

Cartesian coordinates of the larger models in Table 1 (optimized with OLYP potential):

Structure large 4 F:

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C	0.705000	7.351000	24.202000	N	-3.157597	2.537067	22.541029
C	1.512780	6.279027	23.527991	C	-2.320043	3.639133	20.862323
O	2.143573	5.427467	24.186369	C	-1.881317	2.149733	22.355175
H	1.271843	7.736012	25.054795	N	-1.335942	2.789783	21.331577
H	-0.217871	6.901097	24.586424	H	-4.814676	4.892256	20.740376
H	0.438971	8.172590	23.531943	H	-5.238965	4.401249	22.392119
N	1.506703	6.270320	22.182363	H	-3.784908	2.181385	23.271721
C	2.286387	5.311682	21.419771	H	-2.157147	4.282321	20.010442
C	1.764616	5.090584	19.994392	H	-1.393962	1.400969	22.954275
C	2.550441	3.962571	19.414541	C	-8.609531	-3.722032	17.690766
N	2.205064	2.634501	19.614627	C	-8.350594	-2.887470	18.912430
C	3.808908	4.016457	18.885966	O	-8.719589	-1.722092	19.032973
C	3.249903	1.914032	19.245218	O	-7.656484	-3.547508	19.845051
N	4.255108	2.712057	18.786606	H	-7.658731	-3.882071	17.167658
H	1.071798	7.047100	21.694375	H	-9.301625	-3.203495	17.024988
H	2.263924	4.365918	21.965001	C	-10.876610	-3.421599	22.605339
H	0.698148	4.851173	20.015781	C	-10.888852	-2.043256	23.164106
H	1.894256	5.996852	19.391438	N	-9.758607	-1.264655	23.233152
H	4.432326	4.848497	18.597427	C	-11.885631	-1.261201	23.696412
H	3.334204	0.842032	19.309256	C	-10.098634	-0.078851	23.789390
H	3.333260	5.639682	21.371065	N	-11.389949	-0.030735	24.084224
C	9.000672	3.539327	19.833687	H	-10.722501	-3.411657	21.519886
C	7.960813	2.744738	19.098538	H	-11.829174	-3.917644	22.810427
C	8.293761	1.665178	18.277234	H	-8.817130	-1.554848	22.914465
C	6.609637	3.052631	19.242268	H	-12.930811	-1.515625	23.823667
C	7.315884	0.949490	17.600145	H	-9.380954	0.708229	23.966514
C	5.618925	2.340358	18.571230	C	-0.021367	-7.237010	24.210589
C	5.970781	1.286883	17.719740	C	0.718233	-6.151921	23.494937
O	5.067768	0.541106	17.012377	N	1.683930	-6.390426	22.543030
H	8.886920	4.610573	19.631732	C	0.560193	-4.785270	23.478081
H	10.009637	3.235703	19.542635	C	2.071908	-5.221774	21.997067
H	9.335775	1.379188	18.153695	N	1.405816	-4.213996	22.541870
H	6.307843	3.854999	19.907600	H	-0.551203	-7.859711	23.478156
H	7.588640	0.126613	16.946142	H	-0.770961	-6.784100	24.865419
H	4.245914	1.057727	16.883855	H	2.052694	-7.300209	22.279391
C	-3.882662	1.780733	16.251573	H	-0.109571	-4.190959	24.077843
C	-2.554611	1.811721	16.920161	H	2.820224	-5.157266	21.227325
N	-1.363238	1.895544	16.234083	C	-7.107299	-3.024030	29.450503
C	-2.184783	1.757325	18.236956	N	-5.967919	-2.425468	30.114153
C	-0.346749	1.906008	17.119112	C	-5.166678	-1.515805	29.560171
N	-0.812512	1.824515	18.356579	N	-5.346776	-1.126496	28.306506
H	-4.125985	0.769878	15.900393	N	-4.153182	-1.013196	30.283832
H	-3.894552	2.449586	15.384219	H	-6.808813	-3.824249	28.764447
H	-1.258566	1.955867	15.224816	H	-7.673018	-2.261458	28.913072
H	-2.819897	1.689734	19.103427	H	-5.653816	-2.842892	30.984024
H	0.687349	1.987113	16.825615	H	-6.006197	-1.586659	27.681041
C	-4.838046	4.048968	21.435713	H	-4.863523	-0.294243	27.949387
C	-3.471555	3.483933	21.591200	H	-4.241313	-1.023508	31.294128

