332845	C	22.331385	3.365878	57.436611
C	43.569992	6.827568	41.926855	C	21.814710	4.112884	56.361150
C	43.925941	3.723236	39.868137	C	20.430494	4.433315	56.342792
O	46.422267	6.503075	41.412467	C	19.905553	5.122397	55.229090
O	46.061006	4.316655	41.824664	C	20.738391	5.515874	54.186119
C	45.637699	5.493425	41.530975	C	22.103408	5.240684	54.221587
C	47.836682	5.967569	45.772502	C	22.653603	4.531055	55.298055
C	48.802343	6.769820	46.408917	O	22.923247	5.644748	53.173641
C	50.026480	7.183737	32.174797	O	17.802914	5.581415	57.294197

O	17.308407	3.412280	57.669498	C	16.534338	6.475552	48.445884
C	18.152835	4.359713	57.476287	C	15.490026	5.734017	47.861560
C	15.662528	4.204910	53.319571	C	14.198077	5.242813	62.095147
C	16.364660	3.091089	52.823823	C	13.166036	4.552830	61.469195
C	16.401826	2.819133	51.463370	C	12.083071	4.099834	62.213248
C	15.731574	3.648129	50.571999	C	13.327597	4.624418	48.014963
C	14.993402	4.761763	51.022291	C	14.371824	5.327770	48.630804
C	14.947275	5.039276	52.415894	O	12.223508	4.237292	48.766346
C	14.159390	6.115870	52.869970	O	15.767654	6.372257	59.106964
C	13.472402	6.914605	51.963941	O	15.279965	4.202388	59.478482
C	13.533581	6.673194	50.601351	C	15.450129	5.406312	59.892118
C	14.298108	5.593354	50.105068	Cu	31.470730	6.089964	57.124010
O	12.837146	7.552348	49.775038	Cu	30.962626	3.674185	57.573998
O	15.949233	5.644959	55.203030	C	35.209751	4.030578	57.450474
O	15.437734	3.480681	55.578876	C	35.758783	3.329870	58.540296
C	15.684002	4.459534	54.786449	C	37.107532	2.999733	58.571259
C	11.644813	5.800876	56.909215	C	37.932478	3.353083	57.509690
C	11.172845	6.908875	57.603239	C	37.423915	4.037249	56.388988
C	25.312649	7.051276	57.536338	C	36.042479	4.369707	56.347936
C	24.480500	6.226556	56.789097	C	35.524874	4.997223	55.195843
C	24.990857	5.115688	56.086597	C	36.363560	5.316925	54.131816
C	26.384458	4.841494	56.150413	C	37.725887	5.029212	54.185926
C	11.243748	3.934890	55.440215	C	38.269559	4.382587	55.305088
C	26.057588	2.980629	54.625110	O	38.550375	5.357159	53.115533
C	24.691809	3.209777	54.590227	O	33.390685	5.567278	57.253050
C	24.132573	4.280806	55.323153	O	32.927944	3.402429	57.695012
O	23.924339	2.328381	53.831651	C	33.757070	4.355359	57.471452
O	13.943114	6.427961	56.972758	C	31.235812	4.124845	53.347370
O	13.435687	4.267610	57.369719	C	32.000077	3.066114	52.887729
C	13.093312	5.473093	57.085314	C	32.049588	2.788821	51.501546
C	15.283042	5.695809	61.352094	C	31.337987	3.562878	50.611460
C	16.314083	6.385792	61.978046	C	30.518926	4.639082	51.057801
C	17.621572	6.902195	47.692677	C	30.447049	4.933194	52.465668

C	29.555768	5.976835	52.876874	O	31.379699	6.352547	59.099100
C	28.808922	6.686997	51.968911	O	30.902375	4.184349	59.494736
C	28.919091	6.419458	50.581242	C	31.070370	5.393039	59.894622
C	29.761921	5.416287	50.125326	Cu	47.041159	6.239413	57.144022
O	28.179385	7.185292	49.744359	Cu	46.684335	3.784495	57.535287
O	31.481393	5.594824	55.201708	C	50.914826	4.464382	57.493755
O	31.057097	3.407848	55.609435	C	51.500920	3.947352	58.641694
C	31.260389	4.390694	54.803846	C	52.873920	3.732327	58.685568
C	27.223499	5.663416	56.953826	C	53.659827	4.036331	57.580503
C	26.670272	6.774298	57.617673	C	53.073733	4.554362	56.431564
C	40.892089	6.936566	57.544474	C	51.700733	4.768387	56.388690
C	40.072979	6.094916	56.804065	C	51.114640	5.287417	55.239751
C	40.597878	4.982609	56.114668	C	51.901547	5.591423	54.133687
C	41.995687	4.724984	56.184603	C	53.273547	5.377397	54.178561
C	26.904663	3.778168	55.385823	C	53.859639	4.858367	55.326499
C	41.689618	2.834813	54.691945	O	53.987443	5.617405	52.967501
C	40.322337	3.054356	54.642956	O	48.985049	5.853931	57.294632
C	39.749976	4.133285	55.354475	O	48.672424	3.650065	57.667417
O	39.567749	2.152918	53.895566	C	49.435672	4.668883	57.495404
O	29.502059	6.362931	57.016924	C	46.932691	4.340752	53.311499
O	29.046956	4.185950	57.396606	C	47.722039	3.294825	52.799024
C	28.676925	5.386129	57.128132	C	47.757004	3.029094	51.437653
C	30.903116	5.695628	61.351271	C	47.000116	3.797732	50.562037
C	31.934171	6.385605	61.977208	C	46.178663	4.844569	51.028780
C	33.023380	7.123425	47.901539	C	46.132095	5.112665	52.424066
C	31.960066	6.580970	48.593450	C	45.262766	6.116318	52.895714
C	31.014501	5.735151	47.943243	C	44.500650	6.861187	52.004078
C	29.818163	5.242633	62.094342	C	44.561544	6.632291	50.639203
C	28.786109	4.552656	61.468406	C	45.404825	5.621005	50.125483
C	27.703155	4.099663	62.212477	O	43.790054	7.461148	49.827892
C	28.966455	4.413176	47.977730	O	47.110313	5.783802	55.207896
C	29.897407	5.190704	48.658510	O	46.802986	3.577709	55.562589
O	27.916446	3.913578	48.678107	C	46.949031	4.583499	54.779964

C	42.825599	5.575398	56.968765	C	46.419443	6.168348	64.088184
C	42.253075	6.682104	57.624267	C	45.387375	5.478376	63.463264
C	42.526953	3.654374	55.439378	C	43.271365	4.336411	63.580432
O	45.064647	6.382487	57.014453	C	44.303433	5.025383	64.205353
O	44.736822	4.177924	57.354177	O	42.183428	3.908416	64.359522
C	44.294956	5.360895	57.114730	H	12.119209	8.127032	26.935796
C	46.523192	5.695393	61.350166	H	10.573037	6.786761	25.566470
C	47.554258	6.385364	61.976087	H	13.382432	2.322101	22.983375
C	48.688255	7.093533	47.754446	H	9.847358	3.169348	22.676421
C	47.604608	6.628649	48.489723	H	22.126035	2.888480	28.248542
C	46.603256	5.839855	47.891797	H	24.526485	2.359186	28.328640
C	45.438249	5.242399	62.093255	H	26.030432	3.152521	26.577809
C	44.406182	4.552428	61.467335	H	21.547883	5.337340	24.089822
C	43.323240	4.099435	62.211424	H	23.060892	6.066575	22.356358
C	44.491292	4.633936	48.015165	H	19.533761	2.331015	22.589877
C	45.495680	5.380492	48.646895	H	19.680073	1.794626	20.190438
O	43.395429	4.197183	48.750731	H	18.480862	3.171009	18.536745
O	46.913372	6.439947	59.118804	H	16.652300	6.145813	22.827053
O	46.574349	4.235586	59.463603	H	15.507195	7.501699	21.164005
C	46.673479	5.441671	59.889901	H	14.495648	7.508817	27.086856
C	16.262158	6.620778	63.347051	H	27.653793	8.086782	26.947059
C	15.179191	6.168782	64.090104	H	26.154898	6.582540	25.750559
C	14.147152	5.478800	63.465152	H	14.941022	3.631926	24.316734
C	12.031146	4.336820	63.582253	H	29.134287	2.107849	23.255718
C	13.063187	5.025805	64.207205	H	19.768553	6.990271	30.313285
O	10.943183	3.908824	64.361306	H	15.687282	4.568903	29.272836
C	31.882271	6.620587	63.346214	H	13.777778	3.871718	30.578233
C	30.799317	6.168593	64.089284	H	15.672522	6.861922	17.596265
C	29.767262	5.478616	63.464348	H	25.195321	6.222756	21.555567
C	27.651255	4.336645	63.581483	H	25.619993	2.524008	23.038097
C	28.683309	5.025622	64.206418	H	37.800081	2.970183	28.262670
O	26.563304	3.908650	64.360554	H	40.180139	2.359019	28.319884
C	47.502385	6.620342	63.345096	H	41.657269	2.958780	26.473682

H 37.186468 5.149698 23.966941	H 46.908364 6.858734 17.596190
H 38.670065 5.668769 22.128992	H 56.056697 5.974286 21.102333
H 35.151044 2.330348 22.590847	H 10.790906 8.128124 42.498320
H 35.298992 1.793895 20.190282	H 9.244413 6.786909 41.130228
H 34.100505 3.170932 18.536501	H 12.054167 2.324035 38.544699
H 32.266436 6.143584 22.826458	H 8.520658 3.174477 38.234317
H 31.125079 7.500183 21.164020	H 20.727648 2.893424 43.766420
H 30.057496 7.596425 27.098255	H 23.111154 2.341406 43.988079
H 43.091745 7.763871 26.910074	H 24.729658 3.143844 42.349054
H 41.678273 6.258665 25.624674	H 20.438850 5.465381 39.649461
H 30.655638 3.560677 24.458405	H 22.072053 6.198304 38.024788
H 44.849000 1.899688 23.154063	H 18.140167 2.385469 37.880466
H 35.825555 6.880429 30.155193	H 18.125026 1.915588 35.467737
H 31.554800 4.642702 29.584688	H 16.917162 3.369536 33.931283
H 29.733962 4.112206 31.088209	H 15.275174 6.271911 38.396369
H 31.290200 6.860088 17.596456	H 14.053433 7.670599 36.835862
H 40.789506 5.701228 21.270926	H 13.169686 7.511365 42.644994
H 41.334082 2.235770 22.827495	H 26.710912 8.290536 42.362158
H 53.552178 3.700961 28.381637	H 25.103509 6.738392 41.382513
H 55.987801 3.326728 28.455981	H 13.611681 3.633158 39.869895
H 57.384024 3.866288 26.497948	H 27.847509 1.834912 39.316253
H 52.703546 5.453397 24.015259	H 18.554396 6.921323 45.771162
H 54.081375 5.977015 22.117040	H 19.567310 7.552365 32.699065
H 50.777749 2.335333 22.589487	H 17.646863 6.787069 33.994373
H 50.921002 1.795349 20.189763	H 14.452643 4.488707 44.827818
H 49.720251 3.170762 18.536008	H 12.562711 3.817558 46.174393
H 47.864594 6.135361 22.823932	H 12.744811 3.718675 32.612017
H 46.741390 7.497427 21.163783	H 14.018647 7.285775 33.311401
H 45.503916 7.350431 27.104209	H 24.251652 6.303602 37.343572
H 46.294235 3.365579 24.439816	H 24.444698 2.319457 39.060974
H 50.979294 7.233501 30.261509	H 36.702822 3.092454 44.187755
H 47.045245 4.549201 29.307309	H 39.160320 2.578432 44.171212
H 45.190413 3.765850 30.643412	H 40.533326 3.093389 42.213449

H	35.771541	4.742739	39.771363	H	49.654997	7.139267	45.850042
H	37.097217	5.180867	37.767506	H	50.769705	7.822225	32.641329
H	33.620486	2.157777	38.308092	H	48.907273	6.970186	33.968680
H	33.732248	1.705749	35.838058	H	45.669484	4.548278	44.844362
H	32.954507	3.372279	34.237753	H	43.785883	3.800446	46.162497
H	31.762325	6.591883	38.658174	H	44.183112	3.594672	32.689944
H	30.931869	8.261837	37.042022	H	45.299671	7.287789	33.283353
H	29.150726	7.703714	42.468802	H	54.726430	5.966810	36.663207
H	41.753768	7.910861	42.304000	H	9.463380	8.126972	58.063051
H	40.339684	6.334063	41.097806	H	7.916951	6.786648	56.693756
H	29.465624	3.366537	40.386451	H	10.727093	2.324959	54.106596
H	43.547160	2.011011	38.631889	H	7.193490	3.175209	53.796568
H	34.055708	7.248907	45.981656	H	19.533080	2.918092	59.285366
H	35.903622	7.482981	32.535042	H	21.927860	2.354529	59.289260
H	34.077439	6.863389	34.030388	H	23.378715	3.097104	57.473516
H	30.307537	4.406985	44.836726	H	18.850244	5.357799	55.140983
H	28.365093	3.554397	46.068783	H	20.312307	6.045944	53.345281
H	28.875384	4.119080	33.208958	H	16.892927	2.433723	53.505447
H	30.883215	7.914250	33.607130	H	16.952128	1.959172	51.095784
H	39.121451	5.646572	37.032156	H	15.780621	3.399832	49.521388
H	40.002960	2.173742	38.515460	H	14.050068	6.351433	53.922531
H	52.223115	3.706137	43.946076	H	12.874767	7.743138	52.319949
H	54.659218	3.327404	44.019633	H	11.840793	7.509325	58.211844
H	56.055251	3.865868	42.061090	H	24.900165	7.906830	58.061075
H	51.375049	5.456877	39.580965	H	23.429309	6.474421	56.751556
H	52.752686	5.977183	37.680421	H	12.284827	3.635359	55.428807
H	49.574429	2.629118	37.964751	H	26.464369	2.161984	54.046478
H	49.637414	2.152367	35.554591	H	17.168702	6.738690	61.410823
H	48.382738	3.530546	33.986704	H	18.409586	7.484834	48.158935
H	46.501965	6.368410	38.398987	H	16.508156	6.742487	49.493844
H	45.253955	7.702667	36.804820	H	13.130250	4.374771	60.400657
H	44.175333	7.537535	42.479258	H	11.278280	3.573241	61.719710
H	44.995421	3.548806	39.828415	H	11.554598	3.711416	48.223835

H	12.913185	7.319183	48.799679	H	48.372506	2.220571	51.057092
H	22.421906	6.172227	52.474552	H	47.049066	3.553830	49.510626
H	22.944082	2.552749	53.840077	H	45.147485	6.335637	53.951098
H	35.127440	3.043594	59.373914	H	43.841851	7.635665	52.373793
H	37.516863	2.463708	59.421365	H	42.876143	7.351003	58.207371
H	38.976166	3.074271	57.564317	H	43.588577	3.439620	55.408186
H	34.470505	5.238136	55.095150	H	48.405868	6.743806	61.407837
H	35.943411	5.798702	53.259374	H	49.444163	7.708226	48.232236
H	32.580412	2.440807	53.574998	H	47.546657	6.902760	49.534488
H	32.658750	1.954788	51.139545	H	44.382681	4.361771	60.399774
H	31.382562	3.345111	49.541485	H	42.519209	3.571538	61.717843
H	29.439633	6.226411	53.934844	H	42.756780	3.643562	48.199176
H	28.121418	7.472962	52.291251	H	43.848494	7.220956	48.853290
H	27.303378	7.420928	58.215201	H	53.398601	5.964634	52.224812
H	40.467999	7.793081	58.058298	H	17.068788	7.157005	63.836247
H	39.019761	6.332566	56.761021	H	15.148347	6.357085	65.155561
H	27.966081	3.555062	55.349270	H	10.261922	3.422172	63.798223
H	42.105259	2.009485	54.129132	H	32.688523	7.157528	63.835064
H	32.789260	6.736549	61.409577	H	30.768381	6.356720	65.154688
H	33.730293	7.781527	48.415884	H	25.879845	3.426648	63.796001
H	31.823573	6.803817	49.654348	H	48.307237	7.159615	63.833645
H	28.748169	4.377083	60.399333	H	46.387898	6.357360	65.153446
H	26.898366	3.573626	61.718197	H	41.496445	3.432062	63.794251
H	27.352421	3.375379	48.098092	H	54.922472	4.682717	55.325506
H	28.340893	6.887358	48.828775	H	56.250017	4.683119	39.763406
H	38.054322	5.843041	52.383279	H	57.578845	4.683521	24.200325
H	38.587518	2.377414	53.881729	H	32.654321	5.043722	18.026509
H	50.894624	3.699033	59.505777	H	17.034742	5.043886	18.026663
H	53.331520	3.325457	59.581299	H	10.176533	4.915001	24.089415
H	54.727794	3.865701	57.623291	H	8.847895	4.915082	39.653409
H	50.047758	5.460950	55.145938	H	7.520500	4.915149	55.216502
H	51.425100	5.978061	53.243311	H	12.998700	5.198788	65.268980
H	48.317941	2.684408	53.468641	H	28.618566	5.198773	65.268037

H	44.238294	5.198790	65.266945		
H	48.273684	5.043270	18.026083	RCext2	
C	34.018274	9.494937	41.700310	C	12.487000 7.261000 26.395000
C	33.387591	9.308365	40.373125	C	11.616000 6.503000 25.622000
C	31.883340	9.414561	40.190012	C	12.086000 5.395000 24.927000
C	31.178383	10.078763	41.385538	C	13.428000 5.043000 25.007000
C	31.691787	9.536431	42.725547	C	13.027000 3.179000 23.539000
C	33.188282	9.832366	42.918103	C	11.685000 3.529000 23.460000
O	33.842692	8.178092	41.150751	C	11.215000 4.638000 24.154000
C	36.667895	7.782851	38.948484	O	10.782000 2.793000 22.654000
C	37.805132	8.057336	38.159657	Cu	18.545764 6.084974 26.019232
C	37.763341	7.902602	36.770514	Cu	17.951770 3.697366 26.530411
C	36.590312	7.479751	36.129795	C	22.218764 3.946423 26.385605
C	35.450748	7.228776	36.907567	C	22.756430 3.177863 27.434202
C	35.481798	7.382886	38.293365	C	24.109043 2.861444 27.465799
N	36.709654	7.894719	40.332853	C	24.949067 3.299886 26.447726
H	31.673023	9.967215	39.257323	C	24.449813 4.044515 25.362497
H	34.012827	9.459727	39.484119	C	23.064566 4.356336 25.315727
H	35.078474	9.783068	41.724387	C	22.557292 5.035127 24.186996
H	30.088884	9.917891	41.298737	C	23.408232 5.430922 23.159682
H	31.341850	11.174396	41.349805	C	24.773819 5.166909 23.224795
H	31.126196	9.981299	43.563575	C	25.306488 4.465738 24.315163
H	31.528070	8.447613	42.772143	O	25.611974 5.568694 22.190504
H	33.342321	10.909411	43.126665	O	20.438063 5.517506 26.193311
H	33.579781	9.270068	43.785074	O	19.915082 3.371878 26.654411
H	31.491821	8.391481	40.056635	C	20.771962 4.299723 26.421599
H	38.737455	8.363252	38.646361	C	18.226925 4.022012 22.293999
H	38.663563	8.119160	36.183632	C	18.992913 2.941010 21.873981
H	36.564929	7.348306	35.044353	C	19.081888 2.638015 20.519979
H	34.521508	6.883357	36.444055	C	18.404874 3.417021 19.587993
H	34.603394	7.118220	38.885369	C	17.639886 4.497022 20.008011
H	35.994040	7.370410	40.835919	C	17.550911 4.800017 21.362013
H	37.631596	7.780527	40.746126	C	16.783922 5.881019 21.784030

C	16.107908	6.659025	20.850045	C	39.712958	2.837862	27.531449
C	16.197883	6.355030	19.497042	C	40.556548	3.211531	26.491775
C	16.963873	5.274029	19.076025	C	40.068152	3.918256	25.376636
O	15.523870	7.185036	18.539057	C	38.689289	4.257046	25.320054
O	18.566534	5.529570	24.113655	C	38.192527	4.905150	24.170223
O	18.025015	3.388223	24.574921	C	39.048338	5.238778	23.124636
C	18.266357	4.336562	23.746351	C	40.408854	4.947102	23.196246
C	14.301000	5.801000	25.782000	C	40.931314	4.279916	24.313002
C	13.829000	6.909000	26.476000	O	41.252643	5.294875	22.147178
C	27.966528	7.051758	26.483030	O	36.044931	5.467760	26.187696
C	27.131058	6.198881	25.770703	O	35.545310	3.316565	26.649179
C	27.640691	5.069379	25.098257	C	36.391546	4.252560	26.418840
C	29.034707	4.800106	25.164982	C	33.846853	4.021969	22.293716
C	13.900000	3.935000	24.313000	C	34.612830	2.940966	21.873681
C	28.706723	2.892328	23.697696	C	34.701779	2.637975	20.519676
C	27.341572	3.120084	23.657666	C	34.024751	3.416985	19.587706
C	26.782975	4.211684	24.359730	C	33.259774	4.496987	20.007739
O	26.575122	2.219336	22.921445	C	33.170824	4.799980	21.361745
O	16.597542	6.403167	25.853699	C	32.403846	5.880983	21.783779
O	16.056233	4.263416	26.319556	C	31.727819	6.658993	20.849808
C	15.736620	5.461753	25.985866	C	31.817769	6.355001	19.496803
C	17.906535	5.817457	30.234791	C	32.583746	5.273997	19.075769
C	18.894319	6.582246	30.882075	O	31.143739	7.185012	18.538833
C	16.754362	5.404587	30.961996	O	34.121248	5.512664	24.152966
C	15.684120	4.729172	30.337285	O	33.631044	3.355331	24.584281
C	14.575875	4.326476	31.076435	C	33.856409	4.318205	23.763140
O	18.432915	6.401630	27.981558	C	29.876192	5.648583	25.938714
O	17.897799	4.256947	28.433372	C	29.325970	6.781763	26.564838
C	18.096348	5.470965	28.799269	C	43.535124	6.873148	26.527664
Cu	34.136340	6.025557	26.076638	C	42.719170	6.012265	25.805002
Cu	33.584103	3.625683	26.563096	C	43.249992	4.891207	25.134132
C	37.839027	3.904609	26.404577	C	44.647795	4.639954	25.211281
C	38.366726	3.176574	27.487106	C	29.553528	3.714115	24.430861

C	44.351943	2.716544	23.759565	C	50.321667	2.637886	20.519091
C	42.985308	2.936168	23.696040	C	49.644624	3.416901	19.587136
C	42.408782	4.027859	24.383353	C	48.879658	4.496905	20.007187
O	42.235125	2.024284	22.956971	C	48.790735	4.799894	21.361195
O	32.167427	6.327119	25.985084	C	48.023770	5.880898	21.783247
O	31.681682	4.167563	26.415259	C	47.347728	6.658913	20.849290
C	31.327181	5.365772	26.123827	C	47.437652	6.354926	19.496283
C	33.759079	5.677045	30.328447	C	48.203617	5.273922	19.075230
C	34.805783	6.446233	30.872377	O	46.763610	7.184943	18.538326
C	32.690464	5.263671	31.175960	O	49.725059	5.588715	24.095214
C	31.577149	4.558327	30.675386	O	49.386251	3.420849	24.607756
C	30.541268	4.182336	31.526875	C	49.523214	4.366323	23.751286
O	34.090500	6.300919	28.049397	C	45.474186	5.514003	25.971044
O	33.573240	4.150463	28.487974	C	44.898771	6.630681	26.605649
C	33.806104	5.354898	28.869558	C	45.184125	3.550902	24.496588
Cu	49.689524	6.197107	25.991956	O	47.709181	6.325062	25.895638
Cu	49.345031	3.777034	26.565009	O	47.393076	4.154907	26.421469
C	53.571003	4.464794	26.367934	C	46.944816	5.315309	26.100137
C	54.157057	3.947776	27.515897	C	49.192289	5.966345	30.228543
C	55.530059	3.732762	27.559821	C	50.131478	6.811527	30.847255
C	56.316002	4.036764	26.454782	C	48.080988	5.488972	30.979280
C	55.729945	4.554783	25.305818	C	47.057146	4.723133	30.382246
C	54.356946	4.768798	25.262894	C	45.983678	4.266659	31.140774
C	53.770889	5.287815	24.113932	O	49.600942	6.549949	27.950181
C	54.557833	5.591817	23.007892	O	49.296359	4.373113	28.459161
C	55.929833	5.377802	23.052816	C	49.382498	5.608814	28.795532
C	56.515888	4.858784	24.200779	C	11.158287	7.260976	41.959132
O	56.643769	5.617808	21.841779	C	10.287269	6.502982	41.186144
O	51.633385	5.833718	26.127071	C	10.757253	5.394981	40.491132
O	51.336466	3.655106	26.634966	C	12.099253	5.042976	40.571108
C	52.092183	4.663324	26.381411	C	11.698221	3.178982	39.103110
C	49.466778	4.021877	22.293151	C	10.356221	3.528988	39.024135
C	50.232744	2.940873	21.873099	C	9.886237	4.637987	39.718145

O	9.453203	2.792994	38.218148	C	26.898567	7.141350	42.502684
Cu	17.245085	6.098385	41.492382	C	26.037884	6.342993	41.777227
Cu	16.667150	3.706620	41.989849	C	26.498828	5.206434	41.037822
C	20.944972	3.972125	41.896673	C	27.904814	4.899475	41.106659
C	21.407649	3.085296	42.888309	C	12.571237	3.934977	39.877096
C	22.754328	2.758965	42.987995	C	27.558724	3.032778	39.587413
C	23.669679	3.310201	42.099994	C	26.168549	3.319395	39.520461
C	23.254155	4.172473	41.069908	C	25.630760	4.385173	40.236655
C	21.873918	4.497463	40.950394	O	25.482123	2.458912	38.711539
C	21.458848	5.297902	39.864979	O	15.282302	6.414295	41.363474
C	22.390998	5.800904	38.961987	O	14.761347	4.269972	41.822693
C	23.745809	5.516541	39.102247	C	14.424123	5.470809	41.513815
C	24.186042	4.694643	40.143863	C	16.726969	5.799000	45.717570
O	24.661690	6.017146	38.185687	C	17.767925	6.514968	46.337434
O	19.147757	5.535880	41.648179	C	18.785893	6.892377	32.231598
O	18.633566	3.386551	42.090092	C	17.686230	6.450742	32.958755
C	19.489967	4.319386	41.875476	C	16.658601	5.708038	32.346142
C	16.875190	4.090603	37.741706	C	15.575228	5.444499	46.474034
C	17.557336	2.972687	37.228497	C	14.469020	4.799763	45.881824
C	17.555080	2.700970	35.866920	C	13.355495	4.465475	46.646740
C	16.870760	3.538747	34.993475	C	14.502474	4.578578	32.443903
C	16.147303	4.653536	35.465337	C	15.531899	5.276872	33.089416
C	16.129877	4.921375	36.860230	O	13.390580	4.167269	33.170469
C	15.344429	5.989047	37.339480	O	17.167132	6.399745	43.455582
C	14.635533	6.792069	36.454732	O	16.641900	4.251549	43.902452
C	14.678214	6.567903	35.088711	C	16.857013	5.461687	44.273956
C	15.443023	5.499515	34.568530	Cu	33.047998	6.084993	41.931283
O	13.966285	7.454006	34.283440	Cu	32.381674	3.612985	42.411172
O	17.248955	5.560603	39.580399	C	36.544641	3.603770	42.144512
O	16.724205	3.411762	40.022621	C	37.087975	2.781561	43.112798
C	16.957302	4.369274	39.200736	C	38.474331	2.506853	43.107064
C	12.972270	5.800971	41.346095	C	39.290114	3.036451	42.130085
C	12.500287	6.908971	42.040107	C	38.767947	3.856012	41.075933

C	37.354159	4.132397	41.085376	O	40.841419	2.198840	38.588718
C	36.802060	4.887515	40.012135	O	31.048269	6.363011	41.794218
C	37.599557	5.358695	38.997252	O	30.522586	4.247165	42.355583
C	39.002150	5.135962	39.005328	C	30.225066	5.431487	42.010244
C	39.590098	4.391143	40.026505	C	32.268409	5.685256	46.088216
O	39.775074	5.654126	38.009273	C	33.220777	6.366125	46.824212
O	34.819623	5.196304	42.146307	C	34.832375	6.770246	32.222753
O	34.260121	3.039280	42.441272	C	33.804891	6.348362	33.057919
C	35.097313	3.970241	42.249309	C	32.720662	5.605405	32.557819
C	32.658095	4.063914	38.186426	C	31.015898	5.304437	46.671890
C	33.170722	2.839912	37.789651	C	29.959450	4.728542	45.907063
C	33.243598	2.516691	36.419071	C	28.738988	4.469711	46.486729
C	32.769484	3.396524	35.468135	C	30.578687	4.500034	32.882526
C	32.186960	4.655486	35.822978	C	31.657730	5.218809	33.406538
C	32.146442	4.996181	37.223831	O	29.530386	4.128537	33.714684
C	31.546174	6.232135	37.604040	O	32.889604	6.325550	43.903356
C	31.037155	7.087127	36.660445	O	32.441505	4.153375	44.307433
C	31.086805	6.767806	35.276479	C	32.558935	5.363626	44.655103
C	31.646470	5.567115	34.848112	Cu	48.399963	6.324745	41.575914
O	30.541058	7.736785	34.481586	Cu	48.001715	3.894445	42.066934
O	33.059222	5.514854	40.020807	C	52.242279	4.464604	41.931330
O	32.342580	3.421418	40.432436	C	52.828353	3.947581	43.079281
C	32.678560	4.362243	39.654165	C	54.201353	3.732560	43.123179
C	28.766738	5.741059	41.880317	C	54.987278	4.036564	42.018127
C	28.278824	6.852172	42.545004	C	54.401204	4.554586	40.869175
C	42.223441	7.041360	42.125442	C	53.028204	4.768608	40.826277
C	41.389577	6.166437	41.439642	C	52.442129	5.287631	39.677326
C	41.910865	5.063746	40.735265	C	53.229056	5.591635	38.571274
C	43.315336	4.835619	40.750223	C	54.601055	5.377613	38.616174
C	28.400753	3.792754	40.356422	C	55.187129	4.858591	39.764123
C	42.983441	2.918178	39.297690	O	55.314972	5.617620	37.405126
C	41.612569	3.113772	39.300313	O	50.339326	5.896497	41.713758
C	41.057024	4.192222	40.015993	O	49.984501	3.717532	42.180298

C	50.767682	4.708589	41.950950	O	47.920887	4.434662	43.979731
C	48.219858	4.299005	37.816717	C	48.046485	5.657051	44.353235
C	48.981109	3.221428	37.328581	C	9.830847	7.260907	57.522288
C	49.030200	2.940692	35.970067	C	8.959814	6.502918	56.749313
C	48.317463	3.727647	35.072927	C	9.429781	5.394919	56.054289
C	47.519294	4.802189	35.516293	C	10.771781	5.042908	56.134240
C	47.454273	5.082432	36.908240	C	10.370715	3.178922	54.666242
C	46.601093	6.111001	37.356256	C	9.028715	3.528931	54.587292
C	45.871905	6.865883	36.445712	C	8.558748	4.637930	55.281316
C	45.954276	6.626468	35.084083	O	8.125681	2.792943	53.781318
C	46.784247	5.593143	34.593892	Cu	15.892890	6.156931	57.133781
O	45.209814	7.460182	34.252527	Cu	15.354562	3.738961	57.538918
O	48.434345	5.795791	39.661285	C	19.612357	4.077974	57.370723
O	48.093042	3.609809	40.098026	C	20.183563	3.269651	58.370635
C	48.249781	4.584871	39.277821	C	21.537433	2.958080	58.348983
C	44.160779	5.711058	41.490206	C	22.345301	3.440280	57.325132
C	43.594071	6.819790	42.146904	C	21.813868	4.231842	56.289503
C	43.836285	3.762410	40.000752	C	20.426858	4.540137	56.296930
O	46.416419	6.498645	41.468814	C	19.886696	5.268244	55.215341
O	46.061147	4.312947	41.891795	C	20.707374	5.717143	54.185289
C	45.632747	5.492166	41.617052	C	22.075685	5.459473	54.201503
C	47.860173	5.987907	45.792034	C	22.640860	4.706920	55.240124
C	48.823842	6.791834	46.428842	O	22.883949	5.921392	53.168480
C	50.015894	7.142909	32.191606	O	17.799485	5.625033	57.289024
C	48.956292	6.643627	32.941364	O	17.324152	3.448734	57.644677
C	47.976101	5.819130	32.357029	C	18.160106	4.403823	57.450481
C	46.723110	5.546775	46.524817	C	15.656580	4.257637	53.307824
C	45.680748	4.820456	45.911089	C	16.340053	3.134709	52.805814
C	44.583339	4.397121	46.654863	C	16.372836	2.868688	51.444262
C	45.900839	4.551826	32.501312	C	15.718224	3.714018	50.557063
C	46.885613	5.333605	33.120765	C	14.999303	4.838229	51.012513
O	44.822887	4.087543	33.246758	C	14.955328	5.108544	52.407731
O	48.306387	6.613777	43.539335	C	14.182470	6.194410	52.866023

C	13.513929	7.011917	51.962727	O	15.289653	4.210902	59.470132
C	13.575107	6.778099	50.598812	C	15.449276	5.414169	59.890231
C	14.320245	5.686794	50.098187	Cu	31.448113	6.143117	57.120058
O	12.897289	7.675007	49.775886	Cu	30.925566	3.725399	57.541177
O	15.944695	5.686290	55.201370	C	35.174971	4.050631	57.409732
O	15.445130	3.517185	55.563663	C	35.710114	3.298963	58.472338
C	15.682921	4.502892	54.776933	C	37.056582	2.959582	58.501298
C	11.644814	5.800897	56.909215	C	37.894197	3.357333	57.465684
C	11.172847	6.908897	57.603238	C	37.399897	4.092041	56.371228
C	25.284002	7.084277	57.652106	C	36.020055	4.431542	56.330528
C	24.456142	6.309034	56.848148	C	35.516094	5.104873	55.198531
C	24.973656	5.254547	56.067206	C	36.367081	5.466694	54.158279
C	26.368036	4.985043	56.113150	C	37.728029	5.173489	54.214594
C	11.243748	3.934910	55.440216	C	38.257414	4.477394	55.310611
C	26.059501	3.244447	54.449560	O	38.564371	5.542433	53.166898
C	24.692620	3.467879	54.426566	O	33.364787	5.601808	57.229644
C	24.122554	4.472069	55.242425	O	32.888593	3.436223	57.651413
O	23.934998	2.646626	53.594364	C	33.723746	4.385126	57.434595
O	13.936271	6.440489	56.976653	C	31.165274	4.225383	53.319567
O	13.443169	4.274893	57.363942	C	32.009793	3.247074	52.827051
C	13.093367	5.479165	57.083849	C	32.003129	2.955464	51.443979
C	15.283043	5.695832	61.352095	C	31.162801	3.638307	50.592065
C	16.314084	6.385815	61.978046	C	30.267264	4.639802	51.067269
C	17.702771	6.845366	47.684728	C	30.248485	4.936314	52.477929
C	16.592742	6.476775	48.436319	C	29.270443	5.870961	52.945284
C	15.518106	5.778130	47.853931	C	28.344132	6.415146	52.091001
C	14.198078	5.242836	62.095148	C	28.369064	6.129788	50.700870
C	13.166036	4.552853	61.469196	C	29.371216	5.319835	50.165335
C	12.083071	4.099857	62.213249	O	27.397926	6.696479	49.942453
C	13.312878	4.756238	48.008229	O	31.436709	5.676614	55.187152
C	14.383050	5.420673	48.623229	O	31.010547	3.485438	55.573409
O	12.193381	4.415685	48.759400	C	31.209882	4.477117	54.777636
O	15.758860	6.386779	59.109924	C	27.200482	5.750794	56.974639

C	26.642934	6.809419	57.714526	C	53.073731	4.554370	56.431571
C	40.902938	6.954447	57.606487	C	51.700732	4.768395	56.388697
C	40.075327	6.133887	56.852058	C	51.114639	5.287425	55.239756
C	40.590629	5.034352	56.135736	C	51.901546	5.591429	54.133692
C	41.986683	4.764257	56.196417	C	53.273545	5.377401	54.178567
C	26.897825	3.983268	55.276002	C	53.859638	4.858374	55.326505
C	41.659914	2.901782	54.673973	O	53.987443	5.617408	52.967507
C	40.295515	3.139284	54.626113	O	48.987960	5.858456	57.298264
C	39.734531	4.209897	55.358421	O	48.670677	3.654117	57.664472
O	39.531592	2.264099	53.857419	C	49.436070	4.671924	57.495906
O	29.481692	6.434619	57.034138	C	46.938414	4.363080	53.310712
O	29.012817	4.253776	57.376923	C	47.732293	3.322578	52.794747
C	28.651117	5.461797	57.133941	C	47.767849	3.061326	51.432600
C	30.903117	5.695647	61.351272	C	47.008162	3.830452	50.559724
C	31.934172	6.385624	61.977208	C	46.183675	4.873678	51.030550
C	32.986267	6.653536	48.187589	C	46.135230	5.135406	52.426564
C	31.810846	6.258474	48.792817	C	45.261405	6.133211	52.902680
C	30.792820	5.572942	48.065779	C	44.495122	6.877712	52.014430
C	29.818163	5.242653	62.094343	C	44.557676	6.655358	50.648695
C	28.786110	4.552676	61.468408	C	45.407690	5.651831	50.130881
C	27.703155	4.099683	62.212479	O	43.780536	7.482386	49.840925
C	28.534281	4.701215	47.871810	O	47.115104	5.799088	55.210962
C	29.552246	5.185168	48.688796	O	46.804230	3.592149	55.558266
O	27.314305	4.469540	48.439339	C	46.953117	4.600454	54.779284
O	31.374750	6.377239	59.102033	C	42.826161	5.596124	56.990013
O	30.878467	4.209109	59.470545	C	42.263382	6.692391	57.671299
C	31.060757	5.410431	59.887298	C	42.506570	3.699724	55.434560
Cu	47.044737	6.248028	57.147671	O	45.068215	6.394153	57.019597
Cu	46.683019	3.792487	57.531295	O	44.735381	4.188993	57.351285
C	50.914824	4.464393	57.493762	C	44.295777	5.374496	57.120377
C	51.500917	3.947364	58.641701	C	46.523189	5.695410	61.350170
C	52.873917	3.732338	58.685576	C	47.554256	6.385382	61.976090
C	53.659825	4.036341	57.580511	C	48.701543	7.123757	47.771690

C	47.612192	6.664446	48.502683	H	22.116425	2.835979	28.240064
C	46.612606	5.874729	47.902384	H	24.511336	2.276571	28.286696
C	45.438246	5.242418	62.093259	H	25.997305	3.039206	26.506517
C	44.406178	4.552447	61.467340	H	21.501759	5.257050	24.071932
C	43.323236	4.099455	62.211428	H	22.995421	5.952262	22.306721
C	44.497118	4.673508	48.017142	H	19.532559	2.329838	22.589817
C	45.500631	5.418156	48.652396	H	19.679746	1.794368	20.190483
O	43.398068	4.238659	48.749105	H	18.480860	3.170986	18.536738
O	46.915979	6.443255	59.121699	H	16.654048	6.146427	22.827183
O	46.572658	4.238611	59.460841	H	15.507701	7.502086	21.163872
C	46.673421	5.443620	59.889965	H	14.495440	7.507876	27.087987
C	16.262157	6.620800	63.347051	H	27.554899	7.924087	26.980228
C	15.179191	6.168806	64.090104	H	26.078321	6.440723	25.733625
C	14.147152	5.478824	63.465153	H	14.941227	3.633089	24.313586
C	12.031146	4.336844	63.582254	H	29.112148	2.056633	23.142965
C	13.063186	5.025829	64.207206	H	19.762724	6.925998	30.330980
O	10.943182	3.908848	64.361307	H	15.678145	4.514880	29.273937
C	31.882272	6.620606	63.346214	H	13.770148	3.807475	30.575281
C	30.799319	6.168612	64.089285	H	15.672379	6.861994	17.596215
C	29.767263	5.478636	63.464349	H	25.121589	6.089291	21.478589
C	27.651256	4.336666	63.581485	H	25.594951	2.444635	22.920840
C	28.683310	5.025642	64.206420	H	37.722219	2.878521	28.306703
O	26.563304	3.908672	64.360557	H	40.106603	2.282707	28.376812
C	47.502383	6.620361	63.345099	H	41.599129	2.931379	26.558979
C	46.419440	6.168369	64.088187	H	37.142178	5.153356	24.057073
C	45.387372	5.478397	63.463268	H	38.644428	5.737771	22.254340
C	43.271361	4.336433	63.580436	H	35.147773	2.327072	22.590528
C	44.303429	5.025405	64.205357	H	35.298435	1.793452	20.190356
O	42.183423	3.908440	64.359527	H	34.100021	3.170534	18.536539
H	12.119161	8.126831	26.936091	H	32.268226	6.144807	22.826213
H	10.573006	6.786710	25.566637	H	31.125495	7.500495	21.163875
H	13.382328	2.322301	22.983028	H	29.961546	7.450302	27.134600
H	9.847423	3.169510	22.676405	H	43.106849	7.736693	27.026316

H	41.663999	6.241208	25.761433	H	20.415598	5.529239	39.680143
H	30.613412	3.489872	24.396038	H	22.047449	6.414371	38.139924
H	44.770340	1.877757	23.219412	H	18.103795	2.315452	37.895613
H	35.615613	6.787019	30.236143	H	18.090324	1.838195	35.483774
H	31.481698	4.300543	29.625489	H	16.894264	3.295223	33.940654
H	29.698422	3.640252	31.119699	H	15.252879	6.212546	38.396326
H	31.288763	6.859196	17.596527	H	14.038501	7.612551	36.829912
H	40.771544	5.802623	21.419791	H	13.169387	7.510054	42.646516
H	41.252922	2.240594	22.946556	H	26.508912	8.007469	43.047607
H	53.552137	3.699826	28.381271	H	24.974150	6.601872	41.769211
H	55.987719	3.325987	28.455683	H	13.611835	3.633431	39.869060
H	57.384051	3.866381	26.497950	H	27.933565	2.192343	38.997161
H	52.703583	5.454744	24.016451	H	18.639902	6.810532	45.764363
H	54.081457	5.977278	22.117122	H	19.561290	7.473970	32.719694
H	50.776969	2.334564	22.589419	H	17.636502	6.707689	34.008293
H	50.920580	1.795012	20.189812	H	14.441642	4.554044	44.825343
H	49.720365	3.170798	18.535983	H	12.520643	3.969539	46.170736
H	47.864296	6.135485	22.823720	H	12.737305	3.641950	32.608478
H	46.741603	7.497600	21.163657	H	14.005623	7.215987	33.307100
H	45.521588	7.316931	27.168792	H	24.232682	6.615986	37.495298
H	46.245677	3.331566	24.485050	H	24.541992	2.683432	38.633009
H	50.966621	7.203770	30.277570	H	36.440756	2.369466	43.891563
H	47.060949	4.477604	29.325650	H	38.902814	1.873138	43.890264
H	45.212211	3.680417	30.660286	H	40.360647	2.810569	42.161101
H	46.907584	6.858320	17.596187	H	35.733557	5.104882	39.990605
H	56.056786	5.973719	21.101979	H	37.153317	5.933011	38.175872
H	10.790872	8.127964	42.498587	H	33.528748	2.140162	38.548743
H	9.244520	6.787292	41.129779	H	33.675110	1.559615	36.109289
H	12.054201	2.324433	38.544124	H	32.840577	3.107504	34.414617
H	8.520615	3.174370	38.234517	H	31.482781	6.496222	38.660033
H	20.711600	2.655818	43.600768	H	30.566666	8.032017	36.946182
H	23.093970	2.080240	43.764537	H	28.966143	7.485383	43.112059
H	24.712550	3.040931	42.213516	H	41.802706	7.894121	42.648455

H 40.326829 6.368135 41.451046	H 7.917006 6.786887 56.693606
H 29.462994 3.546485 40.387672	H 10.726903 2.324683 54.106960
H 43.390145 2.090840 38.730947	H 7.192569 3.172857 53.799874
H 34.155785 6.669156 46.343742	H 19.568459 2.888113 59.177902
H 35.654617 7.353430 32.625742	H 21.966101 2.340270 59.131316
H 33.858844 6.616802 34.105582	H 23.394623 3.177946 57.340960
H 30.106123 4.503003 44.848970	H 18.828349 5.491088 55.139980
H 27.918753 4.059677 45.888675	H 20.268608 6.275605 53.369621
H 28.826345 3.587918 33.233781	H 16.857803 2.465300 53.483712
H 30.568520 7.510153 33.538904	H 16.908746 2.001315 51.072283
H 39.214353 6.119570 37.367691	H 15.764705 3.470281 49.505382
H 39.852438 2.393594 38.629246	H 14.069773 6.423320 53.919566
H 52.223426 3.706219 43.946354	H 12.929184 7.848140 52.322156
H 54.659178 3.327005 44.019474	H 11.840433 7.509792 58.211907
H 56.055346 3.866418 42.061264	H 24.867557 7.898884 58.235744
H 51.374881 5.455348 39.580372	H 23.403793 6.553155 56.828145
H 52.752615 5.976726 37.680284	H 12.284781 3.635338 55.429434
H 49.550566 2.603565 38.014027	H 26.473935 2.476881 53.809136
H 49.626859 2.109648 35.608166	H 17.168793 6.738849 61.411006
H 48.380498 3.476527 34.023659	H 18.516507 7.391607 48.150578
H 46.470483 6.339740 38.407780	H 16.573585 6.753477 49.481691
H 45.222359 7.656382 36.797539	H 13.133819 4.372040 60.400841
H 44.227248 7.507693 42.696574	H 11.278470 3.573158 61.719532
H 44.900646 3.565478 39.933278	H 11.506545 3.910918 48.219180
H 49.679858 7.157309 45.872301	H 12.966689 7.443227 48.799699
H 50.753283 7.788455 32.657653	H 22.376068 6.491997 52.509615
H 48.898486 6.920196 33.985587	H 22.954257 2.866122 53.612798
H 45.689853 4.579817 44.853417	H 35.069047 2.979880 59.286297
H 43.797166 3.841150 46.162444	H 37.454041 2.382757 59.330065
H 44.197855 3.512012 32.702166	H 38.936229 3.072324 57.517788
H 45.288422 7.217039 33.279836	H 34.462774 5.348166 55.093549
H 54.726535 5.966285 36.662888	H 35.956899 5.984050 53.301798
H 9.463421 8.127169 58.062817	H 32.683660 2.688540 53.485921

H	32.662046	2.174335	51.052267	H	44.382398	4.361986	60.399736
H	31.160858	3.389488	49.529351	H	42.519236	3.571622	61.717720
H	29.217086	6.141537	54.003980	H	42.760706	3.684768	48.196242
H	27.559603	7.082464	52.456878	H	43.832969	7.240881	48.866334
H	27.273574	7.413309	58.357666	H	53.398489	5.963910	52.224563
H	40.485949	7.801069	58.142059	H	17.068384	7.157736	63.836136
H	39.022819	6.376960	56.820647	H	15.148310	6.357045	65.155581
H	27.960635	3.766172	55.234408	H	10.262139	3.421942	63.798186
H	42.065723	2.080312	54.098699	H	32.688191	7.158119	63.835003
H	32.787148	6.739803	61.408511	H	30.768397	6.356730	65.154696
H	33.740033	7.197294	48.766209	H	25.880609	3.425393	63.796175
H	31.641311	6.493214	49.844630	H	48.307667	7.158864	63.833786
H	28.746629	4.376792	60.399763	H	46.387448	6.358028	65.153328
H	26.897814	3.574114	61.718588	H	41.497052	3.431033	63.794363
H	26.622549	4.212713	47.771687	H	54.922459	4.682604	55.325501
H	27.168040	6.049606	49.238248	H	56.250018	4.683007	39.763369
H	38.076766	6.058672	52.449771	H	57.578857	4.683485	24.200316
H	38.555645	2.506613	53.839447	H	32.654154	5.043609	18.026506
H	50.894658	3.699348	59.505914	H	17.034688	5.043879	18.026654
H	53.331500	3.325387	59.581284	H	10.176533	4.915018	24.089462
H	54.727811	3.865796	57.623315	H	8.847927	4.915211	39.653227
H	50.047827	5.461177	55.145837	H	7.520504	4.915235	55.216509
H	51.425187	5.978068	53.243281	H	12.998810	5.198730	65.269021
H	48.330827	2.713020	53.462707	H	28.618806	5.198511	65.268116
H	48.386015	2.256006	51.049442	H	44.238275	5.198802	65.266960
H	47.057698	3.589928	49.507460	H	48.273871	5.043411	18.026041
H	45.145558	6.347463	53.959057	C	22.884648	5.079798	47.466822
H	43.831227	7.646214	52.387594	C	24.373992	5.336293	47.525238
H	42.893978	7.346915	58.262893	C	25.124393	5.723395	46.314404
H	43.565845	3.472738	55.402002	C	24.442461	5.869382	44.966094
H	48.405407	6.744820	61.407784	C	22.906188	5.829465	45.052413
H	49.455169	7.740622	48.250464	C	22.405208	4.767559	46.040384
H	47.547810	6.944242	49.545495	O	25.198720	4.373272	46.834728

C	27.966528	7.051758	26.483030	O	36.044931	5.467760	26.187696
C	27.131058	6.198881	25.770703	O	35.545310	3.316565	26.649179
C	27.640691	5.069379	25.098257	C	36.391546	4.252560	26.418840
C	29.034707	4.800106	25.164982	C	33.846853	4.021969	22.293716
C	13.900000	3.935000	24.313000	C	34.612830	2.940966	21.873681
C	28.706723	2.892328	23.697696	C	34.701779	2.637975	20.519676
C	27.341572	3.120084	23.657666	C	34.024751	3.416985	19.587706
C	26.782975	4.211684	24.359730	C	33.259774	4.496987	20.007739
O	26.575122	2.219336	22.921445	C	33.170824	4.799980	21.361745
O	16.597542	6.403167	25.853699	C	32.403846	5.880983	21.783779
O	16.056233	4.263416	26.319556	C	31.727819	6.658993	20.849808
C	15.736620	5.461753	25.985866	C	31.817769	6.355001	19.496803
C	17.906535	5.817457	30.234791	C	32.583746	5.273997	19.075769
C	18.894319	6.582246	30.882075	O	31.143739	7.185012	18.538833
C	16.754362	5.404587	30.961996	O	34.121248	5.512664	24.152966
C	15.684120	4.729172	30.337285	O	33.631044	3.355331	24.584281
C	14.575875	4.326476	31.076435	C	33.856409	4.318205	23.763140
O	18.432915	6.401630	27.981558	C	29.876192	5.648583	25.938714
O	17.897799	4.256947	28.433372	C	29.325970	6.781763	26.564838
C	18.096348	5.470965	28.799269	C	43.535124	6.873148	26.527664
Cu	34.136340	6.025557	26.076638	C	42.719170	6.012265	25.805002
Cu	33.584103	3.625683	26.563096	C	43.249992	4.891207	25.134132
C	37.839027	3.904609	26.404577	C	44.647795	4.639954	25.211281
C	38.366726	3.176574	27.487106	C	29.553528	3.714115	24.430861
C	39.712958	2.837862	27.531449	C	44.351943	2.716544	23.759565
C	40.556548	3.211531	26.491775	C	42.985308	2.936168	23.696040
C	40.068152	3.918256	25.376636	C	42.408782	4.027859	24.383353
C	38.689289	4.257046	25.320054	O	42.235125	2.024284	22.956971
C	38.192527	4.905150	24.170223	O	32.167427	6.327119	25.985084
C	39.048338	5.238778	23.124636	O	31.681682	4.167563	26.415259
C	40.408854	4.947102	23.196246	C	31.327181	5.365772	26.123827
C	40.931314	4.279916	24.313002	C	33.759079	5.677045	30.328447
O	41.252643	5.294875	22.147178	C	34.805783	6.446233	30.872377

C	32.690464	5.263671	31.175960	O	49.725059	5.588715	24.095214
C	31.577149	4.558327	30.675386	O	49.386251	3.420849	24.607756
C	30.541268	4.182336	31.526875	C	49.523214	4.366323	23.751286
O	34.090500	6.300919	28.049397	C	45.474186	5.514003	25.971044
O	33.573240	4.150463	28.487974	C	44.898771	6.630681	26.605649
C	33.806104	5.354898	28.869558	C	45.184125	3.550902	24.496588
Cu	49.689524	6.197107	25.991956	O	47.709181	6.325062	25.895638
Cu	49.345031	3.777034	26.565009	O	47.393076	4.154907	26.421469
C	53.571003	4.464794	26.367934	C	46.944816	5.315309	26.100137
C	54.157057	3.947776	27.515897	C	49.192289	5.966345	30.228543
C	55.530059	3.732762	27.559821	C	50.131478	6.811527	30.847255
C	56.316002	4.036764	26.454782	C	48.080988	5.488972	30.979280
C	55.729945	4.554783	25.305818	C	47.057146	4.723133	30.382246
C	54.356946	4.768798	25.262894	C	45.983678	4.266659	31.140774
C	53.770889	5.287815	24.113932	O	49.600942	6.549949	27.950181
C	54.557833	5.591817	23.007892	O	49.296359	4.373113	28.459161
C	55.929833	5.377802	23.052816	C	49.382498	5.608814	28.795532
C	56.515888	4.858784	24.200779	C	11.158287	7.260976	41.959132
O	56.643769	5.617808	21.841779	C	10.287269	6.502982	41.186144
O	51.633385	5.833718	26.127071	C	10.757253	5.394981	40.491132
O	51.336466	3.655106	26.634966	C	12.099253	5.042976	40.571108
C	52.092183	4.663324	26.381411	C	11.698221	3.178982	39.103110
C	49.466778	4.021877	22.293151	C	10.356221	3.528988	39.024135
C	50.232744	2.940873	21.873099	C	9.886237	4.637987	39.718145
C	50.321667	2.637886	20.519091	O	9.453203	2.792994	38.218148
C	49.644624	3.416901	19.587136	Cu	17.245085	6.098385	41.492382
C	48.879658	4.496905	20.007187	Cu	16.667150	3.706620	41.989849
C	48.790735	4.799894	21.361195	C	20.944972	3.972125	41.896673
C	48.023770	5.880898	21.783247	C	21.407649	3.085296	42.888309
C	47.347728	6.658913	20.849290	C	22.754328	2.758965	42.987995
C	47.437652	6.354926	19.496283	C	23.669679	3.310201	42.099994
C	48.203617	5.273922	19.075230	C	23.254155	4.172473	41.069908
O	46.763610	7.184943	18.538326	C	21.873918	4.497463	40.950394

C	21.458848	5.297902	39.864979	O	15.282302	6.414295	41.363474
C	22.390998	5.800904	38.961987	O	14.761347	4.269972	41.822693
C	23.745809	5.516541	39.102247	C	14.424123	5.470809	41.513815
C	24.186042	4.694643	40.143863	C	16.726969	5.799000	45.717570
O	24.661690	6.017146	38.185687	C	17.767925	6.514968	46.337434
O	19.147757	5.535880	41.648179	C	18.785893	6.892377	32.231598
O	18.633566	3.386551	42.090092	C	17.686230	6.450742	32.958755
C	19.489967	4.319386	41.875476	C	16.658601	5.708038	32.346142
C	16.875190	4.090603	37.741706	C	15.575228	5.444499	46.474034
C	17.557336	2.972687	37.228497	C	14.469020	4.799763	45.881824
C	17.555080	2.700970	35.866920	C	13.355495	4.465475	46.646740
C	16.870760	3.538747	34.993475	C	14.502474	4.578578	32.443903
C	16.147303	4.653536	35.465337	C	15.531899	5.276872	33.089416
C	16.129877	4.921375	36.860230	O	13.390580	4.167269	33.170469
C	15.344429	5.989047	37.339480	O	17.167132	6.399745	43.455582
C	14.635533	6.792069	36.454732	O	16.641900	4.251549	43.902452
C	14.678214	6.567903	35.088711	C	16.857013	5.461687	44.273956
C	15.443023	5.499515	34.568530	Cu	33.047998	6.084993	41.931283
O	13.966285	7.454006	34.283440	Cu	32.381674	3.612985	42.411172
O	17.248955	5.560603	39.580399	C	36.544641	3.603770	42.144512
O	16.724205	3.411762	40.022621	C	37.087975	2.781561	43.112798
C	16.957302	4.369274	39.200736	C	38.474331	2.506853	43.107064
C	12.972270	5.800971	41.346095	C	39.290114	3.036451	42.130085
C	12.500287	6.908971	42.040107	C	38.767947	3.856012	41.075933
C	26.898567	7.141350	42.502684	C	37.354159	4.132397	41.085376
C	26.037884	6.342993	41.777227	C	36.802060	4.887515	40.012135
C	26.498828	5.206434	41.037822	C	37.599557	5.358695	38.997252
C	27.904814	4.899475	41.106659	C	39.002150	5.135962	39.005328
C	12.571237	3.934977	39.877096	C	39.590098	4.391143	40.026505
C	27.558724	3.032778	39.587413	O	39.775074	5.654126	38.009273
C	26.168549	3.319395	39.520461	O	34.819623	5.196304	42.146307
C	25.630760	4.385173	40.236655	O	34.260121	3.039280	42.441272
O	25.482123	2.458912	38.711539	C	35.097313	3.970241	42.249309

C	32.658095	4.063914	38.186426	C	31.015898	5.304437	46.671890
C	33.170722	2.839912	37.789651	C	29.959450	4.728542	45.907063
C	33.243598	2.516691	36.419071	C	28.738988	4.469711	46.486729
C	32.769484	3.396524	35.468135	C	30.578687	4.500034	32.882526
C	32.186960	4.655486	35.822978	C	31.657730	5.218809	33.406538
C	32.146442	4.996181	37.223831	O	29.530386	4.128537	33.714684
C	31.546174	6.232135	37.604040	O	32.889604	6.325550	43.903356
C	31.037155	7.087127	36.660445	O	32.441505	4.153375	44.307433
C	31.086805	6.767806	35.276479	C	32.558935	5.363626	44.655103
C	31.646470	5.567115	34.848112	Cu	48.399963	6.324745	41.575914
O	30.541058	7.736785	34.481586	Cu	48.001715	3.894445	42.066934
O	33.059222	5.514854	40.020807	C	52.242279	4.464604	41.931330
O	32.342580	3.421418	40.432436	C	52.828353	3.947581	43.079281
C	32.678560	4.362243	39.654165	C	54.201353	3.732560	43.123179
C	28.766738	5.741059	41.880317	C	54.987278	4.036564	42.018127
C	28.278824	6.852172	42.545004	C	54.401204	4.554586	40.869175
C	42.223441	7.041360	42.125442	C	53.028204	4.768608	40.826277
C	41.389577	6.166437	41.439642	C	52.442129	5.287631	39.677326
C	41.910865	5.063746	40.735265	C	53.229056	5.591635	38.571274
C	43.315336	4.835619	40.750223	C	54.601055	5.377613	38.616174
C	28.400753	3.792754	40.356422	C	55.187129	4.858591	39.764123
C	42.983441	2.918178	39.297690	O	55.314972	5.617620	37.405126
C	41.612569	3.113772	39.300313	O	50.339326	5.896497	41.713758
C	41.057024	4.192222	40.015993	O	49.984501	3.717532	42.180298
O	40.841419	2.198840	38.588718	C	50.767682	4.708589	41.950950
O	31.048269	6.363011	41.794218	C	48.219858	4.299005	37.816717
O	30.522586	4.247165	42.355583	C	48.981109	3.221428	37.328581
C	30.225066	5.431487	42.010244	C	49.030200	2.940692	35.970067
C	32.268409	5.685256	46.088216	C	48.317463	3.727647	35.072927
C	33.220777	6.366125	46.824212	C	47.519294	4.802189	35.516293
C	34.832375	6.770246	32.222753	C	47.454273	5.082432	36.908240
C	33.804891	6.348362	33.057919	C	46.601093	6.111001	37.356256
C	32.720662	5.605405	32.557819	C	45.871905	6.865883	36.445712