H	-3.594147	-0.251594	29.875453	H	-7.746921	-3.426171	30.227401
Fe	1.638557	-2.117351	21.959248	O	1.717398	-0.319232	21.448216
C	-1.292751	-1.454647	23.527629	O	0.795679	0.601972	21.723205
C	0.015114	-2.550614	19.009158	O	-7.908716	1.066645	20.275115
C	4.615135	-2.796683	20.387537	H	-7.606724	1.406165	19.411995
C	3.331335	-1.521219	24.849647	H	-8.076899	0.122517	20.082023
N	1.118017	-1.612211	23.820465	O	-7.277564	-2.001468	26.116212
C	-0.148831	-1.389848	24.293424	H	-6.942015	-1.733114	25.222342
C	-0.115083	-1.052473	25.700754	H	-7.399115	-2.966675	26.030905
C	1.202250	-1.047488	26.065103	O	1.942551	4.153935	28.293551
C	1.952170	-1.403091	24.881058	H	1.617284	3.834105	27.417310
C	1.790459	-0.735338	27.399091	H	1.279220	3.787383	28.915503
O	-2.807302	-2.315320	17.794917	O	-7.248548	3.087764	25.132194
C	-1.293412	-0.761504	26.569666	H	-6.494350	2.480288	24.941934
C	-1.631747	0.741078	26.670412	H	-7.668069	3.212453	24.259510
C	-2.765289	0.955497	27.664636	O	-4.981025	1.375528	24.623161
O	-2.481864	0.888873	28.888853	H	-4.554377	1.238648	25.509965
O	-3.947625	1.127658	27.202152	H	-5.322171	0.495446	24.355197
N	2.204168	-2.646478	20.086269	O	-5.806603	2.607459	28.932594
C	1.378260	-2.754431	18.999501	H	-5.145268	2.143777	28.366651
C	2.130195	-3.096732	17.811408	H	-5.648963	3.551534	28.727222
C	3.437078	-3.201774	18.200963	O	0.956015	3.365186	25.667381
C	3.467851	-2.888427	19.620007	H	1.372086	4.069123	25.113795
C	1.527050	-3.284180	16.460699	H	1.258546	2.535394	25.253849
N	3.584327	-2.166061	22.513285	H	-7.501390	-2.970580	20.679986
C	4.669797	-2.452298	21.726672	H	-1.904181	1.134731	25.688096
C	5.897595	-2.341570	22.478459	H	-0.750462	1.284264	27.024923
C	5.536403	-1.976965	23.754608	H	-1.085664	-1.136365	27.578334
C	4.088124	-1.882222	23.753130	H	-2.171962	-1.312061	26.213291
C	7.258738	-2.613579	21.941418	H	2.646264	-1.379226	27.623938
C	6.358765	-1.764531	24.934866	H	2.141926	0.303751	27.442734
C	7.611999	-1.287998	24.977709	H	1.053709	-0.869198	28.195349
N	-0.284685	-2.079287	21.386154	H	-2.227289	-1.256330	24.032115
C	-0.751356	-2.221747	20.115336	H	3.861182	-1.298214	25.764601
C	-2.166467	-1.940959	20.078006	H	5.889618	-2.021734	25.884171
C	-2.542838	-1.619398	21.372047	H	8.125235	-1.192443	25.932071
C	-1.355315	-1.721447	22.165808	H	8.148612	-0.963466	24.091688
C	-3.061602	-1.936289	18.941165	H	7.941662	-2.896672	22.746829
C	-3.890827	-1.208980	21.860645	H	7.245341	-3.426188	21.209047
C	-4.896540	-2.362180	22.006607	H	7.674328	-1.724026	21.448039
C	-6.197030	-1.913930	22.674103	H	5.552949	-2.969659	19.884460
O	-7.295133	-2.293150	22.152053	H	4.229145	-3.606129	16.290605
O	-6.107410	-1.227071	23.726634	H	4.364930	-5.727762	17.516756
C	4.594126	-3.593389	17.324409	H	5.553158	-5.039056	18.645287
O	5.693865	-2.657438	17.401567	H	2.291615	-3.424850	15.693848
C	5.154950	-4.977119	17.627462	H	0.866522	-4.160236	16.442145
H	5.959435	-5.205686	16.918159	H	0.925713	-2.412386	16.177201
Cu	0.280884	1.898048	20.175042	H	-0.516332	-2.638139	18.073615
H	8.891071	3.392424	20.913367	H	-4.070257	-1.546312	19.164971
H	-4.673317	2.104938	16.938341	H	-4.309673	-0.455022	21.183636
H	-5.531461	3.294705	21.032081	H	-3.798228	-0.719205	22.827810
H	-9.006488	-4.710142	17.956796	H	-4.461309	-3.140908	22.649215
H	-10.071118	-4.017669	23.050776	H	-5.100829	-2.822154	21.037159
H	0.595658	-7.919074	24.825696	H	5.319185	-1.770445	17.234057

Structure large 4 AF:

204

C	0.705000	7.351000	24.202000	C	-1.936204	2.023011	22.423909
C	1.484798	6.257047	23.527617	N	-1.373374	2.631677	21.390414
O	2.133219	5.421400	24.187779	H	-4.760295	4.877884	20.814388
H	1.270542	7.704258	25.068548	H	-5.237562	4.343069	22.438176
H	-0.241231	6.930925	24.563522	H	-3.837142	2.130379	23.340522
H	0.480380	8.188989	23.536484	H	-2.145430	4.135290	20.051831
N	1.424548	6.206341	22.183097	H	-1.465794	1.276432	23.037183
C	2.180884	5.223989	21.424850	C	-8.625595	-3.713001	17.702666
C	1.669434	5.016092	19.993755	C	-8.365912	-2.900995	18.938907
C	2.469210	3.897436	19.411300	O	-8.767443	-1.751202	19.097603
N	2.153690	2.565991	19.631753	O	-7.634747	-3.563826	19.839661
C	3.723468	3.972359	18.874437	H	-7.678482	-3.851658	17.167095
C	3.210744	1.864322	19.267681	H	-9.332612	-3.193206	17.053967
N	4.197795	2.676073	18.790949	C	-10.870199	-3.417989	22.599079
H	0.978155	6.972122	21.687647	C	-10.873665	-2.038841	23.153345
H	2.128907	4.277656	21.966989	N	-9.733301	-1.275420	23.233521
H	0.603886	4.772363	20.002744	C	-11.866150	-1.238559	23.666495
H	1.801910	5.928110	19.400438	C	-10.064554	-0.081270	23.776682
H	4.326914	4.813980	18.571795	N	-11.357946	-0.013604	24.055294
H	3.319874	0.795765	19.351135	H	-10.709168	-3.412491	21.514543
H	3.237133	5.521884	21.384845	H	-11.827122	-3.907548	22.799489
C	8.914484	3.627584	19.844222	H	-8.794817	-1.582011	22.922771
C	7.897474	2.793201	19.122530	H	-12.916714	-1.476583	23.779608
C	8.257075	1.680939	18.358099	H	-9.337648	0.696507	23.958047
C	6.541470	3.085116	19.239960	C	-0.027718	-7.254827	24.200621
C	7.297780	0.918999	17.706127	C	0.711317	-6.172537	23.482419
C	5.568768	2.326070	18.594953	N	1.699786	-6.411363	22.553143
C	5.947097	1.241536	17.796746	C	0.546846	-4.807023	23.454712
O	5.063317	0.451276	17.114887	C	2.091995	-5.239316	22.013133
H	8.695473	4.694997	19.734259	N	1.409074	-4.232998	22.536833
H	9.923476	3.435813	19.469759	H	-0.547485	-7.892330	23.474096
H	9.304019	1.404098	18.261175	H	-0.783695	-6.801130	24.846895
H	6.220796	3.909677	19.867207	H	2.077699	-7.320267	22.303007
H	7.590926	0.068928	17.096748	H	-0.139435	-4.215024	24.036946
H	4.229258	0.942074	16.967043	H	2.858150	-5.172315	21.259978
C	-3.880696	1.754103	16.265920	C	-7.091505	-3.053897	29.449347
C	-2.560720	1.788600	16.949117	N	-5.938155	-2.477297	30.108520
N	-1.363392	1.928144	16.283083	C	-5.144801	-1.558027	29.562239
C	-2.205724	1.683780	18.266373	N	-5.338875	-1.152879	28.314907
C	-0.357867	1.918907	17.180233	N	-4.125402	-1.062140	30.283346
N	-0.837452	1.772086	18.406365	H	-6.812652	-3.870726	28.775351
H	-4.131583	0.736526	15.941451	H	-7.633842	-2.283085	28.900739
H	-3.876636	2.399436	15.381618	H	-5.620548	-2.906519	30.971652
H	-1.249188	2.036404	15.278886	H	-5.979738	-1.628272	27.681452
H	-2.851258	1.560000	19.118997	H	-4.855245	-0.320035	27.960121
H	0.677771	2.037875	16.905864	H	-4.220488	-1.064989	31.294548
C	-4.826042	4.012412	21.478981	H	-3.583266	-0.286198	29.881921
C	-3.481359	3.400269	21.643646	Fe	1.614437	-2.038495	21.933144
N	-3.197953	2.455213	22.605167	C	-1.328559	-1.478261	23.519563
C	-2.327530	3.509109	20.911430	C	0.014761	-2.467373	18.984323

C	4.605746	-2.775960	20.387827	O	0.970120	0.653441	21.827342
C	3.302100	-1.484199	24.833567	O	-7.854001	1.029748	20.201378
N	1.083448	-1.598740	23.807886	H	-7.626561	1.368878	19.312994
C	-0.185809	-1.405428	24.287674	H	-8.075082	0.093853	20.018744
C	-0.153588	-1.087048	25.697385	O	-7.240667	-2.110572	26.131629
C	1.166541	-1.067472	26.058413	H	-6.910523	-1.843329	25.235597
C	1.919693	-1.391892	24.867681	H	-7.340718	-3.079326	26.056662
C	1.746480	-0.763810	27.397652	O	1.753328	4.047228	27.963558
O	-2.809324	-2.251701	17.765264	H	1.516506	3.649113	27.093933
C	-1.329329	-0.799493	26.571701	H	1.054507	3.709726	28.556686
C	-1.665517	0.704396	26.661463	O	-7.395782	3.032165	25.040167
C	-2.783572	0.939145	27.668715	H	-6.613531	2.445291	24.917052
O	-2.485857	0.898350	28.889889	H	-7.745680	3.138641	24.133900
O	-3.972454	1.100913	27.216467	O	-5.046516	1.347772	24.669823
N	2.195966	-2.584654	20.070358	H	-4.609783	1.219479	25.554344
C	1.376068	-2.685576	18.980196	H	-5.363924	0.459392	24.404242
C	2.130151	-3.048266	17.800007	O	-6.008258	2.547884	28.729648
C	3.431963	-3.178985	18.200445	H	-5.276733	2.096019	28.244057
C	3.459683	-2.857210	19.616559	H	-5.796803	3.495256	28.608001
C	1.534289	-3.228165	16.445922	O	0.988693	3.081770	25.307672
N	3.572470	-2.131161	22.502930	H	1.422108	3.815294	24.812548
C	4.659969	-2.419591	21.723322	H	1.344244	2.270803	24.885740
C	5.887472	-2.296066	22.476901	H	-7.487484	-3.008393	20.692392
C	5.520435	-1.920949	23.747046	H	-1.953001	1.085431	25.678696
C	4.068901	-1.833764	23.739891	H	-0.777133	1.250732	26.991991
C	7.249290	-2.571061	21.941990	H	-1.112969	-1.166150	27.581656
C	6.339244	-1.695853	24.927551	H	-2.208521	-1.355084	26.224350
C	7.585643	-1.202989	24.967163	H	2.664043	-1.329860	27.581680
N	-0.293865	-2.007187	21.363938	H	1.994497	0.302179	27.489207
C	-0.756798	-2.149069	20.090150	H	1.039383	-1.007154	28.195668
C	-2.179194	-1.908218	20.056461	H	-2.268816	-1.317735	24.025556
C	-2.566595	-1.624654	21.355201	H	3.826266	-1.258692	25.750616
C	-1.378705	-1.707454	22.151506	H	5.873082	-1.955302	25.877930
C	-3.078747	-1.922495	18.922801	H	8.099100	-1.096639	25.920645
C	-3.922687	-1.253767	21.849815	H	8.115737	-0.873733	24.079194
C	-4.893640	-2.431529	22.010846	H	7.941110	-2.818449	22.750219
C	-6.192240	-1.997295	22.690103	H	7.240826	-3.408436	21.238088
O	-7.293044	-2.368515	22.167990	H	7.652205	-1.696173	21.414718
O	-6.096823	-1.320674	23.748682	H	5.542785	-2.964097	19.888227
C	4.584922	-3.597602	17.331211	H	4.221921	-3.611793	16.297404
O	5.699685	-2.679613	17.404783	H	4.319838	-5.726489	17.531893
C	5.121770	-4.988887	17.643813	H	5.514770	-5.052912	18.663081
H	5.924907	-5.233937	16.938528	H	2.303187	-3.347690	15.679212
Cu	0.211328	1.778724	20.260893	H	0.886873	-4.114002	16.414874
H	8.891071	3.392424	20.913367	H	0.920904	-2.362229	16.170988
H	-4.673317	2.104938	16.938341	H	-0.514926	-2.555366	18.047434
H	-5.531461	3.294705	21.032081	H	-4.106443	-1.594694	19.160778
H	-9.006488	-4.710142	17.956796	H	-4.368039	-0.514967	21.172544
H	-10.071118	-4.017669	23.050776	H	-3.837122	-0.757081	22.813635
H	0.595658	-7.919074	24.825696	H	-4.434168	-3.195656	22.654376
H	-7.746921	-3.426171	30.227401	H	-5.099809	-2.901743	21.047008
O	1.871554	-0.284555	21.501937	H	5.336739	-1.784150	17.258831

Structure large 5 F:

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C	0.705000	7.351000	24.202000	C	-1.880005	2.062570	22.304210
C	1.511164	6.236871	23.596709	N	-1.341840	2.626197	21.232926
O	2.179901	5.460678	24.309365	H	-4.748975	4.830432	20.615595
H	1.322012	7.869451	24.942505	H	-5.134531	4.467107	22.308760
H	-0.151975	6.912014	24.726344	H	-3.754670	2.222805	23.265738
H	0.336086	8.067726	23.463651	H	-2.139302	4.083401	19.859942
N	1.461802	6.104289	22.259754	H	-1.399816	1.332453	22.930780
C	2.227793	5.086466	21.557194	C	-8.642590	-3.715793	17.671452
C	1.760122	4.881475	20.112653	C	-8.385766	-2.869904	18.881888
C	2.559272	3.770717	19.516222	O	-8.704840	-1.688712	18.979777
N	2.169278	2.441623	19.548918	O	-7.747454	-3.547529	19.845597
C	3.853163	3.832808	19.079511	H	-7.694082	-3.853179	17.136954
C	3.219419	1.729409	19.156065	H	-9.354447	-3.219546	17.009553
N	4.273738	2.534875	18.870970	C	-10.877363	-3.429241	22.601032
H	0.992466	6.822376	21.717888	C	-10.847480	-2.045570	23.129838
H	2.132002	4.149012	22.110340	N	-9.688227	-1.296728	23.164345
H	0.693176	4.644505	20.093720	C	-11.825746	-1.254489	23.661171
H	1.906137	5.803201	19.536528	C	-9.939578	-0.103885	23.690519
H	4.506970	4.674950	18.918096	N	-11.232614	-0.063210	23.995310
H	3.267067	0.659307	19.067074	H	-10.742434	-3.435580	21.513987
H	3.290118	5.361739	21.556493	H	-11.834396	-3.900477	22.836030
C	9.023524	3.437128	19.823397	H	-8.733512	-1.629693	22.821899
C	7.983303	2.613450	19.112075	H	-12.876639	-1.434952	23.826994
C	8.308213	1.525702	18.290438	H	-9.229383	0.687615	23.860052
C	6.625389	2.893548	19.266705	C	-0.034822	-7.214604	24.252933
C	7.329843	0.760962	17.672241	C	0.700204	-6.136701	23.523540
C	5.632975	2.144752	18.637452	N	1.692161	-6.379508	22.600093
C	5.930683	1.004908	17.814817	C	0.517073	-4.774951	23.469712
O	5.024013	0.273889	17.262159	C	2.068947	-5.215158	22.034099
H	8.964054	4.494233	19.532840	N	1.369999	-4.209743	22.538067
H	10.031938	3.080740	19.590929	H	-0.613792	-7.813789	23.537909
H	9.354917	1.265909	18.137489	H	-0.741794	-6.755126	24.949526
H	6.328665	3.710194	19.917503	H	2.085039	-7.287807	22.369711
H	7.623769	-0.078098	17.044475	H	-0.174640	-4.178288	24.041550
H	-11.697887	0.732322	24.426172	H	2.836192	-5.151773	21.282261
C	-3.894790	1.825336	16.217064	C	-7.098235	-3.040185	29.449088
C	-2.559826	1.779942	16.872077	N	-5.966968	-2.426563	30.113703
N	-1.369931	1.887499	16.185262	C	-5.158994	-1.525638	29.556297
C	-2.183708	1.647040	18.180716	N	-5.321786	-1.152693	28.292736
C	-0.348578	1.839770	17.063011	N	-4.150611	-1.019099	30.280317
N	-0.810391	1.697397	18.297284	H	-6.791251	-3.853306	28.782016
H	-4.159962	0.854309	15.780574	H	-7.659609	-2.289529	28.891468
H	-3.902199	2.568680	15.412154	H	-5.656455	-2.837155	30.988439
H	-1.268303	1.996198	15.179648	H	-6.019308	-1.580190	27.687216
H	-2.816979	1.536602	19.043555	H	-4.862885	-0.303233	27.946152
H	0.685702	1.924042	16.770234	H	-4.230101	-1.043757	31.291299
C	-4.786065	4.034611	21.364305	H	-3.590080	-0.256005	29.876621
C	-3.440303	3.416964	21.510782	Fe	1.553513	-2.102142	21.946321
N	-3.134611	2.509242	22.501374	C	-1.369939	-1.442708	23.524382
C	-2.305209	3.489017	20.745624	C	-0.078969	-2.596231	19.014202

C	4.537606	-2.704971	20.358671	O	0.843390	0.522652	21.651979
C	3.252182	-1.601681	24.858079	O	-7.910209	1.088147	20.193097
N	1.039880	-1.620389	23.813478	H	-7.602637	1.449988	19.339297
C	-0.225721	-1.389047	24.289322	H	-8.094651	0.153440	19.970311
C	-0.187643	-1.075159	25.701675	O	-7.354859	-1.937964	26.131750
C	1.129025	-1.108228	26.069343	H	-7.011146	-1.655592	25.247906
C	1.875288	-1.455359	24.881455	H	-7.452886	-2.904808	26.033490
C	1.727346	-0.840186	27.407992	O	2.103593	3.912541	28.354505
O	-2.925024	-2.423467	17.821408	H	1.757059	3.665215	27.465138
C	-1.361043	-0.766165	26.571378	H	1.314059	3.841041	28.924536
C	-1.671704	0.742210	26.675443	O	-7.414200	3.078148	25.131622
C	-2.789598	0.976320	27.683119	H	-6.602715	2.541210	24.968770
O	-2.494173	0.903905	28.903591	H	-7.698455	3.342269	24.236187
O	-3.976444	1.166377	27.236087	O	-5.012964	1.498890	24.671961
N	2.118689	-2.637233	20.073157	H	-4.581875	1.346008	25.555351
C	1.290552	-2.757378	18.991399	H	-5.348543	0.621556	24.394415
C	2.051909	-3.028303	17.790182	O	-5.758525	2.574824	29.055391
C	3.366982	-3.049292	18.163407	H	-5.124222	2.117907	28.451794
C	3.389185	-2.794118	19.592361	H	-5.677659	3.512075	28.788415
C	1.448891	-3.232735	16.441253	O	1.051007	3.280550	25.714836
N	3.509546	-2.176903	22.509847	H	1.452457	4.005043	25.180073
C	4.592784	-2.430555	21.712533	H	1.402043	2.466937	25.305266
C	5.823359	-2.355782	22.468645	H	-7.586144	-2.962241	20.659885
C	5.462654	-2.044640	23.757564	H	-1.947024	1.140989	25.695860
C	4.012025	-1.942560	23.756524	H	-0.776250	1.268075	27.019867
C	7.184105	-2.610927	21.921629	H	-1.161093	-1.147972	27.578871
C	6.287697	-1.868576	24.941205	H	-2.249498	-1.299653	26.213148
C	7.546736	-1.407223	24.991015	H	2.451827	-1.614690	27.683836
N	-0.365997	-2.078417	21.383534	H	2.257043	0.121334	27.419392
C	-0.842351	-2.258593	20.120555	H	0.961089	-0.806508	28.185697
C	-2.261460	-1.987950	20.087441	H	-2.303518	-1.242438	24.030008
C	-2.628593	-1.635928	21.376662	H	3.776936	-1.413599	25.783751
C	-1.436217	-1.716420	22.164241	H	5.816944	-2.137829	25.886652
C	-3.168770	-2.022637	18.963382	H	8.063120	-1.336525	25.945832
C	-3.971613	-1.206300	21.864911	H	8.084859	-1.070014	24.110614
C	-4.978354	-2.346684	22.074492	H	7.858916	-2.951350	22.711760
C	-6.278267	-1.853397	22.703231	H	7.166112	-3.376067	21.140040
O	-7.374518	-2.255775	22.176587	H	7.614609	-1.698126	21.486969
O	-6.211313	-1.112521	23.714778	H	5.473013	-2.819850	19.834437
C	4.548924	-3.318717	17.266473	H	4.194252	-3.217965	16.231875
O	5.642758	-2.419295	17.469124	H	4.301434	-5.470592	17.222002
C	5.091114	-4.738148	17.422644	H	5.471973	-4.906361	18.435901
H	5.908666	-4.895603	16.708580	H	2.214183	-3.347864	15.670841
Cu	0.285217	1.719984	20.117039	H	0.820269	-4.132123	16.424004
H	8.891071	3.392424	20.913367	H	0.815530	-2.383347	16.158936
H	-4.673317	2.104938	16.938341	H	-0.615493	-2.705924	18.083899
H	-5.531461	3.294705	21.032081	H	-4.180009	-1.641137	19.190472
H	-9.006488	-4.710142	17.956796	H	-4.397597	-0.480477	21.161860
H	-10.071118	-4.017669	23.050776	H	-3.864118	-0.673772	22.808259
H	0.595658	-7.919074	24.825696	H	-4.550360	-3.087486	22.765250
H	-7.746921	-3.426171	30.227401	H	-5.180484	-2.865320	21.134592
O	1.827626	-0.356781	21.328247	H	5.324443	-1.474391	17.388489