C	45.954276	6.626468	35.084083	O	8.125681	2.792943	53.781318
C	46.784247	5.593143	34.593892	Cu	15.892890	6.156931	57.133781
O	45.209814	7.460182	34.252527	Cu	15.354562	3.738961	57.538918
O	48.434345	5.795791	39.661285	C	19.612357	4.077974	57.370723
O	48.093042	3.609809	40.098026	C	20.183563	3.269651	58.370635
C	48.249781	4.584871	39.277821	C	21.537433	2.958080	58.348983
C	44.160779	5.711058	41.490206	C	22.345301	3.440280	57.325132
C	43.594071	6.819790	42.146904	C	21.813868	4.231842	56.289503
C	43.836285	3.762410	40.000752	C	20.426858	4.540137	56.296930
O	46.416419	6.498645	41.468814	C	19.886696	5.268244	55.215341
O	46.061147	4.312947	41.891795	C	20.707374	5.717143	54.185289
C	45.632747	5.492166	41.617052	C	22.075685	5.459473	54.201503
C	47.860173	5.987907	45.792034	C	22.640860	4.706920	55.240124
C	48.823842	6.791834	46.428842	O	22.883949	5.921392	53.168480
C	50.015894	7.142909	32.191606	O	17.799485	5.625033	57.289024
C	48.956292	6.643627	32.941364	O	17.324152	3.448734	57.644677
C	47.976101	5.819130	32.357029	C	18.160106	4.403823	57.450481
C	46.723110	5.546775	46.524817	C	15.656580	4.257637	53.307824
C	45.680748	4.820456	45.911089	C	16.340053	3.134709	52.805814
C	44.583339	4.397121	46.654863	C	16.372836	2.868688	51.444262
C	45.900839	4.551826	32.501312	C	15.718224	3.714018	50.557063
C	46.885613	5.333605	33.120765	C	14.999303	4.838229	51.012513
O	44.822887	4.087543	33.246758	C	14.955328	5.108544	52.407731
O	48.306387	6.613777	43.539335	C	14.182470	6.194410	52.866023
O	47.920887	4.434662	43.979731	C	13.513929	7.011917	51.962727
C	48.046485	5.657051	44.353235	C	13.575107	6.778099	50.598812
C	9.830847	7.260907	57.522288	C	14.320245	5.686794	50.098187
C	8.959814	6.502918	56.749313	O	12.897289	7.675007	49.775886
C	9.429781	5.394919	56.054289	O	15.944695	5.686290	55.201370
C	10.771781	5.042908	56.134240	O	15.445130	3.517185	55.563663
C	10.370715	3.178922	54.666242	C	15.682921	4.502892	54.776933
C	9.028715	3.528931	54.587292	C	11.644814	5.800897	56.909215
C	8.558748	4.637930	55.281316	C	11.172847	6.908897	57.603238

C	25.284002	7.084277	57.652106	C	36.020055	4.431542	56.330528
C	24.456142	6.309034	56.848148	C	35.516094	5.104873	55.198531
C	24.973656	5.254547	56.067206	C	36.367081	5.466694	54.158279
C	26.368036	4.985043	56.113150	C	37.728029	5.173489	54.214594
C	11.243748	3.934910	55.440216	C	38.257414	4.477394	55.310611
C	26.059501	3.244447	54.449560	O	38.564371	5.542433	53.166898
C	24.692620	3.467879	54.426566	O	33.364787	5.601808	57.229644
C	24.122554	4.472069	55.242425	O	32.888593	3.436223	57.651413
O	23.934998	2.646626	53.594364	C	33.723746	4.385126	57.434595
O	13.936271	6.440489	56.976653	C	31.165274	4.225383	53.319567
O	13.443169	4.274893	57.363942	C	32.009793	3.247074	52.827051
C	13.093367	5.479165	57.083849	C	32.003129	2.955464	51.443979
C	15.283043	5.695832	61.352095	C	31.162801	3.638307	50.592065
C	16.314084	6.385815	61.978046	C	30.267264	4.639802	51.067269
C	17.702771	6.845366	47.684728	C	30.248485	4.936314	52.477929
C	16.592742	6.476775	48.436319	C	29.270443	5.870961	52.945284
C	15.518106	5.778130	47.853931	C	28.344132	6.415146	52.091001
C	14.198078	5.242836	62.095148	C	28.369064	6.129788	50.700870
C	13.166036	4.552853	61.469196	C	29.371216	5.319835	50.165335
C	12.083071	4.099857	62.213249	O	27.397926	6.696479	49.942453
C	13.312878	4.756238	48.008229	O	31.436709	5.676614	55.187152
C	14.383050	5.420673	48.623229	O	31.010547	3.485438	55.573409
O	12.193381	4.415685	48.759400	C	31.209882	4.477117	54.777636
O	15.758860	6.386779	59.109924	C	27.200482	5.750794	56.974639
O	15.289653	4.210902	59.470132	C	26.642934	6.809419	57.714526
C	15.449276	5.414169	59.890231	C	40.902938	6.954447	57.606487
Cu	31.448113	6.143117	57.120058	C	40.075327	6.133887	56.852058
Cu	30.925566	3.725399	57.541177	C	40.590629	5.034352	56.135736
C	35.174971	4.050631	57.409732	C	41.986683	4.764257	56.196417
C	35.710114	3.298963	58.472338	C	26.897825	3.983268	55.276002
C	37.056582	2.959582	58.501298	C	41.659914	2.901782	54.673973
C	37.894197	3.357333	57.465684	C	40.295515	3.139284	54.626113
C	37.399897	4.092041	56.371228	C	39.734531	4.209897	55.358421

O	39.531592	2.264099	53.857419	C	49.436070	4.671924	57.495906
O	29.481692	6.434619	57.034138	C	46.938414	4.363080	53.310712
O	29.012817	4.253776	57.376923	C	47.732293	3.322578	52.794747
C	28.651117	5.461797	57.133941	C	47.767849	3.061326	51.432600
C	30.903117	5.695647	61.351272	C	47.008162	3.830452	50.559724
C	31.934172	6.385624	61.977208	C	46.183675	4.873678	51.030550
C	32.986267	6.653536	48.187589	C	46.135230	5.135406	52.426564
C	31.810846	6.258474	48.792817	C	45.261405	6.133211	52.902680
C	30.792820	5.572942	48.065779	C	44.495122	6.877712	52.014430
C	29.818163	5.242653	62.094343	C	44.557676	6.655358	50.648695
C	28.786110	4.552676	61.468408	C	45.407690	5.651831	50.130881
C	27.703155	4.099683	62.212479	O	43.780536	7.482386	49.840925
C	28.534281	4.701215	47.871810	O	47.115104	5.799088	55.210962
C	29.552246	5.185168	48.688796	O	46.804230	3.592149	55.558266
O	27.314305	4.469540	48.439339	C	46.953117	4.600454	54.779284
O	31.374750	6.377239	59.102033	C	42.826161	5.596124	56.990013
O	30.878467	4.209109	59.470545	C	42.263382	6.692391	57.671299
C	31.060757	5.410431	59.887298	C	42.506570	3.699724	55.434560
Cu	47.044737	6.248028	57.147671	O	45.068215	6.394153	57.019597
Cu	46.683019	3.792487	57.531295	O	44.735381	4.188993	57.351285
C	50.914824	4.464393	57.493762	C	44.295777	5.374496	57.120377
C	51.500917	3.947364	58.641701	C	46.523189	5.695410	61.350170
C	52.873917	3.732338	58.685576	C	47.554256	6.385382	61.976090
C	53.659825	4.036341	57.580511	C	48.701543	7.123757	47.771690
C	53.073731	4.554370	56.431571	C	47.612192	6.664446	48.502683
C	51.700732	4.768395	56.388697	C	46.612606	5.874729	47.902384
C	51.114639	5.287425	55.239756	C	45.438246	5.242418	62.093259
C	51.901546	5.591429	54.133692	C	44.406178	4.552447	61.467340
C	53.273545	5.377401	54.178567	C	43.323236	4.099455	62.211428
C	53.859638	4.858374	55.326505	C	44.497118	4.673508	48.017142
O	53.987443	5.617408	52.967507	C	45.500631	5.418156	48.652396
O	48.987960	5.858456	57.298264	O	43.398068	4.238659	48.749105
O	48.670677	3.654117	57.664472	O	46.915979	6.443255	59.121699

O	46.572658	4.238611	59.460841	H	15.507701	7.502086	21.163872
C	46.673421	5.443620	59.889965	H	14.495440	7.507876	27.087987
C	16.262157	6.620800	63.347051	H	27.554899	7.924087	26.980228
C	15.179191	6.168806	64.090104	H	26.078321	6.440723	25.733625
C	14.147152	5.478824	63.465153	H	14.941227	3.633089	24.313586
C	12.031146	4.336844	63.582254	H	29.112148	2.056633	23.142965
C	13.063186	5.025829	64.207206	H	19.762724	6.925998	30.330980
O	10.943182	3.908848	64.361307	H	15.678145	4.514880	29.273937
C	31.882272	6.620606	63.346214	H	13.770148	3.807475	30.575281
C	30.799319	6.168612	64.089285	H	15.672379	6.861994	17.596215
C	29.767263	5.478636	63.464349	H	25.121589	6.089291	21.478589
C	27.651256	4.336666	63.581485	H	25.594951	2.444635	22.920840
C	28.683310	5.025642	64.206420	H	37.722219	2.878521	28.306703
O	26.563304	3.908672	64.360557	H	40.106603	2.282707	28.376812
C	47.502383	6.620361	63.345099	H	41.599129	2.931379	26.558979
C	46.419440	6.168369	64.088187	H	37.142178	5.153356	24.057073
C	45.387372	5.478397	63.463268	H	38.644428	5.737771	22.254340
C	43.271361	4.336433	63.580436	H	35.147773	2.327072	22.590528
C	44.303429	5.025405	64.205357	H	35.298435	1.793452	20.190356
O	42.183423	3.908440	64.359527	H	34.100021	3.170534	18.536539
H	12.119161	8.126831	26.936091	H	32.268226	6.144807	22.826213
H	10.573006	6.786710	25.566637	H	31.125495	7.500495	21.163875
H	13.382328	2.322301	22.983028	H	29.961546	7.450302	27.134600
H	9.847423	3.169510	22.676405	H	43.106849	7.736693	27.026316
H	22.116425	2.835979	28.240064	H	41.663999	6.241208	25.761433
H	24.511336	2.276571	28.286696	H	30.613412	3.489872	24.396038
H	25.997305	3.039206	26.506517	H	44.770340	1.877757	23.219412
H	21.501759	5.257050	24.071932	H	35.615613	6.787019	30.236143
H	22.995421	5.952262	22.306721	H	31.481698	4.300543	29.625489
H	19.532559	2.329838	22.589817	H	29.698422	3.640252	31.119699
H	19.679746	1.794368	20.190483	H	31.288763	6.859196	17.596527
H	18.480860	3.170986	18.536738	H	40.771544	5.802623	21.419791
H	16.654048	6.146427	22.827183	H	41.252922	2.240594	22.946556

H	53.552137	3.699826	28.381271	H	24.974150	6.601872	41.769211
H	55.987719	3.325987	28.455683	H	13.611835	3.633431	39.869060
H	57.384051	3.866381	26.497950	H	27.933565	2.192343	38.997161
H	52.703583	5.454744	24.016451	H	18.639902	6.810532	45.764363
H	54.081457	5.977278	22.117122	H	19.561290	7.473970	32.719694
H	50.776969	2.334564	22.589419	H	17.636502	6.707689	34.008293
H	50.920580	1.795012	20.189812	H	14.441642	4.554044	44.825343
H	49.720365	3.170798	18.535983	H	12.520643	3.969539	46.170736
H	47.864296	6.135485	22.823720	H	12.737305	3.641950	32.608478
H	46.741603	7.497600	21.163657	H	14.005623	7.215987	33.307100
H	45.521588	7.316931	27.168792	H	24.232682	6.615986	37.495298
H	46.245677	3.331566	24.485050	H	24.541992	2.683432	38.633009
H	50.966621	7.203770	30.277570	H	36.440756	2.369466	43.891563
H	47.060949	4.477604	29.325650	H	38.902814	1.873138	43.890264
H	45.212211	3.680417	30.660286	H	40.360647	2.810569	42.161101
H	46.907584	6.858320	17.596187	H	35.733557	5.104882	39.990605
H	56.056786	5.973719	21.101979	H	37.153317	5.933011	38.175872
H	10.790872	8.127964	42.498587	H	33.528748	2.140162	38.548743
H	9.244520	6.787292	41.129779	H	33.675110	1.559615	36.109289
H	12.054201	2.324433	38.544124	H	32.840577	3.107504	34.414617
H	8.520615	3.174370	38.234517	H	31.482781	6.496222	38.660033
H	20.711600	2.655818	43.600768	H	30.566666	8.032017	36.946182
H	23.093970	2.080240	43.764537	H	28.966143	7.485383	43.112059
H	24.712550	3.040931	42.213516	H	41.802706	7.894121	42.648455
H	20.415598	5.529239	39.680143	H	40.326829	6.368135	41.451046
H	22.047449	6.414371	38.139924	H	29.462994	3.546485	40.387672
H	18.103795	2.315452	37.895613	H	43.390145	2.090840	38.730947
H	18.090324	1.838195	35.483774	H	34.155785	6.669156	46.343742
H	16.894264	3.295223	33.940654	H	35.654617	7.353430	32.625742
H	15.252879	6.212546	38.396326	H	33.858844	6.616802	34.105582
H	14.038501	7.612551	36.829912	H	30.106123	4.503003	44.848970
H	13.169387	7.510054	42.646516	H	27.918753	4.059677	45.888675
H	26.508912	8.007469	43.047607	H	28.826345	3.587918	33.233781

H	30.568520	7.510153	33.538904	H	16.908746	2.001315	51.072283
H	39.214353	6.119570	37.367691	H	15.764705	3.470281	49.505382
H	39.852438	2.393594	38.629246	H	14.069773	6.423320	53.919566
H	52.223426	3.706219	43.946354	H	12.929184	7.848140	52.322156
H	54.659178	3.327005	44.019474	H	11.840433	7.509792	58.211907
H	56.055346	3.866418	42.061264	H	24.867557	7.898884	58.235744
H	51.374881	5.455348	39.580372	H	23.403793	6.553155	56.828145
H	52.752615	5.976726	37.680284	H	12.284781	3.635338	55.429434
H	49.550566	2.603565	38.014027	H	26.473935	2.476881	53.809136
H	49.626859	2.109648	35.608166	H	17.168793	6.738849	61.411006
H	48.380498	3.476527	34.023659	H	18.516507	7.391607	48.150578
H	46.470483	6.339740	38.407780	H	16.573585	6.753477	49.481691
H	45.222359	7.656382	36.797539	H	13.133819	4.372040	60.400841
H	44.227248	7.507693	42.696574	H	11.278470	3.573158	61.719532
H	44.900646	3.565478	39.933278	H	11.506545	3.910918	48.219180
H	49.679858	7.157309	45.872301	H	12.966689	7.443227	48.799699
H	50.753283	7.788455	32.657653	H	22.376068	6.491997	52.509615
H	48.898486	6.920196	33.985587	H	22.954257	2.866122	53.612798
H	45.689853	4.579817	44.853417	H	35.069047	2.979880	59.286297
H	43.797166	3.841150	46.162444	H	37.454041	2.382757	59.330065
H	44.197855	3.512012	32.702166	H	38.936229	3.072324	57.517788
H	45.288422	7.217039	33.279836	H	34.462774	5.348166	55.093549
H	54.726535	5.966285	36.662888	H	35.956899	5.984050	53.301798
H	9.463421	8.127169	58.062817	H	32.683660	2.688540	53.485921
H	7.917006	6.786887	56.693606	H	32.662046	2.174335	51.052267
H	10.726903	2.324683	54.106960	H	31.160858	3.389488	49.529351
H	7.192569	3.172857	53.799874	H	29.217086	6.141537	54.003980
H	19.568459	2.888113	59.177902	H	27.559603	7.082464	52.456878
H	21.966101	2.340270	59.131316	H	27.273574	7.413309	58.357666
H	23.394623	3.177946	57.340960	H	40.485949	7.801069	58.142059
H	18.828349	5.491088	55.139980	H	39.022819	6.376960	56.820647
H	20.268608	6.275605	53.369621	H	27.960635	3.766172	55.234408
H	16.857803	2.465300	53.483712	H	42.065723	2.080312	54.098699

H	32.787148	6.739803	61.408511	H	30.768397	6.356730	65.154696
H	33.740033	7.197294	48.766209	H	25.880609	3.425393	63.796175
H	31.641311	6.493214	49.844630	H	48.307667	7.158864	63.833786
H	28.746629	4.376792	60.399763	H	46.387448	6.358028	65.153328
H	26.897814	3.574114	61.718588	H	41.497052	3.431033	63.794363
H	26.622549	4.212713	47.771687	H	54.922459	4.682604	55.325501
H	27.168040	6.049606	49.238248	H	56.250018	4.683007	39.763369
H	38.076766	6.058672	52.449771	H	57.578857	4.683485	24.200316
H	38.555645	2.506613	53.839447	H	32.654154	5.043609	18.026506
H	50.894658	3.699348	59.505914	H	17.034688	5.043879	18.026654
H	53.331500	3.325387	59.581284	H	10.176533	4.915018	24.089462
H	54.727811	3.865796	57.623315	H	8.847927	4.915211	39.653227
H	50.047827	5.461177	55.145837	H	7.520504	4.915235	55.216509
H	51.425187	5.978068	53.243281	H	12.998810	5.198730	65.269021
H	48.330827	2.713020	53.462707	H	28.618806	5.198511	65.268116
H	48.386015	2.256006	51.049442	H	44.238275	5.198802	65.266960
H	47.057698	3.589928	49.507460	H	48.273871	5.043411	18.026041
H	45.145558	6.347463	53.959057	C	22.884648	5.079798	47.466822
H	43.831227	7.646214	52.387594	C	24.373992	5.336293	47.525238
H	42.893978	7.346915	58.262893	C	25.124393	5.723395	46.314404
H	43.565845	3.472738	55.402002	C	24.442461	5.869382	44.966094
H	48.405407	6.744820	61.407784	C	22.906188	5.829465	45.052413
H	49.455169	7.740622	48.250464	C	22.405208	4.767559	46.040384
H	47.547810	6.944242	49.545495	O	25.198720	4.373272	46.834728
H	44.382398	4.361986	60.399736	C	35.147709	8.215033	41.949204
H	42.519236	3.571622	61.717720	C	36.145752	8.093221	40.976403
H	42.760706	3.684768	48.196242	C	37.490714	8.047994	41.353270
H	43.832969	7.240881	48.866334	C	37.850464	8.132277	42.701222
H	53.398489	5.963910	52.224563	C	36.848635	8.255131	43.672139
H	17.068384	7.157736	63.836136	C	35.502874	8.290157	43.303883
H	15.148310	6.357045	65.155581	N	33.768351	8.143981	41.583496
H	10.262139	3.421942	63.798186	H	24.775937	6.810597	44.498335
H	32.688191	7.158119	63.835003	H	24.775928	5.632773	48.506458

H	26.065951	6.276436	46.447166	C	22.529919	4.998496	24.166664
H	22.488496	5.655886	44.045469	C	23.370560	5.386960	23.128625
H	22.532286	6.818716	45.382481	C	24.737093	5.126566	23.184225
H	21.301858	4.713849	46.024293	C	25.280643	4.434689	24.275390
H	22.782958	3.773479	45.742822	O	25.565526	5.524592	22.140774
H	22.632265	4.256102	48.159851	O	20.437332	5.506397	26.195132
H	22.376088	5.985955	47.850195	O	19.909990	3.361518	26.655617
H	24.815807	5.060699	44.312664	C	20.768289	4.287470	26.421987
H	35.866713	7.997401	39.921989	C	18.226927	4.022014	22.293999
H	38.258906	7.928946	40.583192	C	18.992915	2.941012	21.873981
H	38.903450	8.090973	42.995692	C	19.081890	2.638017	20.519979
H	37.115941	8.309639	44.732474	C	18.404876	3.417024	19.587993
H	34.716072	8.332143	44.062994	C	17.639888	4.497025	20.008011
H	33.601167	8.357939	40.598905	C	17.550913	4.800019	21.362013
H	33.168358	8.730687	42.166662	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355032	19.497042
				C	16.963876	5.274031	19.076025
				O	15.523872	7.185038	18.539057
				O	18.566061	5.526425	24.115771
				O	18.021125	3.385519	24.574827
				C	18.264463	4.334421	23.747076
				C	14.301000	5.801000	25.782000
				C	13.829000	6.909000	26.476000
				C	27.923368	7.014460	26.470942
				C	27.093476	6.164458	25.748631
				C	27.610959	5.048070	25.060126
				C	29.007172	4.790068	25.119921
				C	13.900000	3.935000	24.313000
				C	28.692192	2.897509	23.630416
				C	27.324767	3.112799	23.597630
				C	26.758794	4.191593	24.313604
				O	26.563739	2.211177	22.856690
 (<i>R,R</i>)-1-RC (QM(B3LYP)/MM)							
C	12.487000	7.261000	26.395000				
C	11.616000	6.503000	25.622000				
C	12.086000	5.395000	24.927000				
C	13.428000	5.043000	25.007000				
C	13.027000	3.179000	23.539000				
C	11.685000	3.529000	23.460000				
C	11.215000	4.638000	24.154000				
O	10.782000	2.793000	22.654000				
Cu	18.546773	6.079553	26.021782				
Cu	17.948161	3.692683	26.531675				
C	22.213300	3.930369	26.377596				
C	22.759923	3.170687	27.427977				
C	24.113016	2.854892	27.450187				
C	24.943615	3.284687	26.420565				
C	24.434040	4.019629	25.333239				
C	23.048577	4.329986	25.296337				

O	16.598558	6.401421	25.856933	C	32.403849	5.880988	21.783783
O	16.054015	4.262157	26.321133	C	31.727822	6.658998	20.849812
C	15.736235	5.460870	25.987605	C	31.817772	6.355006	19.496807
C	17.909987	5.813879	30.236582	C	32.583750	5.274004	19.075773
C	18.901844	6.572025	30.885679	O	31.143744	7.185017	18.538837
C	16.752885	5.410865	30.960821	O	34.113758	5.509316	24.154401
C	15.679239	4.743737	30.333255	O	33.625040	3.349455	24.577023
C	14.565951	4.350157	31.069395	C	33.852825	4.315111	23.761099
O	18.436767	6.395910	27.983731	C	29.843336	5.634920	25.902837
O	17.896428	4.252443	28.435387	C	29.285306	6.754701	26.546093
C	18.098874	5.466034	28.801386	C	43.542082	6.891091	26.568458
Cu	34.102915	6.022291	26.077308	C	42.717685	6.028764	25.857041
Cu	33.551549	3.618548	26.550916	C	43.241285	4.909125	25.178389
C	37.810057	3.911674	26.435705	C	44.640190	4.658656	25.238942
C	38.332190	3.172666	27.513700	C	29.533639	3.718024	24.371325
C	39.679522	2.838281	27.565043	C	44.327750	2.732791	23.794035
C	40.529700	3.223963	26.535008	C	42.960634	2.953113	23.744737
C	40.047191	3.939142	25.422832	C	42.391983	4.046656	24.435756
C	38.668065	4.277660	25.361072	O	42.202246	2.041306	23.013889
C	38.178750	4.938357	24.215064	O	32.133577	6.317997	25.961401
C	39.040805	5.282746	23.178246	O	31.649349	4.155282	26.377524
C	40.400307	4.987959	23.253772	C	31.294421	5.354355	26.090073
C	40.916081	4.308497	24.366280	C	33.559518	5.674999	30.301712
O	41.249930	5.345580	22.212667	C	34.597535	6.370941	30.948156
O	36.011822	5.470538	26.212932	C	32.386040	5.336150	31.032573
O	35.514224	3.316519	26.662721	C	31.280714	4.717437	30.412230
C	36.360273	4.255529	26.442388	C	30.139188	4.413834	31.148949
C	33.846855	4.021974	22.293721	O	34.023399	6.296881	28.047806
C	34.612832	2.940971	21.873686	O	33.502329	4.142729	28.470580
C	34.701783	2.637980	20.519681	C	33.710248	5.350058	28.855584
C	34.024755	3.416991	19.587710	Cu	49.694877	6.206760	25.985362
C	33.259777	4.496993	20.007743	Cu	49.345408	3.788930	26.565607
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945

C	54.157059	3.947781	27.515908	C	49.206046	5.990064	30.220104
C	55.530060	3.732767	27.559832	C	50.151318	6.829250	30.837732
C	56.316003	4.036770	26.454793	C	48.092759	5.519089	30.970604
C	55.729947	4.554788	25.305829	C	47.064367	4.758642	30.373854
C	54.356948	4.768802	25.262905	C	45.990950	4.304455	31.133638
C	53.770890	5.287820	24.113942	O	49.610589	6.566950	27.940995
C	54.557834	5.591822	23.007903	O	49.302679	4.391963	28.456855
C	55.929834	5.377808	23.052827	C	49.392841	5.628529	28.788961
C	56.515890	4.858790	24.200790	C	11.158284	7.260965	41.959133
O	56.643771	5.617813	21.841791	C	10.287267	6.502972	41.186144
O	51.637482	5.837795	26.122160	C	10.757252	5.394972	40.491132
O	51.335480	3.660886	26.634835	C	12.099252	5.042967	40.571107
C	52.093272	4.666993	26.380510	C	11.698220	3.178974	39.103108
C	49.466780	4.021882	22.293161	C	10.356220	3.528979	39.024133
C	50.232747	2.940878	21.873109	C	9.886236	4.637978	39.718145
C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.240749	6.122556	41.483736
C	48.879663	4.496911	20.007197	Cu	16.677841	3.727727	41.986564
C	48.790739	4.799899	21.361205	C	20.946118	4.019015	41.878686
C	48.023773	5.880903	21.783256	C	21.455610	3.274302	42.958596
C	47.347732	6.658919	20.849300	C	22.806867	2.960943	43.037246
C	47.437657	6.354932	19.496292	C	23.675137	3.375824	42.033962
C	48.203622	5.273928	19.075240	C	23.207562	4.096469	40.919643
O	46.763615	7.184949	18.538336	C	21.824139	4.411835	40.828632
O	49.728122	5.591957	24.090965	C	21.351305	5.073096	39.675938
O	49.383984	3.426249	24.609313	C	22.232846	5.436798	38.661558
C	49.523885	4.369008	23.750430	C	23.593351	5.160148	38.765849
C	45.475703	5.534457	25.986745	C	24.090107	4.488069	39.887279
C	44.907286	6.651290	26.627454	O	24.457488	5.517886	37.738951
C	45.168336	3.568605	24.519841	O	19.146825	5.569485	41.624243
O	47.713651	6.339614	25.892213	O	18.644543	3.421256	42.094405
O	47.394306	4.171724	26.425086	C	19.493495	4.357470	41.867882
C	46.947340	5.332598	26.103879	C	16.880354	4.110050	37.735709

C	17.580761	3.005032	37.219334	C	14.485180	4.741533	45.884233
C	17.587339	2.740383	35.856347	C	13.393039	4.353722	46.654479
C	16.891312	3.570759	34.985041	C	14.491435	4.602204	32.436846
C	16.149915	4.672638	35.459740	C	15.524625	5.292550	33.085130
C	16.125726	4.934282	36.855673	O	13.375259	4.197851	33.160663
C	15.325501	5.989808	37.337355	O	17.163727	6.425079	43.449336
C	14.608187	6.787350	36.454426	O	16.642866	4.276728	43.897874
C	14.657315	6.570087	35.087547	C	16.849150	5.488698	44.268791
C	15.435616	5.512593	34.564717	Cu	32.921107	6.348855	41.577806
O	13.939426	7.453468	34.284417	Cu	32.432137	3.861543	42.072419
O	17.239702	5.583410	39.572739	C	36.637348	4.133332	41.757057
O	16.741512	3.429013	40.018444	C	37.159611	3.465031	42.850620
C	16.961057	4.388747	39.194982	C	38.532031	3.135090	42.889121
C	12.972269	5.800962	41.346096	C	39.364021	3.463756	41.840401
C	12.500284	6.908961	42.040108	C	38.873241	4.132365	40.672157
C	26.763498	7.109895	42.084413	C	37.466652	4.447451	40.629974
C	25.918459	6.264018	41.397284	C	36.943361	5.032041	39.443323
C	26.399705	5.091585	40.728479	C	37.756767	5.340274	38.381095
C	27.809292	4.801685	40.828598	C	39.156845	5.114888	38.448101
C	12.571236	3.934968	39.877095	C	39.718613	4.500057	39.567320
C	27.481765	2.844179	39.417766	O	39.945763	5.496597	37.406800
C	26.091608	3.114272	39.320348	O	34.852879	5.706943	41.553747
C	25.543472	4.216751	39.968775	O	34.380750	3.585073	42.129608
O	25.415589	2.197667	38.565440	C	35.181788	4.505824	41.805963
O	15.276764	6.426139	41.362847	C	32.490140	4.274905	37.856621
O	14.768883	4.276761	41.813962	C	33.128408	3.124011	37.423511
C	14.424786	5.476819	41.510084	C	33.129398	2.790674	36.054138
C	16.702656	5.829369	45.712460	C	32.474634	3.589375	35.140566
C	17.710096	6.594356	46.329660	C	31.765934	4.770742	35.536241
C	18.791816	6.885033	32.234473	C	31.777713	5.113606	36.936446
C	17.686795	6.452531	32.958906	C	31.033034	6.252786	37.360725
C	16.655764	5.716145	32.344337	C	30.320673	7.004319	36.462280
C	15.569353	5.425443	46.473620	C	30.325922	6.694042	35.076702

C	31.050389	5.604414	34.602998	Cu	48.429298	6.365056	41.555352
O	29.593147	7.569355	34.326022	Cu	47.998671	3.937920	42.037088
O	32.813349	5.783875	39.667556	C	52.242277	4.464616	41.931345
O	32.437432	3.611780	40.115233	C	52.828352	3.947593	43.079296
C	32.578246	4.587970	39.318957	C	54.201352	3.732573	43.123194
C	28.659847	5.696987	41.561249	C	54.987277	4.036578	42.018142
C	28.145336	6.839081	42.152576	C	54.401202	4.554601	40.869191
C	42.233103	7.134146	41.830827	C	53.028202	4.768621	40.826292
C	41.442834	6.281215	41.069673	C	52.442128	5.287645	39.677341
C	41.999268	5.173743	40.399672	C	53.229054	5.591649	38.571289
C	43.397793	4.935611	40.506162	C	54.601054	5.377629	38.616189
C	28.312063	3.653810	40.148556	C	55.187129	4.858606	39.764139
C	43.157495	3.056081	38.988419	O	55.314970	5.617636	37.405141
C	41.787442	3.246849	38.917872	O	50.359117	5.916996	41.721020
C	41.187378	4.310490	39.621937	O	49.977383	3.740395	42.178775
O	41.061800	2.334721	38.156417	C	50.772035	4.723441	41.954873
O	30.904846	6.439577	41.593718	C	48.277542	4.342268	37.795346
O	30.504971	4.263441	41.982083	C	49.059605	3.282199	37.302084
C	30.130939	5.447352	41.716414	C	49.110772	3.008231	35.942081
C	32.368628	5.846499	45.794108	C	48.377615	3.783107	35.050510
C	33.294818	6.666401	46.413754	C	47.559095	4.839785	35.500868
C	34.509422	6.694896	32.296193	C	47.494558	5.113922	36.893208
C	33.377647	6.341726	33.021800	C	46.626524	6.126500	37.349066
C	32.303660	5.665010	32.412962	C	45.882668	6.874058	36.445060
C	31.241040	5.334127	46.522206	C	45.963088	6.641015	35.082473
C	30.227714	4.543480	45.907370	C	46.805593	5.621052	34.585462
C	29.145170	4.092127	46.622683	O	45.207546	7.470711	34.256917
C	30.069414	4.705669	32.508486	O	48.488747	5.833785	39.642025
C	31.143483	5.331858	33.149899	O	48.119879	3.650513	40.071827
O	28.914663	4.415708	33.223921	C	48.298688	4.624447	39.255692
O	32.930336	6.469874	43.582021	C	44.195395	5.787375	41.322481
O	32.402215	4.322520	43.983005	C	43.594400	6.890731	41.956504
C	32.580535	5.522271	44.344108	C	43.964527	3.880187	39.765177

O	46.451860	6.560835	41.410438	C	19.909656	5.135651	55.250169
O	46.064905	4.378132	41.822689	C	20.745720	5.528135	54.209585
C	45.656508	5.560277	41.528826	C	22.109489	5.249806	54.248685
C	47.851956	6.023016	45.769465	C	22.655006	4.539064	55.326646
C	48.815163	6.829354	46.404377	O	22.933248	5.650052	53.202540
C	50.039256	7.160496	32.182282	O	17.799899	5.589030	57.304306
C	48.977045	6.667361	32.932237	O	17.307036	3.418255	57.673736
C	47.991647	5.848470	32.348089	C	18.150156	4.367660	57.486974
C	46.726241	5.565912	46.510202	C	15.678761	4.213606	53.319345
C	45.684655	4.834318	45.901481	C	16.394258	3.108806	52.822567
C	44.599993	4.392946	46.653182	C	16.443663	2.845062	51.460684
C	45.912717	4.587091	32.494747	C	15.771040	3.672498	50.569213
C	46.901215	5.365419	33.112520	C	15.018753	4.776361	51.020717
O	44.836564	4.123247	33.242934	C	14.961858	5.046074	52.415370
O	48.309621	6.653705	43.518374	C	14.162495	6.113507	52.870619
O	47.896850	4.477930	43.949005	C	13.475920	6.912962	51.965081
C	48.034468	5.697316	44.327945	C	13.547216	6.679692	50.601628
C	9.830844	7.260885	57.522289	C	14.320721	5.606639	50.104015
C	8.959813	6.502896	56.749314	O	12.850963	7.559840	49.776081
C	9.429780	5.394897	56.054290	O	15.954196	5.650858	55.205834
C	10.771780	5.042887	56.134240	O	15.443542	3.485594	55.577370
C	10.370715	3.178901	54.666241	C	15.692595	4.465495	54.786887
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.317853	7.032674	57.590409
Cu	15.897777	6.133874	57.134774	C	24.482520	6.213477	56.840382
Cu	15.343303	3.720885	57.551211	C	24.990666	5.110262	56.123773
C	19.599508	4.033023	57.444536	C	26.383820	4.835382	56.180407
C	20.149947	3.265359	58.487029	C	11.243748	3.934890	55.440215
C	21.501829	2.945525	58.499586	C	26.052826	2.984023	54.644683
C	22.326531	3.375898	57.465913	C	24.688132	3.217461	54.610541
C	21.813590	4.122677	56.387996	C	24.131576	4.283500	55.352860
C	20.430489	4.444592	56.365024	O	23.919605	2.343333	53.845011

O	13.941736	6.429914	56.971202	C	31.255437	4.095314	53.338565
O	13.436331	4.268786	57.367077	C	32.038201	3.032184	52.852469
C	13.093019	5.474151	57.083659	C	32.107323	2.760667	51.492434
C	15.283042	5.695809	61.352094	C	31.391998	3.541419	50.592000
C	16.314083	6.385792	61.978046	C	30.573361	4.600102	51.033075
C	17.637120	6.917442	47.678607	C	30.489942	4.872395	52.425582
C	16.551564	6.492709	48.435806	C	29.620327	5.887852	52.869673
C	15.505967	5.749737	47.855953	C	28.890696	6.636594	51.952373
C	14.198077	5.242813	62.095147	C	28.993772	6.406484	50.590418
C	13.166036	4.552830	61.469195	C	29.836811	5.383794	50.111703
C	12.083071	4.099834	62.213248	O	28.257320	7.237628	49.750629
C	13.347973	4.632559	48.018245	O	31.491296	5.573219	55.199074
C	14.391711	5.340575	48.629790	O	31.054364	3.398889	55.610508
O	12.250729	4.236256	48.774934	C	31.265465	4.372822	54.802048
O	15.761402	6.375983	59.108314	C	27.226231	5.653150	56.983207
O	15.278479	4.204490	59.477709	C	26.676626	6.757911	57.659587
C	15.447592	5.408274	59.892375	C	40.901177	6.943743	57.615258
Cu	31.473740	6.080527	57.125770	C	40.079357	6.118624	56.858928
Cu	30.966367	3.663736	57.582143	C	40.603423	5.027209	56.135814
C	35.214477	4.026628	57.452663	C	42.002106	4.773679	56.187990
C	35.763618	3.296627	58.523091	C	26.900925	3.775553	55.409054
C	37.113795	2.971051	58.547161	C	41.693082	2.920856	54.650249
C	37.939264	3.357208	57.497295	C	40.324876	3.135891	54.617242
C	37.429828	4.068619	56.394296	C	39.753945	4.194177	55.360117
C	36.047796	4.397990	56.360772	O	39.567779	2.250494	53.853292
C	35.530509	5.054748	55.224671	O	29.506308	6.349391	57.012207
C	36.368375	5.404956	54.170428	O	29.052508	4.176217	57.409349
C	37.730992	5.120005	54.218246	C	28.680440	5.375965	57.142666
C	38.274537	4.444216	55.319928	C	30.903116	5.695628	61.351271
O	38.555902	5.480687	53.158846	C	31.934171	6.385605	61.977208
O	33.391257	5.558835	57.261014	C	33.166576	6.973850	47.785386
O	32.932167	3.392716	57.695006	C	32.105252	6.485842	48.516133
C	33.760622	4.347773	57.478512	C	31.097629	5.658968	47.919812

C	29.818163	5.242633	62.094342	C	44.569637	6.642553	50.642964
C	28.786109	4.552656	61.468406	C	45.432800	5.649524	50.126110
C	27.703155	4.099663	62.212477	O	43.788164	7.464940	49.834349
C	29.011321	4.380278	48.005927	O	47.124391	5.806332	55.212025
C	29.970215	5.155504	48.655883	O	46.813366	3.598879	55.556263
O	27.940204	3.898325	48.695417	C	46.967591	4.607409	54.778777
O	31.377132	6.347620	59.098111	C	42.834437	5.606116	56.987190
O	30.910229	4.178225	59.500364	C	42.264036	6.693101	57.676762
C	31.072372	5.389283	59.896641	C	42.532561	3.724627	55.412140
Cu	47.051219	6.254007	57.149528	O	45.075724	6.405409	57.020809
Cu	46.686308	3.797923	57.529573	O	44.741056	4.199429	57.346979
C	50.914826	4.464382	57.493755	C	44.303100	5.386154	57.119709
C	51.500920	3.947352	58.641694	C	46.523192	5.695393	61.350166
C	52.873920	3.732327	58.685568	C	47.554258	6.385364	61.976087
C	53.659827	4.036331	57.580503	C	48.704708	7.147287	47.751645
C	53.073733	4.554362	56.431564	C	47.626242	6.673507	48.489228
C	51.700733	4.768387	56.388690	C	46.626349	5.882306	47.891601
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.523083	4.660782	48.017647
O	53.987443	5.617405	52.967501	C	45.523958	5.413115	48.648022
O	48.992167	5.860582	57.300821	O	43.435171	4.209768	48.756487
O	48.671994	3.656284	57.666437	O	46.920152	6.445583	59.123755
C	49.438007	4.673275	57.497434	O	46.572057	4.241054	59.459292
C	46.964360	4.371390	53.309688	C	46.674446	5.445197	59.890139
C	47.775932	3.343820	52.794890	C	16.262158	6.620778	63.347051
C	47.824143	3.089000	51.431623	C	15.179191	6.168782	64.090104
C	47.057947	3.850031	50.557018	C	14.147152	5.478800	63.465152
C	46.215710	4.879384	51.026858	C	12.031146	4.336820	63.582253
C	46.156617	5.135866	52.423382	C	13.063187	5.025805	64.207205
C	45.267710	6.120558	52.898397	O	10.943183	3.908824	64.361306
C	44.497040	6.858885	52.009033	C	31.882271	6.620587	63.346214

C	30.799317	6.168593	64.089284	H	15.672947	6.862243	17.596210
C	29.767262	5.478616	63.464348	H	25.068243	6.042231	21.431423
C	27.651255	4.336645	63.581483	H	25.580431	2.422010	22.869129
C	28.683309	5.025622	64.206418	H	37.682612	2.863059	28.324931
O	26.563304	3.908650	64.360554	H	40.068761	2.276627	28.408310
C	47.502385	6.620342	63.345096	H	41.572757	2.946600	26.607285
C	46.419443	6.168348	64.088184	H	37.129434	5.188308	24.097372
C	45.387375	5.478376	63.463264	H	38.642206	5.791312	22.311008
C	43.271365	4.336411	63.580432	H	35.147311	2.326586	22.590500
C	44.303433	5.025383	64.205353	H	35.298290	1.793349	20.190389
O	42.183428	3.908416	64.359522	H	34.100116	3.170555	18.536552
H	12.119120	8.126706	26.936267	H	32.267693	6.144918	22.826020
H	10.572991	6.786676	25.566765	H	31.126229	7.501053	21.163829
H	13.382274	2.321977	22.983502	H	29.916254	7.419609	27.125325
H	9.847369	3.169383	22.676819	H	43.119001	7.753339	27.073812
H	22.126909	2.835535	28.242093	H	41.661351	6.254868	25.829339
H	24.522952	2.277277	28.272509	H	30.595605	3.504317	24.332093
H	25.992382	3.024641	26.471936	H	44.739936	1.893144	23.250468
H	21.473139	5.218434	24.059527	H	35.485909	6.656280	30.395705
H	22.949062	5.900851	22.275450	H	31.274819	4.475071	29.354105
H	19.532426	2.329731	22.589838	H	29.300870	3.946719	30.649389
H	19.679872	1.794466	20.190467	H	31.287715	6.858288	17.596681
H	18.480924	3.171002	18.536740	H	40.773586	5.862970	21.488974
H	16.654530	6.146244	22.827305	H	41.218919	2.252830	23.021272
H	15.508366	7.502562	21.163861	H	53.552053	3.700251	28.381333
H	14.495393	7.507686	27.088242	H	55.987753	3.326311	28.455815
H	27.505331	7.876132	26.981392	H	57.384054	3.866433	26.498003
H	26.038700	6.398175	25.717356	H	52.703548	5.453423	24.015311
H	14.941350	3.633524	24.313418	H	54.081257	5.977706	22.117412
H	29.103619	2.072173	23.064740	H	50.777079	2.334871	22.589591
H	19.773800	6.909470	30.336407	H	50.920638	1.795061	20.189822
H	15.674510	4.529295	29.269867	H	49.720324	3.170750	18.536003
H	13.757514	3.837649	30.566037	H	47.863488	6.134936	22.823748

H 46.741948 7.497853 21.163692	H 13.998976 7.232010 33.305283
H 45.536264 7.338488 27.182524	H 23.994510 6.032055 37.003645
H 46.229838 3.349997 24.496268	H 24.478821 2.422172 38.453222
H 50.988490 7.216033 30.267398	H 36.505087 3.205729 43.686700
H 47.065023 4.514915 29.316801	H 38.937771 2.614819 43.762082
H 45.216442 3.721408 30.654145	H 40.422354 3.193584 41.907983
H 46.905310 6.856607 17.596437	H 35.877828 5.251861 39.369371
H 56.056534 5.972755 21.101719	H 37.326971 5.799705 37.484078
H 10.790905 8.127918 42.498655	H 33.637899 2.487551 38.151001
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H 8.521129 3.175680 38.233122	H 31.019675 6.526504 38.415817
H 20.793418 2.947804 43.752892	H 29.731015 7.864926 36.788440
H 23.185668 2.394528 43.882291	H 28.818755 7.517233 42.682355
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H 20.300059 5.302344 39.532993	H 40.388034 6.507507 40.991703
H 21.846358 5.939449 37.784994	H 29.373589 3.415731 40.206480
H 18.136414 2.353927 37.884802	H 43.599603 2.243766 38.426087
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H 16.921737 3.332209 33.931353	H 35.321856 7.225508 32.783134
H 15.229715 6.208320 38.394840	H 33.341389 6.618404 34.067891
H 14.000308 7.598842 36.831829	H 30.307327 4.286809 44.851772
H 13.169415 7.510814 42.645861	H 28.376649 3.490821 46.121585
H 26.360022 8.000573 42.576154	H 28.232307 3.916519 32.671526
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H 13.611882 3.633719 39.869022	H 39.421866 6.019330 36.776628
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H 18.565248 6.931474 45.754312	H 52.223689 3.708193 43.947076
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H 17.635545 6.711884 34.007754	H 56.055358 3.866492 42.061303
H 14.456273 4.507770 44.825369	H 51.374847 5.454265 39.580034
H 12.576461 3.826611 46.180183	H 52.752455 5.977694 37.680766
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H 45.223936 7.654237 36.802627	H 13.129813 4.375030 60.400673
H 44.193884 7.562774 42.560482	H 11.278537 3.573053 61.719504
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H 49.663631 7.205132 45.843357	H 12.944240 7.340240 48.799048
H 50.781548 7.800412 32.648369	H 22.436162 6.179586 52.501854
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H 45.683895 4.603234 44.841651	H 35.132103 2.984225 59.347317
H 43.815665 3.830894 46.164742	H 37.524089 2.413808 59.383145
H 44.208152 3.549928 32.699908	H 38.984491 3.083308 57.546703
H 45.290341 7.236983 33.282316	H 34.477597 5.297690 55.128101
H 54.726166 5.964390 36.662271	H 35.948624 5.909657 53.310924
H 9.463491 8.127327 58.062561	H 32.608670 2.418175 53.540433
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H 21.914682 2.360825 59.315282	H 27.312732 7.401467 58.257098
H 23.373702 3.108120 57.507485	H 40.477528 7.783557 58.156516
H 18.855113 5.372600 55.158232	H 39.024760 6.352069 56.831798
H 20.323193 6.059024 53.367351	H 27.960205 3.548696 55.371427
H 16.925390 2.453772 53.504193	H 42.107452 2.111883 54.063514
H 17.006722 1.993726 51.091900	H 32.789462 6.736463 61.409876
H 15.831143 3.431564 49.517426	H 33.915836 7.606989 48.270585
H 14.044740 6.341412 53.923868	H 32.036386 6.750010 49.576007
H 12.870334 7.735235 52.322211	H 28.749379 4.375496 60.399737
H 11.840824 7.509348 58.211819	H 26.898317 3.573349 61.718611
H 24.907173 7.883346 58.124734	H 27.382657 3.366442 48.104116
H 23.430875 6.460673 56.811326	H 28.372347 7.019269 48.772800
H 12.284899 3.635864 55.427859	H 38.061342 5.988869 52.440775
H 26.456885 2.168112 54.060324	H 38.586299 2.469192 53.855395

H	50.894934	3.699955	59.506278	H	17.034610	5.043821	18.026662
H	53.331535	3.325382	59.581268	H	10.176547	4.915072	24.089446
H	54.727793	3.865573	57.623256	H	8.847927	4.915173	39.653379
H	50.047717	5.460507	55.146286	H	7.520456	4.915050	55.216666
H	51.425072	5.978864	53.243679	H	12.998637	5.198788	65.268991
H	48.379273	2.740275	53.463931	H	28.618505	5.198767	65.268128
H	48.457699	2.295408	51.048854	H	44.238385	5.198699	65.266999
H	47.117599	3.614942	49.504061	H	48.274069	5.043586	18.026026
H	45.144285	6.329468	53.954930	C	33.296150	9.414126	42.638061
H	43.822357	7.618304	52.381330	C	33.734725	9.813469	41.282701
H	42.889759	7.347701	58.273372	C	32.943916	10.818819	40.462947
H	43.595165	3.515549	55.368780	C	31.860811	11.554159	41.275055
H	48.405468	6.745011	61.407907	C	31.105232	10.619788	42.230816
H	49.459606	7.763887	48.228859	C	32.057716	10.008139	43.269662
H	47.571264	6.941904	49.535567	O	33.069462	8.547633	41.517110
H	44.382340	4.363449	60.399525	C	36.687423	8.444696	39.218774
H	42.520044	3.570251	61.717943	C	37.838135	9.029240	38.649964
H	42.799651	3.651743	48.205783	C	37.882700	9.343987	37.289721
H	43.866725	7.244406	48.856535	C	36.784602	9.086167	36.459593
H	53.398211	5.961946	52.223871	C	35.636372	8.509466	37.018592
H	17.068429	7.157675	63.836093	C	35.580720	8.193482	38.377670
H	15.148291	6.357090	65.155566	N	36.626100	8.157747	40.579907
H	10.261750	3.422944	63.797744	H	33.648378	11.544878	40.018565
H	32.688664	7.157203	63.835293	H	34.795675	9.681383	41.035154
H	30.768269	6.356964	65.154712	H	34.052212	9.028529	43.334948
H	25.878604	3.428723	63.795722	H	31.157552	12.054450	40.585175
H	48.307414	7.159322	63.833715	H	32.336607	12.358520	41.870546
H	46.387847	6.357470	65.153444	H	30.303859	11.175056	42.750577
H	41.497144	3.431315	63.794112	H	30.615961	9.809989	41.659334
H	54.922516	4.682818	55.325530	H	32.388268	10.785391	43.987133
H	56.250054	4.683211	39.763397	H	31.552774	9.222802	43.860807
H	57.578864	4.683551	24.200319	H	32.487654	10.274587	39.615393
H	32.654273	5.043692	18.026504	H	38.709185	9.227133	39.284251

H	38.791733	9.794795	36.875892	C	18.992915	2.941012	21.873981
H	36.820794	9.337496	35.395476	C	19.081890	2.638017	20.519979
H	34.765796	8.294648	36.389067	C	18.404876	3.417023	19.587993
H	34.680081	7.728104	38.790840	C	17.639888	4.497024	20.008011
H	35.999258	7.398839	40.858421	C	17.550913	4.800019	21.362013
H	37.525645	8.091438	41.049723	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
				C	16.963875	5.274030	19.076025
				O	15.523872	7.185037	18.539057
				O	18.566764	5.537286	24.110694
				O	18.036393	3.394413	24.576951
				C	18.271107	4.341673	23.745942
				C	14.301000	5.801000	25.782000
				C	13.829000	6.909000	26.476000
				C	28.051766	7.316336	26.371830
				C	27.201300	6.424477	25.727011
				C	27.698234	5.262465	25.103148
				C	29.094117	4.997753	25.154882
				C	13.900000	3.935000	24.313000
				C	28.737429	3.010229	23.804732
				C	27.371765	3.236490	23.778964
				C	26.826562	4.366181	24.429243
				O	26.591709	2.300265	23.103594
				O	16.595277	6.407599	25.850543
				O	16.064202	4.266355	26.320377
				C	15.738375	5.463420	25.985119
				C	17.926888	5.822569	30.240392
				C	18.905989	6.608549	30.875739
				C	16.799549	5.374795	30.986684
				C	15.734401	4.677881	30.377141
				C	14.651498	4.240953	31.134132
				O	18.429867	6.416975	27.981029

(*R,R*)-1-TS1(QM(B3LYP)/MM)

C	12.487000	7.261000	26.395000
C	11.616000	6.503000	25.622000
C	12.086000	5.395000	24.927000
C	13.428000	5.043000	25.007000
C	13.027000	3.179000	23.539000
C	11.685000	3.529000	23.460000
C	11.215000	4.638000	24.154000
O	10.782000	2.793000	22.654000
Cu	18.543718	6.099330	26.016739
Cu	17.966260	3.708964	26.530400
C	22.238265	3.999922	26.393549
C	22.775082	3.220760	27.434817
C	24.134118	2.934409	27.484596
C	24.982389	3.412966	26.491520
C	24.485629	4.166804	25.411935
C	23.094424	4.450197	25.347346
C	22.592748	5.141013	24.223458
C	23.452864	5.577632	23.220706
C	24.821933	5.337368	23.302038
C	25.350259	4.622456	24.385501
O	25.668060	5.774838	22.288833
O	20.439316	5.548175	26.192323
O	19.935546	3.397880	26.650487
C	20.785075	4.334156	26.420297
C	18.226927	4.022014	22.293999

O	17.914143	4.268129	28.433208	C	29.414002	7.052540	26.437834
C	18.105305	5.482771	28.800326	C	43.533930	6.863584	26.448658
Cu	34.226489	6.214181	25.943853	C	42.730970	6.003734	25.711114
Cu	33.636730	3.857715	26.582603	C	43.270450	4.874715	25.059941
C	37.890896	4.045547	26.364343	C	44.665580	4.620698	25.164408
C	38.417578	3.362387	27.476284	C	29.598449	3.872214	24.472131
C	39.755444	2.992710	27.519143	C	44.392586	2.692166	23.714771
C	40.591638	3.292336	26.450155	C	43.027114	2.911206	23.629026
C	40.103909	3.955261	25.307678	C	42.440199	4.006363	24.302264
C	38.732011	4.319632	25.250539	O	42.288505	1.993333	22.885886
C	38.232699	4.915285	24.073545	O	32.256651	6.539077	25.846029
C	39.081317	5.177702	23.002151	O	31.743301	4.417357	26.410058
C	40.438090	4.870264	23.075991	C	31.403051	5.600252	26.049733
C	40.962324	4.252951	24.220410	C	33.820412	6.173186	30.185976
O	41.276295	5.152850	22.003208	C	34.935044	6.820401	30.750592
O	36.125708	5.630691	26.078152	C	32.635520	6.024346	30.957439
O	35.591769	3.521983	26.677679	C	31.471742	5.441164	30.416898
C	36.451893	4.424949	26.378737	C	30.315906	5.337774	31.185681
C	33.846854	4.021972	22.293718	O	34.201641	6.621528	27.885793
C	34.612831	2.940969	21.873683	O	33.640301	4.514935	28.469055
C	34.701781	2.637978	20.519678	C	33.896827	5.739348	28.764364
C	34.024753	3.416989	19.587708	Cu	49.687477	6.188798	25.996235
C	33.259776	4.496991	20.007741	Cu	49.347628	3.765038	26.557890
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.192589	5.580956	24.066141	C	53.770890	5.287813	24.113936
O	33.668066	3.459842	24.621499	C	54.557834	5.591815	23.007897
C	33.899942	4.373314	23.747185	C	55.929834	5.377800	23.052821
C	29.951926	5.886818	25.863114	C	56.515889	4.858782	24.200784

O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.631437	5.830409	26.133752	C	10.757253	5.394976	40.491133
O	51.338954	3.648180	26.629277	C	12.099253	5.042971	40.571108
C	52.092358	4.659671	26.381404	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.245094	6.021688	41.553494
C	48.879661	4.496905	20.007192	Cu	16.609955	3.644815	42.059434
C	48.790737	4.799893	21.361200	C	20.878339	3.828750	42.075959
C	48.023772	5.880897	21.783251	C	21.363513	3.199044	43.236546
C	47.347731	6.658913	20.849295	C	22.714066	2.901392	43.374577
C	47.437655	6.354926	19.496287	C	23.603215	3.220636	42.353708
C	48.203620	5.273922	19.075235	C	23.155434	3.817370	41.161027
O	46.763613	7.184943	18.538331	C	21.773354	4.107246	41.007563
O	49.727166	5.586517	24.097154	C	21.318670	4.642896	39.785383
O	49.390596	3.416388	24.602751	C	22.216979	4.897310	38.752802
C	49.525222	4.364825	23.750028	C	23.578824	4.655084	38.917236
C	45.478532	5.495167	25.937949	C	24.058870	4.125214	40.119671
C	44.893868	6.615147	26.558097	O	24.464540	4.925802	37.882105
C	45.213002	3.528833	24.462247	O	19.131323	5.413198	41.732834
O	47.709352	6.312616	25.892647	O	18.561391	3.284276	42.218668
O	47.395337	4.140289	26.411213	C	19.438178	4.197243	42.009151
C	46.946866	5.299995	26.087140	C	16.900247	4.007559	37.807435
C	49.155702	5.928958	30.228352	C	17.584338	2.887515	37.302028
C	50.068413	6.790414	30.863813	C	17.609319	2.624524	35.938578
C	48.053361	5.411468	30.966090	C	16.947399	3.471029	35.055711
C	47.049256	4.632541	30.351700	C	16.220761	4.587006	35.518847
C	45.989170	4.129569	31.099338	C	16.180853	4.850006	36.914595
O	49.589254	6.532046	27.957209	C	15.399413	5.925604	37.383084
O	49.294417	4.350669	28.451940	C	14.715021	6.739048	36.488790
C	49.368064	5.584752	28.795374	C	14.775515	6.515841	35.123496
C	11.158286	7.260970	41.959133	C	15.534836	5.438891	34.613131

O	14.082180	7.408381	34.308921	Cu	32.502092	4.874308	42.072855
O	17.264110	5.474973	39.646306	C	36.583430	3.948594	41.642145
O	16.707912	3.334963	40.091662	C	37.006740	3.459875	42.864597
C	16.963702	4.286317	39.268078	C	38.338360	3.009292	43.026363
C	12.972270	5.800966	41.346096	C	39.234943	3.069626	41.980651
C	12.500286	6.908965	42.040108	C	38.839997	3.535932	40.684414
C	26.329117	7.240881	42.070190	C	37.466207	3.928286	40.511988
C	25.613348	6.219266	41.484184	C	37.019736	4.267817	39.203902
C	26.250231	5.046304	40.962636	C	37.886141	4.281505	38.138044
C	27.682991	4.949148	41.104667	C	39.269286	4.021018	38.324184
C	12.571237	3.934972	39.877096	C	39.751246	3.642956	39.576776
C	27.617930	2.791329	39.975915	O	40.121543	4.137166	37.267123
C	26.209344	2.884329	39.818785	O	35.179999	5.761019	41.018175
C	25.522153	3.991372	40.303021	O	34.260047	4.040461	42.113025
O	25.660629	1.810432	39.176863	C	35.241821	4.638409	41.560028
O	15.291238	6.378762	41.397069	C	32.549386	5.594160	37.890523
O	14.724043	4.243528	41.845810	C	33.149550	4.391491	37.544332
C	14.414625	5.450513	41.534136	C	33.218055	3.987550	36.197537
C	16.622105	5.769222	45.770906	C	32.654632	4.765868	35.209289
C	17.638811	6.513657	46.397708	C	32.000599	6.006628	35.501046
C	18.815026	6.905639	32.229727	C	31.964637	6.432311	36.880888
C	17.741850	6.429203	32.974365	C	31.297861	7.654216	37.189225
C	16.722153	5.665707	32.375202	C	30.707607	8.406057	36.206029
C	15.468357	5.397632	46.517296	C	30.740765	7.997999	34.846060
C	14.375014	4.739376	45.915757	C	31.380518	6.817222	34.481932
C	13.264619	4.379308	46.673561	O	30.114255	8.873577	34.005384
C	14.596438	4.483253	32.504287	O	32.598392	7.106875	39.754814
C	15.619025	5.204261	33.135371	O	32.392140	4.893762	40.114107
O	13.507834	4.040908	33.247744	C	32.503431	5.903464	39.363338
O	17.140657	6.336314	43.514619	C	28.401823	6.039243	41.703486
O	16.548465	4.206857	43.965705	C	27.732146	7.164806	42.158707
C	16.783248	5.414761	44.333010	C	42.133679	6.701880	41.404793
Cu	32.319496	7.727795	41.643145	C	41.385200	5.698553	40.803108