Structure large 5 AF:

204

C	0.705000	7.351000	24.202000	C	-1.882448	2.071956	22.315576
C	1.502092	6.244094	23.565591	N	-1.352897	2.654746	21.250112
O	2.150070	5.434548	24.259132	H	-4.772753	4.865391	20.708402
H	1.302779	7.798947	25.000267	H	-5.174758	4.405109	22.374714
H	-0.192831	6.913953	24.653975	H	-3.755563	2.203258	23.286249
H	0.400202	8.123576	23.490497	H	-2.166880	4.123228	19.898468
N	1.464625	6.155548	22.224034	H	-1.392458	1.341002	22.933312
C	2.230902	5.154564	21.497031	C	-8.625433	-3.716401	17.694230
C	1.765244	4.965031	20.048748	C	-8.377837	-2.885771	18.917865
C	2.554577	3.843551	19.455133	O	-8.707593	-1.708363	19.029009
N	2.170291	2.515781	19.538647	O	-7.735042	-3.567595	19.874514
C	3.838437	3.897978	18.987215	H	-7.669622	-3.858660	17.174566
C	3.214734	1.796472	19.147794	H	-9.320464	-3.203206	17.027611
N	4.261078	2.594953	18.813864	C	-10.872349	-3.425133	22.598443
H	1.009812	6.898611	21.701070	C	-10.843893	-2.043836	23.133077
H	2.139351	4.207864	22.034651	N	-9.681651	-1.300851	23.196953
H	0.694910	4.742617	20.023626	C	-11.829792	-1.249399	23.644101
H	1.926981	5.886430	19.476131	C	-9.939464	-0.107617	23.721055
H	4.484225	4.736876	18.781433	N	-11.238865	-0.061967	23.996139
H	3.267551	0.724086	19.086673	H	-10.730004	-3.426852	21.512411
H	3.292827	5.433337	21.498089	H	-11.832132	-3.895081	22.824454
C	8.986972	3.511952	19.822968	H	-8.726966	-1.632350	22.862142
C	7.964547	2.682040	19.092417	H	-12.884774	-1.426340	23.785737
C	8.302209	1.578992	18.297043	H	-9.230792	0.682653	23.902489
C	6.605013	2.963697	19.218569	C	-0.044352	-7.262201	24.211370
C	7.331716	0.797672	17.684672	C	0.682062	-6.175973	23.489049
C	5.621484	2.199033	18.596832	N	1.677025	-6.409609	22.566229
C	5.929032	1.035317	17.811538	C	0.510628	-4.811394	23.460519
O	5.031330	0.281750	17.274464	C	2.065816	-5.234753	22.027998
H	8.864089	4.580470	19.604088	N	1.374236	-4.233537	22.547808
H	10.004142	3.223382	19.539757	H	-0.569803	-7.903873	23.492321
H	9.351193	1.318494	18.161820	H	-0.794494	-6.815235	24.869498
H	6.297628	3.795478	19.845134	H	2.060223	-7.317339	22.316783
H	7.634326	-0.051156	17.074505	H	-0.182245	-4.221789	24.039144
H	-11.715797	0.735466	24.410662	H	2.835597	-5.163655	21.278942
C	-3.914728	1.798737	16.208986	C	-7.086103	-3.053014	29.453633
C	-2.575994	1.775175	16.852960	N	-5.944389	-2.460518	30.119338
N	-1.388516	1.872200	16.162108	C	-5.148270	-1.543189	29.572659
C	-2.198527	1.668973	18.163246	N	-5.332626	-1.145153	28.321021
C	-0.366533	1.843109	17.041272	N	-4.136403	-1.040682	30.297082
N	-0.826602	1.722203	18.277730	H	-6.792757	-3.871372	28.787076
H	-4.188648	0.812412	15.814335	H	-7.630717	-2.291371	28.894811
H	-3.935899	2.513393	15.379063	H	-5.631008	-2.882144	30.987723
H	-1.289501	1.970198	15.155207	H	-5.994726	-1.601819	27.697163
H	-2.831062	1.576475	19.029507	H	-4.854826	-0.308882	27.967811
H	0.667382	1.927157	16.747091	H	-4.219271	-1.064225	31.308119
C	-4.807051	4.030304	21.413248	H	-3.587761	-0.267444	29.898109
C	-3.455231	3.424798	21.546602	Fe	1.585558	-2.025417	21.946652
N	-3.139475	2.506799	22.524425	C	-1.346803	-1.428510	23.537185
C	-2.324954	3.515270	20.776844	C	-0.034336	-2.503695	19.013679

C	4.577851	-2.694649	20.374526	O	0.932447	0.668288	21.751328
C	3.284116	-1.525971	24.853778	O	-7.910724	1.066251	20.250698
N	1.063932	-1.585399	23.822773	H	-7.575920	1.423747	19.406331
C	-0.201974	-1.371298	24.303556	H	-8.082640	0.129369	20.030697
C	-0.164233	-1.063756	25.715083	O	-7.311497	-2.018687	26.145230
C	1.156064	-1.074432	26.076625	H	-6.970894	-1.726498	25.263283
C	1.903279	-1.403969	24.884410	H	-7.353627	-2.990446	26.056643
C	1.750034	-0.794423	27.414640	O	1.938582	3.914567	28.202544
O	-2.873221	-2.352659	17.820309	H	1.630853	3.616450	27.314210
C	-1.338487	-0.770032	26.589091	H	1.144429	3.801371	28.757544
C	-1.659651	0.736510	26.695664	O	-7.418116	2.993413	25.113180
C	-2.785409	0.966413	27.694928	H	-6.591662	2.473543	24.966906
O	-2.499594	0.912722	28.918282	H	-7.683791	3.254073	24.209432
O	-3.971579	1.135168	27.236799	O	-5.007788	1.449373	24.683018
N	2.159099	-2.558141	20.081227	H	-4.566834	1.294549	25.561868
C	1.332868	-2.682721	18.997672	H	-5.337766	0.570685	24.402768
C	2.092037	-3.001655	17.806828	O	-5.879986	2.518115	28.917130
C	3.404495	-3.055251	18.188259	H	-5.195532	2.075635	28.359820
C	3.428142	-2.767461	19.609355	H	-5.809962	3.454795	28.647243
C	1.489399	-3.223814	16.461096	O	1.005310	3.196101	25.546569
N	3.549239	-2.121344	22.509462	H	1.420758	3.927129	25.032192
C	4.634001	-2.395318	21.722835	H	1.354444	2.386618	25.127886
C	5.862007	-2.316092	22.481163	H	-7.574148	-2.985440	20.693403
C	5.498245	-1.975714	23.762036	H	-1.930531	1.134035	25.714253
C	4.047477	-1.868136	23.755313	H	-0.769145	1.266886	27.045440
C	7.221326	-2.593355	21.941447	H	-1.133461	-1.153265	27.595252
C	6.322862	-1.786013	24.944109	H	-2.222698	-1.310561	26.231183
C	7.583859	-1.329659	24.985318	H	2.558837	-1.494600	27.649836
N	-0.326714	-1.991196	21.383892	H	2.172389	0.218629	27.455441
C	-0.801174	-2.171638	20.120087	H	0.998948	-0.872985	28.204776
C	-2.225838	-1.937853	20.093903	H	-2.282772	-1.249628	24.046031
C	-2.603225	-1.616002	21.387622	H	3.808516	-1.325611	25.777195
C	-1.407529	-1.676223	22.173047	H	5.851364	-2.039864	25.893254
C	-3.131949	-1.978371	18.967129	H	8.102176	-1.247149	25.938120
C	-3.953906	-1.214733	21.881202	H	8.121436	-1.007618	24.098954
C	-4.957906	-2.362198	22.066215	H	7.895063	-2.913435	22.740640
C	-6.254765	-1.883409	22.714941	H	7.198304	-3.381421	21.182877
O	-7.355956	-2.268817	22.193303	H	7.655190	-1.696401	21.478078
O	-6.175561	-1.163322	23.744287	H	5.511851	-2.843579	19.856704
C	4.584207	-3.370951	17.304845	H	4.230301	-3.312869	16.266957
O	5.680594	-2.462576	17.471192	H	4.328692	-5.520971	17.348480
C	5.122652	-4.784969	17.517665	H	5.506479	-4.917105	18.534871
H	5.936458	-4.976107	16.807551	H	2.254285	-3.348979	15.691850
Cu	0.253213	1.798720	20.121931	H	0.862771	-4.124915	16.457460
H	8.891071	3.392424	20.913367	H	0.854900	-2.379268	16.168549
H	-4.673317	2.104938	16.938341	H	-0.570190	-2.616441	18.083544
H	-5.531461	3.294705	21.032081	H	-4.154287	-1.631203	19.199071
H	-9.006488	-4.710142	17.956796	H	-4.382478	-0.476197	21.192970
H	-10.071118	-4.017669	23.050776	H	-3.853034	-0.701617	22.835912
H	0.595658	-7.919074	24.825696	H	-4.526994	-3.119940	22.736373
H	-7.746921	-3.426171	30.227401	H	-5.166296	-2.856451	21.114501
O	1.860738	-0.261788	21.517028	H	5.353491	-1.522528	17.396955

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C	0.705000	7.351000	24.202000	C	-1.913960	2.089570	22.344488
C	1.488720	6.254309	23.545167	N	-1.376802	2.722635	21.309309
O	2.129709	5.419732	24.214851	H	-4.813317	4.899430	20.790339
H	1.293028	7.757016	25.030210	H	-5.254531	4.366948	22.426088
H	-0.213625	6.921807	24.619959	H	-3.798798	2.168659	23.299506
H	0.432739	8.155127	23.513221	H	-2.192088	4.231380	20.003763
N	1.444678	6.206767	22.202342	H	-1.431139	1.335207	22.939322
C	2.209935	5.232715	21.449442	C	-8.631287	-3.714131	17.695977
C	1.705207	5.036620	20.017079	C	-8.384077	-2.890333	18.923952
C	2.500481	3.918896	19.438280	O	-8.741404	-1.722901	19.052516
N	2.133000	2.587800	19.584686	O	-7.711935	-3.566754	19.864225
C	3.779091	3.971479	18.969676	H	-7.677827	-3.851912	17.171161
C	3.173129	1.861497	19.210229	H	-9.333166	-3.202371	17.035591
N	4.209085	2.664794	18.834878	C	-10.866783	-3.425867	22.588729
H	0.997093	6.969917	21.704283	C	-10.844402	-2.047583	23.129329
H	2.158936	4.282739	21.986237	N	-9.684866	-1.300707	23.200554
H	0.637932	4.797113	20.019303	C	-11.833962	-1.259981	23.642972
H	1.841423	5.951884	19.429776	C	-9.947475	-0.111644	23.732984
H	4.417721	4.806554	18.728810	N	-11.247531	-0.073331	24.003945
H	3.238496	0.787731	19.213925	H	-10.709782	-3.423792	21.504727
H	3.265284	5.533223	21.417553	H	-11.829359	-3.896340	22.801238
C	8.925337	3.591454	19.830571	H	-8.732974	-1.625768	22.867113
C	7.903189	2.763834	19.114920	H	-12.889415	-1.440568	23.777666
C	8.258388	1.653250	18.321591	H	-9.241796	0.679913	23.921572
C	6.542566	3.054571	19.253859	C	-0.040076	-7.242614	24.228823
C	7.302448	0.866010	17.721707	C	0.695843	-6.162550	23.508397
C	5.563188	2.289205	18.645273	N	1.684366	-6.405281	22.581215
C	5.893967	1.122179	17.850949	C	0.527451	-4.799278	23.475431
O	5.009539	0.385262	17.313073	C	2.077061	-5.240594	22.034041
H	8.726332	4.661292	19.695926	N	1.390689	-4.233220	22.553471
H	9.935606	3.373256	19.474094	H	-0.583518	-7.864115	23.505625
H	9.310467	1.410589	18.188918	H	-0.774621	-6.789822	24.900189
H	6.246472	3.891062	19.878295	H	2.065694	-7.315227	22.336784
H	7.594318	0.011188	17.117004	H	-0.157724	-4.204767	24.056498
H	-11.727855	0.719205	24.423199	H	2.843196	-5.175278	21.282134
C	-3.901472	1.783119	16.231402	C	-7.092890	-3.042451	29.453410
C	-2.571244	1.807434	16.890800	N	-5.942322	-2.463585	30.115629
N	-1.379243	1.911778	16.210048	C	-5.140030	-1.553788	29.565698
C	-2.207919	1.737506	18.207410	N	-5.327182	-1.155269	28.314189
C	-0.365047	1.922369	17.095874	N	-4.120931	-1.058334	30.284000
N	-0.838322	1.818135	18.328984	H	-6.808733	-3.852075	28.772499
H	-4.152699	0.776867	15.874406	H	-7.639718	-2.270683	28.910245
H	-3.921806	2.463071	15.373040	H	-5.628826	-2.889915	30.981885
H	-1.271671	1.989882	15.202274	H	-5.983296	-1.619096	27.688763
H	-2.845233	1.648676	19.070525	H	-4.845527	-0.323533	27.958714
H	0.670789	2.018369	16.813816	H	-4.196271	-1.080013	31.295329
C	-4.847251	4.039239	21.464015	H	-3.565996	-0.292460	29.878007
C	-3.488598	3.458651	21.610456	Fe	1.624458	-2.150837	21.962636
N	-3.176858	2.504614	22.553710	C	-1.324273	-1.498448	23.540062
C	-2.351255	3.592656	20.859110	C	-0.002098	-2.548924	19.015550