C	41.984702	4.499621	40.368481	C	53.229054	5.591652	38.571278
C	43.387801	4.329651	40.537785	C	54.601054	5.377632	38.616177
C	28.332010	3.787837	40.591322	C	55.187129	4.858609	39.764128
C	43.222422	2.184726	39.405996	O	55.314970	5.617639	37.405129
C	41.849865	2.314125	39.289717	O	50.293010	5.833688	41.694444
C	41.212347	3.480847	39.753727	O	50.014143	3.644762	42.166568
O	41.160379	1.247666	38.719142	C	50.761936	4.662488	41.938979
O	30.450690	7.180046	41.609680	C	48.250601	4.118364	37.774528
O	30.519041	5.009155	42.145040	C	49.048186	3.075882	37.270076
C	29.896464	6.061432	41.824747	C	49.099416	2.815044	35.907120
C	32.148840	6.794541	45.824974	C	48.353670	3.587880	35.023581
C	32.806712	7.821011	46.478320	C	47.517277	4.625006	35.485354
C	34.903203	7.288319	32.057932	C	47.447089	4.880904	36.880877
C	33.751555	7.135497	32.821027	C	46.554575	5.867393	37.348024
C	32.605700	6.511746	32.292617	C	45.794252	6.609057	36.452664
C	31.232444	5.943929	46.534019	C	45.883965	6.397540	35.087283
C	30.468387	4.931011	45.885055	C	46.751486	5.404831	34.578378
C	29.568720	4.161427	46.583166	O	45.108104	7.218441	34.271580
C	30.290168	5.795841	32.500786	O	48.441192	5.624960	39.605782
C	31.428125	6.383532	33.064584	O	48.153492	3.435219	40.063203
O	29.123354	5.700083	33.248116	C	48.287516	4.406860	39.234019
O	32.453273	7.639846	43.634599	C	44.145241	5.344922	41.196845
O	32.600348	5.418255	43.959143	C	43.496283	6.527384	41.601539
C	32.415485	6.601818	44.358735	C	43.994741	3.173900	40.004153
Cu	48.340218	6.177371	41.506314	O	46.353910	6.257774	41.330374
Cu	48.031193	3.741837	42.030633	O	46.081505	4.076600	41.821633
C	52.242278	4.464620	41.931334	C	45.612506	5.216747	41.464688
C	52.828353	3.947597	43.079285	C	47.786322	5.884563	45.727150
C	54.201353	3.732577	43.123183	C	48.710850	6.755393	46.333952
C	54.987278	4.036581	42.018131	C	49.938091	7.097268	32.212747
C	54.401203	4.554604	40.869180	C	48.891423	6.554492	32.950614
C	53.028203	4.768624	40.826281	C	47.937200	5.711850	32.349220
C	52.442128	5.287648	39.677330	C	46.689462	5.391396	46.487596

C	45.683955	4.590675	45.906512	C	16.334804	3.096251	52.812607
C	44.624040	4.120833	46.676714	C	16.349246	2.827250	51.451108
C	45.899720	4.381168	32.465674	C	15.653783	3.651261	50.574256
C	46.861427	5.178132	33.101471	C	14.913652	4.757433	51.040478
O	44.835508	3.870644	33.200652	C	14.887640	5.028893	52.435345
O	48.189421	6.493700	43.461765	C	14.094747	6.094009	52.907334
O	47.908430	4.306061	43.935989	C	13.384827	6.889687	52.016529
C	47.975086	5.538772	44.291000	C	13.429455	6.657541	50.651667
C	9.830848	7.260896	57.522290	C	14.198545	5.588871	50.137902
C	8.959816	6.502907	56.749315	O	12.714528	7.536467	49.841059
C	9.429783	5.394908	56.054291	O	15.942185	5.637769	55.203660
C	10.771783	5.042898	56.134241	O	15.429270	3.474180	55.583015
C	10.370718	3.178911	54.666243	C	15.670990	4.452973	54.789258
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.331566	7.059548	57.499123
Cu	15.898099	6.124595	57.131801	C	24.494219	6.215463	56.780260
Cu	15.338396	3.714002	57.555355	C	25.000150	5.088992	56.099932
C	19.597681	4.015577	57.442983	C	26.394229	4.815871	56.161189
C	20.144592	3.255730	58.493042	C	11.243751	3.934900	55.440217
C	21.495982	2.933511	58.511508	C	26.055812	2.916854	54.685572
C	22.324374	3.354069	57.476652	C	24.690987	3.149648	54.649035
C	21.815511	4.092062	56.391107	C	24.137453	4.238665	55.359033
C	20.432639	4.416753	56.362255	O	23.919431	2.254543	53.911359
C	19.916048	5.099468	55.240626	O	13.942528	6.425726	56.973989
C	20.755035	5.477700	54.196832	O	13.432406	4.266345	57.373584
C	22.118033	5.194933	54.240448	C	13.091876	5.471803	57.087181
C	22.660418	4.495713	55.327431	C	15.283046	5.695821	61.352095
O	22.944237	5.579470	53.190399	C	16.314087	6.385804	61.978046
O	17.800415	5.575036	57.293790	C	17.553380	6.848847	47.742581
O	17.302572	3.407207	57.673164	C	16.448292	6.453117	48.486768
C	18.148211	4.353662	57.481276	C	15.395272	5.727845	47.897366
C	15.629344	4.200964	53.323187	C	14.198081	5.242825	62.095148

C	13.166040	4.552842	61.469196	C	29.906118	5.462946	50.119614
C	12.083075	4.099846	62.213249	O	28.185934	7.190356	49.781554
C	13.212428	4.657044	48.037379	O	31.527229	5.625025	55.206241
C	14.266057	5.339897	48.660434	O	31.105451	3.442222	55.591459
O	12.098501	4.286124	48.782349	C	31.322367	4.426013	54.796379
O	15.768142	6.370167	59.106458	C	27.239356	5.659129	56.936552
O	15.278586	4.201100	59.480606	C	26.689985	6.786219	57.575696
C	15.449934	5.405264	59.892696	C	40.904290	6.945442	57.547925
Cu	31.486357	6.114262	57.132594	C	40.083744	6.109878	56.802533
Cu	30.988223	3.690875	57.564854	C	40.606059	4.998647	56.108932
C	35.231531	4.071836	57.472571	C	42.002880	4.737742	56.176856
C	35.782704	3.366829	58.558246	C	26.907800	3.732889	55.419864
C	37.129823	3.029314	58.579880	C	41.692482	2.856136	54.674377
C	37.949441	3.378258	57.512572	C	40.325677	3.078404	54.627782
C	37.437406	4.065482	56.395353	C	39.756135	4.153793	55.346627
C	36.058680	4.408040	56.365207	O	39.568501	2.182820	53.876075
C	35.537813	5.042122	55.218097	O	29.516725	6.369165	57.000119
C	36.368966	5.352320	54.145929	O	29.072898	4.190282	57.372776
C	37.729054	5.053647	54.188739	C	28.695127	5.388831	57.109645
C	38.276506	4.404548	55.304530	C	30.903120	5.695641	61.351269
O	38.547526	5.374799	53.111804	C	31.934175	6.385618	61.977205
O	33.406602	5.601870	57.279276	C	32.633054	8.006870	47.867293
O	32.952618	3.431365	57.698677	C	31.780665	7.192461	48.580918
C	33.778342	4.390774	57.493226	C	31.032577	6.146318	47.947532
C	31.344016	4.169939	53.331972	C	29.818167	5.242646	62.094340
C	32.206878	3.177318	52.834097	C	28.786113	4.552669	61.468405
C	32.330138	2.962220	51.467448	C	27.703159	4.099675	62.212476
C	31.586777	3.726761	50.574587	C	29.380984	4.338625	47.978662
C	30.678409	4.702937	51.030108	C	30.101039	5.316334	48.661418
C	30.547536	4.922826	52.427433	O	28.490570	3.552975	48.646681
C	29.609761	5.869484	52.884995	O	31.372729	6.365207	59.104455
C	28.843039	6.591068	51.976937	O	30.908164	4.191734	59.487329
C	28.979769	6.403698	50.611549	C	31.068563	5.399806	59.894159

Cu	47.047012	6.240783	57.142256	O	45.072486	6.385149	57.009322
Cu	46.688604	3.785857	57.534565	O	44.742063	4.180381	57.346706
C	50.914829	4.464394	57.493750	C	44.302079	5.364351	57.109038
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.591518	7.104644	47.672517
C	53.073736	4.554373	56.431559	C	47.542261	6.597995	48.429727
C	51.700736	4.768398	56.388685	C	46.580127	5.742128	47.860280
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.538668	4.426186	48.033157
O	53.987445	5.617415	52.967495	C	45.505252	5.242723	48.636170
O	48.988622	5.854618	57.295805	O	43.476456	3.946300	48.790846
O	48.674513	3.651360	57.672758	O	46.915121	6.440480	59.117990
C	49.437655	4.669504	57.497448	O	46.572589	4.236649	59.462374
C	46.981985	4.331210	53.313195	C	46.673465	5.442307	59.889194
C	47.813233	3.310774	52.815919	C	16.262162	6.620790	63.347051
C	47.865553	3.032010	51.457687	C	15.179196	6.168795	64.090104
C	47.082247	3.760008	50.570602	C	14.147156	5.478812	63.465153
C	46.219580	4.780222	51.022665	C	12.031150	4.336833	63.582254
C	46.161042	5.065801	52.413892	C	13.063191	5.025817	64.207206
C	45.259350	6.047195	52.870903	O	10.943187	3.908837	64.361307
C	44.468684	6.748614	51.968688	C	31.882275	6.620600	63.346211
C	44.533533	6.497233	50.607852	C	30.799322	6.168606	64.089282
C	45.414534	5.510975	50.109177	C	29.767267	5.478629	63.464346
O	43.725142	7.277912	49.784680	C	27.651260	4.336658	63.581482
O	47.122431	5.784093	55.205363	C	28.683314	5.025635	64.206417
O	46.819056	3.577624	55.563407	O	26.563309	3.908663	64.360554
C	46.972915	4.581372	54.779769	C	47.502389	6.620356	63.345091
C	42.834008	5.582175	56.965362	C	46.419447	6.168363	64.088179
C	42.264275	6.686535	57.627452	C	45.387379	5.478391	63.463260
C	42.531978	3.669869	55.425949	C	43.271369	4.336426	63.580429

C	44.303437	5.025398	64.205349	H	35.300076	1.794681	20.190221
O	42.183431	3.908432	64.359519	H	34.100323	3.170786	18.536506
H	12.119162	8.126838	26.936090	H	32.260926	6.142272	22.825877
H	10.573005	6.786705	25.566697	H	31.124213	7.499586	21.163979
H	13.382328	2.322275	22.983087	H	30.060408	7.749451	26.959419
H	9.847310	3.169200	22.676938	H	43.098623	7.731622	26.933204
H	22.129558	2.850134	28.223398	H	41.679131	6.240375	25.640858
H	24.535126	2.342875	28.301415	H	30.657812	3.647125	24.427195
H	26.035591	3.176885	26.565426	H	44.819100	1.850574	23.185405
H	21.534704	5.340057	24.091723	H	35.834318	6.964955	30.162049
H	23.043655	6.108159	22.371730	H	31.435427	5.068057	29.397742
H	19.533319	2.330567	22.589828	H	29.432553	4.892553	30.747694
H	19.679989	1.794557	20.190458	H	31.288891	6.859366	17.596503
H	18.480875	3.171002	18.536742	H	40.796890	5.636928	21.258651
H	16.652969	6.146000	22.827113	H	41.308181	2.214888	22.850767
H	15.507330	7.501810	21.163907	H	53.552165	3.699251	28.381138
H	14.495468	7.508117	27.087714	H	55.987742	3.326023	28.455692
H	27.649315	8.213581	26.830725	H	57.384042	3.866297	26.497915
H	26.146608	6.659967	25.703148	H	52.703551	5.455750	24.017529
H	14.941168	3.632679	24.315200	H	54.081447	5.977249	22.117120
H	29.132241	2.145162	23.288740	H	50.777401	2.334493	22.589083
H	19.755678	6.977649	30.312064	H	50.920712	1.795110	20.189787
H	15.711485	4.474097	29.312015	H	49.720280	3.170735	18.535991
H	13.849524	3.705768	30.644187	H	47.865573	6.135759	22.823882
H	15.672431	6.862013	17.596227	H	46.741572	7.497571	21.163651
H	25.178301	6.297757	21.578256	H	45.507248	7.301959	27.130798
H	25.611338	2.525384	23.109486	H	46.274297	3.308439	24.468635
H	37.778333	3.121909	28.318569	H	50.896160	7.212131	30.304547
H	40.148331	2.471466	28.386181	H	47.057074	4.412719	29.289615
H	41.627616	2.988622	26.516670	H	45.233591	3.533739	30.605564
H	37.185681	5.176377	23.958891	H	46.907376	6.858156	17.596208
H	38.675456	5.636467	22.110806	H	56.056768	5.973391	21.101840
H	35.154770	2.334181	22.591120	H	10.790737	8.127277	42.499574

H 9.244446 6.787003 41.130261	H 33.703610 3.041662 35.936765
H 12.054389 2.324855 38.543613	H 32.709260 4.400587 34.178835
H 8.520518 3.174044 38.235215	H 31.256717 7.988029 38.224925
H 20.685424 2.958791 44.047989	H 30.187087 9.338249 36.442518
H 23.077157 2.429703 44.282202	H 28.304901 7.989414 42.588691
H 24.650198 2.983901 42.497189	H 41.652559 7.620105 41.724834
H 20.268929 4.857794 39.607722	H 40.327707 5.876541 40.662996
H 21.844959 5.301009 37.820691	H 29.413279 3.694794 40.686756
H 18.114128 2.224130 37.976398	H 43.695561 1.292513 39.017095
H 18.149252 1.762144 35.561239	H 33.472781 8.475825 45.910697
H 16.992052 3.234882 34.001928	H 35.771924 7.783392 32.480083
H 15.292587 6.148335 38.438630	H 33.757386 7.525235 33.831083
H 14.121320 7.565488 36.856188	H 30.587188 4.763465 44.815261
H 13.168997 7.507346 42.649692	H 28.986542 3.395727 46.056234
H 25.806218 8.122096 42.455183	H 28.390433 5.206270 32.759660
H 24.526313 6.331395 41.418469	H 30.082751 8.555662 33.089872
H 13.612347 3.635283 39.865154	H 39.657851 4.550106 36.520478
H 28.115413 1.903281 39.576343	H 40.161856 1.387160 38.692041
H 18.510519 6.825488 45.832926	H 52.222917 3.698864 43.943969
H 19.584110 7.503675 32.708003	H 54.658980 3.325514 44.018903
H 17.706067 6.675203 34.027190	H 56.055274 3.865870 42.061068
H 14.353351 4.505412 44.856732	H 51.375233 5.456861 39.580712
H 12.440493 3.872705 46.190045	H 52.752707 5.977009 37.680366
H 12.854973 3.507419 32.693241	H 49.646957 2.474062 37.944680
H 14.146843 7.181016 33.331351	H 49.726242 2.013189 35.530691
H 24.012494 5.357477 37.089333	H 48.422215 3.355452 33.970336
H 24.704793 1.906733 39.042535	H 46.417586 6.072980 38.403322
H 36.312789 3.457397 43.709439	H 45.116350 7.368207 36.819369
H 38.665465 2.630910 44.000321	H 44.060357 7.319797 42.081140
H 40.266478 2.742819 42.146612	H 45.066067 3.016576 40.018875
H 35.969930 4.518081 39.042662	H 49.535468 7.159209 45.757024
H 37.518505 4.531430 37.136597	H 50.655757 7.755005 32.692389
H 33.554040 3.755750 38.334282	H 48.823197 6.810601 33.999402

H 45.693062 4.326471 44.854333	H 35.154318 3.080143 59.394134
H 43.866370 3.506553 46.209562	H 37.541814 2.489886 59.426535
H 44.232853 3.281166 32.645891	H 38.991913 3.093860 57.559779
H 45.201284 7.001995 33.293784	H 34.487392 5.298888 55.128274
H 54.726507 5.965274 36.662451	H 35.946437 5.838331 53.276937
H 9.463459 8.127206 58.062743	H 32.803557 2.582662 53.516845
H 7.917054 6.786970 56.693379	H 33.011340 2.203543 51.095460
H 10.726981 2.324881 54.106681	H 31.715422 3.535195 49.517442
H 7.193814 3.175995 53.795754	H 29.447055 6.057092 53.941420
H 19.511848 2.921789 59.307805	H 28.122225 7.314871 52.334390
H 21.905671 2.354635 59.332902	H 27.326647 7.449449 58.150713
H 23.371099 3.084948 57.522800	H 40.482006 7.800538 58.065704
H 18.862438 5.339965 55.146126	H 39.031508 6.351387 56.759562
H 20.335533 6.000984 53.348347	H 27.967033 3.506899 55.379916
H 16.883309 2.444081 53.483094	H 42.105709 2.033220 54.106510
H 16.902684 1.974586 51.071126	H 32.788710 6.738067 61.409705
H 15.685995 3.405248 49.522471	H 33.178850 8.804896 48.380708
H 14.000197 6.323226 53.962665	H 31.671228 7.365649 49.656094
H 12.784010 7.709915 52.386185	H 28.750498 4.373932 60.399915
H 11.840682 7.508973 58.212354	H 26.897911 3.573974 61.718632
H 24.922579 7.928565 58.004220	H 28.081713 2.926804 48.026887
H 23.442578 6.461910 56.745119	H 28.304836 6.980868 48.801700
H 12.284916 3.635685 55.428365	H 38.051107 5.867002 52.383772
H 26.457285 2.083507 54.124445	H 38.590617 2.416173 53.855355
H 17.168871 6.738432 61.410903	H 50.894947 3.699484 59.506164
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H 16.415749 6.730850 49.531614	H 54.727792 3.865562 57.623229
H 13.129687 4.375046 60.400686	H 50.047798 5.460577 55.145945
H 11.277998 3.573907 61.719496	H 51.425149 5.977650 53.243104
H 11.426950 3.767036 48.236495	H 48.426826 2.729625 53.495382
H 12.774566 7.306945 48.863802	H 48.513378 2.243374 51.088961
H 22.449469 6.099904 52.481318	H 47.144016 3.505437 49.522265
H 22.943557 2.497089 53.895214	H 45.141637 6.281244 53.923000

H	43.782040	7.504148	52.326794	C	35.185496	8.867515	40.495495
H	42.889069	7.350568	58.214500	C	35.453101	10.159885	39.783917
H	43.593400	3.453353	55.393298	C	36.209697	11.184610	40.643505
H	48.405443	6.744580	61.407664	C	35.608674	11.306006	42.051729
H	49.316075	7.772348	48.127359	C	35.627339	9.952047	42.774799
H	47.478776	6.892656	49.468558	O	33.638797	9.141225	41.586233
H	44.381996	4.363190	60.399584	C	37.874549	7.934693	39.077344
H	42.519478	3.571111	61.717949	C	39.198047	8.407130	39.123183
H	42.865919	3.342663	48.260352	C	39.927687	8.593405	37.946453
H	43.786096	7.018841	48.815001	C	39.346104	8.324325	36.702625
H	53.398602	5.963928	52.224474	C	38.022627	7.869116	36.651063
H	17.068482	7.157617	63.836093	C	37.289406	7.673640	37.824220
H	15.148272	6.357112	65.155559	N	37.120538	7.765233	40.259307
H	10.261870	3.422484	63.798018	H	35.991437	9.944944	38.843602
H	32.688418	7.157673	63.835188	H	34.762994	8.030508	39.943253
H	30.768132	6.357162	65.154664	H	35.086425	7.857285	42.427875
H	25.879087	3.427627	63.796077	H	36.206378	12.163569	40.132064
H	48.307482	7.159214	63.833732	H	37.271262	10.878733	40.724222
H	46.387827	6.357443	65.153444	H	36.166309	12.055409	42.641769
H	41.497971	3.429464	63.794675	H	34.565215	11.663052	41.980273
H	54.922506	4.682760	55.325534	H	36.672924	9.650217	42.988481
H	56.250046	4.683075	39.763397	H	35.106714	10.013238	43.747246
H	57.578863	4.683490	24.200302	H	34.469929	10.563299	39.478186
H	32.654171	5.043665	18.026504	H	39.666510	8.607850	40.092987
H	17.034675	5.043858	18.026668	H	40.963702	8.941379	38.004942
H	10.176536	4.915034	24.089515	H	39.920024	8.470629	35.782542
H	8.847970	4.915261	39.653287	H	37.549952	7.662661	35.684770
H	7.520547	4.915265	55.216398	H	36.258526	7.309808	37.774158
H	12.998687	5.198806	65.268987	H	36.589694	6.878915	40.349924
H	28.618493	5.198861	65.268098	H	37.675791	7.902426	41.104447
H	44.238361	5.198783	65.266977				
H	48.273891	5.043409	18.026042	(<i>R,R</i>)-1-Int1(QM(B3LYP)/MM)			
C	34.967561	8.846720	41.956163	C	12.487000	7.261000	26.395000

C	11.616000	6.503000	25.622000	O	15.523872	7.185037	18.539057
C	12.086000	5.395000	24.927000	O	18.566867	5.529630	24.111016
C	13.428000	5.043000	25.007000	O	18.023068	3.388865	24.570326
C	13.027000	3.179000	23.539000	C	18.264899	4.337454	23.743465
C	11.685000	3.529000	23.460000	C	14.301000	5.801000	25.782000
C	11.215000	4.638000	24.154000	C	13.829000	6.909000	26.476000
O	10.782000	2.793000	22.654000	C	28.021199	7.174712	26.466282
Cu	18.541005	6.085547	26.019072	C	27.171709	6.306698	25.787129
Cu	17.952304	3.697441	26.526471	C	27.671539	5.165157	25.127232
C	22.218138	3.963576	26.392874	C	29.068273	4.899079	25.175052
C	22.749609	3.184297	27.436449	C	13.900000	3.935000	24.313000
C	24.106882	2.885553	27.482722	C	28.715845	2.960227	23.751745
C	24.958091	3.351830	26.485100	C	27.350933	3.185520	23.730352
C	24.464012	4.106708	25.403980	C	26.803103	4.292545	24.417520
C	23.074193	4.401754	25.343125	O	26.575441	2.270739	23.022203
C	22.576100	5.089841	24.215871	O	16.592685	6.402792	25.852021
C	23.436848	5.518355	23.208793	O	16.053524	4.263613	26.321043
C	24.804000	5.269994	23.287917	C	15.733683	5.460916	25.984876
C	25.329214	4.553561	24.372984	C	17.923420	5.802433	30.237103
O	25.651769	5.701147	22.273383	C	18.906488	6.584482	30.870694
O	20.435127	5.524410	26.197811	C	16.796475	5.357804	30.984231
O	19.918955	3.374875	26.645635	C	15.725262	4.668871	30.376182
C	20.771989	4.307335	26.419216	C	14.641583	4.232146	31.134056
C	18.226927	4.022014	22.293999	O	18.425286	6.399434	27.984244
C	18.992915	2.941012	21.873981	O	17.904642	4.251133	28.432477
C	19.081890	2.638017	20.519979	C	18.097412	5.464570	28.800139
C	18.404876	3.417023	19.587993	Cu	34.183736	6.119025	26.005245
C	17.639888	4.497024	20.008011	Cu	33.620026	3.737715	26.564834
C	17.550913	4.800019	21.362013	C	37.869834	3.986729	26.375881
C	16.783924	5.881020	21.784030	C	38.396831	3.282890	27.474228
C	16.107910	6.659026	20.850045	C	39.742103	2.937671	27.520812
C	16.197885	6.355031	19.497042	C	40.585187	3.280940	26.469041
C	16.963875	5.274030	19.076025	C	40.095310	3.963911	25.338748

C	38.716552	4.306855	25.279671	O	42.271368	2.048041	22.906111
C	38.218908	4.924438	24.113343	O	32.214143	6.427886	25.911281
C	39.071937	5.230465	23.055697	O	31.718911	4.286265	26.413948
C	40.431823	4.939539	23.130555	C	31.370527	5.476623	26.088518
C	40.956309	4.299452	24.263263	C	33.757985	5.920884	30.246000
O	41.273369	5.259549	22.070924	C	34.799065	6.690703	30.797714
O	36.090258	5.554975	26.130365	C	32.638904	5.580536	31.056704
O	35.579976	3.418910	26.647054	C	31.530366	4.880404	30.537105
C	36.428909	4.343684	26.387627	C	30.443217	4.572520	31.351618
C	33.846854	4.021972	22.293718	O	34.140415	6.459722	27.964015
C	34.612831	2.940969	21.873683	O	33.622380	4.324151	28.471587
C	34.701781	2.637978	20.519678	C	33.845740	5.542401	28.810118
C	34.024753	3.416989	19.587708	Cu	49.700141	6.207575	25.980832
C	33.259776	4.496991	20.007741	Cu	49.346534	3.791293	26.560551
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.162978	5.545891	24.103370	C	53.770890	5.287813	24.113936
O	33.652866	3.405857	24.595376	C	54.557834	5.591815	23.007897
C	33.879930	4.345752	23.750071	C	55.929834	5.377800	23.052821
C	29.922427	5.762612	25.916003	C	56.515889	4.858782	24.200784
C	29.383588	6.908012	26.529164	O	56.643771	5.617805	21.841785
C	43.549375	6.898537	26.487857	O	51.642672	5.838949	26.127013
C	42.735479	6.038763	25.759858	O	51.338324	3.661582	26.634248
C	43.270083	4.916598	25.092428	C	52.096362	4.667229	26.380447
C	44.668874	4.667356	25.175299	C	49.466779	4.021876	22.293156
C	29.574601	3.800110	24.451687	C	50.232745	2.940872	21.873104
C	44.380974	2.748001	23.713349	C	50.321669	2.637885	20.519096
C	43.014643	2.962119	23.648518	C	49.644627	3.416901	19.587140
C	42.433023	4.050963	24.337522	C	48.879661	4.496905	20.007192

C	48.790737	4.799893	21.361200	C	20.882005	3.859849	42.086796
C	48.023772	5.880897	21.783251	C	21.338337	3.174692	43.227660
C	47.347731	6.658913	20.849295	C	22.684318	2.861612	43.380907
C	47.437655	6.354926	19.496287	C	23.599134	3.217649	42.394810
C	48.203620	5.273922	19.075235	C	23.181620	3.873379	41.221634
O	46.763613	7.184943	18.538331	C	21.803501	4.184743	41.054190
O	49.738719	5.591850	24.085275	C	21.382646	4.778226	39.846567
O	49.388331	3.427566	24.604383	C	22.306485	5.078770	38.848020
C	49.528321	4.370170	23.746340	C	23.661212	4.812011	39.027049
C	45.489980	5.537977	25.942993	C	24.109894	4.211957	40.209666
C	44.912923	6.654505	26.575649	O	24.570478	5.118704	38.022835
C	45.209176	3.583603	24.455339	O	19.132926	5.439097	41.731471
O	47.720903	6.342657	25.876978	O	18.570283	3.307804	42.211888
O	47.395650	4.176003	26.411962	C	19.443563	4.223995	42.004420
C	46.954545	5.335584	26.081153	C	16.906896	4.010773	37.810476
C	49.193466	5.991037	30.213388	C	17.602708	2.896260	37.309653
C	50.127770	6.845494	30.826194	C	17.631427	2.630696	35.945859
C	48.091309	5.503492	30.969836	C	16.963172	3.469068	35.058456
C	47.066912	4.733823	30.378465	C	16.225487	4.579485	35.519129
C	46.004240	4.260397	31.143681	C	16.179739	4.842805	36.915763
O	49.604101	6.568142	27.938381	C	15.381740	5.907688	37.380758
O	49.297833	4.393382	28.453837	C	14.690933	6.714781	36.484084
C	49.382682	5.629761	28.784900	C	14.759440	6.494033	35.119777
C	11.158286	7.260970	41.959133	C	15.531763	5.424546	34.611418
C	10.287269	6.502976	41.186145	O	14.059371	7.380821	34.305508
C	10.757253	5.394976	40.491133	O	17.264824	5.485181	39.639212
C	12.099253	5.042971	40.571108	O	16.712277	3.345295	40.090198
C	11.698221	3.178978	39.103109	C	16.966393	4.295140	39.265832
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.533421	7.057596	42.403616
Cu	17.241501	6.036945	41.546083	C	25.766348	6.116505	41.749316
Cu	16.615839	3.659841	42.056808	C	26.344264	4.963786	41.124995

C	27.772531	4.795193	41.237840	C	39.128411	5.234507	38.765192
C	12.571237	3.934972	39.877096	C	39.668822	4.427088	39.766501
C	27.612666	2.750519	39.929658	O	39.945478	5.803709	37.835746
C	26.205987	2.910422	39.806734	O	34.991822	5.409547	41.821988
C	25.565888	3.999642	40.389745	O	34.220044	3.359834	42.228461
O	25.611122	1.914062	39.086308	C	35.151227	4.173034	41.935613
O	15.285141	6.385438	41.388429	C	32.721047	4.965344	38.041689
O	14.725657	4.250481	41.846590	C	33.467221	3.850650	37.695292
C	14.412868	5.454493	41.529824	C	33.599455	3.484383	36.340333
C	16.627454	5.788161	45.760711	C	32.951727	4.203667	35.357165
C	17.642660	6.538396	46.382440	C	32.142298	5.346404	35.660061
C	18.817970	6.880438	32.225938	C	32.046142	5.741902	37.043999
C	17.744556	6.406726	32.973664	C	31.233323	6.865717	37.374760
C	16.721284	5.646829	32.374439	C	30.562004	7.559136	36.401687
C	15.481144	5.407086	46.512151	C	30.651792	7.180210	35.035602
C	14.386278	4.746924	45.915329	C	31.427649	6.088898	34.653367
C	13.282441	4.373720	46.678102	O	29.924003	7.988404	34.208322
C	14.589532	4.470455	32.504475	O	32.764563	6.499318	39.850571
C	15.616346	5.187413	33.135249	O	32.449441	4.304020	40.272885
O	13.501162	4.029488	33.249154	C	32.627551	5.289046	39.502721
O	17.134179	6.356631	43.507081	C	28.541041	5.798795	41.914056
O	16.557842	4.224184	43.963201	C	27.933560	6.914646	42.466287
C	16.783951	5.434032	44.326317	C	42.205334	6.872666	42.214557
Cu	32.544664	7.264024	41.663507	C	41.399114	6.055545	41.428491
Cu	32.522556	4.342448	42.244788	C	41.955380	5.035491	40.630564
C	36.545037	3.631734	41.767309	C	43.363604	4.830664	40.656886
C	37.042673	2.760705	42.716594	C	28.373792	3.662259	40.614781
C	38.416188	2.421868	42.715707	C	43.100904	3.053685	39.021144
C	39.273905	2.963602	41.782677	C	41.727997	3.227796	39.005215
C	38.802718	3.842361	40.752768	C	41.135261	4.226477	39.804362
C	37.394387	4.139684	40.728007	O	40.992804	2.372784	38.189582
C	36.887413	4.931877	39.658046	O	30.655887	6.799398	41.763502
C	37.725712	5.458146	38.703617	O	30.579259	4.635766	42.334775

C	30.032407	5.727977	42.006917	C	49.121660	2.982032	35.964015
C	32.450026	6.542046	45.856840	C	48.396290	3.758355	35.066164
C	33.274217	7.436596	46.512533	C	47.563980	4.805628	35.513446
C	34.764470	7.092153	32.127464	C	47.478375	5.068312	36.908946
C	33.682863	6.747521	32.930425	C	46.591133	6.066838	37.358690
C	32.607937	5.996993	32.417815	C	45.851686	6.814648	36.449032
C	31.382580	5.878036	46.547943	C	45.954006	6.594122	35.086552
C	30.464531	5.015403	45.881153	C	46.812905	5.585569	34.592991
C	29.430079	4.421018	46.562176	O	45.196222	7.419344	34.259178
C	30.423302	4.956096	32.689268	O	48.435868	5.784696	39.665038
C	31.494130	5.677631	33.230242	O	48.119434	3.591930	40.086744
O	29.322051	4.659610	33.482073	C	48.269162	4.574157	39.274954
O	32.787067	7.282447	43.638204	C	44.175600	5.648201	41.489799
O	32.748948	5.062852	44.057839	C	43.579789	6.677772	42.239250
C	32.679978	6.276433	44.398717	C	43.921017	3.840327	39.824565
Cu	48.396665	6.300381	41.583816	O	46.412793	6.459851	41.480703
Cu	48.016682	3.863616	42.057702	O	46.074919	4.265097	41.876932
C	52.242278	4.464620	41.931334	C	45.641105	5.443950	41.616464
C	52.828353	3.947597	43.079285	C	47.861159	5.935822	45.792557
C	54.201353	3.732577	43.123183	C	48.824439	6.739398	46.429629
C	54.987278	4.036581	42.018131	C	50.016371	7.174395	32.172478
C	54.401203	4.554604	40.869180	C	48.967301	6.662746	32.930481
C	53.028203	4.768624	40.826281	C	47.992051	5.828605	32.350455
C	52.442128	5.287648	39.677330	C	46.725935	5.491793	46.524974
C	53.229054	5.591652	38.571278	C	45.680930	4.770082	45.910581
C	54.601054	5.377632	38.616177	C	44.583302	4.342631	46.653515
C	55.187129	4.858609	39.764128	C	45.930286	4.536226	32.506076
O	55.314970	5.617639	37.405129	C	46.911648	5.327656	33.120553
O	50.338489	5.886306	41.720010	O	44.865389	4.053960	33.259086
O	49.998209	3.702612	42.175703	O	48.299677	6.576451	43.548833
C	50.772469	4.699939	41.949646	O	47.925684	4.392794	43.975672
C	48.256208	4.297270	37.816198	C	48.044583	5.613345	44.355332
C	49.051335	3.245871	37.325946	C	9.830848	7.260896	57.522290

C	8.959816	6.502907	56.749315	O	12.723895	7.524711	49.836146
C	9.429783	5.394908	56.054291	O	15.941089	5.642761	55.206557
C	10.771783	5.042898	56.134241	O	15.428636	3.478859	55.584991
C	10.370718	3.178911	54.666243	C	15.671739	4.457959	54.793441
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.317185	7.079411	57.558387
Cu	15.892571	6.129113	57.135570	C	24.479463	6.245554	56.825708
Cu	15.336776	3.718257	57.557746	C	24.990069	5.137637	56.117911
C	19.590647	4.027466	57.441808	C	26.387662	4.874947	56.165058
C	20.139638	3.263088	58.486987	C	11.243751	3.934900	55.440217
C	21.493968	2.949361	58.504205	C	26.055805	3.009551	54.642730
C	22.323244	3.384055	57.474489	C	24.689322	3.227966	54.623157
C	21.810178	4.126905	56.393467	C	24.130456	4.296264	55.361240
C	20.423547	4.439838	56.364746	O	23.923249	2.340896	53.870891
C	19.903904	5.119991	55.242836	O	13.936631	6.427924	56.975039
C	20.741511	5.515351	54.203052	O	13.428930	4.268725	57.377123
C	22.107119	5.248878	54.249066	C	13.088397	5.472720	57.087646
C	22.653514	4.546746	55.333291	C	15.283046	5.695821	61.352095
O	22.932301	5.650852	53.204605	C	16.314087	6.385804	61.978046
O	17.796243	5.583138	57.300418	C	17.561855	6.869336	47.729617
O	17.302248	3.413307	57.672312	C	16.464285	6.463130	48.481202
C	18.144614	4.361982	57.482272	C	15.412745	5.732106	47.894850
C	15.640629	4.204372	53.331730	C	14.198081	5.242825	62.095148
C	16.359339	3.106164	52.826302	C	13.166040	4.552842	61.469196
C	16.385778	2.839322	51.463603	C	12.083075	4.099846	62.213249
C	15.690899	3.659043	50.580626	C	13.235852	4.644801	48.042867
C	14.938121	4.758670	51.043648	C	14.288800	5.333778	48.662236
C	14.898697	5.026302	52.440115	O	12.129439	4.262190	48.793123
C	14.089462	6.081285	52.907184	O	15.760635	6.374310	59.110960
C	13.380728	6.875095	52.012272	O	15.280820	4.203286	59.484350
C	13.439659	6.648478	50.648152	C	15.446887	5.407598	59.895730
C	14.221054	5.586363	50.137745	Cu	31.474279	6.145566	57.138444

Cu	30.968633	3.721595	57.552473	C	40.603974	5.025872	56.138085
C	35.209866	4.088117	57.458246	C	42.002767	4.764716	56.193007
C	35.751466	3.365493	58.536839	C	26.905259	3.816512	55.391698
C	37.099113	3.026789	58.562870	C	41.683130	2.912886	54.652960
C	37.929344	3.392877	57.508334	C	40.316577	3.133351	54.620195
C	37.425467	4.098170	56.398084	C	39.750285	4.195721	55.361781
C	36.045224	4.439937	56.362839	O	39.557673	2.250684	53.855690
C	35.533711	5.086211	55.218408	O	29.504281	6.409420	57.014829
C	36.373284	5.415849	54.157267	O	29.054305	4.229716	57.376541
C	37.733557	5.120847	54.206962	C	28.681571	5.430616	57.121563
C	38.272941	4.454988	55.317919	C	30.903120	5.695641	61.351269
O	38.560338	5.461562	53.142280	C	31.934175	6.385618	61.977205
O	33.394547	5.625351	57.276093	C	33.106267	7.665079	47.897083
O	32.933425	3.452123	57.671139	C	32.105506	7.025040	48.597334
C	33.761060	4.410980	57.475680	C	31.196960	6.120747	47.955832
C	31.295403	4.234979	53.324925	C	29.818167	5.242646	62.094340
C	32.099723	3.196107	52.823374	C	28.786113	4.552669	61.468405
C	32.210205	2.979291	51.455247	C	27.703159	4.099675	62.212476
C	31.515406	3.790221	50.563277	C	29.256995	4.628794	47.956525
C	30.668499	4.819163	51.022636	C	30.124504	5.467113	48.653993
C	30.543825	5.035507	52.422700	O	28.236605	4.007268	48.611685
C	29.649337	6.023479	52.880369	O	31.366724	6.380565	59.113218
C	28.932512	6.797924	51.973083	O	30.904188	4.204541	59.481237
C	29.073818	6.620915	50.607737	C	31.063894	5.409405	59.895328
C	29.945186	5.629581	50.113222	Cu	47.048987	6.244385	57.149430
O	28.339999	7.467450	49.782045	Cu	46.688733	3.789862	57.536779
O	31.507076	5.673086	55.206761	C	50.914829	4.464394	57.493750
O	31.070215	3.490891	55.575542	C	51.500923	3.947364	58.641689
C	31.285939	4.480646	54.788528	C	52.873923	3.732339	58.685563
C	27.230218	5.704126	56.956354	C	53.659830	4.036343	57.580498
C	26.678842	6.813601	57.622880	C	53.073736	4.554373	56.431559
C	40.912483	6.945103	57.611651	C	51.700736	4.768398	56.388685
C	40.085211	6.123855	56.855795	C	51.114643	5.287428	55.239746

C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.497768	4.612753	48.016762
O	53.987445	5.617415	52.967495	C	45.502294	5.356012	48.654391
O	48.992472	5.856373	57.300794	O	43.398305	4.175656	48.746884
O	48.676948	3.652321	57.668811	O	46.917668	6.441386	59.125117
C	49.440179	4.670381	57.496804	O	46.577964	4.237028	59.466911
C	46.958343	4.348887	53.320600	C	46.674831	5.442384	59.893497
C	47.780011	3.327322	52.811093	C	16.262162	6.620790	63.347051
C	47.825382	3.063216	51.448779	C	15.179196	6.168795	64.090104
C	47.048804	3.809935	50.569659	C	14.147156	5.478812	63.465153
C	46.197873	4.834553	51.035646	C	12.031150	4.336833	63.582254
C	46.138101	5.096709	52.432497	C	13.063191	5.025817	64.207206
C	45.233668	6.069166	52.903219	O	10.943187	3.908837	64.361307
C	44.449602	6.792455	52.011117	C	31.882275	6.620600	63.346211
C	44.526507	6.574953	50.646234	C	30.799322	6.168606	64.089282
C	45.404706	5.592876	50.131766	C	29.767267	5.478629	63.464346
O	43.732712	7.384708	49.837444	C	27.651260	4.336658	63.581482
O	47.119184	5.792284	55.211222	C	28.683314	5.025635	64.206417
O	46.811675	3.585518	55.563773	O	26.563309	3.908663	64.360554
C	46.962128	4.591992	54.784206	C	47.502389	6.620356	63.345091
C	42.838408	5.593344	56.992114	C	46.419447	6.168363	64.088179
C	42.274027	6.685354	57.678079	C	45.387379	5.478391	63.463260
C	42.526894	3.713060	55.416331	C	43.271369	4.336426	63.580429
O	45.073265	6.391576	57.021074	C	44.303437	5.025398	64.205349
O	44.740521	4.186605	57.355219	O	42.183431	3.908432	64.359519
C	44.303101	5.371693	57.122718	H	12.119370	8.127103	26.935477
C	46.523195	5.695406	61.350162	H	10.572727	6.787268	25.566452
C	47.554262	6.385378	61.976082	H	13.377754	2.322876	22.980214
C	48.702647	7.067445	47.774274	H	9.846122	3.167855	22.675435
C	47.614518	6.605435	48.507003	H	22.102474	2.821734	28.228025
C	46.615308	5.815505	47.905011	H	24.504043	2.292665	28.300132
C	45.438253	5.242413	62.093251	H	26.009213	3.104639	26.555995

H	21.519485	5.291053	24.085747	H	35.645955	6.979279	30.183997
H	23.030247	6.048983	22.359269	H	31.478944	4.575232	29.498659
H	19.532148	2.329264	22.590171	H	29.606512	4.032809	30.929808
H	19.679021	1.794023	20.190610	H	31.291248	6.863217	17.594900
H	18.480548	3.170353	18.536430	H	40.796501	5.750651	21.329269
H	16.650249	6.140419	22.827024	H	41.288726	2.263069	22.885737
H	15.505628	7.501824	21.158911	H	53.552148	3.699851	28.381689
H	14.495782	7.508469	27.087682	H	55.987724	3.326094	28.455521
H	27.618183	8.056914	26.952720	H	57.384426	3.866088	26.498127
H	26.117482	6.545711	25.764969	H	52.704036	5.448100	24.015384
H	14.941677	3.638871	24.310055	H	54.083195	5.976006	22.116677
H	29.108464	2.114211	23.204351	H	50.778385	2.335037	22.589416
H	19.756287	6.952473	30.305618	H	50.920987	1.795422	20.189901
H	15.698463	4.474061	29.310672	H	49.720850	3.170558	18.535633
H	13.836722	3.701636	30.644881	H	47.862913	6.130289	22.823632
H	15.670377	6.862986	17.594960	H	46.740238	7.497712	21.158846
H	25.169504	6.227671	21.560124	H	45.533270	7.339930	27.143323
H	25.594119	2.493335	23.030786	H	46.271551	3.373026	24.442585
H	37.753609	3.008177	28.303520	H	50.956491	7.246041	30.251969
H	40.135207	2.400661	28.377825	H	47.062109	4.500907	29.320220
H	41.626244	2.994563	26.538326	H	45.234801	3.669170	30.667358
H	37.168790	5.166703	23.996965	H	46.912735	6.863905	17.594429
H	38.666968	5.706887	22.173891	H	56.063092	5.977865	21.099171
H	35.151422	2.330072	22.590899	H	10.790899	8.127462	42.499104
H	35.298699	1.793815	20.190412	H	9.244091	6.787402	41.130360
H	34.100181	3.170182	18.536189	H	12.049826	2.325142	38.541278
H	32.261822	6.137874	22.825956	H	8.517974	3.169198	38.238704
H	31.123245	7.500060	21.159045	H	20.640888	2.898646	44.011522
H	30.028761	7.587662	27.075446	H	23.023271	2.344811	44.272902
H	43.119565	7.763134	26.982939	H	24.640620	2.962839	42.549125
H	41.681012	6.270420	25.708440	H	20.339150	5.000813	39.652300
H	30.634321	3.583016	24.399260	H	21.959578	5.530938	37.929141
H	44.798925	1.912701	23.168287	H	18.138062	2.239313	37.986620

H	18.179153	1.771996	35.571806	H	34.062606	7.949857	45.954894
H	17.010888	3.230430	34.005029	H	35.578163	7.681075	32.538197
H	15.266442	6.122985	38.436023	H	33.685938	7.085654	33.959240
H	14.084172	7.533922	36.845217	H	30.573044	4.816173	44.814977
H	13.169252	7.508328	42.649159	H	28.730295	3.770235	46.024332
H	26.054240	7.927751	42.863351	H	28.639167	4.087164	33.007570
H	24.684361	6.277134	41.708001	H	29.960940	7.710102	33.280328
H	13.612641	3.640435	39.863317	H	39.416184	6.294644	37.186283
H	28.068624	1.883439	39.444305	H	39.997555	2.532695	38.235350
H	18.509178	6.858050	45.813242	H	52.223642	3.704278	43.946438
H	19.589194	7.476647	32.702581	H	54.659165	3.326852	44.019235
H	17.710857	6.652999	34.026775	H	56.055723	3.866048	42.061517
H	14.358603	4.524213	44.855267	H	51.375279	5.450197	39.581159
H	12.458986	3.863865	46.198051	H	52.754484	5.976134	37.680116
H	12.840750	3.500867	32.698673	H	49.632256	2.637188	38.010803
H	14.128624	7.157653	33.326865	H	49.745884	2.172618	35.599941
H	24.146979	5.599568	37.242811	H	48.478342	3.521114	34.014661
H	24.655327	2.044177	38.986345	H	46.443070	6.274365	38.411344
H	36.371321	2.372686	43.487306	H	45.177068	7.584170	36.798443
H	38.805577	1.743596	43.481554	H	44.191222	7.320358	42.863983
H	40.336777	2.707456	41.831309	H	44.989987	3.668214	39.773240
H	35.815604	5.121802	39.586035	H	49.679106	7.108693	45.872720
H	37.310035	6.055390	37.883102	H	50.750262	7.827026	32.633846
H	33.944307	3.262554	38.483479	H	48.913766	6.937014	33.975833
H	34.205188	2.613818	36.069245	H	45.688679	4.538701	44.852005
H	33.061938	3.872062	34.319743	H	43.796488	3.789414	46.159993
H	31.142402	7.175639	38.415499	H	44.241647	3.469443	32.722654
H	29.931061	8.417059	36.649513	H	45.305348	7.205576	33.282013
H	28.550220	7.676128	42.949872	H	54.733421	5.973037	36.660950
H	41.762734	7.658933	42.814879	H	9.463506	8.126829	58.063134
H	40.332825	6.232831	41.443582	H	7.916605	6.787083	56.694063
H	29.453241	3.522154	40.676701	H	10.722410	2.324956	54.104727
H	43.532240	2.289896	38.387653	H	7.190376	3.168797	53.802850

H	19.507729	2.919434	59.299049	H	28.248067	7.557075	52.327597
H	21.905318	2.366467	59.321703	H	27.314604	7.466896	58.211005
H	23.371960	3.121702	57.520799	H	40.494279	7.790324	58.148336
H	18.847866	5.342427	55.145215	H	39.032387	6.365988	56.824472
H	20.319110	6.038024	53.356380	H	27.966437	3.606819	55.338434
H	16.908211	2.457548	53.500662	H	42.089228	2.101518	54.064583
H	16.947931	1.990822	51.087584	H	32.788421	6.739923	61.409690
H	15.732494	3.414271	49.528554	H	33.775067	8.358457	48.417075
H	13.980761	6.300379	53.962388	H	32.001760	7.228669	49.667866
H	12.766892	7.688281	52.374810	H	28.749314	4.379529	60.400407
H	11.840497	7.509056	58.213286	H	26.897626	3.574621	61.720244
H	24.905777	7.934179	58.085088	H	27.739004	3.452013	47.989473
H	23.425585	6.485198	56.802431	H	28.479278	7.284617	48.799238
H	12.285084	3.640674	55.426536	H	38.073877	5.967243	52.416946
H	26.456873	2.194068	54.056523	H	38.575402	2.467686	53.862477
H	17.168825	6.739444	61.410817	H	50.895049	3.699562	59.506766
H	18.356642	7.441993	48.196360	H	53.331422	3.325561	59.581254
H	16.435669	6.738015	49.527246	H	54.728193	3.865562	57.623768
H	13.128508	4.380832	60.401068	H	50.048142	5.455201	55.146464
H	11.277598	3.574663	61.721067	H	51.426938	5.977204	53.243093
H	11.453286	3.742541	48.253335	H	48.392173	2.734790	53.482802
H	12.794754	7.302849	48.857450	H	48.464937	2.272584	51.070408
H	22.438971	6.174215	52.496703	H	47.106609	3.566435	49.518236
H	22.941328	2.559820	53.882015	H	45.108848	6.276190	53.959179
H	35.116591	3.066232	59.364051	H	43.761295	7.542138	52.376858
H	37.503289	2.473202	59.403970	H	42.902941	7.338242	58.274127
H	38.971600	3.107165	57.559593	H	43.588195	3.501968	55.373732
H	34.483020	5.334704	55.122664	H	48.406274	6.744633	61.408085
H	35.957353	5.912580	53.291892	H	49.455858	7.684667	48.252912
H	32.659413	2.563509	53.504071	H	47.550999	6.883618	49.550597
H	32.843585	2.181437	51.081393	H	44.382077	4.368277	60.399975
H	31.631070	3.593129	49.505157	H	42.519429	3.571442	61.719562
H	29.480882	6.200760	53.936406	H	42.760239	3.619636	48.196860

H	43.817511	7.167534	48.859142	C	36.786934	9.086809	36.457240
H	53.405536	5.972351	52.223367	C	35.633777	8.503824	37.017072
H	17.068094	7.157953	63.835986	C	35.577577	8.175071	38.379192
H	15.148345	6.357534	65.155915	N	36.631345	8.118329	40.584351
H	10.258596	3.420391	63.803975	H	33.648714	11.553502	40.012804
H	32.688052	7.158042	63.835068	H	34.801743	9.676458	41.037961
H	30.768378	6.357485	65.155053	H	34.047067	9.020049	43.348172
H	25.877478	3.422597	63.802684	H	31.153640	12.079623	40.591909
H	48.307555	7.158926	63.833660	H	32.339407	12.376134	41.887744
H	46.388350	6.357497	65.153875	H	30.287981	11.188682	42.759773
H	41.497299	3.423012	63.801422	H	30.606732	9.817377	41.658752
H	54.923364	4.683318	55.324879	H	32.388111	10.804053	43.995261
H	56.250908	4.683600	39.762528	H	31.538922	9.234962	43.882355
H	57.579678	4.683861	24.199224	H	32.472579	10.277658	39.619025
H	32.653505	5.044465	18.025502	H	38.723897	9.213375	39.299293
H	17.033768	5.044633	18.025670	H	38.802912	9.803974	36.881781
H	10.175615	4.914249	24.088542	H	36.823575	9.346560	35.386573
H	8.847003	4.914442	39.652550	H	34.753935	8.298570	36.384532
H	7.519560	4.914412	55.215976	H	34.670474	7.706112	38.795763
H	12.997579	5.198435	65.269740	H	35.999599	7.351535	40.869167
H	28.617624	5.198373	65.268908	H	37.536538	8.067495	41.061867
H	44.237735	5.198152	65.267813				
H	48.273515	5.044295	18.025049				
C	33.286460	9.413129	42.646493	(<i>R,R</i>)-2-RC(QM(B3LYP)/MM)			
C	33.731135	9.815707	41.285721	C	12.487000	7.261000	26.395000
C	32.939762	10.826940	40.467974	C	11.616000	6.503000	25.622000
C	31.859313	11.569066	41.284398	C	12.086000	5.395000	24.927000
C	31.097293	10.631972	42.237338	C	13.428000	5.043000	25.007000
C	32.049854	10.018263	43.278879	C	13.027000	3.179000	23.539000
O	33.050196	8.545316	41.517232	C	11.685000	3.529000	23.460000
C	36.691654	8.419284	39.226159	C	11.215000	4.638000	24.154000
C	37.847023	9.015610	38.658087	O	10.782000	2.793000	22.654000
C	37.889687	9.341798	37.294153	Cu	18.544164	6.083752	26.015420
				Cu	17.946616	3.696908	26.529265

C	22.209491	3.938305	26.374498	C	29.009481	4.770253	25.123322
C	22.752658	3.180834	27.427770	C	13.900000	3.935000	24.313000
C	24.104561	2.861751	27.453367	C	28.686233	2.888494	23.622832
C	24.937950	3.288450	26.424704	C	27.319386	3.108223	23.594046
C	24.431994	4.023102	25.335190	C	26.758459	4.185455	24.316592
C	23.046926	4.334360	25.293920	O	26.554180	2.214818	22.847346
C	22.531190	4.998498	24.160310	O	16.596802	6.402782	25.849899
C	23.375097	5.384835	23.123852	O	16.053551	4.264178	26.319729
C	24.741630	5.125387	23.184808	C	15.735589	5.462045	25.984420
C	25.281570	4.435519	24.278719	C	17.904585	5.823556	30.228161
O	25.573396	5.517610	22.141800	C	18.896233	6.583785	30.874399
O	20.434440	5.513362	26.188206	C	16.748225	5.421601	30.953636
O	19.907890	3.368599	26.651589	C	15.672712	4.756017	30.327593
C	20.765269	4.294837	26.416046	C	14.561117	4.361565	31.066027
C	18.226927	4.022014	22.293999	O	18.431885	6.402275	27.975876
C	18.992915	2.941012	21.873981	O	17.893272	4.258859	28.431198
C	19.081890	2.638017	20.519979	C	18.093629	5.473402	28.794441
C	18.404876	3.417024	19.587993	Cu	34.102255	5.990715	26.088270
C	17.639888	4.497025	20.008011	Cu	33.554507	3.579779	26.533920
C	17.550913	4.800019	21.362013	C	37.809217	3.886213	26.424333
C	16.783924	5.881020	21.784030	C	38.329671	3.142137	27.498941
C	16.107910	6.659026	20.850045	C	39.677597	2.812450	27.553162
C	16.197885	6.355032	19.497042	C	40.529972	3.210033	26.529311
C	16.963876	5.274031	19.076025	C	40.048860	3.933353	25.421384
O	15.523872	7.185038	18.539057	C	38.668748	4.265570	25.356366
O	18.565413	5.527902	24.112105	C	38.180599	4.933501	24.213878
O	18.019107	3.387724	24.573922	C	39.045584	5.292729	23.184441
C	18.263557	4.335542	23.745622	C	40.406061	5.003376	23.263360
C	14.301000	5.801000	25.782000	C	40.919797	4.316258	24.371768
C	13.829000	6.909000	26.476000	O	41.258532	5.370171	22.227823
C	27.937564	6.995170	26.483726	O	36.010163	5.442052	26.218595
C	27.103333	6.152869	25.757303	O	35.516646	3.279779	26.634368
C	27.614752	5.035197	25.065727	C	36.360079	4.224661	26.430043

C	33.846855	4.021974	22.293721	O	34.018739	6.240585	28.062037
C	34.612832	2.940971	21.873686	O	33.514562	4.076508	28.454843
C	34.701783	2.637980	20.519681	C	33.710795	5.279730	28.855414
C	34.024755	3.416991	19.587710	Cu	49.696873	6.206521	25.982856
C	33.259777	4.496993	20.007743	Cu	49.345882	3.789325	26.565682
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.113633	5.497600	24.161331	C	53.770890	5.287820	24.113942
O	33.619387	3.334367	24.563517	C	54.557834	5.591822	23.007903
C	33.849413	4.307301	23.758678	C	55.929834	5.377808	23.052827
C	29.848466	5.605581	25.911848	C	56.515890	4.858790	24.200790
C	29.296993	6.725234	26.560157	O	56.643771	5.617813	21.841791
C	43.550075	6.892297	26.578103	O	51.638298	5.837591	26.121435
C	42.723616	6.031976	25.866314	O	51.335552	3.661119	26.635495
C	43.245602	4.914183	25.182765	C	52.093473	4.666837	26.380159
C	44.644547	4.664519	25.237134	C	49.466780	4.021882	22.293161
C	29.531611	3.702374	24.365901	C	50.232747	2.940878	21.873109
C	44.329683	2.745835	23.783772	C	50.321671	2.637891	20.519101
C	42.962044	2.963986	23.741488	C	49.644629	3.416907	19.587145
C	42.394986	4.053657	24.439797	C	48.879663	4.496911	20.007197
O	42.201916	2.056787	23.006425	C	48.790739	4.799899	21.361205
O	32.135804	6.285020	25.973167	C	48.023773	5.880903	21.783256
O	31.651851	4.118775	26.373198	C	47.347732	6.658919	20.849300
C	31.297583	5.320368	26.094829	C	47.437657	6.354932	19.496292
C	33.549814	5.577847	30.304366	C	48.203622	5.273928	19.075240
C	34.565460	6.293163	30.964139	O	46.763615	7.184949	18.538336
C	32.393149	5.176810	31.030126	O	49.731242	5.591457	24.089656
C	31.306576	4.535551	30.398272	O	49.385025	3.426357	24.609368
C	30.187512	4.157321	31.134043	C	49.525162	4.368881	23.750088

C	45.480880	5.536503	25.986966	C	24.048888	4.544598	39.811216
C	44.914896	6.650696	26.633592	O	24.390243	5.636708	37.689608
C	45.171843	3.579863	24.509339	O	19.134217	5.585620	41.619457
O	47.717271	6.339248	25.887418	O	18.637935	3.432844	42.076844
O	47.396237	4.171944	26.423352	C	19.482910	4.371782	41.848997
C	46.950985	5.332938	26.101070	C	16.875477	4.126785	37.732928
C	49.213658	5.997327	30.218046	C	17.586282	3.027994	37.218972
C	50.161522	6.841331	30.824606	C	17.598979	2.763153	35.856486
C	48.104581	5.531713	30.978121	C	16.899924	3.589262	34.983342
C	47.072980	4.767326	30.392745	C	16.150487	4.686919	35.456114
C	46.003887	4.318886	31.162072	C	16.118326	4.946383	36.852017
O	49.611036	6.567936	27.937285	C	15.307869	5.994505	37.332543
O	49.301356	4.394083	28.457123	C	14.590728	6.789907	36.447921
C	49.393264	5.631197	28.787002	C	14.647508	6.575661	35.080759
C	11.158284	7.260965	41.959133	C	15.434880	5.523924	34.559524
C	10.287267	6.502972	41.186144	O	13.924792	7.453743	34.275974
C	10.757252	5.394972	40.491132	O	17.229746	5.598727	39.569503
C	12.099252	5.042967	40.571107	O	16.729888	3.443537	40.012026
C	11.698220	3.178974	39.103108	C	16.950805	4.404613	39.190863
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108
O	9.453203	2.792985	38.218146	C	26.652481	6.969900	42.297039
Cu	17.230131	6.133776	41.480402	C	25.832343	6.195295	41.504756
Cu	16.672985	3.735835	41.979770	C	26.339748	5.107201	40.721654
C	20.933278	4.033378	41.834938	C	27.753817	4.840458	40.799474
C	21.455604	3.266556	42.892414	C	12.571236	3.934968	39.877095
C	22.805640	2.944831	42.943014	C	27.477554	3.014068	39.214371
C	23.659592	3.375855	41.934186	C	26.083363	3.269068	39.127441
C	23.178892	4.124829	40.843902	C	25.506503	4.290986	39.876015
C	21.795642	4.444754	40.779506	O	25.432794	2.417361	38.281545
C	21.307855	5.131341	39.647654	O	15.269749	6.431198	41.359311
C	22.176290	5.522584	38.632948	O	14.766097	4.281108	41.815141
C	23.538105	5.246988	38.714954	C	14.421507	5.479750	41.508900

C	16.699640	5.831206	45.705561	C	32.417184	3.267967	35.147896
C	17.703878	6.603753	46.317618	C	31.713512	4.452527	35.542148
C	18.786940	6.901097	32.222001	C	31.674199	4.761375	36.948393
C	17.683661	6.467740	32.948790	C	30.918770	5.894743	37.368788
C	16.653321	5.727637	32.337084	C	30.264464	6.688161	36.461861
C	15.571479	5.420888	46.470109	C	30.337090	6.420445	35.069700
C	14.488708	4.731029	45.884766	C	31.052801	5.322372	34.603421
C	13.402958	4.334755	46.659827	O	29.664761	7.334683	34.308792
C	14.490429	4.611508	32.434088	O	32.699886	5.437553	39.646198
C	15.524454	5.302148	33.080251	O	32.286019	3.291882	40.166523
O	13.375263	4.208869	33.160379	C	32.442725	4.237347	39.337082
O	17.151543	6.432170	43.444494	C	28.582329	5.677078	41.619011
O	16.643067	4.280097	43.891221	C	28.040845	6.723015	42.347331
C	16.843495	5.492708	44.262596	C	42.281338	7.189724	42.155263
Cu	32.855507	6.216785	41.495720	C	41.459712	6.379284	41.380582
Cu	32.358956	3.747242	42.093164	C	41.988696	5.317209	40.620094
C	36.541378	3.997526	41.768861	C	43.387237	5.068231	40.663121
C	37.035693	3.131146	42.728690	C	28.285364	3.768632	40.024698
C	38.410182	2.810869	42.760023	C	43.082174	3.255191	39.078229
C	39.272385	3.334836	41.821727	C	41.713880	3.468067	39.052273
C	38.812067	4.207873	40.783020	C	41.149217	4.507472	39.817455
C	37.409115	4.543271	40.761988	O	40.953682	2.608106	38.264443
C	36.933732	5.376258	39.709035	O	30.828061	6.433861	41.495463
C	37.785093	5.854995	38.741653	O	30.451361	4.277430	42.003711
C	39.172108	5.557178	38.773295	C	30.061737	5.443810	41.710663
C	39.689305	4.743628	39.779234	C	32.304664	5.961967	45.713705
O	39.996091	6.069853	37.817444	C	33.199677	6.847337	46.288584
O	34.727926	5.524294	41.605162	C	34.474899	6.573088	32.321596
O	34.290293	3.380531	42.120414	C	33.361496	6.156660	33.042963
C	35.077757	4.329862	41.828920	C	32.307962	5.461741	32.419329
C	32.350565	3.901566	37.877760	C	31.214000	5.422282	46.478090
C	32.981486	2.747169	37.445276	C	30.220009	4.577494	45.905657
C	33.019596	2.437491	36.069246	C	29.170028	4.105422	46.656088

C	30.116583	4.406458	32.501598	O	48.480874	5.891926	39.678834
C	31.165132	5.065464	33.150901	O	48.100804	3.708944	40.101328
O	28.987841	4.033954	33.219927	C	48.283315	4.685183	39.288506
O	32.803051	6.525249	43.469331	C	44.216817	5.879723	41.484693
O	32.389878	4.369873	43.962610	C	43.646870	6.946078	42.203276
C	32.512469	5.591139	44.274272	C	43.921087	4.040528	39.860622
Cu	48.452802	6.408848	41.597722	O	46.478967	6.626848	41.489484
Cu	48.003828	3.982040	42.069963	O	46.077393	4.443386	41.890007
C	52.242277	4.464616	41.931345	C	45.677280	5.634315	41.625631
C	52.828352	3.947593	43.079296	C	47.881576	6.050131	45.807288
C	54.201352	3.732573	43.123194	C	48.840750	6.852421	46.452355
C	54.987277	4.036578	42.018142	C	50.056504	7.183929	32.166688
C	54.401202	4.554601	40.869191	C	48.998348	6.696632	32.926138
C	53.028202	4.768621	40.826292	C	48.010335	5.872562	32.353886
C	52.442128	5.287645	39.677341	C	46.745332	5.598122	46.534525
C	53.229054	5.591649	38.571289	C	45.701159	4.882103	45.911373
C	54.601054	5.377629	38.616189	C	44.609616	4.439238	46.651877
C	55.187129	4.858606	39.764139	C	45.932336	4.612924	32.521405
O	55.314970	5.617636	37.405141	C	46.923075	5.397066	33.128096
O	50.377127	5.936696	41.734519	O	44.859496	4.155849	33.278468
O	49.976920	3.761805	42.187400	O	48.359454	6.684708	43.562967
C	50.778051	4.737848	41.961287	O	47.927750	4.510460	43.984606
C	48.271790	4.403932	37.827896	C	48.074083	5.727346	44.367663
C	49.057020	3.341912	37.344714	C	9.830844	7.260885	57.522289
C	49.121828	3.063584	35.986641	C	8.959813	6.502896	56.749314
C	48.398641	3.836571	35.085697	C	9.429780	5.394897	56.054290
C	47.576686	4.895326	35.524782	C	10.771780	5.042887	56.134240
C	47.500094	5.175243	36.916020	C	10.370715	3.178901	54.666241
C	46.629741	6.190387	37.360262	C	9.028715	3.528910	54.587291
C	45.891836	6.932252	36.446382	C	8.558747	4.637908	55.281315
C	45.981460	6.691596	35.085177	O	8.125681	2.792922	53.781316
C	46.828815	5.670211	34.599183	Cu	15.894195	6.139667	57.135736
O	45.227370	7.513040	34.249751	Cu	15.342794	3.725445	57.551919

C	19.596827	4.044505	57.441254	C	26.382816	4.877408	56.165844
C	20.149191	3.280487	58.484930	C	11.243748	3.934890	55.440215
C	21.502007	2.965134	58.498883	C	26.056092	3.029651	54.625131
C	22.326069	3.398576	57.465750	C	24.689135	3.251529	54.601884
C	21.810968	4.142143	56.386456	C	24.129384	4.311657	55.350323
C	20.426159	4.456608	56.361076	O	23.922064	2.373597	53.838897
C	19.902333	5.140274	55.243183	O	13.939137	6.432357	56.972663
C	20.737439	5.535446	54.202940	O	13.435937	4.270647	57.369273
C	22.103099	5.266571	54.245323	C	13.092069	5.475327	57.084616
C	22.651524	4.561643	55.325530	C	15.283042	5.695809	61.352094
O	22.925959	5.668584	53.199232	C	16.314083	6.385792	61.978046
O	17.796261	5.597730	57.303283	C	17.632726	6.930638	47.665293
O	17.306382	3.425918	57.672153	C	16.552823	6.499111	48.426865
C	18.147705	4.376739	57.484819	C	15.511341	5.745926	47.852139
C	15.681978	4.217535	53.324172	C	14.198077	5.242813	62.095147
C	16.403637	3.114801	52.832784	C	13.166036	4.552830	61.469195
C	16.458293	2.847180	51.472152	C	12.083071	4.099834	62.213248
C	15.786550	3.671027	50.576553	C	13.362436	4.612832	48.023867
C	15.029279	4.773771	51.023313	C	14.403397	5.328772	48.630310
C	14.964730	5.044958	52.417056	O	12.270507	4.211493	48.785543
C	14.156746	6.107651	52.868014	O	15.757929	6.379589	59.109089
C	13.472055	6.904036	51.958687	O	15.278899	4.206947	59.477460
C	13.551648	6.670625	50.595723	C	15.446193	5.410570	59.892377
C	14.331884	5.600236	50.103020	Cu	31.470523	6.134076	57.133552
O	12.852900	7.544881	49.765777	Cu	30.963382	3.711297	57.559656
O	15.949802	5.657762	55.207634	C	35.208503	4.076720	57.448533
O	15.441122	3.491734	55.579726	C	35.751138	3.341356	58.518121
C	15.690208	4.471745	54.789839	C	37.098802	3.007278	58.544240
C	11.644813	5.800876	56.909215	C	37.928419	3.391774	57.497091
C	11.172845	6.908875	57.603239	C	37.425189	4.109214	56.394836
C	25.311777	7.070918	57.577910	C	36.045048	4.445843	56.358925
C	24.476929	6.245059	56.834511	C	35.532904	5.105764	55.222415
C	24.987614	5.143572	56.116907	C	36.374978	5.453689	54.170538

C	37.736506	5.163354	54.221798	C	28.677575	5.422830	57.130434
C	38.274063	4.482602	55.323151	C	30.903116	5.695628	61.351271
O	38.566312	5.522123	53.165651	C	31.934171	6.385605	61.977208
O	33.388265	5.613254	57.267999	C	33.081915	7.190622	47.653545
O	32.927580	3.441664	57.673859	C	32.062925	6.669233	48.421150
C	33.756172	4.399407	57.471525	C	31.084911	5.778967	47.869398
C	31.281602	4.195101	53.327994	C	29.818163	5.242633	62.094342
C	32.064997	3.132170	52.843739	C	28.786109	4.552656	61.468406
C	32.147792	2.868907	51.483558	C	27.703155	4.099663	62.212477
C	31.442207	3.656168	50.581191	C	29.055299	4.421319	48.034951
C	30.621333	4.714107	51.020703	C	29.997899	5.247532	48.643956
C	30.530774	4.983390	52.413229	O	28.020176	3.915073	48.760675
C	29.668504	6.006578	52.854362	O	31.367640	6.374949	59.106978
C	28.953063	6.764936	51.934420	O	30.903106	4.200220	59.483310
C	29.056181	6.531523	50.572934	C	31.065444	5.406276	59.893587
C	29.888345	5.498884	50.097742	Cu	47.053125	6.252977	57.152937
O	28.327358	7.366052	49.730080	Cu	46.687597	3.796411	57.533600
O	31.498437	5.652478	55.203712	C	50.914826	4.464382	57.493755
O	31.057806	3.473394	55.586977	C	51.500920	3.947352	58.641694
C	31.275299	4.457021	54.792234	C	52.873920	3.732327	58.685568
C	27.223634	5.697945	56.967477	C	53.659827	4.036331	57.580503
C	26.671616	6.801410	57.643237	C	53.073733	4.554362	56.431564
C	40.915375	6.954159	57.632597	C	51.700733	4.768387	56.388690
C	40.088548	6.137053	56.873106	C	51.114640	5.287417	55.239751
C	40.606143	5.046021	56.144273	C	51.901547	5.591423	54.133687
C	42.003393	4.784544	56.193822	C	53.273547	5.377397	54.178561
C	26.903096	3.825021	55.386551	C	53.859639	4.858367	55.326499
C	41.684013	2.944317	54.643728	O	53.987443	5.617405	52.967501
C	40.316694	3.166485	54.613211	O	48.993015	5.860386	57.303286
C	39.751801	4.222499	55.363944	O	48.672889	3.655887	57.668518
O	39.554205	2.290382	53.843678	C	49.438495	4.672984	57.498499
O	29.502237	6.399501	57.014889	C	46.961066	4.371510	53.318746
O	29.050233	4.221525	57.387717	C	47.779587	3.351362	52.801967

C	47.830721	3.101241	51.438304	C	15.179191	6.168782	64.090104
C	47.062227	3.862606	50.565752	C	14.147152	5.478800	63.465152
C	46.212566	4.884839	51.039019	C	12.031146	4.336820	63.582253
C	46.146974	5.132088	52.436368	C	13.063187	5.025805	64.207205
C	45.245423	6.102993	52.915929	O	10.943183	3.908824	64.361306
C	44.469640	6.839005	52.029557	C	31.882271	6.620587	63.346214
C	44.551623	6.635778	50.661962	C	30.799317	6.168593	64.089284
C	45.427832	5.656157	50.141148	C	29.767262	5.478616	63.464348
O	43.766264	7.457613	49.856395	C	27.651255	4.336645	63.581483
O	47.124679	5.805530	55.217523	C	28.683309	5.025622	64.206418
O	46.812852	3.597672	55.562265	O	26.563304	3.908650	64.360554
C	46.966398	4.606675	54.785702	C	47.502385	6.620342	63.345096
C	42.839754	5.608396	56.996712	C	46.419443	6.168348	64.088184
C	42.276214	6.694713	57.691980	C	45.387375	5.478376	63.463264
C	42.528134	3.738065	55.410810	C	43.271365	4.336411	63.580432
O	45.079597	6.403253	57.024918	C	44.303433	5.025383	64.205353
O	44.742856	4.197281	57.351835	O	42.183428	3.908416	64.359522
C	44.306740	5.384563	57.124925	H	12.119249	8.127110	26.935697
C	46.523192	5.695393	61.350166	H	10.573027	6.786843	25.566341
C	47.554258	6.385364	61.976087	H	13.383828	2.323405	22.982345
C	48.718342	7.168316	47.798930	H	9.847429	3.169681	22.677028
C	47.633316	6.692570	48.525932	H	22.117313	2.848975	28.241056
C	46.636538	5.905747	47.916759	H	24.510857	2.284042	28.277764
C	45.438249	5.242399	62.093255	H	25.985870	3.025619	26.478323
C	44.406182	4.552428	61.467335	H	21.474332	5.216094	24.049419
C	43.323240	4.099435	62.211424	H	22.956095	5.895165	22.267159
C	44.528254	4.690385	48.019078	H	19.531962	2.329411	22.589921
C	45.528026	5.433131	48.662031	H	19.679243	1.794008	20.190524
O	43.436185	4.234099	48.748388	H	18.480413	3.170765	18.536729
O	46.922342	6.444427	59.125520	H	16.651533	6.145386	22.827122
O	46.574519	4.239786	59.461952	H	15.506916	7.500980	21.165258
C	46.675852	5.444252	59.891536	H	14.495560	7.508223	27.087552
C	16.262158	6.620778	63.347051	H	27.525527	7.858739	26.996333

H 26.050295 6.394061 25.724532	H 52.703477 5.451863 24.014117
H 14.941512 3.634101 24.311138	H 54.081098 5.975913 22.116776
H 29.094671 2.066158 23.050741	H 50.777474 2.335068 22.589495
H 19.767099 6.920301 30.323372	H 50.920917 1.795283 20.189768
H 15.665667 4.544106 29.263743	H 49.720394 3.170977 18.535924
H 13.750678 3.850652 30.564015	H 47.862836 6.134644 22.823781
H 15.671829 6.861075 17.596372	H 46.741197 7.496784 21.164979
H 25.077712 6.030217 21.427919	H 45.545704 7.334614 27.190095
H 25.573316 2.437101 22.850963	H 46.233911 3.364887 24.477887
H 37.677970 2.824985 28.305235	H 50.994733 7.224702 30.246732
H 40.065030 2.245821 28.394248	H 47.068303 4.516174 29.337468
H 41.573669 2.935635 26.603097	H 45.226803 3.732217 30.691029
H 37.130198 5.177892 24.094002	H 46.913126 6.861861 17.595763
H 38.648568 5.807519 22.320001	H 56.056121 5.977195 21.104215
H 35.146699 2.325378 22.590031	H 10.790923 8.127987 42.498555
H 35.297783 1.792984 20.190399	H 9.244428 6.787037 41.130031
H 34.099808 3.170476 18.536511	H 12.055494 2.324862 38.544365
H 32.268508 6.145143 22.826197	H 8.519393 3.171273 38.239604
H 31.125709 7.500154 21.165125	H 20.804194 2.926689 43.689763
H 29.931862 7.383385 27.142309	H 23.194333 2.359279 43.770611
H 43.129422 7.753993 27.086963	H 24.705490 3.105450 42.005918
H 41.667222 6.258386 25.841584	H 20.255057 5.361722 39.520946
H 30.593082 3.487381 24.320499	H 21.778094 6.047709 37.774955
H 44.741604 1.910758 23.233160	H 18.144867 2.381852 37.886436
H 35.440694 6.623385 30.415967	H 18.158494 1.915775 35.472903
H 31.297294 4.329481 29.332784	H 16.934558 3.350748 33.929815
H 29.367410 3.666622 30.626854	H 15.203600 6.208296 38.390298
H 31.292062 6.861069 17.596316	H 13.974952 7.595646 36.824759
H 40.781741 5.885343 21.503110	H 13.169134 7.511246 42.645856
H 41.219629 2.273444 23.009248	H 26.227259 7.787695 42.887298
H 53.552025 3.700118 28.381287	H 24.764273 6.434486 41.484121
H 55.987722 3.326138 28.455745	H 13.611983 3.633919 39.867874
H 57.384075 3.866339 26.497854	H 27.884464 2.197932 38.611647

H	18.554556	6.945085	45.738529	H	52.224126	3.710619	43.948114
H	19.564278	7.482146	32.708402	H	54.659367	3.328318	44.019965
H	17.632574	6.730187	33.996873	H	56.055413	3.866666	42.061236
H	14.456329	4.499183	44.825647	H	51.374553	5.453017	39.579835
H	12.587493	3.802517	46.189104	H	52.752229	5.975824	37.680139
H	12.716756	3.692007	32.597015	H	49.632293	2.734034	38.033774
H	13.979125	7.226246	33.297904	H	49.737878	2.244703	35.628647
H	23.919664	6.183633	36.983385	H	48.473869	3.587382	34.036809
H	24.495454	2.640124	38.171606	H	46.494158	6.418752	38.411358
H	36.351554	2.708080	43.468100	H	45.228677	7.712381	36.795663
H	38.791993	2.139576	43.535724	H	44.272616	7.583321	42.817949
H	40.331477	3.063271	41.872785	H	44.985085	3.833657	39.815738
H	35.876892	5.638228	39.668281	H	49.693927	7.228411	45.899282
H	37.393462	6.490067	37.938046	H	50.801085	7.828825	32.622926
H	33.466246	2.094385	38.175452	H	48.948263	6.981543	33.968482
H	33.536954	1.534278	35.730407	H	45.703333	4.665290	44.848714
H	32.475836	2.993631	34.089528	H	43.823188	3.889743	46.152392
H	30.852376	6.131135	38.430332	H	44.230473	3.576284	32.743115
H	29.670278	7.547625	36.783793	H	45.321868	7.277700	33.276513
H	28.682104	7.344159	42.977413	H	54.726407	5.972586	36.666003
H	41.855096	8.009829	42.724789	H	9.463379	8.127040	58.062936
H	40.400736	6.600772	41.369920	H	7.916936	6.786690	56.693555
H	29.348859	3.535715	40.079372	H	10.728243	2.325390	54.106750
H	43.498851	2.461856	38.471497	H	7.191665	3.170566	53.803558
H	34.005887	7.265167	45.680318	H	19.519536	2.937647	59.297988
H	35.273225	7.115003	32.819368	H	21.915864	2.382347	59.315863
H	33.324193	6.393732	34.098668	H	23.374411	3.135470	57.508561
H	30.285196	4.299542	44.854220	H	18.846162	5.368827	55.149052
H	28.411821	3.465910	46.188114	H	20.312517	6.060367	53.358047
H	28.329195	3.512225	32.660113	H	16.934926	2.464000	53.517907
H	29.665357	7.111821	33.364837	H	17.025085	1.995952	51.108114
H	39.482502	6.620780	37.204712	H	15.850920	3.427993	49.525467
H	39.965465	2.807840	38.296321	H	14.030050	6.333510	53.920683

H	12.859723	7.722472	52.312882	H	28.748776	4.375566	60.399813
H	11.840564	7.509221	58.212300	H	26.897681	3.574646	61.718370
H	24.900166	7.922191	58.111000	H	27.469953	3.349709	48.194464
H	23.423827	6.486632	56.809872	H	28.451909	7.153202	48.751785
H	12.285074	3.636251	55.427022	H	38.076566	6.036526	52.448840
H	26.463471	2.220690	54.033575	H	38.573828	2.514279	53.847780
H	17.168290	6.739449	61.410650	H	50.894945	3.700187	59.506387
H	18.420522	7.520436	48.123721	H	53.331567	3.325552	59.581318
H	16.530185	6.770922	49.473572	H	54.727847	3.865740	57.623139
H	13.128965	4.375952	60.400578	H	50.047610	5.459474	55.145472
H	11.277844	3.574443	61.719246	H	51.424864	5.977040	53.243048
H	11.603196	3.678723	48.248171	H	48.385861	2.750106	53.469925
H	12.944987	7.319635	48.789854	H	48.469090	2.311878	51.054121
H	22.426715	6.194865	52.497826	H	47.125027	3.632553	49.511876
H	22.941449	2.596489	53.849242	H	45.115069	6.301482	53.973741
H	35.115583	3.029367	59.339023	H	43.783779	7.586340	52.405735
H	37.503274	2.444216	59.379504	H	42.906464	7.343322	58.289834
H	38.971788	3.111225	57.547748	H	43.589708	3.524019	55.365214
H	34.481022	5.352924	55.124629	H	48.405730	6.744627	61.407997
H	35.959449	5.960262	53.309921	H	49.469360	7.784311	48.283621
H	32.625534	2.511685	53.533786	H	47.569738	6.957609	49.572646
H	32.764017	2.050326	51.124692	H	44.381523	4.364263	60.399397
H	31.532002	3.418404	49.529519	H	42.519344	3.571637	61.717687
H	29.525258	6.229838	53.906363	H	42.802976	3.682536	48.188789
H	28.297960	7.553761	52.280495	H	43.851526	7.246813	48.876964
H	27.306981	7.448088	58.237609	H	53.398572	5.970702	52.227733
H	40.497937	7.795224	58.177203	H	17.068253	7.158002	63.836008
H	39.035423	6.377210	56.847213	H	15.148100	6.357237	65.155560
H	27.964185	3.608717	55.338301	H	10.263232	3.421745	63.796998
H	42.094416	2.138339	54.050221	H	32.688294	7.157884	63.835136
H	32.788256	6.738986	61.409544	H	30.768036	6.357127	65.154697
H	33.806817	7.875860	48.104194	H	25.881838	3.424339	63.795579
H	32.000971	6.957390	49.475291	H	48.307515	7.159109	63.833765

H	46.387749	6.357299	65.153495	H	35.702748	8.997073	37.331856
H	41.501143	3.425394	63.794316	H	35.697277	8.189832	38.913015
H	54.922550	4.682775	55.325798	H	33.260130	9.177797	37.298978
H	56.250091	4.683154	39.763725	H	33.645976	7.500401	37.732067
H	57.578896	4.683428	24.200651	H	35.319047	9.814216	41.139259
H	32.654286	5.043320	18.026523	H	28.565695	11.632213	42.191871
H	17.034805	5.043573	18.026679	H	28.607408	12.763213	44.397547
H	10.176551	4.915329	24.089633	H	30.041692	11.878404	46.250959
H	8.847994	4.915610	39.653324	H	31.428652	9.829965	45.845635
H	7.520561	4.915564	55.216460	H	31.397547	8.702313	43.646433
H	12.998962	5.198994	65.269022	H	30.247820	8.479933	41.493895
H	28.618775	5.198984	65.268149	H	29.191039	9.667760	40.913419
H	44.238625	5.198845	65.267032				
H	48.274018	5.043179	18.026059				
C	32.880132	8.692929	39.332430	(<i>R,R</i>)-2-TS1(QM(B3LYP)/MM)			
C	33.313582	9.549169	40.457539	C	12.487000	7.261000	26.395000
C	34.636928	10.295680	40.413614	C	11.616000	6.503000	25.622000
C	35.276631	10.317385	39.012031	C	12.086000	5.395000	24.927000
C	35.182778	8.957298	38.306347	C	13.428000	5.043000	25.007000
C	33.718924	8.544816	38.083914	C	13.027000	3.179000	23.539000
O	33.422407	8.108168	40.527177	C	11.685000	3.529000	23.460000
C	29.977728	10.085552	42.756910	C	11.215000	4.638000	24.154000
C	29.197830	11.236665	42.995015	O	10.782000	2.793000	22.654000
C	29.225266	11.872435	44.238711	Cu	18.544517	6.097334	26.016163
C	30.025199	11.380907	45.276501	Cu	17.961592	3.708242	26.531724
C	30.800289	10.237463	45.046454	C	22.230803	3.984814	26.388071
C	30.783381	9.594111	43.807250	C	22.769987	3.204941	27.427672
N	29.994606	9.470727	41.504572	C	24.127298	2.909209	27.467792
H	34.476400	11.327497	40.773852	C	24.970578	3.378901	26.466407
H	32.527763	9.944314	41.113138	C	24.470379	4.133595	25.388726
H	31.802447	8.517993	39.215150	C	23.081060	4.425903	25.333897
H	36.330298	10.639619	39.092026	C	22.574743	5.116568	24.211808
H	34.763585	11.076699	38.389083	C	23.429862	5.546793	23.202427
				C	24.798037	5.299846	23.275088

C	25.329763	4.582723	24.355414	C	17.919029	5.830915	30.234792
O	25.639691	5.733675	22.256718	C	18.916401	6.579139	30.886723
O	20.438277	5.540927	26.192978	C	16.763473	5.425707	30.959964
O	19.928513	3.392537	26.654213	C	15.685315	4.768498	30.329871
C	20.780091	4.325707	26.421354	C	14.571994	4.374822	31.065845
C	18.226927	4.022014	22.293999	O	18.433073	6.418231	27.978657
C	18.992915	2.941012	21.873981	O	17.908022	4.271661	28.433688
C	19.081890	2.638017	20.519979	C	18.104200	5.486486	28.798204
C	18.404876	3.417023	19.587993	Cu	34.189095	6.116780	26.012130
C	17.639888	4.497024	20.008011	Cu	33.608804	3.736792	26.567718
C	17.550913	4.800019	21.362013	C	37.866049	3.959642	26.374845
C	16.783924	5.881020	21.784030	C	38.393539	3.244342	27.466077
C	16.107910	6.659026	20.850045	C	39.737688	2.897082	27.509931
C	16.197885	6.355031	19.497042	C	40.578937	3.248893	26.460796
C	16.963875	5.274030	19.076025	C	40.090269	3.941563	25.336748
O	15.523872	7.185037	18.539057	C	38.713272	4.287207	25.280096
O	18.566870	5.535298	24.110940	C	38.215290	4.918539	24.121241
O	18.033466	3.393208	24.577329	C	39.068795	5.231859	23.067794
C	18.269969	4.340313	23.746242	C	40.428444	4.937309	23.140491
C	14.301000	5.801000	25.782000	C	40.951906	4.285377	24.265830
C	13.829000	6.909000	26.476000	O	41.270417	5.267665	22.084387
C	28.015672	7.188499	26.472832	O	36.089774	5.538157	26.130017
C	27.170262	6.326305	25.782861	O	35.566966	3.407826	26.658090
C	27.671911	5.192346	25.112174	C	36.422866	4.325783	26.393155
C	29.067155	4.926042	25.160937	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.721114	3.000188	23.721870	C	34.701781	2.637978	20.519678
C	27.355317	3.225724	23.698736	C	34.024753	3.416989	19.587708
C	26.805497	4.325924	24.394295	C	33.259776	4.496991	20.007741
O	26.579519	2.315799	22.983640	C	33.170826	4.799983	21.361747
O	16.595646	6.407825	25.850289	C	32.403848	5.880986	21.783781
O	16.061929	4.267235	26.320395	C	31.727821	6.658997	20.849810
C	15.737875	5.464106	25.984703	C	31.817771	6.355005	19.496805

C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.158390	5.546329	24.109508	C	53.770890	5.287813	24.113936
O	33.648402	3.405474	24.599207	C	54.557834	5.591815	23.007897
C	33.878283	4.345288	23.753824	C	55.929834	5.377800	23.052821
C	29.919440	5.783143	25.912749	C	56.515889	4.858782	24.200784
C	29.377454	6.922111	26.535533	O	56.643771	5.617805	21.841785
C	43.534679	6.873338	26.511256	O	51.636701	5.836697	26.126453
C	42.725992	6.016130	25.776099	O	51.336494	3.658399	26.634436
C	43.263830	4.900409	25.101325	C	52.093310	4.665684	26.381482
C	44.661490	4.652957	25.185115	C	49.466779	4.021876	22.293156
C	29.576974	3.832338	24.432298	C	50.232745	2.940872	21.873104
C	44.381689	2.740534	23.715906	C	50.321669	2.637885	20.519096
C	43.014417	2.954531	23.647579	C	49.644627	3.416901	19.587140
C	42.429897	4.038676	24.340413	C	48.879661	4.496905	20.007192
O	42.271742	2.043680	22.899692	C	48.790737	4.799893	21.361200
O	32.220528	6.439773	25.923755	C	48.023772	5.880897	21.783251
O	31.712979	4.296810	26.407788	C	47.347731	6.658913	20.849295
C	31.370099	5.491713	26.091124	C	47.437655	6.354926	19.496287
C	33.772826	5.904799	30.252006	C	48.203620	5.273922	19.075235
C	34.894507	6.495030	30.862122	O	46.763613	7.184943	18.538331
C	32.582950	5.719664	31.006987	O	49.729701	5.591256	24.092321
C	31.411792	5.196259	30.422179	O	49.387104	3.424553	24.607636
C	30.251627	5.055237	31.178975	C	49.525506	4.368645	23.750230
O	34.159574	6.452883	27.970782	C	45.480001	5.522911	25.957451
O	33.602535	4.323824	28.472032	C	44.898223	6.633285	26.596870
C	33.855824	5.535677	28.814033	C	45.206219	3.571894	24.464701
Cu	49.694040	6.203203	25.988476	O	47.714430	6.334273	25.890161
Cu	49.346365	3.783809	26.563479	O	47.395618	4.164953	26.418512
C	53.571003	4.464792	26.367939	C	46.949363	5.325194	26.094106
C	54.157058	3.947774	27.515902	C	49.189083	5.974486	30.223847
C	55.530059	3.732759	27.559826	C	50.119391	6.828670	30.843752
C	56.316002	4.036762	26.454787	C	48.084312	5.482249	30.974308

C	47.067340	4.707771	30.376007	C	16.122468	4.628398	35.460526
C	46.003987	4.230914	31.135989	C	16.095090	4.876588	36.859033
O	49.603795	6.558498	27.946221	C	15.338312	5.962186	37.343826
O	49.299255	4.381841	28.455767	C	14.666414	6.799838	36.462129
C	49.383866	5.617681	28.791471	C	14.718231	6.592804	35.093671
C	11.158286	7.260970	41.959133	C	15.453952	5.507120	34.567634
C	10.287269	6.502976	41.186145	O	14.043999	7.511428	34.292270
C	10.757253	5.394976	40.491133	O	17.219595	5.455111	39.585549
C	12.099253	5.042971	40.571108	O	16.628378	3.321691	40.017725
C	11.698221	3.178978	39.103109	C	16.889989	4.276122	39.200019
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.299068	6.338941	43.116953
Cu	17.246780	5.980673	41.499841	C	25.599827	5.707181	42.111341
Cu	16.595546	3.605711	41.990128	C	26.242644	4.842462	41.165816
C	20.864572	3.714381	41.824373	C	27.672810	4.679058	41.285592
C	21.336980	2.850189	42.830157	C	12.571237	3.934972	39.877096
C	22.675891	2.485059	42.888854	C	27.635108	3.180493	39.366488
C	23.571337	2.979825	41.948122	C	26.227780	3.326642	39.245004
C	23.143623	3.833549	40.914809	C	25.525513	4.148879	40.121791
C	21.767095	4.175270	40.823980	O	25.698210	2.586575	38.226642
C	21.327883	4.939236	39.722702	O	15.295279	6.364159	41.385190
C	22.239122	5.401711	38.778550	O	14.714238	4.234485	41.842833
C	23.598475	5.133170	38.909249	C	14.412457	5.443799	41.533003
C	24.063221	4.350207	39.972267	C	16.715814	5.686430	45.725172
O	24.495185	5.614393	37.963596	C	17.750395	6.413646	46.343097
O	19.127948	5.346575	41.631094	C	18.814074	6.877657	32.239722
O	18.544164	3.213213	42.071100	C	17.710860	6.441177	32.965003
C	19.427729	4.116082	41.845380	C	16.673083	5.717651	32.346878
C	16.802586	4.010478	37.738098	C	15.564080	5.331559	46.482516
C	17.457059	2.879831	37.217002	C	14.457549	4.685692	45.891648
C	17.467651	2.629877	35.851102	C	13.347649	4.345042	46.658536
C	16.820758	3.500819	34.981350	C	14.502037	4.616832	32.435506

C	15.541429	5.294668	33.086938	O	32.224254	4.035428	40.129972
O	13.384979	4.213803	33.158685	C	32.468640	5.012080	39.365577
O	17.188614	6.274776	43.465211	C	28.382629	5.390930	42.311411
O	16.601901	4.141562	43.905765	C	27.696391	6.189928	43.213002
C	16.848640	5.344765	44.281121	C	42.179960	6.862149	42.049022
Cu	33.547236	6.699198	41.546132	C	41.408298	6.040970	41.235525
Cu	32.417331	4.099226	42.090884	C	41.993163	5.010483	40.472177
C	36.561915	3.649007	41.446186	C	43.395626	4.798755	40.560525
C	37.004207	2.676232	42.324849	C	28.335772	3.834384	40.346115
C	38.357373	2.270356	42.311922	C	43.194340	3.006855	38.933573
C	39.249941	2.836986	41.427973	C	41.824170	3.192996	38.852794
C	38.836919	3.815873	40.465856	C	41.205793	4.199057	39.619495
C	37.449757	4.205470	40.462331	O	41.116373	2.342697	38.007848
C	37.009552	5.112098	39.455573	O	30.471863	6.468751	42.637461
C	37.882843	5.624187	38.526430	O	30.483994	4.259332	42.289389
C	39.263846	5.300357	38.567263	C	29.890325	5.386810	42.420139
C	39.745377	4.409859	39.524885	C	32.730932	6.210145	45.731822
O	40.117791	5.865505	37.669433	C	33.571972	7.122534	46.346177
O	35.001814	5.411630	41.484771	C	34.867255	6.861860	32.201671
O	34.247297	3.352336	41.922969	C	33.712936	6.664817	32.951127
C	35.163552	4.162052	41.620603	C	32.557619	6.104578	32.374375
C	32.358240	4.729882	37.891961	C	31.641910	5.615552	46.464257
C	32.772247	3.471297	37.482276	C	30.706680	4.720051	45.867905
C	32.768440	3.129709	36.115249	C	29.655089	4.201011	46.583676
C	32.320664	4.030300	35.173170	C	30.229448	5.415556	32.524487
C	31.841247	5.330159	35.537436	C	31.375619	5.939569	33.130810
C	31.871979	5.683015	36.935127	O	29.060678	5.281115	33.262679
C	31.369624	6.960650	37.315599	O	33.417253	6.811598	43.543718
C	30.867065	7.833662	36.384543	O	32.778857	4.686461	43.926596
C	30.845495	7.500828	35.004328	C	32.992075	5.876504	44.287470
C	31.333363	6.272326	34.572729	Cu	48.395095	6.294276	41.571282
O	30.331587	8.491281	34.214801	Cu	48.017910	3.857612	42.053746
O	32.831873	6.166263	39.747932	C	52.242278	4.464620	41.931334

C	52.828353	3.947597	43.079285	C	47.854775	5.942825	45.785108
C	54.201353	3.732577	43.123183	C	48.811940	6.756472	46.419658
C	54.987278	4.036581	42.018131	C	50.002632	7.153512	32.189629
C	54.401203	4.554604	40.869180	C	48.950666	6.638397	32.939309
C	53.028203	4.768624	40.826281	C	47.979435	5.804256	32.353641
C	52.442128	5.287648	39.677330	C	46.725970	5.487855	46.521587
C	53.229054	5.591652	38.571278	C	45.690904	4.748340	45.911366
C	54.601054	5.377632	38.616177	C	44.602045	4.310535	46.658962
C	55.187129	4.858609	39.764128	C	45.923435	4.505833	32.498550
O	55.314970	5.617639	37.405129	C	46.898665	5.299268	33.118136
O	50.334834	5.883804	41.714713	O	44.856669	4.019878	33.246186
O	49.996875	3.700778	42.178505	O	48.292873	6.577972	43.534085
C	50.770338	4.698682	41.950287	O	47.921800	4.394867	43.967368
C	48.263532	4.276553	37.806954	C	48.039656	5.617005	44.344774
C	49.064684	3.231121	37.313007	C	9.830848	7.260896	57.522290
C	49.130689	2.966326	35.951763	C	8.959816	6.502907	56.749315
C	48.393345	3.735739	35.058969	C	9.429783	5.394908	56.054291
C	47.555168	4.776815	35.509025	C	10.771783	5.042898	56.134241
C	47.475794	5.041598	36.902770	C	10.370718	3.178911	54.666243
C	46.588970	6.038082	37.357516	C	9.028718	3.528920	54.587293
C	45.841044	6.779765	36.451836	C	8.558750	4.637919	55.281317
C	45.934707	6.555388	35.088546	O	8.125684	2.792932	53.781319
C	46.796310	5.551202	34.591925	Cu	15.896957	6.130335	57.133641
O	45.170715	7.376475	34.262024	Cu	15.343014	3.718176	57.555128
O	48.443581	5.768943	39.656391	C	19.601536	4.035625	57.442993
O	48.127600	3.577282	40.084917	C	20.154869	3.267310	58.483441
C	48.279347	4.556421	39.268865	C	21.509560	2.958686	58.499025
C	44.175389	5.624434	41.417677	C	22.334393	3.401248	57.470431
C	43.550958	6.661791	42.133823	C	21.818658	4.147179	56.393563
C	43.983417	3.795344	39.764612	C	20.432709	4.457270	56.367264
O	46.412712	6.448344	41.455940	C	19.909416	5.146813	55.252654
O	46.077707	4.255062	41.862918	C	20.745247	5.549212	54.215767
C	45.641650	5.430556	41.587069	C	22.111136	5.281562	54.257676

C	22.659618	4.572964	55.335514	C	15.283046	5.695821	61.352095
O	22.934040	5.690249	53.214005	C	16.314087	6.385804	61.978046
O	17.798843	5.587237	57.303090	C	17.683009	6.749178	47.689157
O	17.308503	3.416493	57.675184	C	16.576415	6.374872	48.442240
C	18.150753	4.366653	57.486391	C	15.505955	5.668178	47.861918
C	15.666745	4.198505	53.323644	C	14.198081	5.242825	62.095148
C	16.366386	3.081515	52.831500	C	13.166040	4.552842	61.469196
C	16.402031	2.804239	51.472152	C	12.083075	4.099846	62.213249
C	15.732371	3.631277	50.578486	C	13.306496	4.634431	48.020152
C	14.998414	4.749555	51.025095	C	14.372977	5.307067	48.632533
C	14.953156	5.031495	52.417603	O	12.191186	4.284958	48.773413
C	14.167565	6.110835	52.868751	O	15.760967	6.375009	59.107409
C	13.486220	6.911729	51.960597	O	15.280157	4.203570	59.480105
C	13.549254	6.668437	50.598514	C	15.448019	5.407827	59.892814
C	14.307125	5.582146	50.105376	Cu	31.493229	6.166581	57.140626
O	12.862739	7.553160	49.769720	Cu	30.980124	3.741220	57.541332
O	15.951999	5.642505	55.205194	C	35.224796	4.101424	57.472975
O	15.439659	3.478834	55.583195	C	35.770934	3.382404	58.552001
C	15.687138	4.456438	54.789882	C	37.117401	3.041866	58.573712
C	11.644816	5.800887	56.909216	C	37.940519	3.401015	57.512444
C	11.172849	6.908886	57.603240	C	37.432836	4.101807	56.401586
C	25.331306	7.112378	57.539057	C	36.055282	4.447858	56.371798
C	24.492633	6.275286	56.812944	C	35.538487	5.096661	55.230970
C	24.999883	5.164836	56.107538	C	36.372859	5.418149	54.164899
C	26.395782	4.899857	56.152365	C	37.732026	5.115698	54.207584
C	11.243751	3.934900	55.440217	C	38.275075	4.451870	55.316898
C	26.058114	3.023021	54.648676	O	38.554041	5.448825	53.137027
C	24.691614	3.246495	54.628152	O	33.408936	5.642702	57.295096
C	24.137128	4.321344	55.358892	O	32.942108	3.468091	57.677745
O	23.919780	2.356745	53.884198	C	33.773363	4.426631	57.492608
O	13.941741	6.427403	56.970065	C	31.395073	4.256839	53.314992
O	13.435243	4.267524	57.371435	C	32.172156	3.177986	52.854367
C	13.092592	5.472587	57.085029	C	32.317925	2.931620	51.496201

C	31.679413	3.748766	50.571370	C	29.475255	4.518460	47.953734
C	30.861751	4.819405	50.984626	C	30.360335	5.386845	48.589548
C	30.712622	5.077521	52.374170	O	28.436680	3.971614	48.644703
C	29.862144	6.123750	52.784138	O	31.368156	6.391796	59.113878
C	29.207535	6.907184	51.839149	O	30.898690	4.214666	59.469686
C	29.355444	6.671753	50.482469	C	31.062618	5.416831	59.891226
C	30.188344	5.627412	50.037632	Cu	47.050011	6.245486	57.147657
O	28.662569	7.509789	49.613088	Cu	46.687934	3.790000	57.535560
O	31.550690	5.701704	55.207583	C	50.914829	4.464394	57.493750
O	31.102310	3.520492	55.565304	C	51.500923	3.947364	58.641689
C	31.339063	4.509390	54.781714	C	52.873923	3.732339	58.685563
C	27.242426	5.733657	56.935557	C	53.659830	4.036343	57.580498
C	26.692503	6.846716	57.598363	C	53.073736	4.554373	56.431559
C	40.908547	6.948047	57.604877	C	51.700736	4.768398	56.388685
C	40.085230	6.125726	56.847607	C	51.114643	5.287428	55.239746
C	40.605186	5.027150	56.131980	C	51.901549	5.591433	54.133681
C	42.001847	4.765209	56.190534	C	53.273549	5.377407	54.178555
C	26.910388	3.833065	55.388822	C	53.859642	4.858378	55.326493
C	41.686853	2.906556	54.661044	O	53.987445	5.617415	52.967495
C	40.320063	3.129903	54.621946	O	48.990680	5.856371	57.298541
C	39.753251	4.195246	55.357878	O	48.674005	3.652645	57.671141
O	39.559971	2.244494	53.861099	C	49.438132	4.670426	57.497775
O	29.524717	6.434179	56.999616	C	46.966792	4.346688	53.316152
O	29.069322	4.254245	57.352820	C	47.788400	3.324753	52.806444
C	28.697937	5.457257	57.101800	C	47.835450	3.060767	51.445053
C	30.903120	5.695641	61.351269	C	47.058023	3.807041	50.567788
C	31.934175	6.385618	61.977205	C	46.206569	4.831185	51.032983
C	33.402065	7.447201	47.709669	C	46.148654	5.096509	52.427571
C	32.378929	6.883219	48.441371	C	45.251375	6.075286	52.898830
C	31.452099	5.962181	47.852472	C	44.470388	6.799510	52.006893
C	29.818167	5.242646	62.094340	C	44.541563	6.574956	50.641951
C	28.786113	4.552669	61.468405	C	45.414245	5.587965	50.129348
C	27.703159	4.099675	62.212476	O	43.750592	7.384784	49.830053

O	47.122657	5.791045	55.211459	C	28.683314	5.025635	64.206417
O	46.814785	3.584303	55.564229	O	26.563309	3.908663	64.360554
C	46.968354	4.589931	54.783311	C	47.502389	6.620356	63.345091
C	42.835814	5.596584	56.988823	C	46.419447	6.168363	64.088179
C	42.269183	6.688951	57.672903	C	45.387379	5.478391	63.463260
C	42.528628	3.709132	55.421752	C	43.271369	4.336426	63.580429
O	45.075723	6.394140	57.019367	C	44.303437	5.025398	64.205349
O	44.741876	4.189036	57.352493	O	42.183431	3.908432	64.359519
C	44.303759	5.375059	57.121575	H	12.119159	8.126827	26.936072
C	46.523195	5.695406	61.350162	H	10.572984	6.786747	25.566706
C	47.554262	6.385378	61.976082	H	13.382156	2.321981	22.983480
C	48.691839	7.084784	47.763546	H	9.847346	3.169311	22.676901
C	47.609526	6.614109	48.497340	H	22.127848	2.839685	28.221483
C	46.616042	5.814794	47.899484	H	24.530822	2.316733	28.282772
C	45.438253	5.242413	62.093251	H	26.022480	3.134894	26.532055
C	44.406185	4.552442	61.467332	H	21.516963	5.321122	24.086791
C	43.323243	4.099449	62.211421	H	23.017612	6.078578	22.355810
C	44.515454	4.588341	48.020908	H	19.533170	2.330412	22.589857
C	45.510637	5.347289	48.652384	H	19.680014	1.794584	20.190457
O	43.424196	4.139520	48.756095	H	18.480979	3.170983	18.536721
O	46.919520	6.442019	59.121962	H	16.652823	6.145242	22.827204
O	46.573993	4.237901	59.463246	H	15.507812	7.502163	21.163761
C	46.675103	5.443060	59.890815	H	14.495470	7.508172	27.087708
C	16.262162	6.620790	63.347051	H	27.609840	8.064586	26.968306
C	15.179196	6.168795	64.090104	H	26.115919	6.563608	25.761577
C	14.147156	5.478812	63.465153	H	14.941302	3.633425	24.314678
C	12.031150	4.336833	63.582254	H	29.119970	2.158596	23.171370
C	13.063191	5.025817	64.207206	H	19.787995	6.917214	30.337297
O	10.943187	3.908837	64.361307	H	15.677665	4.562373	29.264687
C	31.882275	6.620600	63.346211	H	13.759583	3.870709	30.560534
C	30.799322	6.168606	64.089282	H	15.672801	6.862041	17.596254
C	29.767267	5.478629	63.464346	H	25.148264	6.261100	21.550605
C	27.651260	4.336658	63.581482	H	25.597704	2.533464	23.003070

H	37.751162	2.964211	28.293605	H	50.949458	7.231720	30.274378
H	40.131831	2.353679	28.362854	H	47.068335	4.470653	29.317530
H	41.619966	2.963043	26.527986	H	45.238778	3.636783	30.655271
H	37.165643	5.168665	24.006466	H	46.905492	6.856629	17.596458
H	38.663895	5.718240	22.190857	H	56.056663	5.972847	21.101661
H	35.151163	2.330450	22.590854	H	10.790666	8.127121	42.499746
H	35.299188	1.794023	20.190321	H	9.244381	6.786934	41.130428
H	34.100286	3.170644	18.536512	H	12.054227	2.324769	38.543663
H	32.264504	6.143031	22.826101	H	8.520773	3.174742	38.234340
H	31.125346	7.500398	21.163796	H	20.656016	2.469458	43.583413
H	30.020416	7.596023	27.090474	H	23.025897	1.823598	43.675194
H	43.100826	7.731899	27.013706	H	24.608959	2.680807	42.028320
H	41.670889	6.243968	25.726625	H	20.280690	5.174019	39.562798
H	30.636782	3.610062	24.385483	H	21.877963	5.985530	37.942717
H	44.806410	1.907836	23.171351	H	17.976786	2.198157	37.880896
H	35.799145	6.663525	30.288487	H	17.985696	1.759402	35.461618
H	31.373892	4.900252	29.377816	H	16.854199	3.274079	33.925082
H	29.362648	4.657996	30.707795	H	15.241374	6.173274	38.402738
H	31.288110	6.858506	17.596666	H	14.090991	7.633516	36.841942
H	40.789716	5.770258	21.353139	H	13.169407	7.506551	42.649954
H	41.288191	2.253638	22.889256	H	25.768220	6.972946	43.834584
H	53.552127	3.700083	28.381371	H	24.521602	5.884857	42.057171
H	55.987740	3.326273	28.455788	H	13.612236	3.636038	39.861593
H	57.384073	3.866388	26.498019	H	28.141947	2.531529	38.647279
H	52.703541	5.453680	24.016083	H	18.620588	6.713812	45.769884
H	54.081156	5.977629	22.117498	H	19.596948	7.445477	32.732251
H	50.777317	2.334859	22.589463	H	17.666041	6.687190	34.017422
H	50.920660	1.795085	20.189814	H	14.425301	4.445231	44.834398
H	49.720320	3.170696	18.535982	H	12.514193	3.845953	46.183381
H	47.864072	6.134779	22.823826	H	12.724174	3.703506	32.591798
H	46.741772	7.497709	21.163581	H	14.099991	7.293500	33.311977
H	45.515651	7.316576	27.169424	H	24.052959	6.207354	37.276470
H	46.268662	3.356959	24.458276	H	24.742275	2.714281	38.128101

H 36.303182 2.252371 43.048322	H 45.167161 7.547128 36.808919
H 38.701615 1.512373 43.022659	H 44.137991 7.311019 42.773900
H 40.296129 2.516555 41.459227	H 45.052389 3.611694 39.761507
H 35.961879 5.406728 39.412756	H 49.661435 7.132278 45.860374
H 37.514950 6.310516 37.753885	H 50.733735 7.805095 32.657226
H 33.111757 2.753270 38.231717	H 48.891827 6.909206 33.984928
H 33.118811 2.141318 35.801358	H 45.698879 4.507722 44.853648
H 32.328048 3.721990 34.122718	H 43.822423 3.742806 46.169493
H 31.387925 7.241502 38.367334	H 44.238280 3.437018 32.701881
H 30.470557 8.809968 36.677152	H 45.266051 7.150642 33.286705
H 28.244952 6.705342 44.005084	H 54.726277 5.964590 36.662270
H 41.710196 7.658881 42.617085	H 9.463471 8.127242 58.062677
H 40.343784 6.230804 41.196235	H 7.917013 6.786968 56.693503
H 29.414410 3.698987 40.416622	H 10.726750 2.324424 54.107290
H 43.652037 2.236156 38.327263	H 7.193971 3.176463 53.795181
H 34.376731 7.577521 45.763745	H 19.525093 2.917590 59.293808
H 35.744061 7.305928 32.662438	H 21.924738 2.374128 59.313640
H 33.725447 6.968110 33.990486	H 23.383992 3.143404 57.514614
H 30.826763 4.430364 44.827419	H 18.852991 5.373979 55.157456
H 28.948574 3.522712 46.090199	H 20.320611 6.078516 53.373652
H 28.321302 4.836971 32.737796	H 16.893904 2.425625 53.515113
H 30.260555 8.226292 33.284489	H 16.951229 1.942306 51.107131
H 39.632050 6.485877 37.101966	H 15.780258 3.378383 49.528904
H 40.127375 2.540768 37.982456	H 14.056655 6.347416 53.920669
H 52.223553 3.704450 43.946028	H 12.892203 7.743768 52.314430
H 54.659162 3.326903 44.019411	H 11.840840 7.509112 58.212090
H 56.055345 3.866258 42.061246	H 24.920988 7.968486 58.064840
H 51.374898 5.455144 39.580821	H 23.438719 6.513772 56.793396
H 52.752355 5.977675 37.680876	H 12.284929 3.636004 55.428338
H 49.653585 2.628247 37.995229	H 26.460596 2.201131 54.071655
H 49.760225 2.162369 35.584267	H 17.168637 6.738882 61.410809
H 48.471038 3.498193 34.007572	H 18.493200 7.302635 48.153202
H 46.448329 6.252366 38.410675	H 16.556877 6.653796 49.487073

H	13.129886	4.375280	60.400688	H	50.047733	5.460083	55.146221
H	11.278530	3.573284	61.719392	H	51.424943	5.978593	53.243684
H	11.508991	3.772563	48.234503	H	48.399592	2.732237	53.478118
H	12.949052	7.325522	48.793932	H	48.476268	2.271325	51.065939
H	22.432863	6.212315	52.510688	H	47.116379	3.564350	49.516506
H	22.939559	2.581520	53.895015	H	45.130063	6.290326	53.954363
H	35.139653	3.087928	59.382842	H	43.789093	7.554547	52.376027
H	37.526131	2.492298	59.415498	H	42.896660	7.342608	58.268620
H	38.982316	3.114189	57.559103	H	43.589937	3.493204	55.383473
H	34.488848	5.356362	55.141244	H	48.405632	6.744712	61.407899
H	35.953705	5.915608	53.300840	H	49.441028	7.708395	48.240627
H	32.683025	2.534190	53.561862	H	47.545915	6.891982	49.540645
H	32.931713	2.103525	51.156022	H	44.382265	4.363741	60.399533
H	31.817932	3.523762	49.522025	H	42.520045	3.570487	61.717812
H	29.677439	6.342710	53.830312	H	42.791572	3.579309	48.204113
H	28.556004	7.709026	52.160957	H	43.823712	7.153949	48.854153
H	27.329938	7.501859	58.181569	H	53.398323	5.962111	52.223839
H	40.488060	7.792878	58.140667	H	17.068432	7.157664	63.836093
H	39.032715	6.367301	56.813869	H	15.148320	6.357113	65.155593
H	27.970911	3.615792	55.336811	H	10.261871	3.422767	63.797768
H	42.098175	2.091864	54.080124	H	32.688170	7.158104	63.835112
H	32.787754	6.740463	61.409645	H	30.768185	6.357209	65.154692
H	34.088437	8.152666	48.188674	H	25.878843	3.428365	63.795764
H	32.275526	7.157092	49.496215	H	48.307461	7.159245	63.833714
H	28.750420	4.374011	60.400069	H	46.387892	6.357470	65.153466
H	26.898505	3.573238	61.718568	H	41.497433	3.430873	63.794145
H	27.936718	3.375786	48.062979	H	54.922567	4.682846	55.325478
H	28.731063	7.222937	48.647949	H	56.250101	4.683220	39.763356
H	38.060431	5.949432	52.412877	H	57.578915	4.683550	24.200270
H	38.580999	2.474050	53.852663	H	32.654261	5.043700	18.026448
H	50.894972	3.699559	59.506234	H	17.034621	5.043815	18.026611
H	53.331514	3.325299	59.581218	H	10.176491	4.915057	24.089421
H	54.727814	3.865552	57.623269	H	8.847860	4.915122	39.653415

H	7.520401	4.915037	55.216677	H	30.363639	8.166258	45.361626
H	12.998593	5.198764	65.269045	H	29.690296	8.214552	42.965295
H	28.618469	5.198756	65.268177	H	29.045067	9.624832	42.289282
H	44.238356	5.198674	65.267044				
H	48.274031	5.043552	18.025976				
C	31.753376	8.907526	41.007037	(R,R)-2-Int1(QM(B3LYP)/MM)			
C	31.811583	9.287648	42.430664	C	12.487000	7.261000	26.395000
C	32.268290	10.653124	42.846404	C	11.616000	6.503000	25.622000
C	31.958905	11.745848	41.811579	C	12.086000	5.395000	24.927000
C	32.336584	11.307626	40.389282	C	13.428000	5.043000	25.007000
C	31.581698	10.032137	39.990446	C	13.027000	3.179000	23.539000
O	33.102891	8.561755	41.240503	C	11.685000	3.529000	23.460000
C	29.364785	9.776949	44.304600	C	11.215000	4.638000	24.154000
C	28.693914	11.005227	44.445723	O	10.782000	2.793000	22.654000
C	28.492768	11.559966	45.712487	Cu	18.543389	6.093520	26.011808
C	28.961513	10.906025	46.856921	Cu	17.953971	3.705471	26.529203
C	29.634516	9.686328	46.719141	C	22.219053	3.968720	26.386829
C	29.834880	9.119605	45.457844	C	22.758962	3.211516	27.442034
N	29.635790	9.245504	43.028853	C	24.114194	2.908019	27.481615
H	31.824190	10.887457	43.830793	C	24.954265	3.348633	26.464252
H	31.874953	8.471424	43.145930	C	24.452113	4.081250	25.371842
H	31.111681	8.041310	40.779563	C	23.064379	4.379308	25.317552
H	32.488513	12.674763	42.089006	C	22.554478	5.044938	24.182159
H	30.876970	11.981857	41.844455	C	23.405523	5.444627	23.156624
H	32.115080	12.115137	39.668483	C	24.773257	5.194055	23.228558
H	33.424232	11.117638	40.335496	C	25.307941	4.502928	24.324206
H	30.497905	10.247392	39.895668	O	25.611528	5.596432	22.194616
H	31.920804	9.662197	39.006656	O	20.435204	5.531625	26.186759
H	33.357917	10.583815	43.022608	O	19.917759	3.385421	26.652888
H	28.323570	11.524379	43.554589	C	20.771687	4.315563	26.418487
H	27.962512	12.513805	45.802263	C	18.226927	4.022014	22.293999
H	28.805122	11.340525	47.848621	C	18.992915	2.941012	21.873981
H	30.017409	9.170324	47.605141	C	19.081890	2.638017	20.519979
				C	18.404876	3.417023	19.587993

C	17.639888	4.497024	20.008011	Cu	33.584785	3.688078	26.554784
C	17.550913	4.800019	21.362013	C	37.839710	3.949002	26.405318
C	16.783924	5.881020	21.784030	C	38.362469	3.237486	27.500731
C	16.107910	6.659026	20.850045	C	39.707458	2.896101	27.554433
C	16.197885	6.355031	19.497042	C	40.554268	3.250257	26.510314
C	16.963875	5.274030	19.076025	C	40.070124	3.940205	25.382336
O	15.523872	7.185037	18.539057	C	38.692505	4.281332	25.316938
O	18.565768	5.532734	24.109215	C	38.199412	4.911047	24.155116
O	18.026774	3.391676	24.575316	C	39.058031	5.226056	23.106213
C	18.266858	4.338639	23.745095	C	40.417656	4.933222	23.186189
C	14.301000	5.801000	25.782000	C	40.936107	4.283011	24.314717
C	13.829000	6.909000	26.476000	O	41.264380	5.259399	22.132544
C	27.983603	7.128254	26.428545	O	36.054710	5.515562	26.161815
C	27.141849	6.260995	25.740761	O	35.544016	3.372797	26.651694
C	27.646938	5.121530	25.081443	C	36.394509	4.302275	26.410990
C	29.042088	4.857007	25.136739	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.704528	2.927036	23.701556	C	34.701781	2.637978	20.519678
C	27.337923	3.147930	23.675939	C	34.024753	3.416989	19.587708
C	26.784049	4.249480	24.366207	C	33.259776	4.496991	20.007741
O	26.565752	2.233356	22.962602	C	33.170826	4.799983	21.361747
O	16.595425	6.406541	25.846065	C	32.403848	5.880986	21.783781
O	16.058107	4.267003	26.318225	C	31.727821	6.658997	20.849810
C	15.736670	5.464001	25.982331	C	31.817771	6.355005	19.496805
C	17.908463	5.833300	30.225366	C	32.583748	5.274002	19.075771
C	18.908446	6.576167	30.878530	O	31.143743	7.185016	18.538835
C	16.746342	5.439795	30.945650	O	34.144575	5.530088	24.122906
C	15.664944	4.790826	30.312393	O	33.635689	3.382650	24.586431
C	14.546055	4.406248	31.045034	C	33.868136	4.332575	23.753903
O	18.430777	6.414945	27.972245	C	29.888974	5.717225	25.890201
O	17.898427	4.270165	28.429535	C	29.343999	6.860397	26.501960
C	18.096819	5.485196	28.791654	C	43.544603	6.867001	26.536788
Cu	34.150830	6.078667	26.030080	C	42.726436	6.007778	25.814562

C	43.255156	4.887901	25.139193	C	52.093032	4.660900	26.379880
C	44.653138	4.637704	25.209532	C	49.466779	4.021876	22.293156
C	29.556695	3.763670	24.410985	C	50.232745	2.940872	21.873104
C	44.354515	2.720668	23.750486	C	50.321669	2.637885	20.519096
C	42.987099	2.937149	23.695284	C	49.644627	3.416901	19.587140
C	42.412146	4.026039	24.388689	C	48.879661	4.496905	20.007192
O	42.235099	2.027064	22.955463	C	48.790737	4.799893	21.361200
O	32.183323	6.385534	25.921334	C	48.023772	5.880897	21.783251
O	31.686099	4.236278	26.389852	C	47.347731	6.658913	20.849295
C	31.338413	5.430921	26.076916	C	47.437655	6.354926	19.496287
C	33.692082	5.814365	30.263540	C	48.203620	5.273922	19.075235
C	34.753652	6.524763	30.853207	O	46.763613	7.184943	18.538331
C	32.546227	5.495874	31.044228	O	49.728668	5.587428	24.094527
C	31.422745	4.853163	30.483990	O	49.389147	3.418678	24.604135
C	30.310402	4.568113	31.271272	C	49.525187	4.365626	23.749813
O	34.092730	6.391453	27.990966	C	45.480619	5.508628	25.970297
O	33.565131	4.248988	28.463869	C	44.907929	6.623419	26.609861
C	33.791871	5.461315	28.821582	C	45.188540	3.554091	24.486034
Cu	49.691371	6.192763	25.991549	O	47.713164	6.319089	25.892417
Cu	49.348445	3.770712	26.559601	O	47.397499	4.147956	26.416162
C	53.571003	4.464792	26.367939	C	46.949843	5.308847	26.096228
C	54.157058	3.947774	27.515902	C	49.186914	5.948110	30.224814
C	55.530059	3.732759	27.559826	C	50.116639	6.801052	30.846542
C	56.316002	4.036762	26.454787	C	48.084368	5.450596	30.974620
C	55.729946	4.554780	25.305823	C	47.065487	4.680804	30.373652
C	54.356947	4.768795	25.262899	C	46.005228	4.196950	31.133553
C	53.770890	5.287813	24.113936	O	49.599567	6.540952	27.949839
C	54.557834	5.591815	23.007897	O	49.299883	4.361840	28.452845
C	55.929834	5.377800	23.052821	C	49.381545	5.596779	28.791855
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.633905	5.831480	26.128575	C	10.757253	5.394976	40.491133
O	51.338818	3.650684	26.629128	C	12.099253	5.042971	40.571108