C	4.599278	-2.839889	20.390191	O	-7.862014	1.043151	20.230869
C	3.310631	-1.563674	24.845937	H	-7.596358	1.407507	19.363986
N	1.089236	-1.664962	23.830506	H	-8.066867	0.111316	20.013748
C	-0.176951	-1.437179	24.302267	O	-7.287720	-2.056193	26.139976
C	-0.137923	-1.092586	25.705651	H	-6.947883	-1.771841	25.255254
C	1.182989	-1.086689	26.066026	H	-7.340611	-3.027972	26.058226
C	1.930154	-1.449551	24.882795	O	1.855950	3.959774	28.047792
C	1.770531	-0.772034	27.398940	H	1.555218	3.635282	27.167038
O	-2.828582	-2.329493	17.801620	H	1.090934	3.765511	28.625701
C	-1.314926	-0.790283	26.575241	O	-7.407055	2.984488	25.095916
C	-1.651040	0.712232	26.661757	H	-6.589069	2.451932	24.946373
C	-2.774982	0.942865	27.664385	H	-7.670419	3.252223	24.192242
O	-2.484451	0.881938	28.886604	O	-5.028150	1.410517	24.669005
O	-3.961092	1.120253	27.211052	H	-4.578110	1.268529	25.545282
N	2.182743	-2.699225	20.089922	H	-5.350266	0.525238	24.397238
C	1.358421	-2.769268	19.003435	O	-5.929860	2.530761	28.835684
C	2.113343	-3.083071	17.808638	H	-5.229411	2.081157	28.306420
C	3.420909	-3.194359	18.197063	H	-5.862392	3.462767	28.537798
C	3.449674	-2.922161	19.622469	O	0.972704	3.119728	25.383578
C	1.512944	-3.242119	16.453013	H	1.403229	3.861961	24.898959
N	3.575100	-2.259642	22.530652	H	1.443173	2.327005	25.067595
C	4.657412	-2.512839	21.733644	H	-7.557532	-2.989183	20.689489
C	5.889173	-2.362612	22.476330	H	-1.932256	1.094870	25.677293
C	5.526692	-1.996240	23.750120	H	-0.765522	1.260072	26.998856
C	4.073118	-1.938221	23.757545	H	-1.105783	-1.157435	27.586531
C	7.251919	-2.595946	21.925871	H	-2.194169	-1.344454	26.225247
C	6.349594	-1.744472	24.921830	H	2.632826	-1.409564	27.620134
C	7.591172	-1.237906	24.948371	H	2.111253	0.271351	27.446377
N	-0.306032	-2.078281	21.391838	H	1.035331	-0.916071	28.195560
C	-0.771273	-2.224269	20.121023	H	-2.257831	-1.309878	24.047318
C	-2.191883	-1.964065	20.087161	H	3.841078	-1.317531	25.756897
C	-2.575227	-1.659993	21.383036	H	5.890004	-1.993504	25.878382
C	-1.384236	-1.751157	22.177007	H	8.106373	-1.111886	25.897620
C	-3.091107	-1.972107	18.951707	H	8.115653	-0.917812	24.053101
C	-3.926533	-1.252361	21.871863	H	7.952987	-2.848580	22.725615
C	-4.940141	-2.389541	22.041885	H	7.255855	-3.415368	21.201016
C	-6.231515	-1.908453	22.701978	H	7.632222	-1.697927	21.419264
O	-7.339960	-2.267986	22.174049	H	5.534639	-2.986366	19.877325
O	-6.139770	-1.211426	23.744178	H	4.221081	-3.543872	16.279973
C	4.583439	-3.561446	17.315716	H	4.324734	-5.698587	17.464534
O	5.687708	-2.641889	17.427706	H	5.523322	-5.045906	18.603361
C	5.124112	-4.959582	17.587052	H	2.278153	-3.367247	15.684868
H	5.925544	-5.186232	16.873242	H	0.853742	-4.118762	16.416639
Cu	0.200391	2.016851	20.096190	H	0.910915	-2.365517	16.186224
H	8.891071	3.392424	20.913367	H	-0.533522	-2.621783	18.075927
H	-4.673317	2.104938	16.938341	H	-4.109913	-1.613782	19.182223
H	-5.531461	3.294705	21.032081	H	-4.344649	-0.503869	21.185991
H	-9.006488	-4.710142	17.956796	H	-3.827118	-0.745457	22.831903
H	-10.071118	-4.017669	23.050776	H	-4.515164	-3.163428	22.699004
H	0.595658	-7.919074	24.825696	H	-5.154362	-2.868787	21.082010
H	-7.746921	-3.426171	30.227401	H	5.337104	-1.729584	17.329300
O	1.979725	-0.475138	21.530839	H	1.427396	1.132630	22.407709
O	0.888261	0.564984	21.812577				