C	11.698221	3.178978	39.103109	C	16.885806	4.304917	39.172206
C	10.356221	3.528983	39.024134	C	12.972270	5.800966	41.346096
C	9.886237	4.637982	39.718146	C	12.500286	6.908965	42.040108
O	9.453204	2.792989	38.218147	C	26.265794	6.458305	43.049293
Cu	17.246459	6.010552	41.467935	C	25.586300	5.828153	42.029322
Cu	16.616358	3.630615	41.961735	C	26.244465	4.959156	41.098373
C	20.885131	3.770470	41.751175	C	27.672615	4.790913	41.245811
C	21.367964	2.896405	42.743166	C	12.571237	3.934972	39.877096
C	22.709238	2.539352	42.792047	C	27.667256	3.313901	39.311664
C	23.598405	3.054094	41.856042	C	26.260673	3.455196	39.170564
C	23.160873	3.915274	40.833268	C	25.541179	4.266923	40.043903
C	21.780681	4.246864	40.750714	O	25.749980	2.719340	38.141301
C	21.331456	5.014432	39.656377	O	15.291573	6.378441	41.369245
C	22.235898	5.489443	38.711198	O	14.728670	4.244833	41.830724
C	23.598560	5.231707	38.835312	C	14.416135	5.452053	41.523041
C	24.074505	4.447532	39.892491	C	16.744720	5.709265	45.695745
O	24.488130	5.727502	37.890685	C	17.777188	6.444907	46.306379
O	19.134645	5.392131	41.580146	C	18.801880	6.882153	32.229114
O	18.569816	3.254360	42.022961	C	17.692395	6.455829	32.951087
C	19.445186	4.163117	41.787528	C	16.652883	5.735620	32.331192
C	16.795854	4.038052	37.712589	C	15.599171	5.348379	46.459571
C	17.461713	2.915397	37.189554	C	14.492765	4.696158	45.875469
C	17.472129	2.666722	35.823759	C	13.388405	4.351198	46.648615
C	16.814929	3.532604	34.956544	C	14.474610	4.648528	32.414505
C	16.106299	4.652887	35.438845	C	15.516823	5.319349	33.068270
C	16.076817	4.897090	36.837484	O	13.352507	4.255403	33.135342
C	15.306234	5.971059	37.326399	O	17.200218	6.302036	43.433950
C	14.624472	6.803518	36.447957	O	16.632888	4.164064	43.877507
C	14.679186	6.602331	35.078762	C	16.871717	5.369033	44.251384
C	15.428448	5.527509	34.549120	Cu	33.687550	6.758913	41.515715
O	13.992410	7.514611	34.280656	Cu	32.444789	4.139643	42.157863
O	17.208464	5.486550	39.554994	C	36.602564	3.596623	41.569473
O	16.634906	3.348598	39.990596	C	37.047761	2.706403	42.529742

C	38.398272	2.288530	42.538061	C	43.237707	2.782589	39.014468
C	39.285136	2.762237	41.595221	C	41.863404	2.935432	38.934974
C	38.866149	3.648871	40.549776	C	41.228366	3.964469	39.656458
C	37.481592	4.043561	40.525011	O	41.169165	2.030025	38.137271
C	37.030192	4.847512	39.439267	O	30.435031	6.509806	42.840357
C	37.892035	5.262140	38.453015	O	30.469489	4.352328	42.294948
C	39.273926	4.945249	38.513748	C	29.859414	5.447740	42.482595
C	39.765661	4.151335	39.548182	C	32.714644	6.308235	45.750183
O	40.118572	5.425059	37.558305	C	33.559339	7.220633	46.359749
O	35.091729	5.398961	41.500158	C	34.716833	6.881761	32.194380
O	34.281870	3.388092	42.059483	C	33.610516	6.552622	32.968709
C	35.217250	4.159933	41.711119	C	32.511243	5.869811	32.415015
C	32.400957	4.513250	37.986982	C	31.612951	5.738072	46.482601
C	32.894204	3.275108	37.604598	C	30.672308	4.845631	45.889837
C	32.929125	2.911376	36.243351	C	29.599357	4.360557	46.596903
C	32.435888	3.765305	35.280334	C	30.283144	4.915132	32.619946
C	31.873668	5.038867	35.617224	C	31.372790	5.573398	33.197913
C	31.875599	5.420806	37.007530	O	29.160703	4.635709	33.388716
C	31.310872	6.680507	37.360685	O	33.432282	6.855291	43.553528
C	30.762090	7.503496	36.410563	O	32.759079	4.749237	43.980323
C	30.752770	7.135318	35.039488	C	32.988056	5.948764	44.309766
C	31.312508	5.928704	34.633553	Cu	48.378076	6.249313	41.563076
O	30.173551	8.073144	34.229086	Cu	48.030271	3.810421	42.058321
O	32.754005	5.997707	39.836022	C	52.242278	4.464620	41.931334
O	32.244439	3.849431	40.232932	C	52.828353	3.947597	43.079285
C	32.463642	4.830207	39.457103	C	54.201353	3.732577	43.123183
C	28.361389	5.488723	42.296167	C	54.987278	4.036581	42.018131
C	27.658029	6.294195	43.181098	C	54.401203	4.554604	40.869180
C	42.160701	6.755857	41.956308	C	53.028203	4.768624	40.826281
C	41.402597	5.886981	41.180528	C	52.442128	5.287648	39.677330
C	42.002930	4.828628	40.468548	C	53.229054	5.591652	38.571278
C	43.408563	4.644430	40.564644	C	54.601054	5.377632	38.616177
C	28.352324	3.954698	40.310978	C	55.187129	4.858609	39.764128

O	55.314970	5.617639	37.405129	C	46.905324	5.251601	33.120489
O	50.321621	5.864246	41.710638	O	44.865523	3.969327	33.246355
O	50.008401	3.678521	42.180243	O	48.269408	6.541011	43.523442
C	50.769704	4.684382	41.948127	O	47.929318	4.355151	43.969579
C	48.260021	4.218727	37.810204	C	48.029922	5.581112	44.339391
C	49.063098	3.175131	37.316882	C	9.830848	7.260896	57.522290
C	49.131607	2.911493	35.955735	C	8.959816	6.502907	56.749315
C	48.397195	3.683217	35.062134	C	9.429783	5.394908	56.054291
C	47.556745	4.722666	35.512092	C	10.771783	5.042898	56.134241
C	47.470661	4.982074	36.906346	C	10.370718	3.178911	54.666243
C	46.575115	5.970646	37.361476	C	9.028718	3.528920	54.587293
C	45.829113	6.713634	36.455602	C	8.558750	4.637919	55.281317
C	45.932779	6.498226	35.091642	O	8.125684	2.792932	53.781319
C	46.800726	5.499610	34.594697	Cu	15.890937	6.152073	57.134072
O	45.170088	7.320668	34.264985	Cu	15.350561	3.735115	57.547093
O	48.435434	5.717102	39.652394	C	19.606234	4.078938	57.423649
O	48.139515	3.524168	40.090219	C	20.167493	3.307747	58.457181
C	48.279383	4.502127	39.270350	C	21.524124	3.008142	58.467320
C	44.173061	5.516298	41.389230	C	22.343913	3.465943	57.441033
C	43.532994	6.576172	42.055936	C	21.820561	4.217087	56.371228
C	44.013812	3.622237	39.805885	C	20.431480	4.513705	56.348562
O	46.395742	6.375343	41.440768	C	19.899497	5.201674	55.237208
O	46.088763	4.181704	41.868088	C	20.730187	5.620758	54.202826
C	45.638884	5.347380	41.575569	C	22.099410	5.370500	54.243598
C	47.843017	5.913485	45.777117	C	22.656475	4.659666	55.315535
C	48.792428	6.741465	46.404061	O	22.917148	5.795124	53.202212
C	50.001697	7.120485	32.193710	O	17.795326	5.620464	57.298377
C	48.953116	6.598301	32.943657	O	17.317985	3.445430	57.663349
C	47.982924	5.763832	32.356216	C	18.154166	4.401108	57.474831
C	46.719350	5.453300	46.517616	C	15.683846	4.229100	53.319381
C	45.689298	4.702307	45.913208	C	16.391935	3.114410	52.834791
C	44.605668	4.259136	46.665427	C	16.444036	2.837277	51.476228
C	45.929582	4.460833	32.498558	C	15.782664	3.663002	50.575130

C	15.039333	4.778335	51.013910	C	14.418821	5.321964	48.615715
C	14.977329	5.059593	52.406149	O	12.241413	4.293413	48.769064
C	14.180728	6.133981	52.849200	O	15.753926	6.386484	59.109254
C	13.506683	6.932604	51.933839	O	15.284370	4.211205	59.473953
C	13.584774	6.689727	50.572399	C	15.446097	5.414616	59.891138
C	14.352394	5.606673	50.086962	Cu	31.486666	6.231051	57.150008
O	12.898779	7.568572	49.736670	Cu	30.971762	3.799755	57.513766
O	15.947136	5.673073	55.203853	C	35.215240	4.161427	57.458876
O	15.447229	3.505098	55.575162	C	35.755978	3.424542	58.528160
C	15.691024	4.486267	54.785269	C	37.101005	3.079531	58.548821
C	11.644816	5.800887	56.909216	C	37.928540	3.453997	57.496235
C	11.172849	6.908886	57.603240	C	37.426456	4.175386	56.395705
C	25.327078	7.165495	57.563765	C	36.049885	4.524886	56.366659
C	24.488938	6.341543	56.821684	C	35.538488	5.192970	55.234484
C	24.997634	5.246696	56.093024	C	36.378143	5.534032	54.178664
C	26.394647	4.986281	56.127767	C	37.736543	5.228427	54.221676
C	11.243751	3.934900	55.440217	C	38.272955	4.541309	55.319726
C	26.062171	3.149671	54.575063	O	38.564307	5.579470	53.161406
C	24.693759	3.363296	54.568568	O	33.401421	5.705562	57.299300
C	24.135793	4.415517	55.329449	O	32.933126	3.525353	57.648006
O	23.923925	2.487298	53.806101	C	33.764716	4.486566	57.478968
O	13.936151	6.437457	56.972400	C	31.380760	4.380980	53.300285
O	13.440616	4.273490	57.366409	C	32.151546	3.305174	52.823510
C	13.092576	5.477597	57.083334	C	32.281881	3.068128	51.462762
C	15.283046	5.695821	61.352095	C	31.635802	3.894182	50.551416
C	16.314087	6.385804	61.978046	C	30.826813	4.965360	50.981399
C	17.714209	6.784473	47.651397	C	30.691029	5.211773	52.374140
C	16.614453	6.403631	48.411549	C	29.845125	6.255207	52.801117
C	15.546131	5.687492	47.838707	C	29.184280	7.048851	51.868803
C	14.198081	5.242825	62.095148	C	29.321910	6.826944	50.508516
C	13.166040	4.552842	61.469196	C	30.147437	5.783872	50.047679
C	12.083075	4.099846	62.213249	O	28.629590	7.678390	49.650777
C	13.352755	4.642887	48.009914	O	31.545632	5.797600	55.211537

O	31.094450	3.611454	55.536815	C	51.500923	3.947364	58.641689
C	31.330960	4.612254	54.768816	C	52.873923	3.732339	58.685563
C	27.238859	5.802148	56.931129	C	53.659830	4.036343	57.580498
C	26.688122	6.899390	57.617963	C	53.073736	4.554373	56.431559
C	40.930188	6.980598	57.641697	C	51.700736	4.768398	56.388685
C	40.098676	6.176687	56.873636	C	51.114643	5.287428	55.239746
C	40.608196	5.083612	56.141786	C	51.901549	5.591433	54.133681
C	42.002423	4.808381	56.194302	C	53.273549	5.377407	54.178555
C	26.912722	3.943681	55.334120	C	53.859642	4.858378	55.326493
C	41.670250	2.978257	54.635155	O	53.987445	5.617415	52.967495
C	40.305265	3.213789	54.601516	O	48.994031	5.859112	57.300907
C	39.748497	4.271350	55.356045	O	48.672766	3.655533	57.670916
O	39.536428	2.348147	53.826582	C	49.438759	4.672150	57.498439
O	29.519373	6.500439	57.009755	C	46.976405	4.354199	53.320191
O	29.061839	4.315213	57.329232	C	47.809487	3.339161	52.816432
C	28.692455	5.522107	57.095369	C	47.859826	3.067710	51.456936
C	30.903120	5.695641	61.351269	C	47.075499	3.801700	50.575347
C	31.934175	6.385618	61.977205	C	46.213289	4.819654	51.034925
C	33.380743	7.566876	47.717600	C	46.150914	5.090760	52.428275
C	32.346015	7.023798	48.449251	C	45.240954	6.059717	52.894900
C	31.414082	6.105834	47.863547	C	44.450633	6.768894	51.999240
C	29.818167	5.242646	62.094340	C	44.526270	6.540006	50.635051
C	28.786113	4.552669	61.468405	C	45.412509	5.562609	50.127262
C	27.703159	4.099675	62.212476	O	43.725148	7.335733	49.818944
C	29.407904	4.702159	47.959470	O	47.126635	5.800595	55.213524
C	30.306966	5.554450	48.596751	O	46.814793	3.593791	55.565398
O	28.345225	4.190699	48.641908	C	46.971718	4.599527	54.785634
O	31.359405	6.423889	59.124702	C	42.843610	5.620610	57.003138
O	30.889138	4.241855	59.448579	C	42.287920	6.707193	57.704547
C	31.055058	5.437257	59.887529	C	42.519619	3.760248	55.408545
Cu	47.055601	6.252104	57.150191	O	45.084245	6.406028	57.023421
Cu	46.687134	3.796558	57.534986	O	44.742369	4.200949	57.352264
C	50.914829	4.464394	57.493750	C	44.309262	5.389775	57.126301

C	46.523195	5.695406	61.350162	H	10.573047	6.786874	25.566268
C	47.554262	6.385378	61.976082	H	13.383775	2.323335	22.982404
C	48.669936	7.080524	47.744773	H	9.847477	3.169806	22.676771
C	47.593802	6.603552	48.483786	H	22.118752	2.869614	28.247310
C	46.608508	5.788274	47.893483	H	24.518066	2.332301	28.308675
C	45.438253	5.242413	62.093251	H	26.004815	3.098963	26.529412
C	44.406185	4.552442	61.467332	H	21.496872	5.253186	24.061004
C	43.323243	4.099449	62.211421	H	22.990816	5.956528	22.298788
C	44.520079	4.542606	48.026351	H	19.532554	2.329888	22.589875
C	45.509528	5.314006	48.651540	H	19.679466	1.794166	20.190511
O	43.434657	4.088387	48.766789	H	18.480535	3.170829	18.536728
O	46.924559	6.444489	59.124241	H	16.650717	6.144995	22.827083
O	46.573256	4.240688	59.462164	H	15.506774	7.500891	21.165215
C	46.676061	5.444947	59.891076	H	14.495640	7.508514	27.087169
C	16.262162	6.620790	63.347051	H	27.576521	8.009426	26.914446
C	15.179196	6.168795	64.090104	H	26.088038	6.499509	25.711312
C	14.147156	5.478812	63.465153	H	14.941499	3.633926	24.311686
C	12.031150	4.336833	63.582254	H	29.107495	2.085994	23.153302
C	13.063191	5.025817	64.207206	H	19.784506	6.905371	30.331298
O	10.943187	3.908837	64.361307	H	15.659808	4.584151	29.247356
C	31.882275	6.620600	63.346211	H	13.730909	3.908408	30.537550
C	30.799322	6.168606	64.089282	H	15.672144	6.861259	17.596350
C	29.767267	5.478629	63.464346	H	25.118308	6.106799	21.477506
C	27.651260	4.336658	63.581482	H	25.584261	2.452958	22.972851
C	28.683314	5.025635	64.206417	H	37.715029	2.954746	28.323107
O	26.563309	3.908663	64.360554	H	40.097049	2.354599	28.410993
C	47.502389	6.620356	63.345091	H	41.595829	2.968218	26.584743
C	46.419447	6.168363	64.088179	H	37.149715	5.158641	24.035325
C	45.387379	5.478391	63.463260	H	38.656877	5.710535	22.226325
C	43.271369	4.336426	63.580429	H	35.149560	2.328663	22.590600
C	44.303437	5.025398	64.205349	H	35.298571	1.793555	20.190385
O	42.183431	3.908432	64.359519	H	34.099980	3.170601	18.536509
H	12.119285	8.127201	26.935565	H	32.264388	6.143607	22.826049

H	31.124884	7.499551	21.165199	H	20.692599	2.499996	43.493067
H	29.984275	7.537658	27.055513	H	23.065436	1.867446	43.567013
H	43.118749	7.729762	27.039544	H	24.638201	2.760875	41.928679
H	41.671264	6.237229	25.775561	H	20.281302	5.240086	39.502123
H	30.617458	3.545754	24.364095	H	21.866112	6.074272	37.879456
H	44.772461	1.885919	23.203926	H	17.989931	2.239113	37.851888
H	35.620664	6.795682	30.261137	H	17.998644	1.801655	35.432764
H	31.381611	4.573145	29.436076	H	16.848519	3.307295	33.900005
H	29.460912	4.073308	30.819640	H	15.204840	6.176272	38.386112
H	31.292527	6.861345	17.596311	H	14.037777	7.627533	36.831459
H	40.785835	5.756352	21.396299	H	13.169655	7.507824	42.648372
H	41.252512	2.241812	22.949648	H	25.722438	7.095877	43.754322
H	53.552012	3.699277	28.381064	H	24.510252	6.010731	41.951253
H	55.987668	3.325945	28.455683	H	13.612105	3.635520	39.860889
H	57.384055	3.866280	26.497847	H	28.187165	2.674809	38.593219
H	52.703431	5.453208	24.015550	H	18.641579	6.749789	45.727437
H	54.081130	5.976275	22.116913	H	19.586663	7.447753	32.721747
H	50.777430	2.334662	22.589226	H	17.644033	6.707761	34.001881
H	50.920806	1.795194	20.189784	H	14.456386	4.454503	44.818670
H	49.720316	3.170916	18.535937	H	12.554338	3.848085	46.178404
H	47.863593	6.134730	22.823902	H	12.689007	3.750906	32.566674
H	46.741225	7.496811	21.164949	H	14.042770	7.295310	33.300404
H	45.532698	7.307649	27.172772	H	24.037612	6.320039	37.208439
H	46.250802	3.339034	24.465794	H	24.795737	2.846005	38.025942
H	50.944516	7.207905	30.277154	H	36.353457	2.359854	43.299583
H	47.062839	4.453540	29.313071	H	38.745844	1.597981	43.313215
H	45.237885	3.607230	30.650554	H	40.329894	2.438627	41.644028
H	46.912818	6.861624	17.595799	H	35.982281	5.139046	39.381878
H	56.056080	5.976926	21.104118	H	37.515748	5.867305	37.619347
H	10.790733	8.127451	42.499273	H	33.264597	2.591068	38.371162
H	9.244367	6.786863	41.130211	H	33.344565	1.941527	35.951135
H	12.055629	2.325628	38.543218	H	32.472726	3.440852	34.235176
H	8.519225	3.170850	38.239933	H	31.323341	6.988509	38.405253

H	30.318940	8.465942	36.680812	H	45.273877	7.103049	33.288669
H	28.191235	6.793211	43.993925	H	54.726131	5.971183	36.665528
H	41.679442	7.573057	42.484553	H	9.463348	8.127006	58.062993
H	40.336178	6.062003	41.128765	H	7.916914	6.786641	56.693639
H	29.429056	3.813474	40.400290	H	10.728123	2.325207	54.106956
H	43.709470	1.996654	38.439246	H	7.191270	3.169558	53.804778
H	34.375136	7.656900	45.778011	H	19.542027	2.948064	59.266204
H	35.549122	7.420529	32.636909	H	21.944494	2.419420	59.276724
H	33.615073	6.848990	34.010125	H	23.395492	3.215591	57.481362
H	30.810133	4.532759	44.859119	H	18.839984	5.414036	55.142854
H	28.887356	3.686643	46.105251	H	20.298463	6.148230	53.363014
H	28.468896	4.103782	32.881490	H	16.913168	2.459966	53.524179
H	30.112432	7.780458	33.306432	H	16.999911	1.976332	51.118152
H	39.625957	5.994698	36.945349	H	15.843946	3.411007	49.526069
H	40.174199	2.196549	38.122309	H	14.054072	6.367372	53.900161
H	52.223450	3.702331	43.945401	H	12.903359	7.760250	52.282080
H	54.659057	3.326348	44.019213	H	11.840423	7.509421	58.212278
H	56.055321	3.866127	42.061023	H	24.916885	8.010885	58.107171
H	51.374792	5.454626	39.580183	H	23.434618	6.578548	56.807632
H	52.752274	5.976114	37.680229	H	12.285021	3.636031	55.427623
H	49.651827	2.573195	37.999733	H	26.467671	2.347523	53.972952
H	49.762098	2.107462	35.589351	H	17.168091	6.739963	61.410673
H	48.477939	3.448173	34.010397	H	18.522624	7.346663	48.108486
H	46.424568	6.176575	38.415021	H	16.597916	6.685902	49.455557
H	45.148066	7.474207	36.813551	H	13.130661	4.374603	60.400649
H	44.109177	7.260461	42.668449	H	11.278047	3.574058	61.719337
H	45.086468	3.462416	39.799033	H	11.556584	3.781437	48.233372
H	49.636739	7.121773	45.840404	H	12.988331	7.336319	48.762256
H	50.732228	7.772919	32.661805	H	22.408809	6.314625	52.502438
H	48.895779	6.864321	33.990639	H	22.940997	2.698019	53.835498
H	45.697526	4.457550	44.856372	H	35.120981	3.118205	59.351568
H	43.829150	3.683312	46.180225	H	37.504711	2.514391	59.383103
H	44.246258	3.389665	32.699926	H	38.969288	3.163048	57.541646

H	34.489184	5.453291	55.144055	H	48.405738	6.744655	61.408001
H	35.963473	6.047851	53.321940	H	49.412677	7.717529	48.214813
H	32.666995	2.654141	53.520706	H	47.527928	6.889954	49.524662
H	32.888465	2.239411	51.110517	H	44.381389	4.364423	60.399374
H	31.761695	3.675264	49.499295	H	42.519352	3.571630	61.717689
H	29.668840	6.464707	53.850775	H	42.804775	3.521851	48.218335
H	28.536675	7.848024	52.204680	H	43.803478	7.103566	48.843690
H	27.325200	7.541425	58.215621	H	53.398514	5.969997	52.227413
H	40.519117	7.822964	58.189166	H	17.068200	7.158084	63.836027
H	39.048500	6.428796	56.843717	H	15.148096	6.357229	65.155567
H	27.974724	3.734795	55.272437	H	10.263239	3.421563	63.797160
H	42.074540	2.170883	54.039362	H	32.687835	7.158729	63.835001
H	32.786486	6.743246	61.409436	H	30.767983	6.357274	65.154675
H	34.071529	8.270728	48.193018	H	25.882281	3.423333	63.795946
H	32.237005	7.312322	49.499775	H	48.307555	7.159071	63.833760
H	28.750205	4.373407	60.400223	H	46.387794	6.357265	65.153494
H	26.897947	3.574106	61.718541	H	41.501618	3.424510	63.794521
H	27.849609	3.587537	48.064026	H	54.922541	4.682751	55.325740
H	28.691161	7.395554	48.684166	H	56.250057	4.683068	39.763666
H	38.074596	6.092855	52.443788	H	57.578880	4.683407	24.200650
H	38.559295	2.585624	53.823298	H	32.654301	5.043328	18.026548
H	50.894958	3.700009	59.506335	H	17.034860	5.043593	18.026685
H	53.331565	3.325492	59.581282	H	10.176560	4.915311	24.089593
H	54.727841	3.865705	57.623105	H	8.847985	4.915557	39.653281
H	50.047620	5.459136	55.145109	H	7.520543	4.915521	55.216490
H	51.424884	5.976937	53.242966	H	12.998951	5.198960	65.269033
H	48.425407	2.756239	53.491781	H	28.618830	5.198896	65.268175
H	48.507967	2.281238	51.083255	H	44.238671	5.198790	65.267033
H	47.136189	3.553412	49.525485	H	48.273947	5.043132	18.026076
H	45.116268	6.277523	53.949650	C	31.864299	8.828983	41.151853
H	43.757786	7.514799	52.365255	C	31.514469	9.345404	42.580973
H	42.922458	7.346593	58.307787	C	31.943482	10.794149	42.818626
H	43.579153	3.535562	55.366265	C	31.544877	11.763638	41.696637

C	32.042958	11.255518	40.336768	C	13.027000	3.179000	23.539000
C	31.491432	9.855045	40.055561	C	11.685000	3.529000	23.460000
O	33.205156	8.524209	41.122537	C	11.215000	4.638000	24.154000
C	29.446309	9.581147	44.077774	O	10.782000	2.793000	22.654000
C	28.348747	10.443408	44.020468	Cu	18.542525	6.087424	26.013160
C	27.786758	10.925883	45.207370	Cu	17.946930	3.700374	26.529360
C	28.328490	10.553973	46.441576	C	22.207587	3.946228	26.375600
C	29.429872	9.690979	46.486571	C	22.751385	3.188691	27.428415
C	29.990930	9.193652	45.306457	C	24.103363	2.870497	27.453332
N	30.027739	9.067519	42.837954	C	24.935590	3.297281	26.423832
H	31.591981	11.150142	43.803074	C	24.428604	4.032543	25.335015
H	32.034721	8.680430	43.282423	C	23.043935	4.344279	25.295243
H	31.246504	7.924143	40.961719	C	22.527664	5.011898	24.163730
H	31.953946	12.766449	41.916761	C	23.371138	5.402262	23.128633
H	30.441621	11.886371	41.665996	C	24.737332	5.141057	23.187567
H	31.752364	11.954051	39.530690	C	25.277116	4.446109	24.278393
H	33.147391	11.209748	40.343994	O	25.568939	5.538020	22.146272
H	30.384266	9.909744	39.958232	O	20.432125	5.519217	26.189125
H	31.868013	9.459168	39.097226	O	19.907562	3.373572	26.651305
H	33.045869	10.756168	42.875175	C	20.763745	4.301028	26.416986
H	27.926553	10.736571	43.053124	C	18.226927	4.022014	22.293999
H	26.923665	11.597011	45.161730	C	18.992915	2.941012	21.873981
H	27.894090	10.935525	47.370593	C	19.081890	2.638017	20.519979
H	29.862730	9.401017	47.448706	C	18.404876	3.417023	19.587993
H	30.844070	8.511497	45.347110	C	17.639888	4.497024	20.008011
H	29.991105	7.964320	42.820180	C	17.550913	4.800019	21.362013
H	29.473902	9.406574	42.042783	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
				C	16.963875	5.274030	19.076025
				O	15.523872	7.185037	18.539057
				O	18.565764	5.528932	24.110832
				O	18.018572	3.389292	24.574345
(S,S)-1-RC(QM(B3LYP)/MM)							
C	12.487000	7.261000	26.395000				
C	11.616000	6.503000	25.622000				
C	12.086000	5.395000	24.927000				
C	13.428000	5.043000	25.007000				

C	18.263697	4.336317	23.745359	C	40.397067	4.970711	23.263137
C	14.301000	5.801000	25.782000	C	40.913825	4.292969	24.376148
C	13.829000	6.909000	26.476000	O	41.247308	5.332366	22.224046
C	27.937190	6.993563	26.490419	O	36.006895	5.421845	26.221887
C	27.101427	6.154871	25.761796	O	35.508359	3.260617	26.636880
C	27.610822	5.038279	25.066950	C	36.354175	4.203630	26.434151
C	29.004679	4.769584	25.124748	C	33.846854	4.021972	22.293718
C	13.900000	3.935000	24.313000	C	34.612831	2.940969	21.873683
C	28.677698	2.893924	23.617159	C	34.701781	2.637978	20.519678
C	27.311401	3.116805	23.588879	C	34.024753	3.416989	19.587708
C	26.753116	4.193211	24.314477	C	33.259776	4.496991	20.007741
O	26.543771	2.226391	22.841015	C	33.170826	4.799983	21.361747
O	16.595609	6.404230	25.846134	C	32.403848	5.880986	21.783781
O	16.053890	4.266077	26.320505	C	31.727821	6.658997	20.849810
C	15.735311	5.463150	25.983300	C	31.817771	6.355005	19.496805
C	17.910418	5.830055	30.225920	C	32.583748	5.274002	19.075771
C	18.902715	6.592910	30.868017	O	31.143743	7.185016	18.538835
C	16.758389	5.424499	30.955846	O	34.110983	5.490745	24.164801
C	15.682953	4.754539	30.334260	O	33.613424	3.327250	24.561719
C	14.576240	4.355460	31.077316	C	33.845561	4.302268	23.759290
O	18.429538	6.408568	27.972378	C	29.845153	5.600873	25.915947
O	17.895526	4.264475	28.430331	C	29.295943	6.720240	26.566764
C	18.095087	5.479543	28.792171	C	43.546946	6.888125	26.558517
Cu	34.100133	5.976820	26.091668	C	42.719570	6.020461	25.856779
Cu	33.546614	3.566634	26.534190	C	43.241276	4.898433	25.180190
C	37.803292	3.862929	26.429490	C	44.640801	4.650101	25.234399
C	38.324931	3.122834	27.506448	C	29.524542	3.702561	24.364422
C	39.674339	2.798378	27.563245	C	44.324609	2.721546	23.794309
C	40.526674	3.196115	26.539229	C	42.956903	2.939295	23.751326
C	40.043830	3.912637	25.427694	C	42.389830	4.032634	24.443902
C	38.662511	4.239728	25.360550	O	42.196784	2.028237	23.020970
C	38.172134	4.899464	24.214468	O	32.134060	6.275423	25.977526
C	39.035464	5.254366	23.182464	O	31.645361	4.109397	26.373232

C	31.293683	5.312327	26.097844	C	47.437655	6.354926	19.496287
C	33.554884	5.567024	30.305518	C	48.203620	5.273922	19.075235
C	34.570560	6.296411	30.949639	O	46.763613	7.184943	18.538331
C	32.404246	5.170111	31.043070	O	49.731043	5.590382	24.089256
C	31.313934	4.521786	30.425322	O	49.386591	3.424675	24.608054
C	30.196436	4.158226	31.171285	C	49.525514	4.367965	23.749491
O	34.017509	6.223542	28.063320	C	45.478044	5.528597	25.976309
O	33.505539	4.061391	28.456874	C	44.912155	6.648699	26.612686
C	33.706687	5.264208	28.856958	C	45.167398	3.560372	24.513770
Cu	49.694642	6.203953	25.981906	O	47.714524	6.333944	25.883392
Cu	49.345050	3.786405	26.563918	O	47.394838	4.166266	26.418001
C	53.571003	4.464792	26.367939	C	46.948694	5.326422	26.093908
C	54.157058	3.947774	27.515902	C	49.214742	5.993362	30.217302
C	55.530059	3.732759	27.559826	C	50.165080	6.836179	30.821640
C	56.316002	4.036762	26.454787	C	48.107805	5.528012	30.980337
C	55.729946	4.554780	25.305823	C	47.072432	4.767381	30.396756
C	54.356947	4.768795	25.262899	C	46.005060	4.319540	31.168926
C	53.770890	5.287813	24.113936	O	49.607360	6.564657	27.936186
C	54.557834	5.591815	23.007897	O	49.297661	4.390668	28.455556
C	55.929834	5.377800	23.052821	C	49.390487	5.627654	28.785760
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.636817	5.836790	26.121624	C	10.757253	5.394976	40.491133
O	51.335289	3.660256	26.635779	C	12.099253	5.042971	40.571108
C	52.092879	4.666276	26.380236	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.231399	6.166552	41.485739
C	48.879661	4.496905	20.007192	Cu	16.691357	3.765679	41.988006
C	48.790737	4.799893	21.361200	C	20.952388	4.102856	41.891278
C	48.023772	5.880897	21.783251	C	21.462784	3.354364	42.967701
C	47.347731	6.658913	20.849295	C	22.815061	3.048739	43.048749

C	23.683004	3.472808	42.049106	C	26.042177	3.106299	39.433675
C	23.213693	4.193688	40.935534	C	25.543464	4.289437	39.969795
C	21.829944	4.506660	40.845218	O	25.319026	2.136668	38.797867
C	21.357324	5.175986	39.696982	O	15.267287	6.445146	41.355231
C	22.239960	5.551924	38.687973	O	14.778909	4.291535	41.809893
C	23.600366	5.272065	38.789226	C	14.425147	5.487590	41.503913
C	24.095147	4.587248	39.903098	C	16.686984	5.868967	45.711299
O	24.466599	5.645339	37.769667	C	17.686746	6.644985	46.326572
O	19.140904	5.636473	41.636140	C	18.798406	6.909384	32.216112
O	18.659084	3.481969	42.100479	C	17.698955	6.473477	32.947084
C	19.498344	4.427562	41.877696	C	16.668020	5.730766	32.339378
C	16.908281	4.148872	37.741033	C	15.559869	5.451959	46.473802
C	17.622700	3.051148	37.229448	C	14.480450	4.759980	45.885165
C	17.635583	2.782820	35.867521	C	13.394246	4.359365	46.657372
C	16.933054	3.604115	34.992631	C	14.509674	4.606561	32.445335
C	16.178519	4.699201	35.463213	C	15.543181	5.302493	33.086801
C	16.146622	4.962483	36.858359	O	13.399206	4.199389	33.176240
C	15.330316	6.007166	37.336737	O	17.141042	6.469762	43.449477
C	14.606866	6.795275	36.450943	O	16.644455	4.315452	43.898227
C	14.664000	6.578126	35.084409	C	16.836203	5.529890	44.268447
C	15.456515	5.529230	34.565270	Cu	32.994522	6.219466	41.507627
O	13.936896	7.451104	34.277978	Cu	32.390679	3.780311	42.090976
O	17.246078	5.626724	39.576298	C	36.590500	3.851776	41.775289
O	16.763861	3.468133	40.021338	C	37.095649	2.974948	42.718345
C	16.979278	4.429422	39.198933	C	38.467676	2.641372	42.716303
C	12.972270	5.800966	41.346096	C	39.316417	3.174941	41.771601
C	12.500286	6.908965	42.040108	C	38.841477	4.058511	40.748000
C	26.900087	7.354974	41.728805	C	37.437770	4.386160	40.744947
C	26.014899	6.467734	41.152924	C	36.939675	5.199489	39.686360
C	26.443317	5.213431	40.609427	C	37.776614	5.689917	38.710856
C	27.843503	4.887575	40.716524	C	39.170968	5.423743	38.742225
C	12.571237	3.934972	39.877096	C	39.704793	4.613472	39.742346
C	27.426729	2.805556	39.524218	O	39.984894	5.958971	37.790105

O	34.854871	5.467285	41.730900	C	34.487514	6.593410	32.303307
O	34.313578	3.328315	42.149758	C	33.382131	6.178705	33.037231
C	35.146237	4.241308	41.887507	C	32.327735	5.470578	32.429634
C	32.541435	3.975282	37.867232	C	31.175377	5.414638	46.471619
C	33.164207	2.818815	37.430282	C	30.223871	4.512567	45.914700
C	33.159852	2.493976	36.057338	C	29.202301	3.996958	46.675999
C	32.516631	3.307148	35.147765	C	30.134071	4.423031	32.536510
C	31.815393	4.490086	35.551511	C	31.190949	5.080247	33.174034
C	31.830779	4.820840	36.952965	O	29.002139	4.075563	33.262358
C	31.086498	5.955123	37.389930	O	32.823854	6.523406	43.469065
C	30.370229	6.716017	36.502026	O	32.373804	4.377363	43.966627
C	30.375037	6.419002	35.113634	C	32.490323	5.602707	44.271702
C	31.100274	5.334863	34.629210	Cu	48.434751	6.370174	41.599675
O	29.639722	7.298741	34.370508	Cu	48.009634	3.939838	42.077253
O	32.999901	5.489089	39.633818	C	52.242278	4.464620	41.931334
O	32.381212	3.388578	40.149440	C	52.828353	3.947597	43.079285
C	32.641699	4.313673	39.324323	C	54.201353	3.732577	43.123183
C	28.734854	5.821996	41.343923	C	54.987278	4.036581	42.018131
C	28.272153	7.041211	41.812235	C	54.401203	4.554604	40.869180
C	42.248343	7.066973	42.164670	C	53.028203	4.768624	40.826281
C	41.441602	6.253359	41.377303	C	52.442128	5.287648	39.677330
C	41.990424	5.211121	40.602837	C	53.229054	5.591652	38.571278
C	43.392034	4.981610	40.650791	C	54.601054	5.377632	38.616177
C	28.297305	3.660642	40.149083	C	55.187129	4.858609	39.764128
C	43.124820	3.193711	39.030802	O	55.314970	5.617639	37.405129
C	41.754452	3.390260	38.995259	O	50.363683	5.918653	41.730433
C	41.168510	4.403778	39.779395	O	49.984877	3.741507	42.191240
O	41.013763	2.539926	38.178932	C	50.776134	4.724471	41.959754
O	31.011957	6.460416	41.317562	C	48.261462	4.361747	37.833161
O	30.507012	4.358936	41.933061	C	49.041756	3.297424	37.347131
C	30.190626	5.522139	41.537856	C	49.110771	3.026893	35.987613
C	32.237868	5.996596	45.697938	C	48.397350	3.810684	35.087989
C	33.073815	6.949538	46.255267	C	47.580705	4.872363	35.529842

C	47.497917	5.142814	36.922466	C	10.370718	3.178911	54.666243
C	46.630236	6.159537	37.368886	C	9.028718	3.528920	54.587293
C	45.906924	6.916600	36.456050	C	8.558750	4.637919	55.281317
C	46.004839	6.686693	35.093808	O	8.125684	2.792932	53.781319
C	46.844300	5.659933	34.605734	Cu	15.892968	6.142729	57.136149
O	45.264760	7.522049	34.259602	Cu	15.342553	3.727918	57.550881
O	48.463039	5.850377	39.683049	C	19.596182	4.049004	57.445764
O	48.105744	3.664188	40.108258	C	20.145903	3.287579	58.492711
C	48.275873	4.641797	39.294099	C	21.498340	2.970906	58.510095
C	44.205083	5.794096	41.487390	C	22.324928	3.401685	57.477844
C	43.617248	6.844763	42.213800	C	21.812541	4.143445	56.396012
C	43.945926	3.972842	39.837735	C	20.427916	4.458080	56.366507
O	46.458145	6.567473	41.496548	C	19.906554	5.138157	55.245284
O	46.079300	4.379945	41.898215	C	20.744089	5.529853	54.205583
C	45.667207	5.566326	41.632886	C	22.109711	5.261531	54.252321
C	47.889530	6.016244	45.810684	C	22.655385	4.560008	55.335996
C	48.867773	6.795704	46.454677	O	22.935391	5.660704	53.207340
C	50.064492	7.177783	32.164336	O	17.795438	5.601565	57.302284
C	49.009250	6.689166	32.927129	O	17.305976	3.429565	57.671001
C	48.019271	5.865932	32.357177	C	18.147054	4.380800	57.485050
C	46.741078	5.595430	46.536381	C	15.672654	4.225733	53.323127
C	45.682876	4.900998	45.913051	C	16.391036	3.122388	52.828663
C	44.573872	4.497217	46.650167	C	16.444395	2.858081	51.467413
C	45.939968	4.609255	32.529460	C	15.773020	3.684956	50.574280
C	46.934819	5.389383	33.134332	C	15.016200	4.786675	51.024334
O	44.869592	4.151911	33.289913	C	14.954457	5.055527	52.418725
O	48.346934	6.648317	43.563695	C	14.148597	6.118505	52.872881
O	47.930528	4.471968	43.991887	C	13.461705	6.916044	51.966156
C	48.073018	5.690565	44.371478	C	13.537357	6.683944	50.602706
C	9.830848	7.260896	57.522290	C	14.317024	5.614680	50.106610
C	8.959816	6.502907	56.749315	O	12.835979	7.558850	49.775674
C	9.429783	5.394908	56.054291	O	15.946431	5.663121	55.207716
C	10.771783	5.042898	56.134241	O	15.439279	3.496465	55.578357

C	15.685475	4.477769	54.789083	C	37.104482	3.026058	58.551886
C	11.644816	5.800887	56.909216	C	37.932213	3.401308	57.499829
C	11.172849	6.908886	57.603240	C	37.427568	4.111385	56.393393
C	25.320181	7.087302	57.562744	C	36.047764	4.449190	56.357888
C	24.483751	6.256044	56.827137	C	35.533913	5.101845	55.217932
C	24.992564	5.147505	56.119041	C	36.373790	5.439351	54.160829
C	26.387719	4.881493	56.167094	C	37.734970	5.146970	54.210836
C	11.243751	3.934900	55.440217	C	38.274666	4.476021	55.317243
C	26.056642	3.017635	54.646762	O	38.562265	5.493454	53.148631
C	24.689612	3.238514	54.626318	O	33.392995	5.623980	57.270045
C	24.132462	4.307892	55.363261	O	32.932760	3.452037	57.675122
O	23.919808	2.351463	53.876738	C	33.761011	4.410341	57.473839
O	13.938001	6.433997	56.974302	C	31.292567	4.203845	53.328307
O	13.435895	4.271610	57.369071	C	32.079017	3.141263	52.848250
C	13.091677	5.476171	57.084962	C	32.156501	2.867839	51.489972
C	15.283046	5.695821	61.352095	C	31.441364	3.643642	50.585450
C	16.314087	6.385804	61.978046	C	30.614551	4.698511	51.021314
C	17.613355	6.966731	47.675559	C	30.532137	4.980699	52.411779
C	16.535210	6.527390	48.435102	C	29.667339	6.003458	52.849190
C	15.497084	5.772345	47.856889	C	28.936100	6.744595	51.927235
C	14.198081	5.242825	62.095148	C	29.027887	6.495379	50.567630
C	13.166040	4.552842	61.469196	C	29.866965	5.466761	50.096620
C	12.083075	4.099846	62.213249	O	28.280591	7.310135	49.721557
C	13.351168	4.632851	48.022347	O	31.505664	5.664424	55.203080
C	14.389869	5.348824	48.632746	O	31.066840	3.484791	55.585952
O	12.258733	4.227055	48.780878	C	31.284403	4.468561	54.791596
O	15.757751	6.380853	59.109660	C	27.230054	5.707698	56.961138
O	15.278905	4.207925	59.476736	C	26.679665	6.816680	57.629211
C	15.446069	5.411329	59.892318	C	40.912422	6.963378	57.613821
Cu	31.475437	6.143683	57.134090	C	40.087238	6.142537	56.856625
Cu	30.968605	3.720256	57.557545	C	40.606208	5.047408	56.135021
C	35.213165	4.088514	57.451735	C	42.003667	4.787229	56.187592
C	35.757187	3.361422	58.526081	C	26.906067	3.822600	55.395190

C	41.687121	2.939554	54.645593	O	53.987445	5.617415	52.967495
C	40.319453	3.159325	54.613949	O	48.993600	5.862758	57.303999
C	39.752963	4.218560	55.358905	O	48.671129	3.657919	57.664318
O	39.558297	2.277498	53.849667	C	49.438074	4.674550	57.497699
O	29.508034	6.409143	57.012815	C	46.947820	4.386387	53.312802
O	29.055990	4.230714	57.382881	C	47.750282	3.355876	52.791065
C	28.683562	5.432195	57.125908	C	47.789834	3.104445	51.427243
C	30.903120	5.695641	61.351269	C	47.026989	3.875836	50.558733
C	31.934175	6.385618	61.977205	C	46.195810	4.911382	51.035791
C	32.934022	7.314822	47.611710	C	46.140038	5.158672	52.433875
C	31.951866	6.744489	48.391611	C	45.253475	6.141366	52.917300
C	31.028412	5.787784	47.857184	C	44.486087	6.890165	52.034266
C	29.818167	5.242646	62.094340	C	44.560721	6.688142	50.666025
C	28.786113	4.552669	61.468405	C	45.419644	5.695538	50.140848
C	27.703159	4.099675	62.212476	O	43.787077	7.524832	49.864477
C	29.077385	4.323054	48.051616	O	47.124597	5.814774	55.216127
C	29.975847	5.207607	48.644336	O	46.808865	3.607037	55.556318
O	28.074895	3.770369	48.789806	C	46.961208	4.617631	54.781285
O	31.369050	6.380025	59.108501	C	42.838581	5.614806	56.988591
O	30.903776	4.204736	59.480976	C	42.273123	6.703907	57.678068
C	31.065500	5.409863	59.893188	C	42.529956	3.738087	55.409140
Cu	47.053443	6.257932	57.152866	O	45.079327	6.409849	57.023749
Cu	46.685613	3.801409	57.529222	O	44.741206	4.203887	57.348364
C	50.914829	4.464394	57.493750	C	44.305698	5.391321	57.121131
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.749249	7.121816	47.799068
C	53.073736	4.554373	56.431559	C	47.649461	6.678715	48.524617
C	51.700736	4.768398	56.388685	C	46.635249	5.913480	47.916435
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.492293	4.760308	48.015393

C	45.512655	5.473139	48.660510	H	19.679284	1.794038	20.190523
O	43.380686	4.346379	48.740455	H	18.480436	3.170780	18.536728
O	46.922251	6.446501	59.125910	H	16.651305	6.145384	22.827088
O	46.573344	4.241666	59.459160	H	15.506883	7.500937	21.165313
C	46.675317	5.445521	59.890714	H	14.495570	7.508372	27.087405
C	16.262162	6.620790	63.347051	H	27.526867	7.857178	27.004363
C	15.179196	6.168795	64.090104	H	26.048886	6.398352	25.729606
C	14.147156	5.478812	63.465153	H	14.941481	3.633900	24.311559
C	12.031150	4.336833	63.582254	H	29.084381	2.072655	23.042307
C	13.063191	5.025817	64.207206	H	19.770564	6.931522	30.313506
O	10.943187	3.908837	64.361307	H	15.672276	4.542099	29.270554
C	31.882275	6.620600	63.346211	H	13.766344	3.840225	30.578837
C	30.799322	6.168606	64.089282	H	15.671825	6.861031	17.596382
C	29.767267	5.478629	63.464346	H	25.073412	6.055815	21.436022
C	27.651260	4.336658	63.581482	H	25.562179	2.445292	22.853354
C	28.683314	5.025635	64.206417	H	37.673540	2.805679	28.312928
O	26.563309	3.908663	64.360554	H	40.063209	2.236115	28.406677
C	47.502389	6.620356	63.345091	H	41.571513	2.926503	26.615269
C	46.419447	6.168363	64.088179	H	37.120828	5.139429	24.093373
C	45.387379	5.478391	63.463260	H	38.635873	5.760630	22.314188
C	43.271369	4.336426	63.580429	H	35.145978	2.324667	22.589977
C	44.303437	5.025398	64.205349	H	35.297511	1.792784	20.190416
O	42.183431	3.908432	64.359519	H	34.099656	3.170375	18.536522
H	12.119253	8.127124	26.935677	H	32.269359	6.145498	22.826255
H	10.573026	6.786833	25.566349	H	31.125759	7.500166	21.165188
H	13.383863	2.323359	22.982438	H	29.932039	7.375704	27.150552
H	9.847426	3.169681	22.677075	H	43.126757	7.753836	27.060882
H	22.116529	2.856361	28.241905	H	41.662704	6.244789	25.833650
H	24.510574	2.293495	28.277794	H	30.585317	3.484207	24.319988
H	25.983641	3.035051	26.476981	H	44.736162	1.883112	23.248523
H	21.470970	5.230437	24.053630	H	35.438280	6.628388	30.390605
H	22.951976	5.917118	22.274705	H	31.298914	4.302488	29.362538
H	19.532034	2.329525	22.589957	H	29.370620	3.667145	30.673828

H	31.291862	6.860908	17.596336	H	13.986208	7.597860	36.826445
H	40.768116	5.841706	21.496737	H	13.169153	7.512246	42.644872
H	41.214881	2.246637	23.019625	H	26.535941	8.307953	42.125705
H	53.552015	3.700006	28.381241	H	24.957754	6.749316	41.109118
H	55.987716	3.326086	28.455723	H	13.611953	3.633479	39.869933
H	57.384072	3.866312	26.497839	H	27.774916	1.870469	39.077675
H	52.703478	5.452004	24.014268	H	18.536379	6.992041	45.749462
H	54.081085	5.975911	22.116779	H	19.576824	7.491397	32.699687
H	50.777546	2.334972	22.589378	H	17.651943	6.735132	33.995525
H	50.920908	1.795271	20.189760	H	14.450981	4.530560	44.825409
H	49.720393	3.170972	18.535918	H	12.580306	3.827582	46.183521
H	47.862963	6.134710	22.823776	H	12.740934	3.679166	32.615709
H	46.741246	7.496798	21.165012	H	14.001003	7.228646	33.299357
H	45.543486	7.338724	27.160980	H	24.002767	6.167109	37.040663
H	46.229445	3.345445	24.482426	H	24.380539	2.365390	38.709240
H	50.996742	7.219392	30.241412	H	36.426573	2.563258	43.477954
H	47.063337	4.519527	29.340673	H	38.860548	1.962504	43.479516
H	45.224155	3.736904	30.699256	H	40.376367	2.904538	41.806392
H	46.913303	6.861969	17.595738	H	35.875446	5.432214	39.636612
H	56.056057	5.977090	21.104215	H	37.366695	6.299851	37.896362
H	10.790991	8.128206	42.498255	H	33.668812	2.172336	38.153010
H	9.244458	6.787119	41.129912	H	33.669557	1.588495	35.712817
H	12.055514	2.324702	38.544638	H	32.535349	3.016220	34.092409
H	8.519386	3.171265	38.239647	H	31.070843	6.216276	38.448338
H	20.800329	3.018400	43.757590	H	29.777375	7.570886	36.837890
H	23.194473	2.481254	43.893057	H	28.977032	7.743271	42.264229
H	24.731420	3.220481	42.147182	H	41.809222	7.871952	42.744889
H	20.306085	5.404848	39.554136	H	40.378918	6.455086	41.370935
H	21.853721	6.064944	37.817321	H	29.352795	3.397455	40.208059
H	18.182969	2.407940	37.898247	H	43.557522	2.418457	38.411873
H	18.197162	1.935951	35.485696	H	33.854457	7.403863	45.640937
H	16.968357	3.363320	33.939621	H	35.284303	7.149558	32.787520
H	15.225666	6.223765	38.393759	H	33.349334	6.432332	34.089034

H	30.297615	4.230813	44.864961	H	18.850472	5.366092	55.148176
H	28.475186	3.314289	46.219559	H	20.321161	6.051356	53.357603
H	28.335224	3.555107	32.711086	H	16.921333	2.468861	53.511956
H	29.546103	7.019891	33.446424	H	17.010047	2.007094	51.101073
H	39.461417	6.499516	37.176557	H	15.836984	3.444838	49.522531
H	40.023384	2.729091	38.200282	H	14.025111	6.343673	53.926082
H	52.224080	3.708504	43.947535	H	12.850837	7.734513	52.322852
H	54.659283	3.327770	44.019752	H	11.840446	7.509302	58.212385
H	56.055390	3.866515	42.061173	H	24.910093	7.943110	58.089745
H	51.374553	5.453432	39.580228	H	23.430832	6.498245	56.801671
H	52.752212	5.975828	37.680147	H	12.285070	3.636221	55.427159
H	49.611936	2.683215	38.034856	H	26.462254	2.202078	54.063123
H	49.724158	2.206965	35.627370	H	17.168253	6.739582	61.410662
H	48.476694	3.568412	34.037793	H	18.398230	7.558203	48.136903
H	46.485296	6.378077	38.420710	H	16.510933	6.795042	49.482905
H	45.248357	7.699745	36.807142	H	13.129062	4.375840	60.400594
H	44.231295	7.484799	42.837283	H	11.277864	3.574436	61.719240
H	45.012597	3.777796	39.801904	H	11.594695	3.692601	48.241063
H	49.731343	7.147496	45.901867	H	12.922057	7.332259	48.799517
H	50.810497	7.822623	32.618374	H	22.437730	6.183663	52.502420
H	48.962619	6.972696	33.970034	H	22.939115	2.574047	53.888482
H	45.688422	4.672189	44.852688	H	35.122865	3.056421	59.350540
H	43.774418	3.967202	46.150114	H	37.509963	2.468823	59.390549
H	44.237194	3.575122	32.755677	H	38.975141	3.119132	57.549897
H	45.369522	7.297945	33.284726	H	34.482340	5.351056	55.121600
H	54.726293	5.972250	36.665931	H	35.957009	5.939886	53.297223
H	9.463375	8.127043	58.062944	H	32.644235	2.527409	53.540424
H	7.916937	6.786694	56.693556	H	32.774363	2.049008	51.134542
H	10.728282	2.325385	54.106799	H	31.527202	3.398299	49.535196
H	7.191610	3.170437	53.803768	H	29.533699	6.238886	53.899806
H	19.514272	2.947311	59.305320	H	28.276721	7.531209	52.270251
H	21.909777	2.389011	59.328955	H	27.316054	7.466561	58.219023
H	23.372938	3.137592	57.523120	H	40.493666	7.807325	58.152977

H	39.034301	6.383091	56.826524	H	15.148102	6.357249	65.155560
H	27.967243	3.607761	55.343162	H	10.263285	3.421738	63.796958
H	42.098861	2.131549	54.055780	H	32.688262	7.157973	63.835111
H	32.788121	6.739517	61.409616	H	30.768063	6.357106	65.154700
H	33.614819	8.054385	48.044744	H	25.881929	3.424290	63.795534
H	31.874470	7.046899	49.440844	H	48.307491	7.159175	63.833744
H	28.749301	4.375204	60.399828	H	46.387735	6.357334	65.153483
H	26.897759	3.574556	61.718362	H	41.501158	3.425505	63.794217
H	27.557372	3.164772	48.234543	H	54.922544	4.682768	55.325791
H	28.388452	7.075770	48.746251	H	56.250088	4.683142	39.763730
H	38.070848	5.999084	52.426636	H	57.578894	4.683407	24.200654
H	38.577838	2.501017	53.850999	H	32.654261	5.043298	18.026526
H	50.894855	3.700383	59.506346	H	17.034822	5.043562	18.026684
H	53.331569	3.325598	59.581325	H	10.176551	4.915331	24.089656
H	54.727847	3.865755	57.623125	H	8.848007	4.915643	39.653297
H	50.047603	5.459480	55.145362	H	7.520571	4.915598	55.216445
H	51.424850	5.977072	53.243058	H	12.998979	5.199005	65.269025
H	48.352200	2.746388	53.455420	H	28.618804	5.198988	65.268149
H	48.414502	2.305806	51.039646	H	44.238629	5.198878	65.267020
H	47.079489	3.643130	49.504896	H	48.274018	5.043157	18.026056
H	45.128224	6.339860	53.975596	C	34.075891	9.578359	41.045847
H	43.812692	7.647144	52.413685	C	34.260424	8.859145	39.762095
H	42.901703	7.354922	58.274977	C	33.296973	9.046690	38.611699
H	43.591806	3.525617	55.364088	C	31.944022	9.612458	39.072081
H	48.405600	6.744845	61.407928	C	32.140940	10.850860	39.956267
H	49.513894	7.721655	48.282673	C	32.909532	10.530670	41.253186
H	47.587985	6.952969	49.569036	O	33.735997	8.184960	40.908959
H	44.381545	4.364253	60.399392	C	37.505546	7.458168	43.628514
H	42.519357	3.571652	61.717664	C	38.801895	7.922241	43.932578
H	42.724387	3.827178	48.176222	C	39.350835	7.729399	45.201991
H	43.863390	7.312701	48.884627	C	38.626868	7.074231	46.204863
H	53.398458	5.970534	52.227735	C	37.336652	6.614742	45.911875
H	17.068243	7.158040	63.836006	C	36.780189	6.800672	44.645587

N	36.935656	7.672499	42.376095	C	24.967554	3.357934	26.466904
H	33.161690	8.076676	38.100037	C	24.466015	4.106272	25.385518
H	35.276591	8.531161	39.496891	C	23.076510	4.398107	25.331023
H	34.960032	9.716037	41.683135	C	22.568676	5.082646	24.206117
H	31.388606	8.836701	39.630510	C	23.422052	5.504812	23.191661
H	31.334677	9.865412	38.186182	C	24.790461	5.257905	23.263387
H	32.700591	11.614109	39.379466	C	25.324378	4.549594	24.348592
H	31.166109	11.305115	40.208697	O	25.630313	5.683673	22.240073
H	32.233186	10.072413	41.998994	O	20.438005	5.523419	26.198059
H	33.289859	11.461878	41.710287	O	19.923562	3.374026	26.649775
H	33.770036	9.734439	37.882819	C	20.777284	4.306691	26.422397
H	39.376872	8.441884	43.157775	C	18.226927	4.022014	22.293999
H	40.362193	8.096401	45.409725	C	18.992915	2.941012	21.873981
H	39.060898	6.923782	47.198194	C	19.081890	2.638017	20.519979
H	36.750304	6.097443	46.679484	C	18.404876	3.417023	19.587993
H	35.773602	6.433827	44.423127	C	17.639888	4.497024	20.008011
H	37.601456	7.803890	41.618658	C	17.550913	4.800019	21.362013
H	36.185501	7.026136	42.119671	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
				C	16.963875	5.274030	19.076025
				O	15.523872	7.185037	18.539057
				O	18.566211	5.530766	24.115823
				O	18.026895	3.388474	24.574641
				C	18.267110	4.337445	23.746915
				C	14.301000	5.801000	25.782000
				C	13.829000	6.909000	26.476000
				C	28.003061	7.205567	26.411163
				C	27.160497	6.327139	25.738602
				C	27.665686	5.181726	25.090778
				C	29.061982	4.920945	25.144679
				C	13.900000	3.935000	24.313000
				C	28.721627	2.965749	23.744422
 (S,S)-1-TS1(QM(B3LYP)/MM)							
C	12.487000	7.261000	26.395000				
C	11.616000	6.503000	25.622000				
C	12.086000	5.395000	24.927000				
C	13.428000	5.043000	25.007000				
C	13.027000	3.179000	23.539000				
C	11.685000	3.529000	23.460000				
C	11.215000	4.638000	24.154000				
O	10.782000	2.793000	22.654000				
Cu	18.544887	6.085274	26.023970				
Cu	17.957100	3.695592	26.529944				
C	22.227527	3.963638	26.388987				
C	22.768062	3.190440	27.432674				
C	24.125409	2.894583	27.472355				

C	27.355013	3.186772	23.716769	C	34.024753	3.416989	19.587708
C	26.801582	4.298624	24.390539	C	33.259776	4.496991	20.007741
O	26.582152	2.261464	23.018613	C	33.170826	4.799983	21.361747
O	16.597200	6.402138	25.857913	C	32.403848	5.880986	21.783781
O	16.058303	4.261509	26.321682	C	31.727821	6.658997	20.849810
C	15.737042	5.460216	25.988474	C	31.817771	6.355005	19.496805
C	17.928321	5.798070	30.246760	C	32.583748	5.274002	19.075771
C	18.910168	6.578925	30.884268	O	31.143743	7.185016	18.538835
C	16.798739	5.353530	30.991402	O	34.165159	5.557496	24.095893
C	15.732004	4.660693	30.380077	O	33.652924	3.421866	24.605763
C	14.647463	4.225630	31.135587	C	33.883680	4.353735	23.751584
O	18.432550	6.396894	27.989154	C	29.911438	5.795528	25.879634
O	17.908085	4.248794	28.434820	C	29.365562	6.944824	26.479549
C	18.105044	5.461456	28.805708	C	43.538202	6.878376	26.514355
Cu	34.179817	6.151136	25.989263	C	42.727526	6.024430	25.777987
Cu	33.608112	3.775676	26.571316	C	43.261479	4.904982	25.106501
C	37.863442	4.011106	26.389270	C	44.658140	4.652083	25.192332
C	38.389606	3.306502	27.487942	C	29.575144	3.814602	24.437807
C	39.731587	2.951645	27.532556	C	44.372041	2.737804	23.726926
C	40.572352	3.285824	26.477316	C	43.005571	2.956815	23.657329
C	40.085477	3.969847	25.347153	C	42.424549	4.045065	24.346790
C	38.710359	4.322713	25.289609	O	42.260013	2.046374	22.911943
C	38.213798	4.944244	24.124968	O	32.209975	6.461640	25.883332
C	39.066998	5.241594	23.066584	O	31.710295	4.324580	26.400811
C	40.425150	4.940403	23.139790	C	31.362927	5.512874	26.064676
C	40.947226	4.297528	24.271073	C	33.725023	6.002897	30.227043
O	41.266871	5.254421	22.078491	C	34.798593	6.701829	30.809149
O	36.083378	5.583527	26.126773	C	32.558103	5.747396	30.999169
O	35.566375	3.455521	26.670132	C	31.425425	5.119263	30.441865
C	36.419793	4.374430	26.401253	C	30.289780	4.901575	31.216719
C	33.846854	4.021972	22.293718	O	34.132212	6.513921	27.941154
C	34.612831	2.940969	21.873683	O	33.594894	4.386844	28.469214
C	34.701781	2.637978	20.519678	C	33.828205	5.607483	28.795709

Cu	49.692226	6.198828	25.992698	O	47.713306	6.329281	25.894979
Cu	49.346310	3.778166	26.563181	O	47.394804	4.159280	26.420796
C	53.571003	4.464792	26.367939	C	46.948279	5.320270	26.098813
C	54.157058	3.947774	27.515902	C	49.184432	5.959134	30.229132
C	55.530059	3.732759	27.559826	C	50.110298	6.815000	30.853347
C	56.316002	4.036762	26.454787	C	48.082627	5.456962	30.977936
C	55.729946	4.554780	25.305823	C	47.069257	4.680752	30.375994
C	54.356947	4.768795	25.262899	C	46.009172	4.193590	31.133804
C	53.770890	5.287813	24.113936	O	49.601311	6.550406	27.952216
C	54.557834	5.591815	23.007897	O	49.300102	4.372177	28.456622
C	55.929834	5.377800	23.052821	C	49.382124	5.607288	28.795423
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.635053	5.834338	26.128959	C	10.757253	5.394976	40.491133
O	51.337148	3.654609	26.632130	C	12.099253	5.042971	40.571108
C	52.092986	4.663321	26.381188	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.245723	6.023685	41.554423
C	48.879661	4.496905	20.007192	Cu	16.611825	3.646934	42.061901
C	48.790737	4.799893	21.361200	C	20.880801	3.828897	42.069571
C	48.023772	5.880897	21.783251	C	21.360547	3.165639	43.213826
C	47.347731	6.658913	20.849295	C	22.706393	2.843549	43.340276
C	47.437655	6.354926	19.496287	C	23.596252	3.167368	42.321871
C	48.203620	5.273922	19.075235	C	23.154592	3.798336	41.144561
O	46.763613	7.184943	18.538331	C	21.777959	4.121610	41.005946
O	49.727819	5.589692	24.095035	C	21.330158	4.699296	39.800165
O	49.385695	3.422120	24.606890	C	22.229863	4.965287	38.771793
C	49.524083	4.367372	23.750843	C	23.585483	4.682197	38.919677
C	45.479062	5.519926	25.964408	C	24.057786	4.102303	40.101706
C	44.900396	6.632538	26.603007	O	24.471681	4.958355	37.886463
C	45.199365	3.567796	24.474104	O	19.132893	5.417813	41.737264

O	18.563600	3.288050	42.219064	C	17.742460	6.402773	32.981067
C	19.440459	4.200932	42.009178	C	16.720734	5.643420	32.380031
C	16.907274	4.002698	37.811036	C	15.469083	5.395501	46.518410
C	17.600060	2.887582	37.306687	C	14.379413	4.731247	45.916908
C	17.626428	2.623273	35.943491	C	13.272622	4.361863	46.675266
C	16.956957	3.463380	35.060184	C	14.591460	4.467035	32.505824
C	16.221988	4.574223	35.522539	C	15.615087	5.185232	33.138636
C	16.180731	4.838208	36.917959	O	13.500819	4.026803	33.247546
C	15.391489	5.908005	37.386215	O	17.138727	6.340995	43.514978
C	14.700798	6.715790	36.491778	O	16.551422	4.210573	43.967641
C	14.763217	6.492664	35.126476	C	16.783475	5.419289	44.334088
C	15.529562	5.420389	34.616411	Cu	32.553362	7.240402	41.582470
O	14.065904	7.381753	34.311580	Cu	32.554659	4.380170	42.094933
O	17.267868	5.473555	39.647770	C	36.634393	3.643267	41.811019
O	16.709718	3.334325	40.095240	C	37.107431	2.752861	42.755699
C	16.968376	4.284062	39.270926	C	38.452663	2.315201	42.706422
C	12.972270	5.800966	41.346096	C	39.308479	2.775244	41.728819
C	12.500286	6.908965	42.040108	C	38.857051	3.665165	40.699563
C	26.553711	7.078046	41.999875	C	37.475932	4.066025	40.727888
C	25.765387	6.103568	41.426713	C	36.980598	4.860119	39.653698
C	26.318582	4.891870	40.899119	C	37.802168	5.270076	38.629968
C	27.743766	4.701349	41.021736	C	39.187632	4.957069	38.644268
C	12.571237	3.934972	39.877096	C	39.718033	4.169090	39.664943
C	27.523103	2.553337	39.893853	O	39.998423	5.437624	37.660443
C	26.121229	2.736265	39.760347	O	35.192161	5.514524	41.936870
C	25.514410	3.885525	40.254017	O	34.291060	3.487044	42.199701
O	25.494558	1.698863	39.129643	C	35.272553	4.268280	41.988327
O	15.291434	6.378836	41.395243	C	32.692389	5.051183	37.885388
O	14.724930	4.244348	41.848224	C	33.345354	3.894680	37.486770
C	14.414970	5.450684	41.534242	C	33.372915	3.526821	36.127431
C	16.620233	5.774357	45.771714	C	32.722880	4.294976	35.185154
C	17.632218	6.525323	46.398398	C	32.008877	5.486483	35.537317
C	18.818788	6.875041	32.238435	C	32.004774	5.871423	36.928001

C	31.267137	7.032787	37.302403	O	32.669181	7.243186	43.572822
C	30.583322	7.768132	36.368950	O	32.542014	5.024567	43.954583
C	30.595713	7.407978	34.995475	C	32.502544	6.233394	44.318704
C	31.302163	6.287914	34.568779	Cu	48.363699	6.228703	41.578534
O	29.882666	8.266417	34.207117	Cu	48.031476	3.785266	42.061351
O	32.832491	6.560083	39.732765	C	52.242278	4.464620	41.931334
O	32.623433	4.352461	40.121932	C	52.828353	3.947597	43.079285
C	32.707669	5.355035	39.357409	C	54.201353	3.732577	43.123183
C	28.539149	5.740866	41.613708	C	54.987278	4.036581	42.018131
C	27.949399	6.908886	42.073628	C	54.401203	4.554604	40.869180
C	42.146879	6.665296	42.153385	C	53.028203	4.768624	40.826281
C	41.377158	5.832992	41.349593	C	52.442128	5.287648	39.677330
C	41.969371	4.818356	40.569595	C	53.229054	5.591652	38.571278
C	43.378123	4.641375	40.625605	C	54.601054	5.377632	38.616177
C	28.308761	3.500954	40.499066	C	55.187129	4.858609	39.764128
C	43.186414	2.849580	38.998029	O	55.314970	5.617639	37.405129
C	41.810365	2.998767	38.950695	O	50.311629	5.853248	41.710101
C	41.183702	3.989107	39.731792	O	50.011826	3.664760	42.174828
O	41.105544	2.124941	38.127730	C	50.767547	4.675722	41.945476
O	30.660714	6.747784	41.572571	C	48.246489	4.215060	37.812485
O	30.583960	4.558855	42.016261	C	49.048453	3.170896	37.317151
C	30.031781	5.661490	41.736901	C	49.118332	2.910770	35.955278
C	32.254293	6.493919	45.778724	C	48.385394	3.684537	35.062667
C	33.017266	7.462803	46.405451	C	47.546402	4.724310	35.513549
C	34.748019	7.114023	32.134210	C	47.460908	4.982990	36.908331
C	33.618690	6.849429	32.899682	C	46.570385	5.976163	37.363390
C	32.512149	6.170871	32.355172	C	45.827615	6.722638	36.457381
C	31.254012	5.765196	46.509357	C	45.929074	6.505462	35.093452
C	30.390589	4.816141	45.889161	C	46.792213	5.503032	34.596233
C	29.416212	4.164835	46.606636	O	45.168832	7.330178	34.267160
C	30.253099	5.289987	32.553490	O	48.409924	5.707188	39.663542
C	31.356890	5.925597	33.132525	O	48.133504	3.510030	40.090791
O	29.105771	5.080076	33.307636	C	48.263724	4.492771	39.274979

C	44.155659	5.481222	41.470250	C	22.327196	3.370974	57.463544
C	43.522961	6.497938	42.207098	C	21.813615	4.118717	56.386876
C	43.973606	3.656250	39.812801	C	20.429034	4.435197	56.362140
O	46.377601	6.346185	41.477209	C	19.907499	5.125764	55.247480
O	46.085394	4.146544	41.884451	C	20.743862	5.523466	54.209215
C	45.626438	5.314446	41.616232	C	22.108738	5.250661	54.250179
C	47.850318	5.868144	45.793005	C	22.655635	4.540766	55.328047
C	48.807951	6.679452	46.429303	O	22.932248	5.654505	53.205283
C	49.992029	7.132169	32.201099	O	17.798652	5.575926	57.299358
C	48.943428	6.607013	32.948847	O	17.303133	3.406870	57.674651
C	47.976621	5.770678	32.359262	C	18.147648	4.354495	57.483714
C	46.716859	5.418790	46.525437	C	15.640359	4.198440	53.325160
C	45.683610	4.679368	45.912564	C	16.359512	3.102712	52.814498
C	44.587518	4.251075	46.655074	C	16.379475	2.836099	51.452521
C	45.927547	4.460534	32.497796	C	15.675879	3.653386	50.575750
C	46.898520	5.256082	33.121551	C	14.922527	4.750445	51.042340
O	44.862938	3.965627	33.242697	C	14.891257	5.019273	52.437474
O	48.268183	6.509421	43.541436	C	14.086379	6.074850	52.910336
O	47.935888	4.320122	43.976460	C	13.369201	6.864336	52.019994
C	48.035663	5.544159	44.353089	C	13.419015	6.635482	50.654699
C	9.830848	7.260896	57.522290	C	14.199718	5.575530	50.140060
C	8.959816	6.502907	56.749315	O	12.697882	7.509653	49.844492
C	9.429783	5.394908	56.054291	O	15.945546	5.636232	55.205294
C	10.771783	5.042898	56.134241	O	15.431822	3.472628	55.584336
C	10.370718	3.178911	54.666243	C	15.676770	4.450798	54.790965
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.318241	7.058901	57.566156
Cu	15.897310	6.124624	57.133100	C	24.483082	6.230148	56.826580
Cu	15.338838	3.713535	57.556376	C	24.992908	5.124834	56.114843
C	19.597362	4.018780	57.439553	C	26.388039	4.857433	56.165826
C	20.148853	3.250039	58.480732	C	11.243751	3.934900	55.440217
C	21.501906	2.934305	58.494261	C	26.057291	2.993534	54.645112

C	24.691239	3.219948	54.617138	O	33.397065	5.603000	57.274231
C	24.133435	4.289001	55.354026	O	32.936181	3.432073	57.683262
O	23.922786	2.337396	53.861361	C	33.764987	4.389444	57.480803
O	13.942269	6.425366	56.972154	C	31.309429	4.188184	53.326931
O	13.432557	4.266242	57.373791	C	32.131339	3.159589	52.832165
C	13.091833	5.471600	57.086640	C	32.238291	2.927779	51.467193
C	15.283046	5.695821	61.352095	C	31.518562	3.711126	50.571994
C	16.314087	6.385804	61.978046	C	30.653231	4.727436	51.023357
C	17.545150	6.859467	47.743496	C	30.539314	4.965604	52.419397
C	16.443139	6.455890	48.488086	C	29.640790	5.952153	52.871852
C	15.394704	5.723915	47.898806	C	28.903273	6.699256	51.959944
C	14.198081	5.242825	62.095148	C	29.025786	6.494052	50.595723
C	13.166040	4.552842	61.469196	C	29.904621	5.506487	50.109172
C	12.083075	4.099846	62.213249	O	28.267536	7.310737	49.761480
C	13.219654	4.637324	48.039461	O	31.512306	5.640193	55.205006
C	14.268738	5.327385	48.662409	O	31.076924	3.459641	55.586243
O	12.109332	4.256670	48.784914	C	31.296096	4.443951	54.792382
O	15.764837	6.371178	59.106887	C	27.230595	5.684224	56.960051
O	15.278703	4.201252	59.481208	C	26.678550	6.791032	57.631025
C	15.449008	5.405654	59.893064	C	40.901338	6.919839	57.625469
Cu	31.478852	6.124032	57.133774	C	40.079613	6.103933	56.859499
Cu	30.972611	3.701303	57.560684	C	40.601299	5.012664	56.134266
C	35.217288	4.065682	57.456783	C	41.998331	4.751451	56.192106
C	35.763856	3.338311	58.530088	C	26.906120	3.795697	55.397598
C	37.110719	2.999741	58.550506	C	41.687055	2.906631	54.645662
C	37.934943	3.370375	57.494144	C	40.320094	3.129826	54.606104
C	37.427855	4.080740	56.389251	C	39.750943	4.187738	55.350964
C	36.049149	4.423427	56.359709	O	39.562089	2.251772	53.834831
C	35.533172	5.079457	55.222816	O	29.509871	6.388053	57.009718
C	36.369686	5.414812	54.162678	O	29.059592	4.209812	57.381203
C	37.729875	5.117227	54.206330	C	28.685572	5.410699	57.123635
C	38.272080	4.443293	55.309949	C	30.903120	5.695641	61.351269
O	38.553495	5.463954	53.141273	C	31.934175	6.385618	61.977205

C	32.862872	7.707466	47.787552	C	46.131075	5.063561	52.427290
C	31.928330	7.009552	48.521279	C	45.230810	6.041399	52.894500
C	31.076775	6.028279	47.915968	C	44.442466	6.754472	51.999683
C	29.818167	5.242646	62.094340	C	44.511131	6.521242	50.635863
C	28.786113	4.552669	61.468405	C	45.388116	5.536032	50.127010
C	27.703159	4.099675	62.212476	O	43.713702	7.321554	49.820634
C	29.249767	4.400153	47.996216	O	47.112132	5.776199	55.208423
C	30.067254	5.318083	48.651855	O	46.810934	3.569742	55.569171
O	28.286783	3.727006	48.685613	C	46.959649	4.573258	54.784520
O	31.371495	6.369453	59.106201	C	42.830744	5.577225	56.997622
O	30.904582	4.195664	59.484742	C	42.262308	6.662033	57.691978
C	31.067221	5.402547	59.893942	C	42.527144	3.702102	55.415669
Cu	47.043620	6.235715	57.144378	O	45.068689	6.379426	57.019792
Cu	46.687758	3.780526	57.539933	O	44.740229	4.174184	57.358578
C	50.914829	4.464394	57.493750	C	44.299167	5.358913	57.126397
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.682175	7.013149	47.771274
C	53.073736	4.554373	56.431559	C	47.593499	6.550531	48.500957
C	51.700736	4.768398	56.388685	C	46.600392	5.751993	47.901262
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.493531	4.535622	48.015253
O	53.987445	5.617415	52.967495	C	45.488873	5.291901	48.650165
O	48.986109	5.851278	57.293116	O	43.393649	4.098395	48.744471
O	48.674848	3.648142	57.672883	O	46.916528	6.437636	59.118945
C	49.436890	4.667091	57.496328	O	46.576139	4.233752	59.466530
C	46.955886	4.323710	53.318419	C	46.675230	5.440257	59.890976
C	47.780799	3.302401	52.812840	C	16.262162	6.620790	63.347051
C	47.822962	3.027757	51.453530	C	15.179196	6.168795	64.090104
C	47.038548	3.763562	50.573809	C	14.147156	5.478812	63.465153
C	46.185445	4.788360	51.034190	C	12.031150	4.336833	63.582254

C	13.063191	5.025817	64.207206	H	19.761969	6.945039	30.321984
O	10.943187	3.908837	64.361307	H	15.708960	4.458494	29.314746
C	31.882275	6.620600	63.346211	H	13.844887	3.692691	30.644201
C	30.799322	6.168606	64.089282	H	15.672755	6.862232	17.596205
C	29.767267	5.478629	63.464346	H	25.137467	6.205802	21.531015
C	27.651260	4.336658	63.581482	H	25.600532	2.480657	23.028238
C	28.683314	5.025635	64.206417	H	37.746911	3.038584	28.319187
O	26.563309	3.908663	64.360554	H	40.123943	2.414688	28.390279
C	47.502389	6.620356	63.345091	H	41.611416	2.992962	26.544931
C	46.419447	6.168363	64.088179	H	37.165484	5.199156	24.009532
C	45.387379	5.478391	63.463260	H	38.662997	5.720969	22.185356
C	43.271369	4.336426	63.580429	H	35.152105	2.331575	22.590966
C	44.303437	5.025398	64.205349	H	35.299378	1.794141	20.190293
O	42.183431	3.908432	64.359519	H	34.100185	3.170662	18.536569
H	12.119162	8.126851	26.936097	H	32.262462	6.142869	22.825988
H	10.573058	6.786744	25.566649	H	31.123931	7.499409	21.164019
H	13.382553	2.322889	22.982209	H	30.006108	7.631306	27.021753
H	9.847319	3.169209	22.676960	H	43.106927	7.739334	27.014892
H	22.126971	2.831599	28.230133	H	41.673865	6.257482	25.725468
H	24.529811	2.307280	28.290556	H	30.635747	3.595058	24.394310
H	26.019514	3.114277	26.532719	H	44.793925	1.902148	23.184531
H	21.510853	5.288362	24.083283	H	35.682567	6.925690	30.222343
H	23.008277	6.031066	22.342245	H	31.395084	4.800506	29.404593
H	19.532595	2.329982	22.589862	H	29.430910	4.422597	30.765849
H	19.679688	1.794311	20.190487	H	31.287803	6.858532	17.596631
H	18.480737	3.170890	18.536796	H	40.787365	5.751516	21.342682
H	16.654033	6.146122	22.827363	H	41.277767	2.261833	22.897646
H	15.506826	7.501473	21.163973	H	53.552136	3.699777	28.381240
H	14.495415	7.507684	27.088153	H	55.987748	3.326089	28.455735
H	27.594316	8.089977	26.889129	H	57.384003	3.866300	26.497924
H	26.105419	6.560431	25.712863	H	52.703422	5.454566	24.016527
H	14.941439	3.633401	24.313924	H	54.081210	5.976643	22.116896
H	29.123062	2.114707	23.210509	H	50.777214	2.334799	22.589378

H	50.920782	1.795151	20.189784	H	14.357524	4.499749	44.857446
H	49.720313	3.170768	18.536027	H	12.451976	3.849754	46.191707
H	47.864632	6.135383	22.823906	H	12.847727	3.494973	32.691695
H	46.740833	7.497068	21.163738	H	14.136987	7.157922	33.333676
H	45.519601	7.313799	27.175963	H	24.026864	5.424117	37.109065
H	46.261063	3.348800	24.467956	H	24.543586	1.852344	39.015352
H	50.938587	7.224716	30.286055	H	36.443101	2.415864	43.556432
H	47.070331	4.450209	29.316148	H	38.822256	1.619779	43.467012
H	45.246982	3.598253	30.649747	H	40.350130	2.439187	41.736013
H	46.905251	6.856655	17.596419	H	35.925160	5.135495	39.630590
H	56.056583	5.972314	21.101465	H	37.390529	5.858684	37.801098
H	10.790729	8.127309	42.499542	H	33.832362	3.271878	38.240553
H	9.244486	6.787007	41.130249	H	33.901549	2.618858	35.819609
H	12.054552	2.325243	38.543046	H	32.754218	3.960560	34.143196
H	8.521095	3.175523	38.233243	H	31.242476	7.335246	38.348286
H	20.681064	2.914653	44.020781	H	30.007051	8.651819	36.656502
H	23.064701	2.345034	44.235397	H	28.580372	7.693130	42.497155
H	24.638963	2.907542	42.455518	H	41.673462	7.442100	42.742683
H	20.284890	4.940030	39.630937	H	40.308458	5.996049	41.338942
H	21.863223	5.405220	37.854033	H	29.382564	3.337592	40.581066
H	18.135507	2.229351	37.981557	H	43.649900	2.090770	38.380945
H	18.173167	1.764926	35.566647	H	33.750620	8.025515	45.822605
H	17.002893	3.226428	34.006664	H	35.586151	7.648035	32.570469
H	15.284012	6.130501	38.441750	H	33.610553	7.194763	33.925624
H	14.101459	7.538258	36.858979	H	30.498421	4.598839	44.827220
H	13.169012	7.507329	42.649630	H	28.759595	3.446297	46.101375
H	26.095032	7.992907	42.388291	H	28.402270	4.558849	32.804614
H	24.686627	6.283312	41.375757	H	29.831920	7.972116	33.284675
H	13.612543	3.635470	39.865579	H	39.475095	5.957278	37.028683
H	27.956470	1.635677	39.486726	H	40.108752	2.278035	38.145283
H	18.501690	6.842685	45.833417	H	52.223433	3.700964	43.944931
H	19.589774	7.469418	32.718261	H	54.659087	3.326013	44.019088
H	17.706304	6.648320	34.033935	H	56.055258	3.866002	42.061101

H 51.374884 5.456905 39.581719	H 23.429927 6.471191 56.801715
H 52.752485 5.976834 37.680304	H 12.285065 3.635911 55.428186
H 49.635964 2.565934 37.998896	H 26.462037 2.175769 54.063789
H 49.748600 2.107724 35.587002	H 17.168767 6.738532 61.410850
H 48.467327 3.451705 34.010529	H 18.338158 7.431903 48.214078
H 46.422124 6.183813 38.416846	H 16.409479 6.732490 49.533224
H 45.151901 7.488309 36.814476	H 13.129544 4.375261 60.400562
H 44.107636 7.153234 42.843209	H 11.277672 3.574415 61.719350
H 45.046820 3.499548 39.785504	H 11.441267 3.733568 48.238603
H 49.661280 7.050460 45.872522	H 12.767718 7.286882 48.866349
H 50.719980 7.785035 32.671924	H 22.433810 6.181029 52.503289
H 48.883999 6.871337 33.996115	H 22.944416 2.570002 53.859483
H 45.699645 4.430926 44.856671	H 35.132246 3.035830 59.357957
H 43.808303 3.684973 46.163031	H 37.519149 2.443582 59.388106
H 44.248552 3.381457 32.695208	H 38.977279 3.085297 57.540290
H 45.271667 7.111311 33.290920	H 34.482516 5.334211 55.131177
H 54.726181 5.963437 36.661825	H 35.950858 5.918975 53.302384
H 9.463416 8.127123 58.062871	H 32.707105 2.546654 53.516677
H 7.917069 6.786908 56.693463	H 32.886648 2.139396 51.098373
H 10.727121 2.325243 54.106135	H 31.631610 3.503135 49.516191
H 7.194644 3.178102 53.792931	H 29.486428 6.153310 53.926909
H 19.518764 2.904901 59.292859	H 28.216113 7.456926 52.313587
H 21.915569 2.348848 59.309041	H 27.313950 7.440735 58.222606
H 23.375411 3.107291 57.506115	H 40.479302 7.758985 58.169010
H 18.852058 5.357713 55.153583	H 39.026849 6.344373 56.827097
H 20.320506 6.053696 53.367018	H 27.966584 3.575923 55.352239
H 16.914484 2.456255 53.485105	H 42.099780 2.097233 54.058279
H 16.943504 1.990595 51.072079	H 32.788539 6.738399 61.409699
H 15.712795 3.409502 49.523711	H 33.489368 8.458628 48.279148
H 13.988447 6.301126 53.966060	H 31.834410 7.225968 49.590099
H 12.758910 7.677283 52.390371	H 28.749938 4.374323 60.399835
H 11.840692 7.508882 58.212359	H 26.897598 3.574432 61.718501
H 24.905964 7.911010 58.096862	H 27.820086 3.122761 48.085328

H	28.384990	7.097811	48.782280	H	56.249989	4.683155	39.763378
H	38.060215	5.973553	52.423291	H	57.578800	4.683540	24.200304
H	38.582399	2.478251	53.830247	H	32.654255	5.043759	18.026566
H	50.894907	3.699180	59.506001	H	17.034637	5.043882	18.026730
H	53.331521	3.325266	59.581236	H	10.176601	4.914999	24.089514
H	54.727762	3.865581	57.623252	H	8.847988	4.915089	39.653448
H	50.047671	5.460308	55.145837	H	7.520533	4.915012	55.216669
H	51.425006	5.977511	53.243045	H	12.998674	5.198779	65.268925
H	48.397406	2.717623	53.486487	H	28.618491	5.198817	65.268043
H	48.465206	2.237714	51.077976	H	44.238386	5.198712	65.266932
H	47.092863	3.512041	49.524485	H	48.274034	5.043592	18.026087
H	45.112924	6.264024	53.949085	C	35.450545	8.525539	42.254206
H	43.758186	7.508344	52.365777	C	35.063811	8.491532	40.828378
H	42.888709	7.310919	58.294107	C	35.575408	9.625419	39.944667
H	43.588713	3.485951	55.379214	C	35.580978	10.977643	40.671162
H	48.405742	6.744156	61.407874	C	36.350300	10.885453	41.997365
H	49.431605	7.635224	48.249996	C	35.752615	9.825541	42.936109
H	47.525385	6.833653	49.542594	O	33.776396	8.727630	41.346530
H	44.382349	4.363055	60.399494	C	38.137175	7.494619	43.458524
H	42.519303	3.571323	61.717859	C	39.169300	8.432658	43.641566
H	42.765667	3.532911	48.192486	C	39.849861	8.504459	44.859989
H	43.786701	7.084397	48.846424	C	39.507979	7.652056	45.915740
H	53.398335	5.961903	52.223775	C	38.474803	6.724411	45.737657
H	17.068438	7.157720	63.836084	C	37.791298	6.641677	44.522368
H	15.148248	6.357173	65.155512	N	37.407494	7.456446	42.254036
H	10.261685	3.422800	63.797965	H	34.944632	9.662139	39.038696
H	32.688381	7.157760	63.835189	H	35.162962	7.510861	40.336302
H	30.768143	6.357166	65.154630	H	35.135745	7.673649	42.852096
H	25.878610	3.428454	63.795950	H	34.538323	11.286454	40.867609
H	48.307585	7.159051	63.833781	H	36.030410	11.751599	40.023232
H	46.387884	6.357377	65.153426	H	37.408102	10.630756	41.786577
H	41.497425	3.430417	63.794534	H	36.363703	11.863617	42.510288
H	54.922456	4.682824	55.325554	H	34.799890	10.184718	43.367765

H	36.416182	9.628941	43.797431	O	19.909908	3.365322	26.649695
H	36.601680	9.369757	39.611037	C	20.765802	4.295528	26.423042
H	39.441966	9.104105	42.819808	C	18.226927	4.022014	22.293999
H	40.654670	9.236522	44.984116	C	18.992915	2.941012	21.873981
H	40.040957	7.710842	46.869554	C	19.081890	2.638017	20.519979
H	38.197423	6.049380	46.553706	C	18.404876	3.417023	19.587993
H	36.991128	5.908934	44.383624	C	17.639888	4.497024	20.008011
H	37.937334	7.746245	41.432505	C	17.550913	4.800019	21.362013
H	36.886874	6.582822	42.077639	C	16.783924	5.881020	21.784030
				C	16.107910	6.659026	20.850045
				C	16.197885	6.355031	19.497042
				C	16.963875	5.274030	19.076025
				O	15.523872	7.185037	18.539057
				O	18.564998	5.527682	24.115723
				O	18.018812	3.386526	24.572728
				C	18.263577	4.335524	23.746366
				C	14.301000	5.801000	25.782000
				C	13.829000	6.909000	26.476000
				C	27.980146	7.119622	26.447788
				C	27.138480	6.249298	25.763794
				C	27.644945	5.112157	25.101249
				C	29.040842	4.851704	25.151490
				C	13.900000	3.935000	24.313000
				C	28.703752	2.917540	23.721924
				C	27.336854	3.136502	23.698327
				C	26.782719	4.238423	24.387703
				O	26.564737	2.220347	22.987043
				O	16.596224	6.400478	25.854837
				O	16.052946	4.260841	26.319692
				C	15.735066	5.459816	25.986593
				C	17.917683	5.794700	30.239899
				C	18.908358	6.559867	30.881883
				C	16.778272	5.366470	30.977729

(S,S)-1-Int1(QM(B3LYP)/MM)

C	12.487000	7.261000	26.395000				
C	11.616000	6.503000	25.622000				
C	12.086000	5.395000	24.927000				
C	13.428000	5.043000	25.007000				
C	13.027000	3.179000	23.539000				
C	11.685000	3.529000	23.460000				
C	11.215000	4.638000	24.154000				
O	10.782000	2.793000	22.654000				
Cu	18.542064	6.080529	26.022368				
Cu	17.947219	3.691609	26.527846				
C	22.212572	3.947077	26.393041				
C	22.748930	3.183035	27.445118				
C	24.104090	2.879635	27.487450				
C	24.947361	3.326438	26.475479				
C	24.448475	4.065368	25.385788				
C	23.061223	4.364534	25.329212				
C	22.555264	5.038987	24.197150				
C	23.409720	5.445804	23.177321				
C	24.776810	5.192898	23.251294				
C	25.307319	4.492968	24.343294				
O	25.618778	5.602616	22.223215				
O	20.431953	5.513392	26.197545				

C	15.702878	4.693486	30.359320	O	33.645930	3.389463	24.592797
C	14.607993	4.274134	31.108859	C	33.872571	4.336743	23.754972
O	18.427727	6.391683	27.985652	C	29.888051	5.716260	25.898930
O	17.895799	4.244827	28.431201	C	29.342047	6.857590	26.513267
C	18.095638	5.457175	28.801001	C	43.547580	6.894018	26.507985
Cu	34.147958	6.094114	26.024557	C	42.729074	6.032347	25.789132
Cu	33.592464	3.704626	26.562292	C	43.256983	4.908687	25.119627
C	37.847269	3.979770	26.407156	C	44.654758	4.656989	25.193027
C	38.374172	3.270733	27.502382	C	29.555917	3.757911	24.426669
C	39.718659	2.926222	27.550607	C	44.355920	2.737106	23.737891
C	40.561507	3.275625	26.501777	C	42.988620	2.954856	23.680102
C	40.073830	3.963186	25.374002	C	42.413330	4.044860	24.371738
C	38.696302	4.306911	25.313790	O	42.237231	2.044508	22.940049
C	38.199329	4.932581	24.151536	O	32.179816	6.391754	25.912867
C	39.053509	5.239098	23.096402	O	31.691910	4.243236	26.394640
C	40.413018	4.944073	23.171278	C	31.338933	5.435379	26.078054
C	40.936110	4.299836	24.301089	C	33.640768	5.869413	30.255735
O	41.254949	5.261896	22.111290	C	34.662482	6.642493	30.837756
O	36.055476	5.540390	26.161564	C	32.495131	5.531092	31.030981
O	35.553504	3.398272	26.662409	C	31.405739	4.826106	30.478258
C	36.400440	4.329425	26.415513	C	30.292836	4.525362	31.259111
C	33.846854	4.021972	22.293718	O	34.079637	6.418051	27.983239
C	34.612831	2.940969	21.873683	O	33.563927	4.276541	28.470513
C	34.701781	2.637978	20.519678	C	33.771708	5.495145	28.819570
C	34.024753	3.416989	19.587708	Cu	49.696207	6.203329	25.982178
C	33.259776	4.496991	20.007741	Cu	49.345520	3.784539	26.559526
C	33.170826	4.799983	21.361747	C	53.571003	4.464792	26.367939
C	32.403848	5.880986	21.783781	C	54.157058	3.947774	27.515902
C	31.727821	6.658997	20.849810	C	55.530059	3.732759	27.559826
C	31.817771	6.355005	19.496805	C	56.316002	4.036762	26.454787
C	32.583748	5.274002	19.075771	C	55.729946	4.554780	25.305823
O	31.143743	7.185016	18.538835	C	54.356947	4.768795	25.262899
O	34.146809	5.536207	24.119385	C	53.770890	5.287813	24.113936

C	54.557834	5.591815	23.007897	O	49.297075	4.384721	28.450293
C	55.929834	5.377800	23.052821	C	49.384297	5.620896	28.783759
C	56.515889	4.858782	24.200784	C	11.158286	7.260970	41.959133
O	56.643771	5.617805	21.841785	C	10.287269	6.502976	41.186145
O	51.637476	5.836432	26.124492	C	10.757253	5.394976	40.491133
O	51.335692	3.658417	26.632709	C	12.099253	5.042971	40.571108
C	52.093213	4.665343	26.380149	C	11.698221	3.178978	39.103109
C	49.466779	4.021876	22.293156	C	10.356221	3.528983	39.024134
C	50.232745	2.940872	21.873104	C	9.886237	4.637982	39.718146
C	50.321669	2.637885	20.519096	O	9.453204	2.792989	38.218147
C	49.644627	3.416901	19.587140	Cu	17.243013	6.033945	41.521634
C	48.879661	4.496905	20.007192	Cu	16.619303	3.656045	42.037011
C	48.790737	4.799893	21.361200	C	20.887972	3.848337	41.998496
C	48.023772	5.880897	21.783251	C	21.365711	3.138864	43.115574
C	47.347731	6.658913	20.849295	C	22.713077	2.822930	43.238416
C	47.437655	6.354926	19.496287	C	23.608434	3.204708	42.245289
C	48.203620	5.273922	19.075235	C	23.170312	3.884760	41.094257
O	46.763613	7.184943	18.538331	C	21.790215	4.193652	40.954636
O	49.734582	5.590533	24.088811	C	21.345638	4.809231	39.766488
O	49.387795	3.424520	24.605606	C	22.252667	5.135869	38.762333
C	49.527206	4.368377	23.748376	C	23.612243	4.876514	38.917853
C	45.482485	5.529388	25.952281	C	24.081063	4.252924	40.078696
C	44.910377	6.648398	26.584950	O	24.506115	5.218456	37.911267
C	45.189818	3.570614	24.473645	O	19.132266	5.433603	41.686525
O	47.717877	6.334443	25.878937	O	18.573218	3.301816	42.170457
O	47.395341	4.166344	26.410732	C	19.445838	4.216786	41.950716
C	46.951283	5.326785	26.084032	C	16.872029	4.007275	37.785787
C	49.195717	5.979744	30.215228	C	17.554813	2.887105	37.279623
C	50.130373	6.832890	30.829281	C	17.575735	2.622486	35.916580
C	48.094428	5.489627	30.971082	C	16.912425	3.469682	35.035163
C	47.070967	4.720304	30.377368	C	16.185221	4.584918	35.500484
C	46.012337	4.242998	31.143532	C	16.145325	4.845304	36.896228
O	49.603766	6.560709	27.937695	C	15.355657	5.912903	37.368465

C	14.666670	6.725105	36.477110	O	16.578390	4.219455	43.942436
C	14.732064	6.509394	35.110809	C	16.810425	5.429026	44.305317
C	15.497546	5.438018	34.597269	Cu	32.459286	7.509872	41.544564
O	14.037063	7.403286	34.298897	Cu	32.543275	4.525281	42.155883
O	17.247001	5.481777	39.615897	C	36.576495	3.524051	41.835269
O	16.694726	3.342406	40.071033	C	37.030208	2.579579	42.735766
C	16.944811	4.291488	39.243740	C	38.374950	2.140998	42.686433
C	12.972270	5.800966	41.346096	C	39.250813	2.655516	41.754913
C	12.500286	6.908965	42.040108	C	38.820375	3.600380	40.766107
C	26.454854	7.138290	42.256699	C	37.438131	4.001542	40.788667
C	25.703779	6.184055	41.604597	C	36.964174	4.844716	39.742004
C	26.303452	5.044449	40.976266	C	37.807376	5.307304	38.758128
C	27.735279	4.902658	41.084382	C	39.191527	4.990792	38.782104
C	12.571237	3.934972	39.877096	C	39.699522	4.149126	39.771334
C	27.602217	2.846559	39.785253	O	40.022685	5.515897	37.840775
C	26.195017	2.987726	39.656170	O	35.150122	5.410279	41.995493
C	25.541050	4.065550	40.242559	O	34.222614	3.418874	42.273068
O	25.612383	1.985806	38.931462	C	35.221214	4.148308	42.040372
O	15.288206	6.384364	41.380006	C	32.613696	4.958618	37.957098
O	14.729794	4.249863	41.843719	C	33.285906	3.798807	37.601754
C	14.415577	5.454523	41.527990	C	33.327915	3.381336	36.256894
C	16.662027	5.783449	45.743674	C	32.667433	4.099810	35.283412
C	17.684327	6.527059	46.361777	C	31.925645	5.285987	35.591142
C	18.816757	6.854537	32.236074	C	31.916030	5.728345	36.965359
C	17.730877	6.395839	32.973579	C	31.165125	6.896097	37.290371
C	16.699768	5.653366	32.366555	C	30.453055	7.569376	36.331482
C	15.513796	5.413604	46.498531	C	30.453794	7.139886	34.978359
C	14.415013	4.756651	45.905253	C	31.195233	6.027278	34.593527
C	13.309336	4.399466	46.671093	O	29.698557	7.932459	34.159260
C	14.551388	4.510872	32.479931	O	32.688970	6.531613	39.762030
C	15.584524	5.209181	33.119142	O	32.606866	4.329651	40.214239
O	13.450131	4.088265	33.216130	C	32.626100	5.320795	39.420015
O	17.153634	6.351922	43.482557	C	28.490986	5.925198	41.750808

C	27.857461	7.024936	42.307901	C	54.401203	4.554604	40.869180
C	42.190278	6.788677	42.036143	C	53.028203	4.768624	40.826281
C	41.398849	5.902122	41.315601	C	52.442128	5.287648	39.677330
C	41.969028	4.825094	40.605404	C	53.229054	5.591652	38.571278
C	43.375939	4.633680	40.656690	C	54.601054	5.377632	38.616177
C	28.348601	3.771622	40.469337	C	55.187129	4.858609	39.764128
C	43.139060	2.733969	39.162261	O	55.314970	5.617639	37.405129
C	41.764656	2.898158	39.121936	O	50.322862	5.864131	41.715183
C	41.161972	3.949319	39.839223	O	50.009954	3.676755	42.177754
O	41.037953	1.985643	38.362543	C	50.770735	4.683626	41.948576
O	30.566764	7.021205	41.689386	C	48.265460	4.230643	37.807180
O	30.583523	4.815929	42.077070	C	49.056218	3.180051	37.308562
C	29.990358	5.909699	41.837860	C	49.125109	2.925151	35.945563
C	32.291725	6.663986	45.799764	C	48.403157	3.712410	35.055355
C	33.076052	7.614779	46.428435	C	47.574952	4.759416	35.510243
C	34.584952	7.051483	32.161781	C	47.488923	5.010812	36.905938
C	33.478922	6.708048	32.928857	C	46.605461	6.008733	37.364848
C	32.421567	5.953265	32.387062	C	45.873379	6.769019	36.462164
C	31.258670	5.978454	46.526710	C	45.977146	6.560520	35.097261
C	30.365896	5.060556	45.901266	C	46.829889	5.551147	34.596514
C	29.354850	4.456813	46.609335	O	45.227206	7.397895	34.274035
C	30.231319	4.915528	32.594668	O	48.442755	5.719723	39.655900
C	31.285045	5.635703	33.166342	O	48.141897	3.526249	40.086344
O	29.103314	4.627953	33.352353	C	48.285284	4.506579	39.269369
O	32.749906	7.357209	43.576493	C	44.173444	5.521657	41.430812
O	32.581900	5.152205	44.011973	C	43.563128	6.603628	42.089584
C	32.552719	6.375918	44.342556	C	43.947837	3.587442	39.904791
Cu	48.380833	6.247323	41.566247	O	46.398861	6.371793	41.443832
Cu	48.032691	3.807326	42.056671	O	46.091584	4.178232	41.870891
C	52.242278	4.464620	41.931334	C	45.641702	5.345017	41.584888
C	52.828353	3.947597	43.079285	C	47.837680	5.909718	45.778391
C	54.201353	3.732577	43.123183	C	48.785339	6.740818	46.403653
C	54.987278	4.036581	42.018131	C	50.021186	7.159750	32.175077

C	48.974017	6.644035	32.931472	O	17.310097	3.436910	57.666233
C	47.999564	5.809265	32.351493	C	18.148566	4.390516	57.478883
C	46.710213	5.456301	46.517830	C	15.652147	4.232425	53.323942
C	45.680298	4.704426	45.914550	C	16.363528	3.128180	52.821492
C	44.592534	4.269250	46.666049	C	16.397400	2.861384	51.460279
C	45.943279	4.512608	32.507700	C	15.714708	3.687646	50.575462
C	46.924425	5.302405	33.122278	C	14.966991	4.792417	51.033869
O	44.882113	4.025215	33.262540	C	14.921944	5.061356	52.428559
O	48.267165	6.535839	43.526120	C	14.120027	6.123212	52.892385
O	47.928648	4.349381	43.970276	C	13.423037	6.921305	51.993945
C	48.027598	5.575371	44.341179	C	13.486260	6.692272	50.629361
C	9.830848	7.260896	57.522290	C	14.260586	5.623248	50.124073
C	8.959816	6.502907	56.749315	O	12.780784	7.571781	49.810771
C	9.429783	5.394908	56.054291	O	15.942045	5.667824	55.207808
C	10.771783	5.042898	56.134241	O	15.437633	3.500473	55.578762
C	10.370718	3.178911	54.666243	C	15.678699	4.482766	54.789496
C	9.028718	3.528920	54.587293	C	11.644816	5.800887	56.909216
C	8.558750	4.637919	55.281317	C	11.172849	6.908886	57.603240
O	8.125684	2.792932	53.781319	C	25.322401	7.127325	57.581508
Cu	15.890397	6.147174	57.136455	C	24.485292	6.302940	56.838901
Cu	15.344831	3.731065	57.550413	C	24.994197	5.204482	56.115362
C	19.598985	4.063477	57.432661	C	26.389901	4.940643	56.156181
C	20.152657	3.288754	58.467735	C	11.243751	3.934900	55.440217
C	21.506744	2.978888	58.480480	C	26.058004	3.095396	54.613098
C	22.331304	3.429764	57.455183	C	24.690584	3.314296	54.598966
C	21.815296	4.185290	56.384688	C	24.133610	4.372656	55.351762
C	20.429044	4.493287	56.359718	O	23.920401	2.436635	53.838798
C	19.904893	5.188060	55.248653	O	13.936125	6.435445	56.975443
C	20.741215	5.602701	54.216940	O	13.436791	4.272392	57.370514
C	22.107951	5.340496	54.259968	C	13.091269	5.476595	57.085756
C	22.656200	4.622385	55.331307	C	15.283046	5.695821	61.352095
O	22.932362	5.761724	53.222654	C	16.314087	6.385804	61.978046
O	17.793319	5.610739	57.300991	C	17.610136	6.863328	47.706944

C	16.510160	6.469238	48.459809	C	29.649590	6.144618	52.896728
C	15.451314	5.745538	47.878514	C	28.931458	6.933031	52.004517
C	14.198081	5.242825	62.095148	C	29.042852	6.754979	50.635167
C	13.166040	4.552842	61.469196	C	29.888703	5.751565	50.123132
C	12.083075	4.099846	62.213249	O	28.306152	7.612222	49.822591
C	13.266798	4.680279	48.034502	O	31.507464	5.734172	55.207858
C	14.325714	5.362449	48.649012	O	31.060090	3.550104	55.553298
O	12.156365	4.315187	48.787569	C	31.275751	4.548227	54.775572
O	15.755561	6.383546	59.110205	C	27.232670	5.758586	56.958459
O	15.282114	4.209199	59.476422	C	26.682546	6.858767	57.640677
C	15.446218	5.412772	59.892355	C	40.917052	6.949472	57.660899
Cu	31.479603	6.183908	57.142790	C	40.090146	6.146656	56.886357
Cu	30.963674	3.756722	57.531748	C	40.606870	5.065843	56.141684
C	35.209588	4.106187	57.432284	C	42.003494	4.801529	56.188773
C	35.749223	3.356113	58.493165	C	26.908019	3.892121	55.369755
C	37.094719	3.012824	58.513374	C	41.684233	2.987675	54.608230
C	37.925245	3.403344	57.469105	C	40.317001	3.211437	54.580409
C	37.425120	4.137019	56.376113	C	39.752453	4.255882	55.347474
C	36.046931	4.481907	56.345674	O	39.554231	2.348927	53.795926
C	35.537211	5.157571	55.217476	O	29.512343	6.456282	57.023787
C	36.380477	5.514900	54.169776	O	29.054203	4.274134	57.363064
C	37.740592	5.217408	54.216581	C	28.685283	5.479600	57.121779
C	38.275369	4.519637	55.308619	C	30.903120	5.695641	61.351269
O	38.571657	5.587807	53.165264	C	31.934175	6.385618	61.977205
O	33.396018	5.653782	57.272494	C	32.914281	7.876062	47.807257
O	32.926284	3.478401	57.646721	C	31.952684	7.212455	48.538031
C	33.758795	4.435534	57.459245	C	31.076249	6.255229	47.930468
C	31.266694	4.320785	53.305746	C	29.818167	5.242646	62.094340
C	32.043604	3.270620	52.785296	C	28.786113	4.552669	61.468405
C	32.129614	3.058683	51.416004	C	27.703159	4.099675	62.212476
C	31.436018	3.887230	50.541179	C	29.184751	4.702960	47.996734
C	30.613776	4.927798	51.017788	C	30.036006	5.583797	48.660646
C	30.516260	5.141380	52.419239	O	28.187393	4.072458	48.677576

O	31.373430	6.396350	59.117292	C	42.839783	5.611177	57.005380
O	30.898497	4.219066	59.464197	C	42.277255	6.686339	57.718432
C	31.063964	5.419555	59.890482	C	42.528200	3.767049	55.390141
Cu	47.052260	6.252187	57.150116	O	45.079252	6.403789	57.026009
Cu	46.687198	3.795911	57.532788	O	44.742205	4.197161	57.349591
C	50.914829	4.464394	57.493750	C	44.306382	5.385469	57.127423
C	51.500923	3.947364	58.641689	C	46.523195	5.695406	61.350162
C	52.873923	3.732339	58.685563	C	47.554262	6.385378	61.976082
C	53.659830	4.036343	57.580498	C	48.657721	7.090023	47.741150
C	53.073736	4.554373	56.431559	C	47.578867	6.618698	48.479608
C	51.700736	4.768398	56.388685	C	46.595952	5.799091	47.891828
C	51.114643	5.287428	55.239746	C	45.438253	5.242413	62.093251
C	51.901549	5.591433	54.133681	C	44.406185	4.552442	61.467332
C	53.273549	5.377407	54.178555	C	43.323243	4.099449	62.211421
C	53.859642	4.858378	55.326493	C	44.505411	4.557670	48.026091
O	53.987445	5.617415	52.967495	C	45.495717	5.328579	48.650595
O	48.992300	5.859213	57.298653	O	43.416732	4.109569	48.765456
O	48.672561	3.655715	57.669604	O	46.923904	6.443859	59.124003
C	49.438153	4.672522	57.497654	O	46.572623	4.240033	59.461004
C	46.972566	4.361411	53.316596	C	46.675850	5.444278	59.890723
C	47.814380	3.356097	52.808132	C	16.262162	6.620790	63.347051
C	47.867321	3.091707	51.447276	C	15.179196	6.168795	64.090104
C	47.077353	3.823500	50.568785	C	14.147156	5.478812	63.465153
C	46.207135	4.832648	51.032648	C	12.031150	4.336833	63.582254
C	46.141208	5.095391	52.427589	C	13.063191	5.025817	64.207206
C	45.222182	6.053438	52.898734	O	10.943187	3.908837	64.361307
C	44.427212	6.761547	52.006031	C	31.882275	6.620600	63.346211
C	44.508217	6.543125	50.640341	C	30.799322	6.168606	64.089282
C	45.401557	5.574571	50.127727	C	29.767267	5.478629	63.464346
O	43.704593	7.339603	49.827044	C	27.651260	4.336658	63.581482
O	47.120465	5.803775	55.212503	C	28.683314	5.025635	64.206417
O	46.815244	3.595618	55.561543	O	26.563309	3.908663	64.360554
C	46.968622	4.603015	54.782978	C	47.502389	6.620356	63.345091

C	46.419447	6.168363	64.088179	H	37.149843	5.183028	24.035944
C	45.387379	5.478391	63.463260	H	38.648900	5.718902	22.215532
C	43.271369	4.336426	63.580429	H	35.150109	2.329245	22.590639
C	44.303437	5.025398	64.205349	H	35.298700	1.793666	20.190363
O	42.183431	3.908432	64.359519	H	34.099976	3.170644	18.536496
H	12.119242	8.126995	26.935874	H	32.263410	6.143093	22.826042
H	10.573019	6.786791	25.566449	H	31.124682	7.499393	21.165272
H	13.383855	2.323457	22.982289	H	29.982566	7.537660	27.063174
H	9.847407	3.169602	22.677258	H	43.122321	7.760382	27.004958
H	22.106177	2.836646	28.246458	H	41.674381	6.263536	25.746865
H	24.505424	2.299585	28.312715	H	30.616989	3.542437	24.376975
H	25.997890	3.077287	26.542984	H	44.773941	1.901280	23.192951
H	21.498322	5.249403	24.074344	H	35.526575	6.930826	30.249987
H	22.998205	5.965215	22.322476	H	31.388817	4.511034	29.440119
H	19.532004	2.329497	22.589957	H	29.468560	3.985836	30.811841
H	19.679371	1.794099	20.190540	H	31.291991	6.861049	17.596337
H	18.480526	3.170838	18.536732	H	40.773719	5.755847	21.374705
H	16.652073	6.145520	22.827187	H	41.255816	2.264181	22.926097
H	15.507041	7.501063	21.165268	H	53.551995	3.699821	28.381166
H	14.495515	7.507892	27.087929	H	55.987720	3.326011	28.455679
H	27.571963	7.998732	26.936655	H	57.384067	3.866269	26.497798
H	26.083430	6.483185	25.740715	H	52.703455	5.452266	24.014537
H	14.941560	3.634300	24.310742	H	54.081110	5.976016	22.116804
H	29.107102	2.076019	23.174706	H	50.777751	2.334988	22.589241
H	19.766955	6.914843	30.323173	H	50.920901	1.795276	20.189738
H	15.682332	4.495159	29.293088	H	49.720330	3.170943	18.535917
H	13.798118	3.756926	30.612430	H	47.863492	6.134720	22.823895
H	15.672239	6.861303	17.596367	H	46.741191	7.496785	21.164950
H	25.128454	6.120430	21.509501	H	45.535222	7.334583	27.145286
H	25.582950	2.438720	22.999177	H	46.251893	3.354213	24.456035
H	37.729852	2.990482	28.328013	H	50.957597	7.234051	30.254815
H	40.110815	2.384717	28.405951	H	47.063735	4.488082	29.317818
H	41.602490	2.990316	26.571509	H	45.241726	3.652996	30.666093

H 46.912592 6.861526 17.595779	H 35.907458 5.112884 39.700451
H 56.056075 5.976781 21.104036	H 37.410857 5.933934 37.950288
H 10.790832 8.127534 42.499202	H 33.775329 3.210212 38.380882
H 9.244421 6.786966 41.130117	H 33.874796 2.472183 35.986740
H 12.055769 2.325581 38.543425	H 32.708140 3.729417 34.253686
H 8.519519 3.171553 38.239287	H 31.154561 7.251726 38.319379
H 20.683013 2.846371 43.905430	H 29.863112 8.455114 36.582842
H 23.068151 2.285290 44.112254	H 28.459597 7.800751 42.785762
H 24.652866 2.950042 42.375951	H 41.739639 7.624568 42.558512
H 20.297496 5.031405 39.590743	H 40.331841 6.074380 41.304404
H 21.888258 5.604154 37.857782	H 29.428274 3.644692 40.542336
H 18.086900 2.225000 37.953007	H 43.585630 1.929671 38.591963
H 18.114656 1.759188 35.538861	H 33.829198 8.155229 45.849343
H 16.955545 3.233834 33.981196	H 35.382535 7.646971 32.595185
H 15.245008 6.128960 38.424959	H 33.447949 7.054462 33.953964
H 14.066256 7.544955 36.848135	H 30.479396 4.831583 44.842199
H 13.169303 7.508117 42.648621	H 28.673221 3.765541 46.099280
H 25.960927 7.997313 42.722146	H 28.444566 4.044431 32.857545
H 24.618677 6.324580 41.569578	H 29.597101 7.558714 33.270367
H 13.612453 3.635511 39.864336	H 39.513548 6.056304 37.214661
H 28.072657 1.983709 39.306097	H 40.045578 2.167197 38.361356
H 18.551326 6.837821 45.789746	H 52.223693 3.702129 43.945489
H 19.595277 7.436570 32.719591	H 54.659164 3.326263 44.019143
H 17.694555 6.639438 34.026889	H 56.055355 3.866084 42.060983
H 14.385870 4.521434 44.846725	H 51.374885 5.455171 39.580474
H 12.480744 3.893888 46.193964	H 52.752391 5.976183 37.680204
H 12.789237 3.571854 32.655305	H 49.636250 2.566247 37.988273
H 14.108101 7.183368 33.320112	H 49.746574 2.115994 35.574847
H 24.063901 5.721848 37.156418	H 48.484685 3.484184 34.002045
H 24.658567 2.117895 38.815465	H 46.453530 6.209565 38.418865
H 36.351046 2.204044 43.506060	H 45.203872 7.538171 36.823218
H 38.728164 1.401664 43.412367	H 44.165301 7.300240 42.662273
H 40.291647 2.316723 41.763836	H 45.018767 3.419748 39.863844

H 49.632164 7.116747 45.840713	H 12.860212 7.349160 48.833214
H 50.755403 7.812537 32.636912	H 22.432689 6.294015 52.526136
H 48.921308 6.915238 33.977340	H 22.939950 2.660388 53.851558
H 45.693124 4.451948 44.859547	H 35.112863 3.039234 59.311587
H 43.815688 3.692879 46.182059	H 37.496707 2.438000 59.341868
H 44.259999 3.444723 32.720147	H 38.966761 3.115170 57.514937
H 45.339091 7.191959 33.295823	H 34.486314 5.410706 55.123532
H 54.726381 5.971166 36.665340	H 35.966752 6.035198 53.316539
H 9.463387 8.127085 58.062879	H 32.599222 2.622728 53.453676
H 7.916958 6.786743 56.693476	H 32.741182 2.250000 51.028236
H 10.728259 2.325438 54.106703	H 31.532082 3.693493 49.480979
H 7.191826 3.170993 53.803015	H 29.501775 6.325957 53.956209
H 19.522913 2.933429 59.275350	H 28.267686 7.701536 52.378808
H 21.921150 2.387013 59.290635	H 27.319482 7.502117 58.236977
H 23.380750 3.170868 57.496878	H 40.500202 7.782371 58.218461
H 18.847623 5.410329 55.152731	H 39.037658 6.389722 56.862214
H 20.316282 6.136584 53.377710	H 27.969383 3.679687 55.312132
H 16.901881 2.474701 53.498471	H 42.094500 2.190696 54.002636
H 16.956322 2.008799 51.087354	H 32.787625 6.740871 61.409715
H 15.762957 3.444296 49.523684	H 33.556109 8.614515 48.298541
H 14.007585 6.347376 53.946964	H 31.853015 7.441326 49.603831
H 12.815729 7.739220 52.357935	H 28.750120 4.374425 60.399947
H 11.840337 7.509399 58.212420	H 26.897830 3.574378 61.718420
H 24.912277 7.975631 58.120349	H 27.700041 3.489047 48.073133
H 23.431687 6.542696 56.820172	H 28.415329 7.418603 48.838375
H 12.285139 3.636324 55.427456	H 38.083637 6.117921 52.459067
H 26.463239 2.288482 54.017200	H 38.572147 2.564584 53.815283
H 17.168177 6.739785 61.410653	H 50.894942 3.700101 59.506355
H 18.411372 7.430619 48.170505	H 53.331585 3.325563 59.581324
H 16.486051 6.747251 49.504796	H 54.727864 3.865765 57.623183
H 13.129795 4.375329 60.400592	H 50.047687 5.459167 55.145063
H 11.277963 3.574260 61.719266	H 51.424948 5.976966 53.242994
H 11.478669 3.799856 48.246122	H 48.436025 2.776064 53.480777

H	48.522743	2.312934	51.070069	H	44.238642	5.198811	65.267058
H	47.141257	3.580805	49.517908	H	48.273932	5.043138	18.026054
H	45.094768	6.263391	53.954957	C	35.713412	8.368786	42.433970
H	43.728181	7.499713	52.376024	C	35.047466	8.408945	41.022639
H	42.907836	7.323557	58.328122	C	35.827732	9.314768	40.041054
H	43.589613	3.551448	55.344777	C	36.127060	10.703875	40.611627
H	48.405769	6.744571	61.408026	C	36.917524	10.583505	41.921697
H	49.398881	7.730509	48.209056	C	36.138747	9.745052	42.946341
H	47.509407	6.912678	49.518208	O	33.746572	8.825188	41.176717
H	44.381351	4.364342	60.399446	C	37.569455	7.112291	43.656864
H	42.519324	3.571614	61.717768	C	38.881054	7.570525	43.790430
H	42.802324	3.518243	48.225973	C	39.569815	7.348823	44.987382
H	43.811520	7.134248	48.848911	C	38.942144	6.681716	46.044001
H	53.398987	5.972009	52.228096	C	37.624416	6.232133	45.900252
H	17.068213	7.158096	63.835984	C	36.931267	6.441181	44.704902
H	15.148085	6.357277	65.155549	N	36.839238	7.327726	42.409442
H	10.263136	3.421945	63.796951	H	35.231910	9.377081	39.114404
H	32.688048	7.158310	63.835081	H	35.086633	7.382843	40.600434
H	30.767943	6.357255	65.154675	H	34.972656	7.930723	43.115923
H	25.881451	3.424973	63.795497	H	35.171939	11.225098	40.806880
H	48.307548	7.159053	63.833809	H	36.684779	11.312044	39.875907
H	46.387778	6.357268	65.153513	H	37.908965	10.125489	41.716121
H	41.501276	3.424928	63.794586	H	37.130319	11.580570	42.347806
H	54.922583	4.682812	55.325861	H	35.193499	10.266188	43.180154
H	56.250108	4.683064	39.763631	H	36.689908	9.655577	43.900060
H	57.578890	4.683389	24.200599	H	36.785385	8.818774	39.766877
H	32.654242	5.043334	18.026542	H	39.360645	8.102050	42.962307
H	17.034872	5.043599	18.026693	H	40.600662	7.700188	45.093269
H	10.176559	4.915326	24.089696	H	39.481095	6.511027	46.981111
H	8.848026	4.915631	39.653295	H	37.127863	5.706871	46.721498
H	7.520592	4.915631	55.216369	H	35.907408	6.077603	44.583498
H	12.998951	5.199019	65.269014	H	37.497106	7.539004	41.650586
H	28.618711	5.199030	65.268140	H	36.294483	6.411211	42.145748

(S,S)-2-RC (QM(B3LYP)/MM)

C	12.487000	7.261000	26.395000	C	16.107910	6.659026	20.850045
C	11.616000	6.503000	25.622000	C	16.197885	6.355032	19.497042
C	12.086000	5.395000	24.927000	C	16.963876	5.274031	19.076025
C	13.428000	5.043000	25.007000	O	15.523872	7.185038	18.539057
C	13.027000	3.179000	23.539000	O	18.566160	5.531975	24.109278
C	11.685000	3.529000	23.460000	O	18.022622	3.391855	24.574856
C	11.215000	4.638000	24.154000	C	18.265636	4.338367	23.744981
O	10.782000	2.793000	22.654000	C	14.301000	5.801000	25.782000
Cu	18.543242	6.092843	26.011721	C	13.829000	6.909000	26.476000
Cu	17.953498	3.705068	26.528957	C	27.985250	7.030605	26.562809
C	22.216638	3.963953	26.382491	C	27.143719	6.198415	25.833116
C	22.751099	3.187946	27.426893	C	27.647156	5.086055	25.127366
C	24.103972	2.874687	27.462700	C	29.040645	4.813561	25.176468
C	24.947287	3.324923	26.452596	C	13.900000	3.935000	24.313000
C	24.450820	4.078573	25.371759	C	28.700444	2.942076	23.666522
C	23.065282	4.386096	25.320432	C	27.335352	3.171900	23.642315
C	22.561126	5.072111	24.194370	C	26.784181	4.248743	24.372557
C	23.416660	5.486600	23.178580	O	26.561727	2.289287	22.891301
C	24.782788	5.228716	23.249869	O	16.595455	6.406056	25.845327
C	25.310480	4.512757	24.332735	O	16.057567	4.267436	26.321349
O	25.626266	5.647616	22.226780	C	15.736458	5.463953	25.983378
O	20.434553	5.530163	26.187604	C	17.933618	5.830233	30.229767
O	19.916035	3.383070	26.648152	C	18.923642	6.606097	30.860016
C	20.770230	4.313213	26.415855	C	16.799739	5.403449	30.976211
C	18.226927	4.022014	22.293999	C	15.725387	4.718735	30.368962
C	18.992915	2.941012	21.873981	C	14.638704	4.295982	31.128136
C	19.081890	2.638017	20.519979	O	18.432169	6.414392	27.971616
C	18.404876	3.417024	19.587993	O	17.905898	4.268786	28.429988
C	17.639888	4.497025	20.008011	C	18.105355	5.483602	28.792741
C	17.550913	4.800019	21.362013	Cu	34.145176	6.011033	26.078243
C	16.783924	5.881020	21.784030	Cu	33.593259	3.605834	26.546907
				C	37.849423	3.892611	26.365643
				C	38.381046	3.139465	27.428549

C	39.729094	2.808008	27.465671	C	44.365912	2.805733	23.685244
C	40.571416	3.215080	26.437447	C	42.997960	3.021134	23.632377
C	40.079504	3.947474	25.340284	C	42.419789	4.093582	24.348414
C	38.698057	4.277478	25.290252	O	42.248681	2.126565	22.871233
C	38.198116	4.948781	24.154887	O	32.177835	6.313205	25.995852
C	39.053380	5.316583	23.120153	O	31.691185	4.149377	26.405499
C	40.416029	5.034296	23.187383	C	31.337853	5.351748	26.130378
C	40.941434	4.342366	24.287273	C	33.683540	5.628848	30.310309
O	41.258901	5.412353	22.148070	C	34.751015	6.289392	30.944574
O	36.052811	5.454780	26.177733	C	32.522694	5.296104	31.063204
O	35.556749	3.299586	26.624439	C	31.388706	4.718145	30.456295
C	36.401216	4.237830	26.394099	C	30.259379	4.421698	31.214636
C	33.846855	4.021974	22.293721	O	34.099452	6.272005	28.052393
C	34.612832	2.940971	21.873686	O	33.575186	4.116995	28.468704
C	34.701783	2.637980	20.519681	C	33.797721	5.319739	28.858361
C	34.024755	3.416991	19.587710	Cu	49.701315	6.215321	25.976291
C	33.259777	4.496993	20.007743	Cu	49.342276	3.800180	26.563630
C	33.170827	4.799985	21.361749	C	53.571004	4.464799	26.367945
C	32.403849	5.880988	21.783783	C	54.157059	3.947781	27.515908
C	31.727822	6.658998	20.849812	C	55.530060	3.732767	27.559832
C	31.817772	6.355006	19.496807	C	56.316003	4.036770	26.454793
C	32.583750	5.274004	19.075773	C	55.729947	4.554788	25.305829
O	31.143744	7.185017	18.538837	C	54.356948	4.768802	25.262905
O	34.123561	5.508281	24.153018	C	53.770890	5.287820	24.113942
O	33.636385	3.347410	24.573771	C	54.557834	5.591822	23.007903
C	33.858009	4.315191	23.759450	C	55.929834	5.377808	23.052827
C	29.887812	5.640793	25.964623	C	56.515890	4.858790	24.200790
C	29.344510	6.756253	26.626854	O	56.643771	5.617813	21.841791
C	43.546957	6.899689	26.544514	O	51.641367	5.841671	26.119366
C	42.729835	6.050217	25.809165	O	51.332404	3.667823	26.640391
C	43.260923	4.943988	25.113776	C	52.093436	4.670497	26.381397
C	44.659454	4.695587	25.179898	C	49.466780	4.021882	22.293161
C	29.553407	3.746512	24.411157	C	50.232747	2.940878	21.873109

C	50.321671	2.637891	20.519101	O	9.453203	2.792985	38.218146
C	49.644629	3.416907	19.587145	Cu	17.236383	6.164325	41.540080
C	48.879663	4.496911	20.007197	Cu	16.685151	3.764315	42.033483
C	48.790739	4.799899	21.361205	C	20.945700	4.111331	42.114353
C	48.023773	5.880903	21.783256	C	21.401305	3.467251	43.279310
C	47.347732	6.658919	20.849300	C	22.742618	3.147162	43.442224
C	47.437657	6.354932	19.496292	C	23.652951	3.442647	42.434404
C	48.203622	5.273928	19.075240	C	23.238464	4.052816	41.236209
O	46.763615	7.184949	18.538336	C	21.869413	4.400381	41.071198
O	49.737015	5.594784	24.085076	C	21.456377	4.985929	39.856776
O	49.387139	3.431294	24.609552	C	22.378063	5.212521	38.836685
C	49.528398	4.371751	23.748555	C	23.717945	4.865534	38.994369
C	45.485225	5.554259	25.955938	C	24.159153	4.294881	40.192179
C	44.911105	6.657659	26.613358	O	24.615000	5.040820	37.949706
C	45.197577	3.625566	24.438726	O	19.147047	5.635818	41.730566
O	47.722727	6.353597	25.875074	O	18.649340	3.486166	42.203195
O	47.393862	4.186978	26.409946	C	19.495254	4.431640	42.007849
C	46.953378	5.348792	26.083771	C	16.988307	4.147540	37.791020
C	49.207329	6.016898	30.210659	C	17.727414	3.062956	37.286928
C	50.160915	6.852612	30.819646	C	17.758811	2.795223	35.925019
C	48.093705	5.558782	30.968440	C	17.047708	3.601852	35.043105
C	47.055960	4.805291	30.379871	C	16.269691	4.683615	35.505818
C	45.982808	4.363056	31.147332	C	16.223322	4.949356	36.900265
O	49.612324	6.581786	27.929675	C	15.389825	5.984414	37.370036
O	49.291355	4.410382	28.453162	C	14.662170	6.760489	36.477332
C	49.388099	5.647743	28.780685	C	14.729217	6.538470	35.112221
C	11.158284	7.260965	41.959133	C	15.537476	5.497543	34.601290
C	10.287267	6.502972	41.186144	O	13.993255	7.397624	34.298763
C	10.757252	5.394972	40.491132	O	17.288019	5.625053	39.632133
C	12.099252	5.042967	40.571107	O	16.807237	3.464465	40.068793
C	11.698220	3.178974	39.103108	C	17.034173	4.426683	39.250186
C	10.356220	3.528979	39.024133	C	12.972269	5.800962	41.346096
C	9.886236	4.637978	39.718145	C	12.500284	6.908961	42.040108

C	27.058169	7.191325	41.624130	C	37.531399	4.335149	40.691336
C	26.142013	6.255249	41.188721	C	36.975155	5.189595	39.696108
C	26.530840	4.925742	40.820488	C	37.760338	5.735016	38.708976
C	27.926588	4.579843	40.954036	C	39.158902	5.495391	38.670611
C	12.571236	3.934968	39.877095	C	39.751896	4.661332	39.615615
C	27.422263	2.356096	40.095901	O	39.919827	6.084108	37.705513
C	26.045975	2.683287	39.974627	O	34.965674	5.292176	41.810621
C	25.592980	3.950505	40.328817	O	34.474793	3.113961	42.077605
O	25.285788	1.655692	39.497443	C	35.282227	4.070191	41.878394
O	15.271573	6.441413	41.374936	C	32.659223	3.945620	37.868339
O	14.775763	4.286093	41.811339	C	33.233037	2.781742	37.386808
C	14.425757	5.484258	41.509458	C	33.227051	2.514685	36.001691
C	16.604046	5.868709	45.755255	C	32.623978	3.389484	35.122637
C	17.582589	6.664746	46.379281	C	31.972279	4.585187	35.569676
C	18.835508	6.915387	32.211008	C	32.000330	4.862976	36.983065
C	17.754240	6.459937	32.956976	C	31.317314	6.019902	37.459263
C	16.725883	5.703543	32.362317	C	30.632856	6.841406	36.599513
C	15.478894	5.428903	46.508535	C	30.606355	6.579867	35.203430
C	14.415406	4.719840	45.911061	C	31.287408	5.487236	34.676721
C	13.334229	4.292541	46.676459	O	29.878499	7.499973	34.499040
C	14.588909	4.542081	32.497693	O	33.130508	5.366035	39.704075
C	15.618570	5.256601	33.124788	O	32.482863	3.253803	40.123438
O	13.496665	4.113950	33.244068	C	32.758339	4.211924	39.341226
O	17.106214	6.466756	43.502317	C	28.853990	5.571525	41.429063
O	16.590376	4.315199	43.941031	C	28.422371	6.854188	41.732375
C	16.778289	5.528921	44.314959	C	42.239986	7.068769	42.135942
Cu	33.122129	6.003598	41.601940	C	41.454414	6.288851	41.294802
Cu	32.550826	3.544424	42.085540	C	42.025645	5.292609	40.477287
C	36.733972	3.728481	41.720815	C	43.429378	5.082320	40.527771
C	37.290884	2.822780	42.605567	C	28.331394	3.268282	40.565817
C	38.670947	2.529389	42.543443	C	43.208583	3.391465	38.800707
C	39.472256	3.126867	41.594534	C	41.833553	3.558767	38.771225
C	38.940679	4.042337	40.628261	C	41.223063	4.509772	39.612632

O	41.113288	2.738048	37.907657	C	50.777191	4.733705	41.957643
O	31.124778	6.236787	41.406765	C	48.279254	4.410604	37.807594
O	30.655169	4.129726	42.018779	C	49.061149	3.349520	37.317162
C	30.316181	5.286893	41.626218	C	49.117400	3.074432	35.958097
C	32.398314	5.570948	45.795390	C	48.389685	3.850538	35.063443
C	33.245667	6.481210	46.402904	C	47.572003	4.909569	35.509973
C	34.705707	6.579246	32.302288	C	47.502416	5.184694	36.902430
C	33.588423	6.225216	33.050690	C	46.633835	6.198088	37.354429
C	32.484250	5.588121	32.453847	C	45.893362	6.944720	36.446805
C	31.319887	4.971235	46.531873	C	45.977855	6.710283	35.084304
C	30.378206	4.089356	45.928076	C	46.821723	5.689665	34.590655
C	29.340558	3.554251	46.652902	O	45.223656	7.538134	34.255377
C	30.231536	4.677833	32.583197	O	48.486077	5.890459	39.665596
C	31.337136	5.258787	33.213236	O	48.116270	3.703703	40.077059
O	29.088972	4.397099	33.321560	C	48.294343	4.684674	39.269294
O	32.913174	6.220046	43.582443	C	44.219346	5.851549	41.424072
O	32.577739	4.035355	43.994640	C	43.610083	6.854203	42.199019
C	32.644613	5.249836	44.348998	C	44.008697	4.133498	39.662568
Cu	48.449495	6.399691	41.586506	O	46.475268	6.614085	41.469670
Cu	48.004626	3.969152	42.045194	O	46.078694	4.424844	41.846568
C	52.242277	4.464616	41.931345	C	45.677349	5.616556	41.588027
C	52.828352	3.947593	43.079296	C	47.885455	6.019492	45.794714
C	54.201352	3.732573	43.123194	C	48.858017	6.806892	46.438286
C	54.987277	4.036578	42.018142	C	50.057105	7.193377	32.162305
C	54.401202	4.554601	40.869191	C	48.995224	6.711499	32.920030
C	53.028202	4.768621	40.826292	C	48.001777	5.895749	32.345201
C	52.442128	5.287645	39.677341	C	46.749607	5.575094	46.526656
C	53.229054	5.591649	38.571289	C	45.697352	4.867965	45.907301
C	54.601054	5.377629	38.616189	C	44.604342	4.435378	46.651727
C	55.187129	4.858606	39.764139	C	45.914356	4.651241	32.508115
O	55.314970	5.617636	37.405141	C	46.911760	5.424380	33.117951
O	50.374040	5.931730	41.730612	O	44.837975	4.200156	33.263661
O	49.977678	3.754902	42.177661	O	48.350090	6.666279	43.552070

O	47.914414	4.490511	43.962044	C	13.364593	6.819756	52.010680
C	48.065837	5.704713	44.351920	C	13.428905	6.592726	50.645649
C	9.830844	7.260885	57.522289	C	14.222733	5.539486	50.137766
C	8.959813	6.502896	56.749314	O	12.704136	7.458140	49.828971
C	9.429780	5.394897	56.054290	O	15.941377	5.607395	55.207673
C	10.771780	5.042887	56.134240	O	15.413251	3.448341	55.594679
C	10.370715	3.178901	54.666241	C	15.665976	4.422137	54.798338
C	9.028715	3.528910	54.587291	C	11.644813	5.800876	56.909215
C	8.558747	4.637908	55.281315	C	11.172845	6.908875	57.603239
O	8.125681	2.792922	53.781316	C	25.341063	6.889531	57.577069
Cu	15.900951	6.101713	57.132348	C	24.499982	6.050995	56.855962
Cu	15.322583	3.696804	57.565883	C	25.001438	4.925815	56.169130
C	19.579207	3.957753	57.474855	C	26.394374	4.648043	56.227014
C	20.106138	3.205451	58.540245	C	11.243748	3.934890	55.440215
C	21.451207	2.860445	58.573543	C	26.048810	2.752099	54.750433
C	22.293253	3.251843	57.538446	C	24.684737	2.991026	54.713484
C	21.803884	3.982285	56.438559	C	24.135927	4.082551	55.423632
C	20.426782	4.328281	56.394213	O	23.908919	2.099072	53.976121
C	19.928178	5.000072	55.258161	O	13.946394	6.415818	56.973624
C	20.780658	5.349870	54.215369	O	13.422444	4.261404	57.382519
C	22.139300	5.048911	54.274872	C	13.089942	5.467304	57.090650
C	22.662744	4.357773	55.376144	C	15.283042	5.695809	61.352094
O	22.980073	5.407905	53.227336	C	16.314083	6.385792	61.978046
O	17.799386	5.535454	57.297850	C	17.492051	6.984026	47.727519
O	17.280474	3.374030	57.687722	C	16.419406	6.518890	48.478992
C	18.134597	4.311920	57.496119	C	15.401667	5.742724	47.892423
C	15.636847	4.165055	53.334253	C	14.198077	5.242813	62.095147
C	16.365464	3.072939	52.830404	C	13.166036	4.552830	61.469195
C	16.404581	2.810242	51.468092	C	12.083071	4.099834	62.213248
C	15.710004	3.628355	50.584358	C	13.280289	4.556343	48.042990
C	14.942735	4.718352	51.045332	C	14.300941	5.290758	48.661369
C	14.893565	4.983551	52.440491	O	12.194769	4.121625	48.795395
C	14.077167	6.033024	52.906997	O	15.773891	6.358124	59.104661

O	15.269457	4.194018	59.487514	C	26.698978	6.613787	57.645413
C	15.449566	5.398662	59.894452	C	40.894786	6.908896	57.568619
Cu	31.485227	5.958919	57.118175	C	40.079287	6.059871	56.832006
Cu	31.001366	3.551734	57.647896	C	40.611702	4.955567	56.134557
C	35.242417	3.951651	57.500954	C	42.012501	4.716019	56.189628
C	35.803212	3.262778	58.591923	C	26.904030	3.563661	55.485690
C	37.155674	2.948042	58.618703	C	41.719502	2.833731	54.684943
C	37.972148	3.307302	57.552244	C	40.348613	3.030889	54.655289
C	37.450659	3.978445	56.429434	C	39.768620	4.096785	55.380132
C	36.065208	4.291252	56.391353	O	39.598576	2.121092	53.913069
C	35.534433	4.898789	55.234187	O	29.516016	6.201422	56.995271
C	36.363621	5.223402	54.165062	O	29.082025	4.036048	57.452987
C	37.730421	4.960399	54.218335	C	28.699250	5.224490	57.153792
C	38.286489	4.329072	55.339805	C	30.903116	5.695628	61.351271
O	38.547229	5.295513	53.144421	C	31.934171	6.385605	61.977208
O	33.407000	5.461607	57.269829	C	33.089184	6.796181	47.770123
O	32.968601	3.306087	57.773861	C	32.076398	6.223805	48.508813
C	33.787221	4.261315	57.524345	C	31.147518	5.301621	47.925544
C	31.329576	3.848234	53.400410	C	29.818163	5.242633	62.094342
C	32.173398	2.813888	52.958048	C	28.786109	4.552656	61.468406
C	32.279717	2.508964	51.607669	C	27.703155	4.099663	62.212477
C	31.541395	3.227831	50.674106	C	29.181377	3.848802	48.032528
C	30.660283	4.252629	51.072878	C	30.067546	4.714379	48.670986
C	30.540037	4.558033	52.455733	O	28.154136	3.287323	48.728763
C	29.613837	5.538911	52.859787	O	31.383875	6.288691	59.081288
C	28.858712	6.220758	51.912278	O	30.933864	4.128213	59.546668
C	28.994121	5.958897	50.558518	C	31.084796	5.351969	59.906782
C	29.898586	4.971144	50.119413	Cu	47.047349	6.241270	57.149678
O	28.225163	6.724242	49.686075	Cu	46.691691	3.784740	57.538648
O	31.511972	5.390817	55.209586	C	50.914826	4.464382	57.493755
O	31.102267	3.224318	55.688271	C	51.500920	3.947352	58.641694
C	31.309679	4.174265	54.851477	C	52.873920	3.732327	58.685568
C	27.242996	5.489451	56.998164	C	53.659827	4.036331	57.580503

C	53.073733	4.554362	56.431564	C	47.658643	6.654915	48.516840
C	51.700733	4.768387	56.388690	C	46.650151	5.881243	47.910021
C	51.114640	5.287417	55.239751	C	45.438249	5.242399	62.093255
C	51.901547	5.591423	54.133687	C	44.406182	4.552428	61.467335
C	53.273547	5.377397	54.178561	C	43.323240	4.099435	62.211424
C	53.859639	4.858367	55.326499	C	44.528784	4.689611	48.018801
O	53.987443	5.617405	52.967501	C	45.538732	5.421284	48.658596
O	48.989074	5.855871	57.301892	O	43.432268	4.248544	48.750814
O	48.676371	3.650928	57.671063	O	46.915585	6.439591	59.122019
C	49.438397	4.669976	57.498478	O	46.579901	4.234267	59.466117
C	46.953678	4.349666	53.319724	C	46.675902	5.440683	59.891814
C	47.755888	3.315315	52.805306	C	16.262158	6.620778	63.347051
C	47.803437	3.060944	51.442262	C	15.179191	6.168782	64.090104
C	47.048003	3.832529	50.567379	C	14.147152	5.478800	63.465152
C	46.214436	4.869069	51.037637	C	12.031146	4.336820	63.582253
C	46.151604	5.120652	52.434560	C	13.063187	5.025805	64.207205
C	45.263999	6.106249	52.910475	O	10.943183	3.908824	64.361306
C	44.502178	6.853476	52.021291	C	31.882271	6.620587	63.346214
C	44.583153	6.646306	50.654333	C	30.799317	6.168593	64.089284
C	45.442804	5.650490	50.137065	C	29.767262	5.478616	63.464348
O	43.813295	7.479799	49.845683	C	27.651255	4.336645	63.581483
O	47.121639	5.788141	55.215793	C	28.683309	5.025622	64.206418
O	46.813704	3.580998	55.566849	O	26.563304	3.908650	64.360554
C	46.963373	4.588288	54.786919	C	47.502385	6.620342	63.345096
C	42.836840	5.569474	56.974482	C	46.419443	6.168348	64.088184
C	42.258577	6.667487	57.638587	C	45.387375	5.478376	63.463264
C	42.552253	3.660090	55.429390	C	43.271365	4.336411	63.580432
O	45.072158	6.382269	57.017748	C	44.303433	5.025383	64.205353
O	44.746723	4.176780	57.357581	O	42.183428	3.908416	64.359522
C	44.304715	5.359323	57.118936	H	12.119271	8.127086	26.935748
C	46.523192	5.695393	61.350166	H	10.573023	6.786801	25.566437
C	47.554258	6.385364	61.976087	H	13.383797	2.323292	22.982513
C	48.746504	7.118851	47.786628	H	9.847411	3.169589	22.677263

H	22.108023	2.837584	28.226303	H	41.673812	6.276923	25.774626
H	24.503207	2.283315	28.280859	H	30.613075	3.524069	24.361593
H	25.995892	3.066660	26.514416	H	44.786123	1.982880	23.122571
H	21.504868	5.286000	24.072575	H	35.630045	6.570579	30.375583
H	23.006703	6.015538	22.328841	H	31.351612	4.504570	29.392320
H	19.532377	2.329869	22.589986	H	29.397909	3.987729	30.724555
H	19.679457	1.794168	20.190523	H	31.291615	6.860768	17.596367
H	18.480537	3.170850	18.536729	H	40.774894	5.933550	21.432424
H	16.650776	6.145064	22.827097	H	41.267097	2.345887	22.860246
H	15.506767	7.500870	21.165269	H	53.552061	3.700686	28.381470
H	14.495601	7.508397	27.087364	H	55.987732	3.326253	28.455790
H	27.579194	7.890348	27.086511	H	57.384077	3.866366	26.497863
H	26.091113	6.442795	25.809769	H	52.703451	5.451151	24.013623
H	14.941524	3.633907	24.312316	H	54.081074	5.975726	22.116704
H	29.101364	2.119898	23.088936	H	50.777952	2.335447	22.589451
H	19.778615	6.959042	30.294498	H	50.920975	1.795332	20.189754
H	15.699533	4.512867	29.304313	H	49.720357	3.170966	18.535925
H	13.830195	3.768289	30.640623	H	47.862837	6.134526	22.823839
H	15.672056	6.861191	17.596385	H	46.741007	7.496651	21.164975
H	25.138528	6.178141	21.520607	H	45.534890	7.332860	27.188073
H	25.581561	2.514707	22.904042	H	46.260420	3.412157	24.418542
H	37.738105	2.816943	28.239685	H	50.997973	7.230099	30.243480
H	40.124820	2.233505	28.297484	H	47.049821	4.558606	29.323467
H	41.615729	2.939923	26.498758	H	45.200450	3.785319	30.673994
H	37.145636	5.188159	24.044012	H	46.912434	6.861363	17.595838
H	38.647047	5.833220	22.261149	H	56.056133	5.977171	21.104189
H	35.147926	2.326545	22.590078	H	10.790960	8.128089	42.498400
H	35.298127	1.793240	20.190382	H	9.244455	6.787086	41.129938
H	34.099828	3.170507	18.536511	H	12.055643	2.325213	38.543938
H	32.267382	6.144104	22.826357	H	8.519716	3.172080	38.238549
H	31.125163	7.499748	21.165184	H	20.703056	3.221888	44.071730
H	29.985627	7.407708	27.209675	H	23.078744	2.661557	44.353274
H	43.119513	7.753191	27.061389	H	24.690005	3.175406	42.593831

H	20.421465	5.258848	39.672833	H	40.390539	6.485116	41.275215
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H	18.292893	2.430429	37.961432	H	43.660450	2.665102	38.137785
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H	17.097300	3.361705	33.990526	H	35.541782	7.081835	32.778864
H	15.276256	6.203924	38.425432	H	33.587015	6.470132	34.105228
H	14.029740	7.556948	36.846096	H	30.474801	3.836957	44.872573
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H	13.612344	3.634839	39.868392	H	39.359037	6.646926	37.147343
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H	19.613227	7.505985	32.685529	H	54.659337	3.328053	44.019861
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H	12.533290	3.746897	46.196236	H	52.752248	5.975782	37.680102
H	12.837771	3.585964	32.691708	H	49.639296	2.738889	38.001412
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H	24.201493	5.529718	37.165892	H	48.457761	3.603395	34.013598
H	24.356167	1.901655	39.367855	H	46.501711	6.422325	38.406687
H	36.657231	2.352506	43.361888	H	45.232371	7.724006	36.802006
H	39.107404	1.824189	43.257924	H	44.207481	7.461844	42.869148
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H	33.701873	1.604061	35.622725	H	45.694923	4.649786	44.844822
H	32.636092	3.138397	34.057185	H	43.811960	3.891685	46.155307
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H	41.781468	7.840055	42.746973	H	9.463316	8.126902	58.063108

H 7.916929 6.786669 56.693543	H 32.941758 1.713139 51.280574
H 10.728289 2.325618 54.106425	H 31.651819 2.961260 49.631226
H 7.191911 3.171197 53.802696	H 29.450888 5.784045 53.904454
H 19.461853 2.892976 59.354123	H 28.149043 6.973503 52.230040
H 21.844547 2.285885 59.406332	H 27.340082 7.274086 58.218369
H 23.334833 2.965569 57.595843	H 40.465842 7.759537 58.088856
H 18.878632 5.253916 55.152825	H 39.023165 6.285489 56.798357
H 20.375366 5.865808 53.355463	H 27.962499 3.332605 55.449016
H 16.915005 2.427897 53.506439	H 42.141675 2.020484 54.109880
H 16.977675 1.967988 51.093328	H 32.791907 6.730940 61.410258
H 15.763480 3.390168 49.531539	H 33.777658 7.501506 48.246305
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H 11.840691 7.508244 58.213054	H 26.897520 3.574952 61.718282
H 24.936344 7.757276 58.088349	H 27.645975 2.701300 48.144454
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H 26.447416 1.917640 54.189023	H 38.613891 2.324818 53.919378
H 17.169052 6.737739 61.410793	H 50.894973 3.699707 59.506285
H 18.260020 7.592670 48.194832	H 53.331554 3.325433 59.581273
H 16.382637 6.783954 49.527070	H 54.727842 3.865695 57.623128
H 13.125526 4.379120 60.400360	H 50.047582 5.459431 55.145591
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H 12.777031 7.230678 48.851931	H 48.429056 2.260367 51.060330
H 22.498436 5.926515 52.508182	H 47.107904 3.599271 49.513998
H 22.931347 2.335542 53.975055	H 45.133336 6.308158 53.967457
H 35.178624 2.973071 59.429262	H 43.828332 7.612981 52.394735
H 37.574519 2.420959 59.470232	H 42.879172 7.338619 58.221485
H 39.019862 3.043714 57.604641	H 43.617030 3.463512 55.382921
H 34.477663 5.121964 55.133067	H 48.405836 6.744138 61.407891
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H 32.763688 2.250950 53.672224	H 47.602976 6.917924 49.564509

H	44.381954	4.363875	60.399399	C	26.001931	7.823443	37.115996
H	42.519440	3.571466	61.717720	C	24.805232	8.201977	37.767163
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H	43.901116	7.269212	48.866397	C	23.701328	8.575264	35.631777
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H	17.068447	7.157633	63.836089	C	26.023526	7.844242	35.702801
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H	10.176556	4.915317	24.089703	H	22.814850	8.864411	35.059202
H	8.848020	4.915634	39.653268	H	24.933537	8.221997	33.885163
H	7.520574	4.915579	55.216386	H	26.949949	7.576903	35.182531
H	12.998943	5.198973	65.269024	H	27.815679	6.900926	37.355961
H	28.618798	5.198884	65.268171	H	26.971690	7.172807	38.801462
H	44.238651	5.198804	65.267041				
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C	32.691186	9.067722	40.736169	C	12.487000	7.261000	26.395000
C	33.308765	9.160509	42.076609	C	11.616000	6.503000	25.622000
C	34.419998	10.148295	42.353744	C	12.086000	5.395000	24.927000
C	35.122229	10.621885	41.070806	C	13.428000	5.043000	25.007000
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Cu	18.545906	6.084099	26.020446	C	27.133618	6.197970	25.777632
Cu	17.951514	3.696709	26.531490	C	27.642875	5.069792	25.102962
C	22.219271	3.946278	26.387989	C	29.037186	4.800937	25.167876
C	22.757463	3.180395	27.438179	C	13.900000	3.935000	24.313000
C	24.110667	2.866431	27.471319	C	28.708248	2.895716	23.697362
C	24.950644	3.304103	26.452862	C	27.342852	3.122615	23.659586
C	24.451104	4.046488	25.366289	C	26.784565	4.213352	24.363301
C	23.065336	4.356141	25.318242	O	26.575904	2.222332	22.923103
C	22.557877	5.033251	24.188691	O	16.597624	6.402718	25.855008
C	23.408887	5.429902	23.161888	O	16.055854	4.262897	26.320011
C	24.774863	5.168009	23.228089	C	15.736546	5.461392	25.986609
C	25.307909	4.467740	24.318937	C	17.908936	5.817224	30.237208
O	25.612724	5.570354	22.193765	C	18.899174	6.579454	30.883831
O	20.437973	5.516343	26.193908	C	16.755276	5.409415	30.965104
O	19.915064	3.370858	26.655501	C	15.683137	4.736289	30.341448
C	20.772081	4.298820	26.423085	C	14.573180	4.339124	31.081089
C	18.226925	4.022012	22.293999	O	18.433546	6.400415	27.983058
C	18.992913	2.941010	21.873981	O	17.896808	4.256248	28.435081
C	19.081888	2.638015	20.519979	C	18.097141	5.470046	28.801222
C	18.404874	3.417021	19.587993	Cu	34.141585	6.026349	26.068786
C	17.639885	4.497022	20.008011	Cu	33.591043	3.625552	26.555653
C	17.550911	4.800017	21.362013	C	37.844803	3.906020	26.392333
C	16.783920	5.881019	21.784030	C	38.371643	3.177982	27.475248
C	16.107906	6.659024	20.850045	C	39.717371	2.837687	27.519849
C	16.197881	6.355028	19.497042	C	40.561086	3.208795	26.479326
C	16.963871	5.274029	19.076025	C	40.073399	3.916020	25.363976
O	15.523868	7.185034	18.539057	C	38.695295	4.257714	25.307928
O	18.566108	5.529220	24.114386	C	38.199450	4.908130	24.158964
O	18.024828	3.387795	24.575376	C	39.054993	5.238303	23.112094
C	18.266193	4.336246	23.746807	C	40.414668	4.942639	23.182560
C	14.301000	5.801000	25.782000	C	40.936641	4.275816	24.299802
C	13.829000	6.909000	26.476000	O	41.258152	5.286236	22.131851

O	36.050503	5.468902	26.176817	C	32.684068	5.260855	31.146323
O	35.552041	3.316196	26.633577	C	31.572049	4.564362	30.629134
C	36.397486	4.253415	26.405924	C	30.529175	4.179758	31.466780
C	33.846852	4.021974	22.293716	O	34.100189	6.302754	28.038808
C	34.612829	2.940971	21.873681	O	33.590003	4.149893	28.476485
C	34.701778	2.637980	20.519676	C	33.818511	5.355030	28.857420
C	34.024750	3.416990	19.587706	Cu	49.689249	6.197404	25.991917
C	33.259772	4.496992	20.007739	Cu	49.344897	3.777506	26.565472
C	33.170822	4.799984	21.361745	C	53.571003	4.464803	26.367930
C	32.403844	5.880987	21.783779	C	54.157056	3.947784	27.515893
C	31.727817	6.658997	20.849809	C	55.530058	3.732771	27.559816
C	31.817767	6.355005	19.496804	C	56.316001	4.036773	26.454777
C	32.583744	5.274001	19.075769	C	55.729944	4.554792	25.305813
O	31.143737	7.185017	18.538834	C	54.356945	4.768807	25.262890
O	34.123767	5.512282	24.147793	C	53.770888	5.287824	24.113928
O	33.630373	3.355196	24.579943	C	54.557831	5.591827	23.007888
C	33.856685	4.318081	23.759985	C	55.929832	5.377811	23.052810
C	29.879513	5.647968	25.942660	C	56.515887	4.858794	24.200774
C	29.329164	6.779252	26.572177	O	56.643767	5.617817	21.841773
C	43.532858	6.867824	26.523596	O	51.633364	5.833992	26.126742
C	42.719536	6.007654	25.797249	O	51.336379	3.655742	26.636091
C	43.252909	4.888279	25.125511	C	52.092137	4.663711	26.381685
C	44.650766	4.638635	25.204738	C	49.466776	4.021885	22.293147
C	29.555562	3.716828	24.430850	C	50.232742	2.940881	21.873096
C	44.359836	2.717268	23.749139	C	50.321665	2.637894	20.519088
C	42.993043	2.935292	23.683693	C	49.644622	3.416909	19.587132
C	42.414125	4.025191	24.371742	C	48.879655	4.496913	20.007183
O	42.245189	2.024050	22.941427	C	48.790732	4.799902	21.361191
O	32.171593	6.326919	25.980605	C	48.023768	5.880906	21.783244
O	31.687547	4.167705	26.414697	C	47.347725	6.658920	20.849287
C	31.331639	5.365830	26.124127	C	47.437649	6.354933	19.496280
C	33.762224	5.674541	30.313559	C	48.203614	5.273930	19.075227
C	34.807930	6.435738	30.869811	O	46.763606	7.184950	18.538323

O	49.724745	5.588884	24.095162	C	21.378138	5.268694	39.813793
O	49.387106	3.420933	24.608010	C	22.287545	5.779235	38.892800
C	49.523312	4.366409	23.751371	C	23.643945	5.484993	38.994302
C	45.474481	5.512254	25.967896	C	24.107194	4.640707	40.011469
C	44.896555	6.626748	26.603971	O	24.541432	5.999265	38.065221
C	45.189761	3.551514	24.488983	O	19.130387	5.515372	41.658902
O	47.708915	6.325073	25.895442	O	18.609581	3.364579	42.089024
O	47.393301	4.154675	26.420690	C	19.466782	4.294834	41.870002
C	46.944888	5.314896	26.099208	C	16.866401	4.092348	37.746780
C	49.195253	5.968233	30.229377	C	17.553465	2.978408	37.231763
C	50.135742	6.814828	30.844367	C	17.559446	2.713627	35.868860
C	48.087392	5.489844	30.984621	C	16.876174	3.552937	34.996096
C	47.062420	4.721892	30.392228	C	16.148246	4.664186	35.469280
C	45.992154	4.265098	31.155291	C	16.124964	4.926682	36.865244
O	49.600959	6.550621	27.950066	C	15.338058	5.992845	37.345285
O	49.295082	4.374193	28.459712	C	14.631892	6.798578	36.460778
C	49.382027	5.609977	28.795860	C	14.678756	6.578505	35.094113
C	11.158285	7.260976	41.959131	C	15.445023	5.511647	34.572779
C	10.287267	6.502982	41.186143	O	13.968209	7.466360	34.289504
C	10.757252	5.394981	40.491131	O	17.237603	5.554737	39.591451
C	12.099252	5.042976	40.571107	O	16.703318	3.406473	40.025556
C	11.698220	3.178982	39.103109	C	16.943239	4.365663	39.207208
C	10.356220	3.528988	39.024134	C	12.972269	5.800972	41.346094
C	9.886236	4.637987	39.718144	C	12.500285	6.908972	42.040106
O	9.453202	2.792994	38.218147	C	26.809485	7.013123	42.354287
Cu	17.235428	6.086650	41.504888	C	25.956515	6.223368	41.592182
Cu	16.648785	3.694490	41.994475	C	26.440867	5.113578	40.868869
C	20.915643	3.939037	41.856356	C	27.823391	4.793861	40.939365
C	21.397381	3.047401	42.834272	C	12.571236	3.934978	39.877095
C	22.742717	2.708606	42.893887	C	27.449755	2.955732	39.396345
C	23.635065	3.251782	41.978329	C	26.096579	3.240989	39.339542
C	23.196152	4.121689	40.962611	C	25.568357	4.324678	40.076148
C	21.818069	4.458845	40.883772	O	25.308873	2.406012	38.549923

O	15.278008	6.409680	41.375446	C	32.711153	4.034463	38.108672
O	14.748902	4.265591	41.830081	C	33.286741	2.837892	37.638854
C	14.418404	5.467549	41.520425	C	33.331458	2.546890	36.282703
C	16.719745	5.778873	45.727997	C	32.795410	3.439509	35.363763
C	17.762403	6.492517	46.347879	C	32.183268	4.637952	35.781111
C	18.790781	6.893326	32.232558	C	32.132373	4.940629	37.171576
C	17.689197	6.457237	32.960051	C	31.469191	6.114411	37.583884
C	16.660085	5.715803	32.348830	C	30.933755	6.987856	36.644716
C	15.565740	5.430537	46.483188	C	31.001016	6.716058	35.289035
C	14.457303	4.790442	45.890037	C	31.616497	5.529863	34.832304
C	13.341636	4.461242	46.653816	O	30.448778	7.662898	34.428639
C	14.500610	4.593393	32.448360	O	32.984452	5.469640	40.010576
C	15.532359	5.288919	33.093142	O	32.482720	3.303122	40.371495
O	13.387299	4.186636	33.175353	C	32.721612	4.287891	39.582575
O	17.158247	6.382814	43.468055	C	28.681995	5.585699	41.750326
O	16.627987	4.234490	43.909590	C	28.157213	6.696622	42.433010
C	16.847599	5.443127	44.284002	C	42.234028	7.026049	42.099691
Cu	32.933802	5.941571	41.945906	C	41.416844	6.144852	41.402658
Cu	32.376298	3.528870	42.348758	C	41.954247	5.040545	40.709450
C	36.632186	3.826600	42.175842	C	43.359011	4.826330	40.739277
C	37.210926	3.038599	43.187398	C	28.314361	3.717734	40.172278
C	38.561288	2.711774	43.152191	C	43.068095	2.911328	39.274025
C	39.357723	3.160009	42.103541	C	41.694422	3.090961	39.262513
C	38.815104	3.925077	41.053862	C	41.112382	4.156208	39.985102
C	37.431540	4.245818	41.074407	O	40.944457	2.170319	38.534263
C	36.878712	4.945200	39.980206	O	30.972433	6.240429	41.801802
C	37.683883	5.346200	38.918607	O	30.474897	4.068669	42.158718
C	39.049437	5.074880	38.919172	C	30.128568	5.279451	41.911254
C	39.627761	4.362200	39.978319	C	32.149874	5.517347	46.107478
O	39.843819	5.491300	37.856404	C	33.089552	6.238186	46.819060
O	34.837756	5.393455	42.093865	C	34.823330	6.751865	32.221946
O	34.342296	3.224187	42.471142	C	33.786156	6.329294	33.044610
C	35.185745	4.170029	42.266751	C	32.704124	5.591886	32.529549

C	30.899443	5.117288	46.692164	C	45.974752	6.635783	35.091904
C	29.820274	4.516593	45.969229	C	46.801555	5.599136	34.603421
C	28.623079	4.230618	46.576811	O	45.234155	7.471308	34.258708
C	30.556787	4.483668	32.826234	O	48.443934	5.799425	39.673155
C	31.631670	5.201631	33.368189	O	48.100091	3.614323	40.112553
O	29.502272	4.101154	33.647807	C	48.256699	4.588431	39.290961
O	32.805718	6.179302	43.914622	C	44.184947	5.708590	41.490501
O	32.277989	4.006274	44.272477	C	43.604430	6.812876	42.141331
C	32.442100	5.214367	44.684682	C	43.901080	3.762132	39.991002
Cu	48.412849	6.330930	41.587233	O	46.433242	6.505900	41.482889
Cu	48.014325	3.900514	42.082112	O	46.079622	4.320862	41.914542
C	52.242277	4.464613	41.931331	C	45.652233	5.497960	41.632337
C	52.828351	3.947590	43.079282	C	47.873583	5.997903	45.803535
C	54.201352	3.732569	43.123180	C	48.835342	6.801241	46.443644
C	54.987276	4.036572	42.018127	C	50.024908	7.146714	32.188985
C	54.401202	4.554594	40.869175	C	48.968593	6.646907	32.942812
C	53.028202	4.768616	40.826278	C	47.987115	5.821210	32.362549
C	52.442127	5.287638	39.677327	C	46.734396	5.556363	46.532495
C	53.229054	5.591642	38.571275	C	45.693040	4.832149	45.914485
C	54.601053	5.377620	38.616175	C	44.593757	4.407560	46.654520
C	55.187127	4.858598	39.764122	C	45.913795	4.552060	32.515791
O	55.314970	5.617627	37.405127	C	46.899954	5.335590	33.130704
O	50.348357	5.900640	41.721040	O	44.838782	4.088409	33.265713
O	49.991741	3.721108	42.188028	O	48.322778	6.622205	43.550749
C	50.773227	4.711397	41.955105	O	47.940841	4.442820	43.994245
C	48.227042	4.301306	37.829679	C	48.063753	5.666050	44.365672
C	48.988240	3.223049	37.342603	C	9.830843	7.260911	57.522287
C	49.042473	2.944756	35.983700	C	8.959811	6.502921	56.749313
C	48.333656	3.733606	35.085162	C	9.429778	5.394922	56.054289
C	47.534050	4.807496	35.527287	C	10.771778	5.042912	56.134240
C	47.465992	5.087105	36.919345	C	10.370714	3.178925	54.666242
C	46.614870	6.118080	37.365482	C	9.028713	3.528933	54.587292
C	45.892026	6.876849	36.453141	C	8.558746	4.637932	55.281315

O	8.125680	2.792944	53.781318	C	25.301497	7.066998	57.646035
Cu	15.893588	6.159078	57.134550	C	24.471235	6.291802	56.845325
Cu	15.356041	3.740708	57.539211	C	24.983407	5.227232	56.075373
C	19.613432	4.082793	57.379115	C	26.376116	4.948619	56.126877
C	20.179428	3.275323	58.382334	C	11.243746	3.934914	55.440217
C	21.531905	2.958054	58.364378	C	26.059684	3.203235	54.470071
C	22.343471	3.432618	57.339674	C	24.693584	3.432585	54.445690
C	21.817274	4.223288	56.300548	C	24.128544	4.445136	55.254410
C	20.431882	4.540064	56.306208	O	23.931662	2.608018	53.620800
C	19.897310	5.271813	55.224400	O	13.936629	6.441162	56.974441
C	20.721727	5.713146	54.194007	O	13.444350	4.275608	57.362743
C	22.087834	5.442765	54.208798	C	13.093963	5.479669	57.082478
C	22.647950	4.689157	55.249657	C	15.283038	5.695841	61.352095
O	22.898794	5.896454	53.174004	C	16.314079	6.385825	61.978046
O	17.800469	5.629791	57.292746	C	17.696157	6.827372	47.694015
O	17.325530	3.452978	57.646375	C	16.584020	6.463999	48.444813
C	18.161252	4.408704	57.454073	C	15.508299	5.766567	47.862309
C	15.662652	4.257703	53.310595	C	14.198074	5.242844	62.095148
C	16.350166	3.137532	52.808411	C	13.166033	4.552860	61.469196
C	16.377749	2.868496	51.447357	C	12.083068	4.099863	62.213249
C	15.714065	3.708344	50.561430	C	13.299460	4.751984	48.015235
C	14.994067	4.831798	51.017649	C	14.371578	5.413101	48.630619
C	14.954989	5.104394	52.412234	O	12.178888	4.414052	48.765946
C	14.180736	6.188434	52.872327	O	15.756867	6.388355	59.110425
C	13.508075	7.004160	51.970950	O	15.289910	4.211809	59.470028
C	13.565852	6.769788	50.607213	C	15.448694	5.415025	59.890355
C	14.310224	5.678437	50.105211	Cu	31.460001	6.112901	57.121269
O	12.887510	7.667627	49.785932	Cu	30.942566	3.696984	57.562987
O	15.949730	5.687121	55.202982	C	35.191951	4.031802	57.416302
O	15.448583	3.518190	55.565137	C	35.731408	3.289540	58.483206
C	15.688356	4.503471	54.778848	C	37.079991	2.959481	58.514603
C	11.644811	5.800902	56.909215	C	37.914629	3.352482	57.474917
C	11.172843	6.908901	57.603238	C	37.415129	4.072587	56.373089

C	36.033891	4.406592	56.331735	O	39.557391	2.247344	53.853417
C	35.526561	5.070437	55.195366	O	29.492799	6.398666	57.033942
C	36.374967	5.427044	54.150739	O	29.027282	4.219492	57.390627
C	37.736957	5.139409	54.208175	C	28.663285	5.425958	57.142244
C	38.269710	4.452391	55.308065	C	30.903113	5.695671	61.351281
O	38.572443	5.508581	53.159967	C	31.934168	6.385649	61.977217
O	33.378123	5.578281	57.231381	C	32.841939	6.556983	48.174867
O	32.907227	3.415988	57.675192	C	31.684542	6.137567	48.792830
C	33.740073	4.364080	57.444929	C	30.686747	5.402111	48.088725
C	31.189636	4.153306	53.346441	C	29.818160	5.242675	62.094350
C	32.062896	3.202122	52.853867	C	28.786107	4.552698	61.468415
C	32.040789	2.887260	51.476185	C	27.703152	4.099704	62.212486
C	31.164696	3.531209	50.630420	C	28.442367	4.468673	47.961581
C	30.242338	4.505796	51.109877	C	29.467751	4.990998	48.741840
C	30.228120	4.812915	52.516145	O	27.243420	4.207819	48.553269
C	29.210592	5.696607	52.997112	O	31.384095	6.362297	59.100502
C	28.246397	6.191789	52.155261	O	30.889254	4.196343	59.485292
C	28.282939	5.911578	50.767040	C	31.067588	5.401066	59.891838
C	29.309592	5.146196	50.217427	Cu	47.047639	6.248626	57.148765
O	27.280509	6.434914	50.005099	Cu	46.684794	3.793008	57.533111
O	31.451286	5.627581	55.194165	C	50.914822	4.464429	57.493771
O	31.033304	3.438043	55.601792	C	51.500915	3.947400	58.641709
C	31.233283	4.421870	54.798332	C	52.873915	3.732375	58.685585
C	27.211723	5.715240	56.984688	C	53.659823	4.036378	57.580520
C	26.658436	6.783083	57.715052	C	53.073729	4.554406	56.431580
C	40.902161	6.948861	57.599451	C	51.700730	4.768431	56.388706
C	40.078425	6.121760	56.847670	C	51.114638	5.287461	55.239765
C	40.599396	5.023974	56.132450	C	51.901544	5.591465	54.133701
C	41.996855	4.762998	56.191490	C	53.273543	5.377438	54.178575
C	26.900881	3.939118	55.296381	C	53.859636	4.858411	55.326514
C	41.682646	2.903502	54.662923	O	53.987441	5.617444	52.967515
C	40.316060	3.128526	54.620575	O	48.989520	5.857957	57.299156
C	39.748091	4.193329	55.356264	O	48.671769	3.653732	57.666720

C	49.436962	4.671381	57.496679	O	46.573925	4.238658	59.461971
C	46.940678	4.361777	53.313046	C	46.674600	5.443648	59.890664
C	47.734914	3.321908	52.796134	C	16.262151	6.620810	63.347051
C	47.770576	3.062174	51.433663	C	15.179185	6.168816	64.090104
C	47.010737	3.832216	50.561734	C	14.147147	5.478833	63.465153
C	46.185778	4.874554	51.033752	C	12.031142	4.336850	63.582254
C	46.136511	5.134013	52.429976	C	13.063181	5.025837	64.207206
C	45.260271	6.129112	52.907411	O	10.943178	3.908854	64.361306
C	44.493135	6.873891	52.020179	C	31.882266	6.620631	63.346223
C	44.557847	6.655145	50.654008	C	30.799313	6.168635	64.089293
C	45.410097	5.654052	50.135056	C	29.767259	5.478659	63.464356
O	43.780229	7.482995	49.847504	C	27.651253	4.336688	63.581492
O	47.117980	5.798383	55.212476	C	28.683306	5.025664	64.206427
O	46.806175	3.591646	55.560635	O	26.563301	3.908693	64.360564
C	46.955818	4.599510	54.781390	C	47.502381	6.620396	63.345107
C	42.831139	5.597925	56.986557	C	46.419438	6.168404	64.088195
C	42.263676	6.692855	57.665834	C	45.387370	5.478430	63.463277
C	42.523963	3.705465	55.424897	C	43.271360	4.336465	63.580445
O	45.072140	6.397120	57.020576	C	44.303429	5.025438	64.205366
O	44.738472	4.191967	57.352711	O	42.183423	3.908472	64.359536
C	44.299864	5.377643	57.121126	H	12.119211	8.126789	26.936182
C	46.523187	5.695444	61.350179	H	10.573025	6.786711	25.566689
C	47.554254	6.385417	61.976098	H	13.382421	2.322409	22.982934
C	48.710071	7.130484	47.786962	H	9.847352	3.169230	22.676979
C	47.619248	6.669377	48.514775	H	22.117847	2.839954	28.244926
C	46.620553	5.881630	47.910307	H	24.513696	2.284842	28.294267
C	45.438244	5.242452	62.093268	H	25.999369	3.045683	26.513407
C	44.406178	4.552479	61.467349	H	21.502138	5.253354	24.072736
C	43.323236	4.099487	62.211437	H	22.995734	5.949962	22.308371
C	44.503992	4.681326	48.017010	H	19.532791	2.330062	22.589870
C	45.506179	5.424290	48.656377	H	19.679967	1.794512	20.190528
O	43.403234	4.244368	48.745188	H	18.480950	3.171020	18.536757
O	46.918286	6.443255	59.122682	H	16.654533	6.146656	22.827199

H	15.507709	7.502061	21.163927	H	53.552114	3.699943	28.381309
H	14.495485	7.507741	27.088116	H	55.987707	3.326262	28.455800
H	27.557884	7.920138	26.991355	H	57.384038	3.866412	26.497977
H	26.080728	6.439350	25.742145	H	52.703570	5.454848	24.016528
H	14.941213	3.632956	24.313856	H	54.081383	5.977194	22.117115
H	29.113568	2.061131	23.140977	H	50.776921	2.334581	22.589459
H	19.769587	6.918380	30.332962	H	50.920600	1.795040	20.189833
H	15.677202	4.519734	29.278555	H	49.720208	3.170723	18.536000
H	13.765737	3.822247	30.580599	H	47.864186	6.135496	22.823710
H	15.673399	6.862582	17.596200	H	46.741322	7.497396	21.163719
H	25.122331	6.092830	21.483302	H	45.517168	7.312264	27.170394
H	25.595261	2.445469	22.926887	H	46.251624	3.333688	24.478926
H	37.726688	2.881335	28.295116	H	50.968376	7.207666	30.271560
H	40.110254	2.283280	28.366128	H	47.062824	4.475120	29.335914
H	41.603065	2.926366	26.546324	H	45.219347	3.677552	30.678541
H	37.149951	5.160754	24.047514	H	46.906369	6.857486	17.596322
H	38.651523	5.737873	22.241901	H	56.056711	5.973851	21.102086
H	35.147698	2.326957	22.590536	H	10.790862	8.127806	42.498795
H	35.298242	1.793310	20.190459	H	9.244502	6.787164	41.129938
H	34.099945	3.170486	18.536580	H	12.054340	2.324549	38.544025
H	32.267949	6.144829	22.826253	H	8.521031	3.175322	38.233337
H	31.125426	7.500419	21.164009	H	20.717948	2.624073	43.565863
H	29.964606	7.445743	27.144611	H	23.099301	2.027047	43.659784
H	43.102335	7.729477	27.023618	H	24.677011	2.971691	42.059212
H	41.664199	6.235536	25.752396	H	20.332668	5.506668	39.656471
H	30.615566	3.493630	24.394431	H	21.926860	6.406808	38.089217
H	44.779998	1.879801	23.208382	H	18.099852	2.320458	37.898242
H	35.624714	6.775819	30.242633	H	18.101360	1.855725	35.484044
H	31.483511	4.317632	29.576647	H	16.906198	3.314503	33.942384
H	29.689799	3.641790	31.047783	H	15.243825	6.213236	38.402565
H	31.288445	6.858872	17.596653	H	14.033594	7.617730	36.836807
H	40.777858	5.796099	21.405434	H	13.169061	7.509649	42.647390
H	41.262999	2.240446	22.928548	H	26.423895	7.873142	42.892128

H 24.912311 6.498667 41.557620	H 30.532379 7.410246 33.458634
H 13.612117 3.634122 39.867835	H 39.323738 6.021101 37.172926
H 27.833302 2.127113 38.815939	H 39.960086 2.377791 38.536123
H 18.635741 6.784364 45.775020	H 52.223744 3.706506 43.946731
H 19.567831 7.473383 32.719994	H 54.659174 3.327335 44.019597
H 17.639686 6.716836 34.008949	H 56.055309 3.866344 42.061207
H 14.429793 4.544877 44.833498	H 51.374671 5.455086 39.580815
H 12.505135 3.968788 46.176899	H 52.752474 5.976899 37.680412
H 12.733192 3.661619 32.614209	H 49.554731 2.603591 38.029025
H 14.017992 7.236148 33.311799	H 49.640495 2.114447 35.622514
H 24.098486 6.617893 37.402588	H 48.401144 3.484859 34.035663
H 24.341351 2.679878 38.530358	H 46.480542 6.345516 38.416881
H 36.603478 2.685768 44.013379	H 45.244261 7.669363 36.803690
H 38.995054 2.108929 43.943415	H 44.226214 7.504655 42.698600
H 40.404753 2.888076 42.107627	H 44.967948 3.579255 39.931812
H 35.821984 5.181580 39.919992	H 49.692068 7.167815 45.889205
H 37.236147 5.883132 38.093485	H 50.763401 7.793024 32.652196
H 33.711220 2.127470 38.339544	H 48.914096 6.923879 33.987141
H 33.783379 1.621711 35.940025	H 45.704049 4.594247 44.856060
H 32.848727 3.176693 34.316737	H 43.808712 3.853008 46.158497
H 31.336483 6.373615 38.626899	H 44.210132 3.514003 32.724223
H 30.440482 7.893876 36.970569	H 45.304318 7.220538 33.287386
H 28.807301 7.312118 43.042997	H 54.726213 5.965600 36.662773
H 41.799921 7.877043 42.614470	H 9.463448 8.127252 58.062701
H 40.354899 6.345171 41.395106	H 7.917015 6.786914 56.693495
H 29.365732 3.455459 40.145440	H 10.726816 2.324453 54.107251
H 43.491687 2.094605 38.704819	H 7.193291 3.174735 53.797293
H 34.024691 6.568007 46.355054	H 19.560547 2.898605 59.189118
H 35.643780 7.329198 32.636072	H 21.955941 2.341020 59.149929
H 33.830055 6.593094 34.092895	H 23.391437 3.164862 57.357557
H 29.908503 4.293551 44.903436	H 18.840639 5.504097 55.149613
H 27.800752 3.796841 46.000145	H 20.287517 6.276792 53.379467
H 28.802340 3.568688 33.153423	H 16.873487 2.471852 53.485836

H 16.915665 2.002569 51.075028	H 32.788689 6.737583 61.409298
H 15.754782 3.460993 49.510282	H 33.578292 7.141842 48.734604
H 14.070906 6.417852 53.925934	H 31.512494 6.394335 49.839018
H 12.923743 7.840096 52.331736	H 28.747123 4.376499 60.399801
H 11.840420 7.509830 58.211866	H 26.897762 3.574448 61.718432
H 24.888071 7.889583 58.220590	H 26.535072 3.977306 47.882594
H 23.420815 6.543826 56.818746	H 27.034917 5.745879 49.340421
H 12.284730 3.635138 55.429515	H 38.086408 6.030312 52.445895
H 26.470760 2.430611 53.833757	H 38.578701 2.478506 53.842676
H 17.168404 6.739649 61.410939	H 50.894795 3.699755 59.506114
H 18.510371 7.373385 48.159313	H 53.331488 3.325353 59.581256
H 16.563971 6.744233 49.489300	H 54.727771 3.865587 57.623202
H 13.133563 4.371731 60.400919	H 50.047739 5.460915 55.146159
H 11.278544 3.572939 61.719668	H 51.425155 5.978041 53.243257
H 11.492374 3.909153 48.225372	H 48.333585 2.711649 53.463222
H 12.959588 7.439079 48.809224	H 48.389273 2.257752 51.049382
H 22.388918 6.452392 52.504089	H 47.060016 3.592914 49.509171
H 22.949585 2.821101 53.650224	H 45.142673 6.340628 53.964076
H 35.092289 2.971978 59.299525	H 43.827091 7.640079 52.394188
H 37.481875 2.394637 59.349308	H 42.891045 7.350617 58.257140
H 38.959118 3.077447 57.531531	H 43.585311 3.488799 55.387757
H 34.473171 5.312516 55.091641	H 48.405513 6.744773 61.407834
H 35.963238 5.938079 53.291012	H 49.462391 7.746663 48.268517
H 32.768505 2.680189 53.508952	H 47.552518 6.946611 49.558113
H 32.715449 2.119420 51.085316	H 44.382342 4.363005 60.399589
H 31.154043 3.270641 49.570937	H 42.519526 3.571042 61.717949
H 29.156047 5.961717 54.056898	H 42.766753 3.693917 48.187853
H 27.426469 6.808848 52.531783	H 43.838187 7.247707 48.871588
H 27.291063 7.390199 58.353029	H 53.398351 5.963020 52.224203
H 40.481120 7.795347 58.132137	H 17.068386 7.157776 63.836094
H 39.024815 6.359447 56.816285	H 15.148295 6.357093 65.155573
H 27.962082 3.714031 55.259380	H 10.262041 3.422115 63.798141
H 42.094464 2.089241 54.081778	H 32.688604 7.157462 63.835082

H	30.768275	6.357019	65.154663	H	26.143150	6.033523	46.482451
H	25.880724	3.425136	63.796284	H	22.597732	5.501253	44.020304
H	48.307438	7.159323	63.833709	H	22.679779	6.675632	45.345836
H	46.387753	6.357559	65.153431	H	21.344993	4.618917	45.984326
H	41.497209	3.430950	63.794299	H	22.803384	3.629864	45.756863
H	54.922468	4.682740	55.325478	H	22.612388	4.176009	48.164717
H	56.249997	4.683114	39.763384	H	22.422910	5.906380	47.799953
H	57.578847	4.683549	24.200360	H	24.891661	4.789993	44.344838
H	32.654139	5.043594	18.026555	H	25.540441	9.821324	45.956986
H	17.034773	5.043885	18.026683	H	27.139793	10.406343	44.153178
H	10.176561	4.915040	24.089519	H	29.492236	9.549267	44.211124
H	8.847984	4.915260	39.653157	H	30.198284	8.053524	46.099080
H	7.520505	4.915220	55.216468	H	28.608843	7.480878	47.906080
H	12.998722	5.198769	65.269007	H	25.258282	8.866310	48.181520
H	28.618680	5.198750	65.268091	H	26.476217	7.955951	48.957438
H	44.238260	5.198921	65.266950				
H	48.273808	5.043409	18.026056	TS _{BINOL}			
C	22.906508	4.971485	47.454165	C	12.487000	7.261000	26.395000
C	24.400902	5.182511	47.533824	C	11.616000	6.503000	25.622000
C	25.193657	5.502375	46.335853	C	12.086000	5.395000	24.927000
C	24.547898	5.634766	44.969559	C	13.428000	5.043000	25.007000
C	23.009984	5.666191	45.030245	C	13.027000	3.179000	23.539000
C	22.448779	4.641005	46.025055	C	11.685000	3.529000	23.460000
O	25.206830	4.159188	46.903588	C	11.215000	4.638000	24.154000
C	26.964087	8.618478	47.069929	O	10.782000	2.793000	22.654000
C	26.565824	9.433964	45.989552	Cu	18.546834	6.089739	26.015783
C	27.469877	9.761625	44.975002	Cu	17.954989	3.702729	26.532258
C	28.784783	9.282157	45.002567	C	22.221721	3.955531	26.379113
C	29.178898	8.452271	46.060672	C	22.766550	3.200697	27.433780
C	28.286450	8.123249	47.082369	C	24.120248	2.888283	27.462080
N	26.066380	8.261022	48.073963	C	24.953817	3.316544	26.434306
H	24.929083	6.553940	44.494372	C	24.447099	4.047483	25.343218
H	24.790848	5.511969	48.507283	C	23.060906	4.355433	25.300399

C	22.546003	5.021406	24.167608	O	16.597377	6.405495	25.852812
C	23.390245	5.407788	23.131334	O	16.058296	4.265621	26.320527
C	24.756825	5.147633	23.191827	C	15.737331	5.463203	25.985713
C	25.297202	4.459639	24.286833	C	17.924415	5.830664	30.234294
O	25.588192	5.540676	22.148733	C	18.924622	6.581551	30.878813
O	20.439608	5.524081	26.186621	C	16.768002	5.435705	30.964223
O	19.919014	3.379438	26.655271	C	15.688000	4.773841	30.342299
C	20.774785	4.307341	26.418337	C	14.574076	4.390798	31.083344
C	18.226925	4.022012	22.293999	O	18.439020	6.410040	27.977569
C	18.992913	2.941010	21.873981	O	17.901760	4.266982	28.434906
C	19.081888	2.638015	20.519979	C	18.105369	5.481156	28.798305
C	18.404874	3.417021	19.587993	Cu	34.124493	6.060838	26.052446
C	17.639885	4.497022	20.008011	Cu	33.573411	3.663737	26.557228
C	17.550911	4.800017	21.362013	C	37.829344	3.950924	26.424446
C	16.783920	5.881019	21.784030	C	38.353953	3.233834	27.515671
C	16.107906	6.659024	20.850045	C	39.699334	2.892302	27.565638
C	16.197881	6.355028	19.497042	C	40.545037	3.250534	26.522097
C	16.963871	5.274029	19.076025	C	40.059967	3.946261	25.398566
O	15.523868	7.185034	18.539057	C	38.682368	4.290171	25.337575
O	18.565144	5.531539	24.111497	C	38.189293	4.929440	24.181178
O	18.027501	3.390061	24.576524	C	39.046602	5.246506	23.131688
C	18.266874	4.337585	23.746256	C	40.405385	4.947803	23.206103
C	14.301000	5.801000	25.782000	C	40.924982	4.291435	24.330667
C	13.829000	6.909000	26.476000	O	41.250258	5.277448	22.151995
C	27.950197	7.075054	26.427358	O	36.033617	5.509694	26.187829
C	27.117424	6.214070	25.721632	O	35.535177	3.360534	26.660689
C	27.630560	5.080714	25.058485	C	36.381026	4.296817	26.429748
C	29.025616	4.817284	25.126059	C	33.846852	4.021974	22.293716
C	13.900000	3.935000	24.313000	C	34.612829	2.940971	21.873681
C	28.703658	2.897126	23.673706	C	34.701778	2.637980	20.519676
C	27.337306	3.118414	23.634416	C	34.024750	3.416990	19.587706
C	26.775168	4.213315	24.328519	C	33.259772	4.496992	20.007739
O	26.573393	2.208352	22.906938	C	33.170822	4.799984	21.361745

C	32.403844	5.880987	21.783779	C	54.157056	3.947784	27.515893
C	31.727817	6.658997	20.849809	C	55.530058	3.732771	27.559816
C	31.817767	6.355005	19.496804	C	56.316001	4.036773	26.454777
C	32.583744	5.274001	19.075769	C	55.729944	4.554792	25.305813
O	31.143737	7.185017	18.538834	C	54.356945	4.768807	25.262890
O	34.128948	5.523957	24.137445	C	53.770888	5.287824	24.113928
O	33.634416	3.370432	24.585422	C	54.557831	5.591827	23.007888
C	33.862092	4.326650	23.758400	C	55.929832	5.377811	23.052810
C	29.864466	5.674049	25.893422	C	56.515887	4.858794	24.200774
C	29.310483	6.809784	26.511614	O	56.643767	5.617817	21.841773
C	43.540297	6.893907	26.520540	O	51.635627	5.836587	26.124696
C	42.720639	6.028940	25.807217	O	51.335017	3.659525	26.636974
C	43.247078	4.901210	25.144283	C	52.092450	4.665946	26.381618
C	44.644792	4.648037	25.218888	C	49.466776	4.021885	22.293147
C	29.548009	3.727943	24.399721	C	50.232742	2.940881	21.873096
C	44.340288	2.713363	23.783919	C	50.321665	2.637894	20.519088
C	42.973802	2.934905	23.723382	C	49.644622	3.416909	19.587132
C	42.401593	4.033594	24.403160	C	48.879655	4.496913	20.007183
O	42.219616	2.018938	22.993449	C	48.790732	4.799902	21.361191
O	32.155192	6.355837	25.938341	C	48.023768	5.880906	21.783244
O	31.670699	4.199985	26.388326	C	47.347725	6.658920	20.849287
C	31.315571	5.394918	26.084276	C	47.437649	6.354933	19.496280
C	33.635602	5.761968	30.289241	C	48.203614	5.273930	19.075227
C	34.658087	6.524595	30.884570	O	46.763606	7.184950	18.538323
C	32.520495	5.357981	31.076690	O	49.727817	5.590654	24.092507
C	31.422881	4.675674	30.511930	O	49.385362	3.424305	24.609098
C	30.347225	4.290913	31.306680	C	49.524005	4.367999	23.750871
O	34.053937	6.361337	28.018779	C	45.475275	5.526728	25.969128
O	33.542052	4.211609	28.470777	C	44.903625	6.649390	26.596620
C	33.752032	5.423401	28.841386	C	45.176689	3.552500	24.510791
Cu	49.692393	6.203175	25.987694	O	47.712059	6.333984	25.890297
Cu	49.343807	3.785031	26.566004	O	47.392621	4.165651	26.421154
C	53.571003	4.464803	26.367930	C	46.945967	5.325926	26.097310

C	49.199258	5.983800	30.224876	C	17.533677	2.977428	37.225235
C	50.142486	6.827829	30.839179	C	17.539490	2.719546	35.861149
C	48.089634	5.509968	30.980005	C	16.869193	3.571942	34.991188
C	47.062006	4.745586	30.387586	C	16.155616	4.690841	35.468159
C	45.990232	4.292550	31.150613	C	16.133138	4.947286	36.865378
O	49.604497	6.561155	27.944603	C	15.360960	6.022934	37.348347
O	49.295823	4.386126	28.458804	C	14.668895	6.843083	36.465763
C	49.385023	5.622490	28.792296	C	14.714585	6.627678	35.098318
C	11.158285	7.260976	41.959131	C	15.465404	5.551455	34.574038
C	10.287267	6.502982	41.186143	O	14.018511	7.529003	34.295980
C	10.757252	5.394981	40.491131	O	17.237938	5.542302	39.601919
C	12.099252	5.042976	40.571107	O	16.687265	3.394719	40.017781
C	11.698220	3.178982	39.103109	C	16.934910	4.358894	39.207495
C	10.356220	3.528988	39.024134	C	12.972269	5.800972	41.346094
C	9.886236	4.637987	39.718144	C	12.500285	6.908972	42.040106
O	9.453202	2.792994	38.218147	C	26.726566	6.744400	42.191115
Cu	17.240471	6.055639	41.520235	C	25.879521	5.965474	41.413695
Cu	16.632994	3.664805	41.989727	C	26.365662	4.858815	40.687315
C	20.898791	3.863413	41.831085	C	27.748248	4.535941	40.764529
C	21.398507	3.015493	42.837334	C	12.571236	3.934978	39.877095
C	22.736401	2.643883	42.859907	C	27.384971	2.737418	39.172824
C	23.604580	3.117707	41.884188	C	26.029952	3.016665	39.120265
C	23.145205	3.943051	40.840774	C	25.495166	4.082015	39.878800
C	21.772135	4.306905	40.797142	O	25.247709	2.191626	38.314972
C	21.304100	5.064138	39.701909	O	15.283953	6.397051	41.393525
C	22.182551	5.487651	38.709228	O	14.738606	4.253319	41.828895
C	23.536817	5.170779	38.774209	C	14.416929	5.459640	41.527252
C	24.029221	4.389725	39.828256	C	16.696255	5.716550	45.741523
O	24.402816	5.601449	37.775515	C	17.722054	6.447986	46.368897
O	19.133179	5.464731	41.661845	C	18.822696	6.896089	32.227936
O	18.590148	3.316678	42.083290	C	17.717563	6.472452	32.957548
C	19.456159	4.238663	41.865390	C	16.678647	5.743383	32.347982
C	16.859791	4.097343	37.744690	C	15.547374	5.340383	46.492940

C	14.450523	4.685763	45.893780	C	31.360277	5.523898	34.740860
C	13.341513	4.327653	46.654303	O	29.897279	7.489537	34.465938
C	14.506011	4.647069	32.450539	O	32.909177	5.366292	39.898470
C	15.547166	5.329859	33.093930	O	32.461152	3.168153	40.125536
O	13.388777	4.254120	33.179069	C	32.687144	4.202858	39.401232
O	17.162772	6.334106	43.487978	C	28.600978	5.308245	41.602817
O	16.612533	4.187087	43.908905	C	28.070201	6.415054	42.292269
C	16.836678	5.391049	44.294865	C	42.218613	7.008806	42.082058
Cu	32.844111	5.711599	41.861518	C	41.405099	6.125636	41.382636
Cu	32.336194	3.267486	42.108760	C	41.947492	5.024380	40.689318
C	36.588772	3.673237	42.047473	C	43.353398	4.813971	40.723032
C	37.164671	2.892791	43.066022	C	28.244569	3.481003	39.972366
C	38.527243	2.618906	43.069848	C	43.071298	2.898752	39.256652
C	39.337710	3.109499	42.050970	C	41.697234	3.073583	39.242548
C	38.798704	3.867183	40.994056	C	41.109801	4.138328	39.961746
C	37.405103	4.142100	40.980209	O	40.952108	2.149132	38.513842
C	36.859378	4.846223	39.886140	O	30.880747	5.986757	41.724715
C	37.678987	5.289097	38.852655	O	30.420245	3.789181	41.941337
C	39.051438	5.054043	38.881843	C	30.052371	5.007399	41.765245
C	39.624072	4.339709	39.943463	C	32.129738	4.977296	46.002666
O	39.858168	5.504707	37.842798	C	33.018283	5.783247	46.693183
O	34.758038	5.194604	41.987913	C	34.616794	6.846284	32.235275
O	34.307813	2.995869	42.228957	C	33.549097	6.421476	33.017408
C	35.131804	3.972226	42.104286	C	32.489867	5.680434	32.461319
C	32.707022	4.032459	37.919950	C	30.970025	4.409276	46.635420
C	33.429805	2.948353	37.387537	C	29.936671	3.685706	45.955758
C	33.489652	2.731796	36.018390	C	28.804233	3.266848	46.607498
C	32.818331	3.585023	35.151876	C	30.334231	4.568134	32.671807
C	32.063223	4.673065	35.635247	C	31.394571	5.270552	33.261434
C	32.003119	4.901147	37.038567	O	29.252987	4.175083	33.452508
C	31.208601	5.959526	37.521706	O	32.706150	5.813923	43.843236
C	30.530921	6.789931	36.636842	O	32.233539	3.610386	44.055999
C	30.595139	6.588756	35.267711	C	32.380059	4.787877	44.551057

Cu	48.406404	6.327334	41.586681	O	46.424806	6.499521	41.479562
Cu	48.010898	3.895300	42.073764	O	46.074437	4.312796	41.903763
C	52.242277	4.464613	41.931331	C	45.644781	5.489759	41.623651
C	52.828351	3.947590	43.079282	C	47.865685	5.981964	45.801966
C	54.201352	3.732569	43.123180	C	48.826131	6.786788	46.442344
C	54.987276	4.036572	42.018127	C	50.032482	7.161146	32.183534
C	54.401202	4.554594	40.869175	C	48.974590	6.664968	32.937631
C	53.028202	4.768616	40.826278	C	47.990574	5.841999	32.357720
C	52.442127	5.287638	39.677327	C	46.728534	5.536357	46.531684
C	53.229054	5.591642	38.571275	C	45.688197	4.810516	45.913894
C	54.601053	5.377620	38.616175	C	44.590224	4.383306	46.654437
C	55.187127	4.858598	39.764122	C	45.913247	4.579419	32.511192
O	55.314970	5.617627	37.405127	C	46.902250	5.359500	33.126003
O	50.344219	5.899153	41.721824	O	44.837204	4.118649	33.261389
O	49.989957	3.718225	42.182578	O	48.313394	6.612843	43.550832
C	50.771204	4.709919	41.953735	O	47.933576	4.431858	43.987741
C	48.225990	4.310401	37.822516	C	48.055123	5.654130	44.362929
C	48.984691	3.231644	37.332707	C	9.830843	7.260911	57.522287
C	49.038618	2.956804	35.973138	C	8.959811	6.502921	56.749313
C	48.332292	3.749961	35.076482	C	9.429778	5.394922	56.054289
C	47.535726	4.825082	35.521125	C	10.771778	5.042912	56.134240
C	47.467619	5.101034	36.913898	C	10.370714	3.178925	54.666242
C	46.618874	6.133126	37.362191	C	9.028713	3.528933	54.587292
C	45.899720	6.897262	36.451338	C	8.558746	4.637932	55.281315
C	45.983113	6.660015	35.089511	O	8.125680	2.792944	53.781318
C	46.806092	5.621394	34.599002	Cu	15.904420	6.102651	57.128626
O	45.246983	7.501055	34.257849	Cu	15.329732	3.697875	57.562102
O	48.440847	5.802375	39.671151	C	19.591759	3.964485	57.440100
O	48.099701	3.615498	40.103231	C	20.132349	3.200616	58.490499
C	48.255178	4.592561	39.284827	C	21.479154	2.859456	58.505063
C	44.175923	5.697398	41.477373	C	22.309895	3.265410	57.466290
C	43.590013	6.799657	42.127093	C	21.808311	4.008079	56.380776
C	43.900158	3.752036	39.975233	C	20.429092	4.350581	56.355137

C	19.917919	5.034895	55.232578	O	13.948284	6.416034	56.971100
C	20.758553	5.398296	54.184801	O	13.426660	4.261319	57.379882
C	22.118970	5.101060	54.226235	C	13.091934	5.467331	57.088966
C	22.656996	4.400184	55.314618	C	15.283038	5.695841	61.352095
O	22.946347	5.476897	53.173350	C	16.314079	6.385825	61.978046
O	17.805331	5.540245	57.289655	C	17.647600	6.770077	47.717728
O	17.291827	3.377996	57.678783	C	16.543021	6.377317	48.464516
C	18.144619	4.316594	57.480726	C	15.481703	5.664123	47.875087
C	15.641363	4.160688	53.327180	C	14.198074	5.242844	62.095148
C	16.336810	3.042299	52.832508	C	13.166033	4.552860	61.469196
C	16.366360	2.765023	51.472876	C	12.083068	4.099863	62.213249
C	15.696428	3.594493	50.581462	C	13.292307	4.606810	48.017839
C	14.966637	4.714135	51.030949	C	14.350005	5.285139	48.639142
C	14.925742	4.994898	52.423880	O	12.176544	4.243829	48.763967
C	14.143521	6.075398	52.878212	O	15.776881	6.358195	59.103104
C	13.460076	6.877451	51.972630	O	15.274752	4.193738	59.485584
C	13.518757	6.635058	50.610142	C	15.452173	5.398609	59.893338
C	14.276231	5.550040	50.113620	Cu	31.474123	5.943667	57.105380
O	12.828289	7.519461	49.784359	Cu	30.989308	3.542706	57.652040
O	15.946323	5.607659	55.202108	C	35.232567	3.933318	57.490070
O	15.419052	3.449327	55.590465	C	35.794650	3.252061	58.585600
C	15.670848	4.422146	54.792441	C	37.147792	2.940345	58.614689
C	11.644811	5.800902	56.909215	C	37.964319	3.293690	57.546536
C	11.172843	6.908901	57.603238	C	37.442107	3.954863	56.418460
C	25.326270	6.882641	57.582402	C	36.055949	4.266037	56.378097
C	24.490373	6.066245	56.830643	C	35.524773	4.864495	55.216457
C	24.995377	4.956342	56.122467	C	36.354497	5.180239	54.144470
C	26.387496	4.673547	56.187137	C	37.721341	4.917116	54.199089
C	11.243746	3.934914	55.440217	C	38.278255	4.295794	55.325883
C	26.053827	2.825773	54.649311	O	38.537438	5.242094	53.121355
C	24.689767	3.065596	54.608883	O	33.397904	5.443970	57.250083
C	24.133958	4.134132	55.348780	O	32.957916	3.295559	57.784436
O	23.920505	2.196886	53.838259	C	33.776840	4.245280	57.514711

C	31.317815	3.793626	53.422166	C	29.818160	5.242675	62.094350
C	32.273227	2.880762	53.014637	C	28.786107	4.552698	61.468415
C	32.318961	2.476693	51.660563	C	27.703152	4.099704	62.212486
C	31.413742	2.983904	50.754852	C	28.614684	3.510232	47.997282
C	30.406642	3.912722	51.146882	C	29.618468	4.149102	48.732113
C	30.340648	4.330062	52.524362	O	27.448907	3.191939	48.584799
C	29.269946	5.196606	52.910881	O	31.385047	6.283120	59.074029
C	28.294836	5.562264	52.013498	O	30.922176	4.127676	59.548174
C	28.367103	5.149758	50.660976	C	31.082402	5.350740	59.904502
C	29.446675	4.402544	50.193908	Cu	47.040617	6.236209	57.145009
O	27.336752	5.488514	49.825465	Cu	46.688711	3.780487	57.537367
O	31.487547	5.369193	55.199084	C	50.914822	4.464429	57.493771
O	31.096789	3.195387	55.705510	C	51.500915	3.947400	58.641709
C	31.300308	4.141224	54.858468	C	52.873915	3.732375	58.685585
C	27.230756	5.490309	56.990031	C	53.659823	4.036378	57.580520
C	26.682635	6.599942	57.659961	C	53.073729	4.554406	56.431580
C	40.882584	6.907888	57.518837	C	51.700730	4.768431	56.388706
C	40.069573	6.049027	56.791490	C	51.114638	5.287461	55.239765
C	40.603258	4.932994	56.115020	C	51.901544	5.591465	54.133701
C	42.003687	4.690739	56.182520	C	53.273543	5.377438	54.178575
C	26.903088	3.609556	55.421613	C	53.859636	4.858411	55.326514
C	41.711929	2.782986	54.709035	O	53.987441	5.617444	52.967515
C	40.341973	2.984921	54.667051	O	48.984896	5.853368	57.297192
C	39.761238	4.064586	55.370266	O	48.675122	3.648970	57.670429
O	39.593439	2.065704	53.935199	C	49.436608	4.668492	57.496838
O	29.504477	6.196292	56.996382	C	46.938709	4.340620	53.314417
O	29.066029	4.030127	57.451106	C	47.735883	3.302969	52.797810
C	28.686613	5.219743	57.149247	C	47.773007	3.043621	51.435263
C	30.903113	5.695671	61.351281	C	47.011420	3.811608	50.562951
C	31.934168	6.385649	61.977217	C	46.183313	4.851561	51.034569
C	32.802354	6.040815	48.065742	C	46.132871	5.110896	52.430841
C	31.721552	5.491086	48.718844	C	45.254446	6.104385	52.907713
C	30.780205	4.657693	48.044474	C	44.486811	6.848153	52.020023

C	44.552527	6.629437	50.653912	C	30.799313	6.168635	64.089293
C	45.406244	5.629361	50.135429	C	29.767259	5.478659	63.464356
O	43.774509	7.456553	49.846981	C	27.651253	4.336688	63.581492
O	47.113769	5.780937	55.210552	C	28.683306	5.025664	64.206427
O	46.809834	3.574080	55.564572	O	26.563301	3.908693	64.360564
C	46.955038	4.580672	54.782521	C	47.502381	6.620396	63.345107
C	42.826963	5.556254	56.957398	C	46.419438	6.168404	64.088195
C	42.245899	6.665959	57.600379	C	45.387370	5.478430	63.463277
C	42.543663	3.619277	55.444275	C	43.271360	4.336465	63.580445
O	45.063253	6.373797	57.011934	C	44.303429	5.025438	64.205366
O	44.741558	4.168852	57.354632	O	42.183423	3.908472	64.359536
C	44.296603	5.349474	57.110897	H	12.119207	8.126810	26.936144
C	46.523187	5.695444	61.350179	H	10.573020	6.786699	25.566687
C	47.554254	6.385417	61.976098	H	13.382385	2.322291	22.983093
C	48.701743	7.113521	47.786318	H	9.847262	3.168990	22.677262
C	47.612921	6.648738	48.514638	H	22.131799	2.867595	28.247404
C	46.615394	5.859574	47.910116	H	24.528577	2.315056	28.288274
C	45.438244	5.242452	62.093268	H	26.003069	3.059377	26.491017
C	44.406178	4.552479	61.467349	H	21.489509	5.240720	24.056823
C	43.323236	4.099487	62.211437	H	22.971488	5.919153	22.275303
C	44.500927	4.655745	48.017262	H	19.532910	2.330185	22.589884
C	45.502545	5.399447	48.656690	H	19.679959	1.794503	20.190531
O	43.400717	4.217549	48.745522	H	18.480914	3.170991	18.536759
O	46.910650	6.438095	59.118722	H	16.653661	6.146412	22.827112
O	46.577509	4.233025	59.465543	H	15.507548	7.501947	21.163930
C	46.673877	5.439896	59.890593	H	14.495474	7.507943	27.087931
C	16.262151	6.620810	63.347051	H	27.535631	7.949383	26.918611
C	15.179185	6.168816	64.090104	H	26.063842	6.451898	25.683297
C	14.147147	5.478833	63.465153	H	14.941178	3.632736	24.314644
C	12.031142	4.336850	63.582254	H	29.111972	2.058886	23.125046
C	13.063181	5.025837	64.207206	H	19.797536	6.910760	30.326012
O	10.943178	3.908854	64.361306	H	15.679532	4.555296	29.279731
C	31.882266	6.620631	63.346223	H	13.760152	3.882882	30.584190

H	15.673136	6.862396	17.596219	H	46.741374	7.497436	21.163713
H	25.092976	6.055288	21.435881	H	45.528939	7.338612	27.153300
H	25.592075	2.428557	22.908305	H	46.237895	3.331837	24.496303
H	37.707365	2.946077	28.337371	H	50.976594	7.217260	30.266173
H	40.090306	2.346197	28.418166	H	47.061602	4.498745	29.331262
H	41.586458	2.966982	26.593190	H	45.215396	3.707692	30.673850
H	37.140566	5.183331	24.065824	H	46.906562	6.857623	17.596299
H	38.645089	5.737764	22.255866	H	56.056703	5.973765	21.102053
H	35.148623	2.328041	22.590729	H	10.790755	8.127468	42.499254
H	35.298498	1.793496	20.190440	H	9.244456	6.787020	41.130134
H	34.099983	3.170505	18.536575	H	12.054400	2.324783	38.543692
H	32.266088	6.144465	22.826001	H	8.520687	3.174423	38.234540
H	31.125188	7.500260	21.163991	H	20.737913	2.644085	43.612974
H	29.943389	7.483085	27.078908	H	23.105506	1.986310	43.640886
H	43.114945	7.761900	27.013950	H	24.641086	2.812059	41.937125
H	41.665770	6.259515	25.765447	H	20.258357	5.325000	39.583076
H	30.608897	3.508157	24.366058	H	21.799965	6.069477	37.881721
H	44.755167	1.869499	23.249034	H	18.069431	2.308542	37.889543
H	35.500548	6.860716	30.290272	H	18.070633	1.856276	35.473358
H	31.371201	4.441762	29.453881	H	16.897979	3.337765	33.936512
H	29.518166	3.766877	30.851012	H	15.267377	6.240203	38.406301
H	31.288284	6.858750	17.596665	H	14.082126	7.669529	36.844000
H	40.771547	5.779740	21.419289	H	13.168940	7.508407	42.648694
H	41.237718	2.236828	22.985160	H	26.337113	7.604514	42.725769
H	53.552100	3.700226	28.381372	H	24.838734	6.251161	41.363487
H	55.987715	3.326303	28.455816	H	13.612197	3.635024	39.864778
H	57.384039	3.866408	26.497975	H	27.773499	1.925226	38.572907
H	52.703575	5.454334	24.015997	H	18.590295	6.761864	45.800174
H	54.081374	5.977058	22.117060	H	19.607366	7.467024	32.713919
H	50.777031	2.334772	22.589528	H	17.673012	6.732058	34.006676
H	50.920645	1.795071	20.189831	H	14.425461	4.451740	44.834812
H	49.720231	3.170731	18.535998	H	12.514873	3.823436	46.172500
H	47.864238	6.135526	22.823731	H	12.727601	3.736949	32.618935

H	14.068441	7.303178	33.317226	H	49.634398	2.125746	35.609981
H	23.941466	6.175986	37.086168	H	48.399424	3.503640	34.026391
H	24.277959	2.457268	38.303814	H	46.483562	6.357570	38.414053
H	36.545916	2.507855	43.869172	H	45.254327	7.690977	36.803510
H	38.959518	2.024770	43.868456	H	44.208173	7.492691	42.686772
H	40.394049	2.879199	42.086004	H	44.967632	3.572424	39.918099
H	35.797377	5.053708	39.806169	H	49.681167	7.156680	45.887497
H	37.236449	5.825819	38.024538	H	50.772990	7.805420	32.646378
H	33.952861	2.266776	38.049223	H	48.920909	6.942552	33.981839
H	34.054771	1.893048	35.624987	H	45.698864	4.573603	44.855241
H	32.882188	3.376538	34.093579	H	43.805694	3.827934	46.158507
H	31.086607	6.156839	38.580536	H	44.207134	3.545645	32.720061
H	29.929382	7.605268	37.015896	H	45.320010	7.254900	33.285526
H	28.713896	7.023288	42.917981	H	54.726168	5.965290	36.662668
H	41.780842	7.858103	42.596528	H	9.463384	8.127028	58.062999
H	40.342168	6.321253	41.373178	H	7.916995	6.786833	56.693556
H	29.296552	3.222668	39.940746	H	10.726902	2.324640	54.106987
H	43.498490	2.083174	38.688553	H	7.193513	3.175245	53.796556
H	33.884316	6.234809	46.197852	H	19.497904	2.876389	59.307879
H	35.418414	7.426609	32.680800	H	21.883459	2.276402	59.326209
H	33.549612	6.688204	34.065818	H	23.352628	2.980458	57.509388
H	29.999646	3.471660	44.886699	H	18.866960	5.287927	55.140812
H	28.010573	2.749132	46.062027	H	20.342186	5.923341	53.335981
H	28.570459	3.648122	32.928491	H	16.866154	2.385774	53.514154
H	29.975397	7.284071	33.484583	H	16.911678	1.901468	51.105795
H	39.339665	6.027738	37.152975	H	15.739688	3.342058	49.531535
H	39.965279	2.344076	38.524182	H	14.036291	6.311616	53.930790
H	52.223594	3.706224	43.946521	H	12.867279	7.709363	52.328865
H	54.659162	3.327249	44.019566	H	11.840898	7.508329	58.212690
H	56.055302	3.866287	42.061191	H	24.918240	7.738070	58.110835
H	51.374702	5.455542	39.581141	H	23.440731	6.320401	56.794406
H	52.752492	5.977009	37.680452	H	12.284838	3.635320	55.428655
H	49.549331	2.608831	38.017625	H	26.457268	2.008791	54.065633

H	17.169444	6.737208	61.411057	H	50.894810	3.699324	59.506020
H	18.450352	7.328004	48.188746	H	53.331465	3.325223	59.581211
H	16.517422	6.647051	49.511634	H	54.727760	3.865509	57.623182
H	13.128333	4.376200	60.400628	H	50.047718	5.460894	55.146272
H	11.277897	3.574059	61.719498	H	51.425153	5.978025	53.243258
H	11.500753	3.729430	48.218831	H	48.336425	2.694774	53.465094
H	12.895015	7.281017	48.809648	H	48.394641	2.241382	51.051184
H	22.448054	5.983058	52.457045	H	47.062284	3.572906	49.510330
H	22.941762	2.426613	53.843477	H	45.135755	6.315668	53.964286
H	35.170147	2.966637	59.424739	H	43.819716	7.613644	52.393581
H	37.567393	2.420197	59.469429	H	42.863784	7.346266	58.175854
H	39.012440	3.032810	57.601580	H	43.607685	3.417139	55.408089
H	34.466721	5.085592	55.113623	H	48.405456	6.744451	61.407611
H	35.923773	5.640057	53.265387	H	49.453133	7.730764	48.267977
H	32.994548	2.454462	53.720668	H	47.546813	6.924220	49.558477
H	33.067393	1.745986	51.338985	H	44.382412	4.362805	60.399586
H	31.445300	2.651326	49.715689	H	42.519551	3.570987	61.717961
H	29.188344	5.553209	53.942158	H	42.764613	3.666659	48.188177
H	27.439301	6.168556	52.321726	H	43.834069	7.222086	48.870966
H	27.319920	7.242927	58.256892	H	53.398286	5.962655	52.224094
H	40.451337	7.766866	58.022610	H	17.068722	7.157168	63.836200
H	39.013953	6.275694	56.748343	H	15.148395	6.356891	65.155609
H	27.962626	3.375344	55.394991	H	10.262421	3.421460	63.798240
H	42.133640	1.957523	54.151180	H	32.689507	7.155789	63.835403
H	32.791737	6.730383	61.409683	H	30.768511	6.356513	65.154755
H	33.494872	6.691194	48.608848	H	25.881286	3.424216	63.796349
H	31.565281	5.721485	49.772907	H	48.307471	7.159256	63.833721
H	28.747587	4.377141	60.399311	H	46.387810	6.357434	65.153454
H	26.897872	3.574342	61.718324	H	41.497526	3.430340	63.794426
H	26.587847	3.089535	47.873525	H	54.922460	4.682685	55.325469
H	27.156338	4.643850	49.314557	H	56.249995	4.683082	39.763378
H	38.032834	5.712692	52.384884	H	57.578846	4.683534	24.200355
H	38.610370	2.277327	53.926626	H	32.654137	5.043583	18.026552

H	17.034744	5.043864	18.026684	H	27.925733	9.899918	44.205205
H	10.176555	4.915023	24.089519	H	30.258676	9.081643	44.592581
H	8.847975	4.915224	39.653217	H	30.699541	7.433417	46.425089
H	7.520503	4.915162	55.216475	H	28.836811	6.615956	47.843569
H	12.998757	5.198690	65.269016	H	25.403771	7.746244	47.561618
H	28.618714	5.198609	65.268102	H	26.531437	6.888973	48.494661
H	44.238270	5.198878	65.266956				
H	48.273830	5.043416	18.026052	PC _{BINOL}			
C	23.510621	4.770401	47.259242	C	12.487000	7.261000	26.395000
C	24.980268	4.534589	47.604918	C	11.616000	6.503000	25.622000
C	25.962896	5.221029	46.733775	C	12.086000	5.395000	24.927000
C	25.651077	5.472056	45.290147	C	13.428000	5.043000	25.007000
C	24.166036	5.754531	45.024135	C	13.027000	3.179000	23.539000
C	23.269426	4.738990	45.745467	C	11.685000	3.529000	23.460000
O	25.507750	3.336737	47.100231	C	11.215000	4.638000	24.154000
C	27.330603	7.791450	46.824154	O	10.782000	2.793000	22.654000
C	27.077456	8.713673	45.796509	Cu	18.547019	6.079847	26.021582
C	28.131595	9.180419	45.004238	Cu	17.950555	3.692538	26.530279
C	29.437545	8.725816	45.221670	C	22.217443	3.935680	26.379525
C	29.686383	7.804991	46.247411	C	22.761244	3.180867	27.434748
C	28.642153	7.341088	47.049261	C	24.113864	2.863528	27.461410
N	26.266735	7.202897	47.551824	C	24.947353	3.286897	26.431530
H	26.301465	6.286144	44.928808	C	24.441764	4.018720	25.340506
H	25.144341	4.678197	48.692462	C	23.056588	4.331616	25.299430
H	27.014140	5.110202	46.987457	C	22.542505	4.999080	24.167251
H	23.980529	5.736862	43.936299	C	23.386482	5.381066	23.129179
H	23.916130	6.777058	45.374523	C	24.752309	5.116314	23.187967
H	22.205751	4.932957	45.518452	C	25.292105	4.427813	24.283041
H	23.505480	3.724670	45.382537	O	25.583506	5.506229	22.143584
H	22.911349	3.996657	47.771166	O	20.438823	5.509151	26.191886
H	23.204169	5.751601	47.676513	O	19.913477	3.363641	26.651316
H	25.970977	4.572397	44.734500	C	20.771322	4.290704	26.419140
H	26.053402	9.057485	45.612754	C	18.226925	4.022012	22.293999

C	18.992913	2.941010	21.873981	O	17.901252	4.249154	28.434643
C	19.081888	2.638015	20.519979	C	18.103926	5.461868	28.802831
C	18.404874	3.417021	19.587993	Cu	34.113164	6.041353	26.061670
C	17.639885	4.497022	20.008011	Cu	33.572536	3.639437	26.553640
C	17.550911	4.800017	21.362013	C	37.826072	3.941337	26.417809
C	16.783920	5.881019	21.784030	C	38.350514	3.211417	27.500596
C	16.107906	6.659024	20.850045	C	39.695750	2.869383	27.547001
C	16.197881	6.355028	19.497042	C	40.541555	3.239436	26.507822
C	16.963871	5.274029	19.076025	C	40.056842	3.948278	25.392390
O	15.523868	7.185034	18.539057	C	38.679390	4.293609	25.335267
O	18.565360	5.527383	24.115166	C	38.186908	4.946750	24.186396
O	18.021328	3.386118	24.573987	C	39.044653	5.275483	23.140822
C	18.264549	4.335037	23.746600	C	40.403223	4.974813	23.211759
C	14.301000	5.801000	25.782000	C	40.922216	4.304979	24.328616
C	13.829000	6.909000	26.476000	O	41.248487	5.316582	22.161840
C	27.935470	7.029671	26.451277	O	36.024799	5.496539	26.193929
C	27.106098	6.173049	25.736358	O	35.534674	3.341831	26.649885
C	27.622866	5.046079	25.065114	C	36.376835	4.282981	26.425879
C	29.018451	4.785234	25.133021	C	33.846852	4.021974	22.293716
C	13.900000	3.935000	24.313000	C	34.612829	2.940971	21.873681
C	28.702950	2.875030	23.666115	C	34.701778	2.637980	20.519676
C	27.336285	3.094398	23.625064	C	34.024750	3.416990	19.587706
C	26.770501	4.182835	24.326417	C	33.259772	4.496992	20.007739
O	26.575819	2.188347	22.889012	C	33.170822	4.799984	21.361745
O	16.598613	6.400995	25.857564	C	32.403844	5.880987	21.783779
O	16.055016	4.261426	26.321290	C	31.727817	6.658997	20.849809
C	15.736569	5.460313	25.988144	C	31.817767	6.355005	19.496804
C	17.925924	5.805591	30.241446	C	32.583744	5.274001	19.075769
C	18.911857	6.582778	30.877078	O	31.143737	7.185017	18.538834
C	16.787931	5.378775	30.983445	O	34.120501	5.516488	24.144069
C	15.718252	4.689939	30.372699	O	33.629795	3.359628	24.580624
C	14.625546	4.272114	31.126283	C	33.856854	4.320614	23.758962
O	18.437548	6.393647	27.984864	C	29.854400	5.638850	25.907256

C	29.296408	6.767577	26.534690	O	56.643767	5.617817	21.841773
C	43.539513	6.883873	26.543994	O	51.634032	5.834684	26.125395
C	42.719174	6.026449	25.822385	O	51.335593	3.657172	26.636862
C	43.244763	4.904791	25.148534	C	52.092100	4.664408	26.381573
C	44.642212	4.649357	25.221431	C	49.466776	4.021885	22.293147
C	29.544263	3.701958	24.400166	C	50.232742	2.940881	21.873096
C	44.336046	2.727373	23.770050	C	50.321665	2.637894	20.519088
C	42.969966	2.951937	23.709542	C	49.644622	3.416909	19.587132
C	42.398703	4.045284	24.398665	C	48.879655	4.496913	20.007183
O	42.215156	2.043807	22.970544	C	48.790732	4.799902	21.361191
O	32.142702	6.328851	25.949764	C	48.023768	5.880906	21.783244
O	31.667214	4.169578	26.393323	C	47.347725	6.658920	20.849287
C	31.306915	5.364334	26.094452	C	47.437649	6.354933	19.496280
C	33.638846	5.717553	30.298304	C	48.203614	5.273930	19.075227
C	34.635271	6.528733	30.874249	O	46.763606	7.184950	18.538323
C	32.553845	5.270095	31.105388	O	49.724663	5.589424	24.094686
C	31.481098	4.530294	30.564571	O	49.385555	3.422073	24.608903
C	30.437719	4.101842	31.379613	C	49.522816	4.366848	23.751541
O	34.040998	6.329641	28.028865	C	45.473528	5.521090	25.978691
O	33.547172	4.174139	28.470636	C	44.902756	6.638043	26.616989
C	33.748439	5.385386	28.847503	C	45.173079	3.558782	24.505101
Cu	49.690191	6.199442	25.990978	O	47.709710	6.328737	25.896157
Cu	49.343896	3.780409	26.566535	O	47.392058	4.159033	26.422770
C	53.571003	4.464803	26.367930	C	46.944413	5.319967	26.102568
C	54.157056	3.947784	27.515893	C	49.202994	5.974851	30.229514
C	55.530058	3.732771	27.559816	C	50.146593	6.820840	30.840699
C	56.316001	4.036773	26.454777	C	48.096326	5.499641	30.988538
C	55.729944	4.554792	25.305813	C	47.068336	4.732739	30.400115
C	54.356945	4.768807	25.262890	C	45.998250	4.280841	31.166378
C	53.770888	5.287824	24.113928	O	49.603771	6.554559	27.948780
C	54.557831	5.591827	23.007888	O	49.295579	4.378994	28.460636
C	55.929832	5.377811	23.052810	C	49.385211	5.614935	28.795762
C	56.515887	4.858794	24.200774	C	11.158285	7.260976	41.959131

C	10.287267	6.502982	41.186143	O	14.011468	7.415213	34.299928
C	10.757252	5.394981	40.491131	O	17.262779	5.566902	39.635148
C	12.099252	5.042976	40.571107	O	16.748283	3.414947	40.074431
C	11.698220	3.178982	39.103109	C	16.986209	4.373059	39.253967
C	10.356220	3.528988	39.024134	C	12.972269	5.800972	41.346094
C	9.886236	4.637987	39.718144	C	12.500285	6.908972	42.040106
O	9.453202	2.792994	38.218147	C	26.609089	6.995556	41.959689
Cu	17.232641	6.108460	41.544465	C	25.784280	6.123757	41.261154
Cu	16.653451	3.715220	42.041685	C	26.305647	4.981971	40.617572
C	20.913487	3.988595	41.951372	C	27.699460	4.717031	40.704292
C	21.454196	3.282429	43.041797	C	12.571236	3.934978	39.877095
C	22.804551	2.957084	43.080836	C	27.390710	2.781447	39.269950
C	23.637879	3.328415	42.032025	C	26.025611	3.004901	39.212080
C	23.133758	4.010146	40.907827	C	25.458263	4.109845	39.885346
C	21.752436	4.333963	40.856254	O	25.267482	2.085958	38.489730
C	21.240748	4.961428	39.700212	O	15.274973	6.417094	41.389207
C	22.083998	5.288914	38.643531	O	14.751948	4.269799	41.836109
C	23.446090	5.007066	38.707172	C	14.418600	5.470426	41.524801
C	23.982299	4.359655	39.828981	C	16.642562	5.824836	45.761941
O	24.277037	5.340348	37.643554	C	17.655700	6.574262	46.388396
O	19.128989	5.549261	41.720297	C	18.815279	6.893722	32.227350
O	18.614080	3.401175	42.181814	C	17.729813	6.439788	32.967930
C	19.466874	4.334748	41.962656	C	16.704992	5.683012	32.368675
C	16.928108	4.094197	37.793759	C	15.494287	5.441049	46.509718
C	17.636346	2.989216	37.288598	C	14.405959	4.774449	45.908417
C	17.657620	2.719934	35.926655	C	13.299199	4.404661	46.666933
C	16.967449	3.544671	35.045161	C	14.565640	4.525044	32.494304
C	16.219459	4.646791	35.508170	C	15.592235	5.240040	33.125894
C	16.183664	4.915994	36.902650	O	13.468206	4.099733	33.234684
C	15.382009	5.976359	37.371682	O	17.125183	6.415074	43.505501
C	14.672532	6.769313	36.478473	O	16.590048	4.269006	43.951151
C	14.728219	6.540616	35.113802	C	16.799465	5.480539	44.321995
C	15.508122	5.478417	34.603165	Cu	32.754038	6.068103	41.868996

Cu	32.270260	3.633463	42.225455	C	41.920403	5.154211	40.846074
C	36.508373	4.085778	42.306164	C	43.320377	4.903020	40.857906
C	37.064149	3.382346	43.389738	C	28.229163	3.622218	39.991963
C	38.421996	3.087770	43.426388	C	42.941191	2.907074	39.526305
C	39.245695	3.474269	42.373667	C	41.573254	3.122617	39.537434
C	38.726271	4.154239	41.255719	C	41.038337	4.253102	40.194015
C	37.339941	4.460290	41.214425	O	40.780740	2.173551	38.895332
C	36.814529	5.094959	40.068956	O	30.795760	6.304049	41.625428
C	37.646561	5.438510	39.008550	O	30.358123	4.115919	41.951211
C	39.011040	5.165397	39.057542	C	29.979666	5.315756	41.690666
C	39.562725	4.515348	40.170565	C	31.796479	5.563519	45.998880
O	39.830256	5.513016	37.989139	C	32.454276	6.619756	46.611670
O	34.667375	5.586180	42.115927	C	34.597388	6.862051	32.221707
O	34.233454	3.395371	42.445105	C	33.557280	6.402975	33.020646
C	35.049637	4.375193	42.305491	C	32.524602	5.610115	32.486147
C	32.779941	4.193737	38.020743	C	30.744179	4.848131	46.675251
C	33.557423	3.121763	37.545037	C	29.946264	3.789828	46.122263
C	33.645265	2.851773	36.186320	C	28.960583	3.164963	46.848195
C	32.944677	3.634897	35.276244	C	30.426079	4.401605	32.739557
C	32.134140	4.705997	35.704921	C	31.454340	5.169356	33.303481
C	32.049951	4.991775	37.095868	O	29.373912	3.970115	33.539470
C	31.206597	6.035211	37.526683	O	32.507087	6.276767	43.830357
C	30.499980	6.794393	36.602656	O	32.079035	4.080796	44.145950
C	30.583752	6.535850	35.244649	C	32.159479	5.287783	44.579058
C	31.400108	5.483814	34.769978	Cu	48.428951	6.371448	41.591955
O	29.852461	7.368582	34.400164	Cu	48.005038	3.949133	42.101760
O	32.918670	5.618077	39.935662	C	52.242277	4.464613	41.931331
O	32.480737	3.429346	40.257163	C	52.828351	3.947590	43.079282
C	32.723050	4.429187	39.490581	C	54.201352	3.732569	43.123180
C	28.528837	5.582180	41.471280	C	54.987276	4.036572	42.018127
C	27.966155	6.729797	42.061431	C	54.401202	4.554594	40.869175
C	42.283350	7.207900	42.110423	C	53.028202	4.768616	40.826278
C	41.427827	6.310953	41.483629	C	52.442127	5.287638	39.677327

C	53.229054	5.591642	38.571275	C	45.693847	4.914486	45.916181
C	54.601053	5.377620	38.616175	C	44.591486	4.494850	46.654470
C	55.187127	4.858598	39.764122	C	45.922716	4.572203	32.526178
O	55.314970	5.617627	37.405127	C	46.912375	5.354317	33.137270
O	50.360827	5.919651	41.723675	O	44.846834	4.114938	33.278856
O	49.982338	3.745832	42.198557	O	48.344535	6.675313	43.553983
C	50.774359	4.726503	41.959680	O	47.945876	4.501780	44.011005
C	48.214205	4.325467	37.845225	C	48.076242	5.726685	44.374555
C	48.962489	3.235227	37.364919	C	9.830843	7.260911	57.522287
C	49.017260	2.950343	36.007405	C	8.959811	6.502921	56.749313
C	48.321236	3.744154	35.103266	C	9.429778	5.394922	56.054289
C	47.534433	4.830179	35.538221	C	10.771778	5.042912	56.134240
C	47.466738	5.117705	36.928844	C	10.370714	3.178925	54.666242
C	46.630133	6.163674	37.367388	C	9.028713	3.528933	54.587292
C	45.919700	6.927386	36.449206	C	8.558746	4.637932	55.281315
C	46.001459	6.677321	35.089481	O	8.125680	2.792944	53.781318
C	46.814654	5.626649	34.608502	Cu	15.899106	6.134775	57.132039
O	45.273175	7.517537	34.250102	Cu	15.344757	3.722065	57.548639
O	48.450176	5.830246	39.680814	C	19.603518	4.029006	57.413464
O	48.077931	3.652411	40.132576	C	20.161535	3.269719	58.457962
C	48.246427	4.620075	39.305249	C	21.511841	2.942723	58.459553
C	44.187918	5.806224	41.535689	C	22.328083	3.357801	57.412935
C	43.648572	6.960667	42.134496	C	21.808877	4.097059	56.333092
C	43.814711	3.781770	40.161351	C	20.426510	4.425728	56.321293
O	46.450378	6.567519	41.491475	C	19.898227	5.108494	55.205533
O	46.072660	4.392157	41.945780	C	20.724919	5.480294	54.149466
C	45.656435	5.571965	41.656936	C	22.088118	5.195672	54.177053
C	47.880574	6.069587	45.809025	C	22.643680	4.500152	55.259892
C	48.840427	6.875972	46.448201	O	22.901937	5.577271	53.115874
C	50.040184	7.154778	32.185154	O	17.803922	5.589362	57.287692
C	48.984931	6.658204	32.942580	O	17.310332	3.419923	57.662981
C	47.999903	5.834140	32.366063	C	18.154114	4.367366	57.467507
C	46.736951	5.635300	46.535534	C	15.644873	4.222268	53.318341

C	16.358979	3.123331	52.807426	C	13.166033	4.552860	61.469196
C	16.383342	2.860795	51.444824	C	12.083068	4.099863	62.213249
C	15.689333	3.685495	50.567398	C	13.246461	4.680079	48.031172
C	14.940623	4.785669	51.034164	C	14.295961	5.369584	48.654126
C	14.905678	5.051340	52.429771	O	12.136070	4.299705	48.776861
C	14.107210	6.112302	52.901698	O	15.769361	6.374181	59.107718
C	13.400616	6.910124	52.010315	O	15.281671	4.203903	59.476385
C	13.452452	6.682619	50.645019	C	15.450865	5.407474	59.891653
C	14.226564	5.617556	50.131366	Cu	31.431513	6.055879	57.111198
O	12.739518	7.562606	49.833810	Cu	30.946072	3.641661	57.596863
O	15.944770	5.654739	55.203029	C	35.193648	4.027408	57.420190
O	15.437839	3.488568	55.575445	C	35.743790	3.292641	58.487010
C	15.678824	4.470102	54.784994	C	37.096098	2.976877	58.516242
C	11.644811	5.800902	56.909215	C	37.924968	3.377981	57.475084
C	11.172843	6.908901	57.603238	C	37.416384	4.093808	56.374808
C	25.275033	6.985925	57.567666	C	36.031088	4.412727	56.335375
C	24.452701	6.175587	56.794364	C	35.515539	5.071290	55.199920
C	24.971896	5.076511	56.079224	C	36.357879	5.434503	54.153269
C	26.364209	4.801015	56.156575	C	37.722200	5.158545	54.206593
C	11.243746	3.934914	55.440217	C	38.264873	4.479955	55.306921
C	26.062926	2.982448	54.576967	O	38.548792	5.526299	53.150947
C	24.697217	3.210495	54.529084	O	33.356488	5.545949	57.219927
C	24.124643	4.258228	55.285980	O	32.916099	3.384253	57.694822
O	23.944521	2.350962	53.732502	C	33.736102	4.339979	57.449136
O	13.941894	6.430981	56.976255	C	31.155403	4.025784	53.370404
O	13.437083	4.269117	57.367964	C	32.078252	3.112635	52.891763
C	13.093311	5.474551	57.085567	C	32.083667	2.786112	51.517723
C	15.283038	5.695841	61.352095	C	31.170176	3.363905	50.662332
C	16.314079	6.385825	61.978046	C	30.190803	4.285189	51.132503
C	17.571307	6.904008	47.734690	C	30.171550	4.629437	52.527415
C	16.470709	6.497772	48.480196	C	29.141532	5.522162	52.970071
C	15.421497	5.766985	47.890595	C	28.208552	6.028539	52.102886
C	14.198074	5.242844	62.095148	C	28.247380	5.722456	50.710258

C	29.233995	4.866336	50.224756	Cu	47.054592	6.269777	57.152900
O	27.301470	6.321845	49.965623	Cu	46.680768	3.813404	57.519839
O	31.411420	5.537028	55.190241	C	50.914822	4.464429	57.493771
O	31.016824	3.351319	55.638617	C	51.500915	3.947400	58.641709
C	31.199914	4.323074	54.816737	C	52.873915	3.732375	58.685585
C	27.191294	5.606316	56.987329	C	53.659823	4.036378	57.580520
C	26.630774	6.705620	57.663164	C	53.073729	4.554406	56.431580
C	40.906662	6.994205	57.570749	C	51.700730	4.768431	56.388706
C	40.080709	6.164537	56.824049	C	51.114638	5.287461	55.239765
C	40.598895	5.061149	56.116003	C	51.901544	5.591465	54.133701
C	41.996397	4.798606	56.174554	C	53.273543	5.377438	54.178575
C	26.896615	3.755804	55.375907	C	53.859636	4.858411	55.326514
C	41.677085	2.933998	54.653000	O	53.987441	5.617444	52.967515
C	40.310339	3.158115	54.614769	O	48.995291	5.868321	57.306073
C	39.744613	4.226086	55.347381	O	48.667034	3.663361	57.659070
O	39.549177	2.273168	53.854208	C	49.437336	4.678398	57.497344
O	29.462436	6.316876	57.028850	C	46.948365	4.414927	53.304454
O	29.023727	4.140893	57.434232	C	47.746884	3.382963	52.778953
C	28.645003	5.337126	57.158798	C	47.784241	3.135819	51.414317
C	30.903113	5.695671	61.351281	C	47.021251	3.910357	50.549111
C	31.934168	6.385649	61.977217	C	46.192032	4.945390	51.029839
C	32.117223	7.007940	47.926771	C	46.142158	5.192853	52.428103
C	31.127856	6.343087	48.612724	C	45.263788	6.182089	52.913994
C	30.423432	5.260720	48.018493	C	44.493704	6.931630	52.033131
C	29.818160	5.242675	62.094350	C	44.557732	6.723430	50.665189
C	28.786107	4.552698	61.468415	C	45.412783	5.729188	50.137830
C	27.703152	4.099704	62.212486	O	43.777066	7.555126	49.865608
C	28.698731	3.545627	48.185390	O	47.128389	5.834577	55.214462
C	29.401022	4.584541	48.769674	O	46.807629	3.626423	55.545577
O	27.730567	2.848893	48.847503	C	46.962298	4.639843	54.774303
O	31.365801	6.338332	59.087913	C	42.833174	5.634545	56.967050
O	30.906080	4.171375	59.509929	C	42.267421	6.734137	57.640384
C	31.069490	5.384699	59.896185	C	42.520858	3.738453	55.409940

O	45.078575	6.426567	57.018644	C	44.303429	5.025438	64.205366
O	44.735955	4.220701	57.334556	O	42.183423	3.908472	64.359536
C	44.301796	5.409011	57.107977	H	12.119182	8.126714	26.936293
C	46.523187	5.695444	61.350179	H	10.573002	6.786635	25.566800
C	47.554254	6.385417	61.976098	H	13.382424	2.322414	22.982938
C	48.710770	7.211680	47.789576	H	9.847237	3.168919	22.677402
C	47.618402	6.752779	48.516590	H	22.126507	2.851402	28.249846
C	46.620614	5.963906	47.912219	H	24.521400	2.290219	28.287946
C	45.438244	5.242452	62.093268	H	25.995662	3.025571	26.486722
C	44.406178	4.552479	61.467349	H	21.486822	5.223358	24.058724
C	43.323236	4.099487	62.211437	H	22.968303	5.893676	22.273610
C	44.501317	4.768259	48.016983	H	19.532564	2.329874	22.589886
C	45.505316	5.507694	48.657605	H	19.679826	1.794411	20.190552
O	43.398767	4.334053	48.744142	H	18.480863	3.170961	18.536769
O	46.921389	6.452042	59.127063	H	16.654843	6.146944	22.827187
O	46.566357	4.247206	59.452534	H	15.507666	7.502036	21.163935
C	46.672696	5.449223	59.888972	H	14.495419	7.507531	27.088398
C	16.262151	6.620810	63.347051	H	27.517763	7.898428	26.949808
C	15.179185	6.168816	64.090104	H	26.052121	6.409156	25.698087
C	14.147147	5.478833	63.465153	H	14.941176	3.632825	24.314054
C	12.031142	4.336850	63.582254	H	29.113911	2.041438	23.112353
C	13.063181	5.025837	64.207206	H	19.770155	6.936048	30.316215
O	10.943178	3.908854	64.361306	H	15.700094	4.476534	29.309420
C	31.882266	6.620631	63.346223	H	13.820683	3.741846	30.635735
C	30.799313	6.168635	64.089293	H	15.673245	6.862474	17.596218
C	29.767259	5.478659	63.464356	H	25.089220	6.023402	21.431914
C	27.651253	4.336688	63.581492	H	25.594046	2.406432	22.890299
C	28.683306	5.025664	64.206427	H	37.703516	2.913145	28.318229
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C	47.502381	6.620396	63.345107	H	41.582724	2.954333	26.575544
C	46.419438	6.168404	64.088195	H	37.138427	5.202852	24.073749
C	45.387370	5.478430	63.463277	H	38.643531	5.777200	22.270781
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H 45.528733 7.321852 27.179536	H 23.788428 5.838901 36.914919
H 46.233944 3.336125 24.490982	H 24.289645 2.318712 38.463170
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H 45.222925 3.694338 30.692452	H 40.296829 3.225635 42.432534
H 46.906415 6.857530 17.596309	H 35.759298 5.325885 39.970086
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H 40.371251 6.538466 41.487361	H 7.917030 6.786923 56.693410
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H 33.558875 6.682813 34.065465	H 23.373461 3.082432 57.445571
H 30.071436 3.447805 45.094604	H 18.844410 5.353224 55.125265
H 28.361052 2.365988 46.405286	H 20.295454 6.002041 53.305051
H 28.710343 3.404265 33.032034	H 16.907129 2.471196 53.478333
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H 39.328003 6.001419 37.262867	H 15.730039 3.444768 49.514628
H 39.798734 2.388282 38.935426	H 14.005832 6.336670 53.957344
H 52.223954 3.708821 43.947495	H 12.796107 7.727602 52.380016
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H 56.055342 3.866532 42.061269	H 24.856693 7.833971 58.099910
H 51.374537 5.454189 39.580498	H 23.402946 6.427595 56.745010
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H 50.781158 7.800455 32.645326	H 22.394412 6.085805 52.407174
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H	38.971864	3.110766	57.528400	H	43.581992	3.521714	55.370243
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H	35.939106	5.941308	53.294700	H	49.461708	7.829846	48.270705
H	32.811755	2.640012	53.553425	H	47.549214	7.033093	49.558974
H	32.815913	2.069157	51.133367	H	44.381545	4.363548	60.399562
H	31.185729	3.101942	49.602782	H	42.519788	3.570628	61.718002
H	29.079254	5.816663	54.021913	H	42.761326	3.785431	48.186165
H	27.418916	6.699578	52.450067	H	43.837275	7.329226	48.887579
H	27.257883	7.343088	58.276585	H	53.398456	5.963496	52.224344
H	40.487843	7.845194	58.098087	H	17.068503	7.157553	63.836130
H	39.027665	6.404405	56.790458	H	15.148388	6.356890	65.155605
H	27.957565	3.528443	55.357630	H	10.261923	3.422363	63.798053
H	42.086995	2.117685	54.073463	H	32.689061	7.156643	63.835271
H	32.789308	6.735546	61.409148	H	30.768422	6.356741	65.154751
H	32.639541	7.849096	48.391675	H	25.880553	3.425738	63.795966
H	30.860724	6.650785	49.625625	H	48.307452	7.159311	63.833721
H	28.748018	4.375219	60.399923	H	46.387683	6.357709	65.153410
H	26.897838	3.574478	61.718314	H	41.497626	3.430184	63.794469
H	26.051044	2.687539	47.720988	H	54.922479	4.682742	55.325487
H	27.677583	3.170225	49.770713	H	56.250002	4.683110	39.763375
H	38.053484	6.035092	52.433741	H	57.578847	4.683537	24.200346
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H	50.047784	5.461369	55.146518	H	7.520517	4.915191	55.216425
H	51.425244	5.978249	53.243299	H	12.998699	5.198773	65.268995
H	48.348044	2.769632	53.441023	H	28.618657	5.198752	65.268129
H	48.406838	2.337799	51.023092	H	44.238277	5.198914	65.266967
H	47.072529	3.680802	49.494613	H	48.273815	5.043414	18.026050
H	45.147245	6.385507	53.972403	C	23.815057	4.954228	47.672452

C 25.266024 4.457090 47.652750
C 26.144032 5.260710 46.655870
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C 24.029136 5.831276 45.312808
C 23.195424 4.967268 46.269171
O 25.265003 3.084420 47.302029
C 27.434976 7.439064 46.735644
C 27.480604 8.755692 47.238243
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C 29.403946 9.264236 45.848292
C 29.362515 7.960767 45.346685
C 28.389178 7.053266 45.777072
N 26.496462 6.541998 47.280144
H 26.087922 5.979467 44.598854
H 25.699298 4.590008 48.662483
H 27.082426 4.700779 46.552098
H 23.597902 5.811588 44.295526
H 23.998360 6.887588 45.649590
H 22.151156 5.326839 46.313803
H 23.164612 3.929231 45.894735
H 23.241187 4.303231 48.354820
H 23.783817 5.975501 48.103453
H 25.501983 4.323593 44.838834
H 26.754506 9.062801 47.999208
H 28.468058 10.668909 47.210048
H 30.171633 9.964792 45.506560
H 30.108350 7.638259 44.613745
H 28.386931 6.039440 45.375156
H 25.695274 7.024381 47.682130
H 27.343535 6.165351 48.986091