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C	0.705000	7.351000	24.202000	C	-1.865248	2.124798	22.216679
C	1.518834	6.270001	23.562162	N	-1.365644	2.778976	21.175045
O	2.160959	5.441987	24.239048	H	-4.842470	4.908401	20.764126
H	1.297868	7.814745	24.997774	H	-5.225124	4.375393	22.415059
H	-0.177812	6.896747	24.668462	H	-3.720516	2.186160	23.232573
H	0.374447	8.117665	23.497424	H	-2.230909	4.297994	19.914570
N	1.505812	6.234729	22.219436	H	-1.361687	1.361824	22.783346
C	2.281795	5.268435	21.470385	C	-8.637493	-3.713191	17.686333
C	1.794811	5.104814	20.028495	C	-8.382767	-2.876288	18.904296
C	2.568773	3.977464	19.443413	O	-8.708008	-1.697739	19.011323
N	2.142621	2.658297	19.533045	O	-7.737997	-3.555896	19.862266
C	3.862954	3.992292	19.023402	H	-7.687059	-3.848535	17.154907
C	3.166486	1.900113	19.173472	H	-9.345315	-3.208849	17.026354
N	4.246497	2.673157	18.864479	C	-10.867795	-3.418220	22.599357
H	1.046104	6.988548	21.718746	C	-10.833912	-2.038145	23.137162
H	2.215678	4.309311	21.990166	N	-9.673071	-1.291573	23.183461
H	0.722490	4.887529	20.014134	C	-11.814307	-1.246815	23.663946
H	1.957481	6.025980	19.457703	C	-9.925943	-0.100242	23.713906
H	4.540986	4.808049	18.832484	N	-11.221172	-0.058175	24.008415
H	3.188295	0.825311	19.144031	H	-10.723787	-3.417976	21.513548
H	3.339136	5.563300	21.460976	H	-11.830543	-3.883314	22.822992
C	8.980007	3.511058	19.824707	H	-8.719119	-1.622350	22.843915
C	7.940413	2.691957	19.127812	H	-12.867080	-1.425077	23.819367
C	8.271163	1.580310	18.324575	H	-9.215797	0.690048	23.889948
C	6.586424	3.003545	19.285913	C	-0.064650	-7.248231	24.255928
C	7.296890	0.811219	17.733813	C	0.666592	-6.185336	23.513520
C	5.588434	2.261993	18.680528	N	1.665080	-6.445051	22.602225
C	5.893869	1.090649	17.880077	C	0.507288	-4.823563	23.466117
O	4.992794	0.372299	17.350126	C	2.071366	-5.288511	22.047440
H	8.841292	4.577664	19.607572	N	1.383712	-4.273300	22.549306
H	9.989245	3.218709	19.523715	H	-0.640362	-7.869302	23.557953
H	9.318110	1.322867	18.179945	H	-0.766255	-6.784492	24.954379
H	6.313740	3.840057	19.920224	H	2.045015	-7.359853	22.375452
H	7.567710	-0.047037	17.124197	H	-0.180349	-4.220099	24.034706
H	-11.690362	0.736974	24.435627	H	2.847601	-5.235221	21.305234
C	-3.929346	1.815763	16.188303	C	-7.097133	-3.030429	29.455409
C	-2.581304	1.811086	16.808523	N	-5.959821	-2.431507	30.124652
N	-1.401869	1.884396	16.102206	C	-5.145929	-1.535593	29.571491
C	-2.193267	1.760964	18.118149	N	-5.311031	-1.154587	28.309146
C	-0.370465	1.898567	16.968633	N	-4.130071	-1.038824	30.292803
N	-0.821350	1.825427	18.212277	H	-6.795560	-3.834817	28.775574
H	-4.195265	0.828261	15.792017	H	-7.656047	-2.268254	28.910697
H	-3.976528	2.537648	15.365660	H	-5.658069	-2.844045	31.001842
H	-1.312656	1.940357	15.091226	H	-6.005933	-1.581835	27.701021
H	-2.815814	1.696625	18.993932	H	-4.836929	-0.315443	27.958515
H	0.660983	1.974341	16.663682	H	-4.209568	-1.060761	31.304422
C	-4.844169	4.050468	21.441410	H	-3.568531	-0.277646	29.889356
C	-3.474609	3.487828	21.545658	Fe	1.620757	-2.216359	21.988947
N	-3.125379	2.525009	22.466732	C	-1.316470	-1.504453	23.566944
C	-2.361057	3.645984	20.764970	C	-0.022354	-2.632501	19.052352

C	4.588128	-2.896966	20.399600	O	-7.968375	1.110782	20.210912
C	3.315168	-1.654223	24.872520	H	-7.565817	1.433938	19.383075
N	1.093237	-1.709182	23.852322	H	-8.122422	0.164995	20.012759
C	-0.168143	-1.458823	24.327661	O	-7.334317	-1.934698	26.140135
C	-0.122992	-1.114212	25.732467	H	-6.986512	-1.660012	25.255935
C	1.196527	-1.135643	26.091985	H	-7.431095	-2.902666	26.050756
C	1.936815	-1.514503	24.907589	O	2.018800	3.910073	28.211311
C	1.798845	-0.824108	27.418905	H	1.693355	3.625423	27.326187
O	-2.846130	-2.378172	17.841159	H	1.226735	3.827204	28.775962
C	-1.295925	-0.797070	26.601050	O	-7.396622	3.029359	25.123721
C	-1.630346	0.708260	26.674229	H	-6.578769	2.506459	24.957067
C	-2.751289	0.946726	27.678381	H	-7.683656	3.302640	24.231542
O	-2.458901	0.880589	28.899885	O	-4.949851	1.472961	24.642525
O	-3.936345	1.137106	27.227307	H	-4.534181	1.320217	25.533278
N	2.173698	-2.768756	20.113370	H	-5.304140	0.599561	24.373569
C	1.340495	-2.843914	19.032879	O	-5.762151	2.544735	29.023270
C	2.090489	-3.135708	17.828176	H	-5.108912	2.092668	28.438783
C	3.402285	-3.227634	18.203231	H	-5.816852	3.445098	28.639732
C	3.437026	-2.974051	19.633916	O	1.057267	3.177481	25.536796
C	1.480184	-3.279952	16.475311	H	1.460045	3.927051	25.039468
N	3.570105	-2.329010	22.545693	H	1.527881	2.393085	25.196482
C	4.650340	-2.582356	21.745644	H	-7.574483	-2.971984	20.677341
C	5.883590	-2.444205	22.487409	H	-1.912647	1.081645	25.686472
C	5.524902	-2.091214	23.766371	H	-0.743456	1.257077	27.005196
C	4.071445	-2.027003	23.777304	H	-1.087817	-1.153964	27.615943
C	7.246313	-2.662540	21.930173	H	-2.178299	-1.351253	26.259012
C	6.353765	-1.839476	24.934372	H	2.571664	-1.551687	27.690317
C	7.585441	-1.309293	24.952101	H	2.270254	0.167846	27.415147
N	-0.315500	-2.133538	21.425704	H	1.041647	-0.828150	28.206903
C	-0.785560	-2.290165	20.158576	H	-2.245912	-1.291682	24.074612
C	-2.201293	-2.006155	20.123473	H	3.847601	-1.427961	25.785347
C	-2.575495	-1.675223	21.415881	H	5.907722	-2.104141	25.892934
C	-1.385515	-1.774762	22.207074	H	8.109239	-1.181234	25.896862
C	-3.100341	-2.005783	18.988701	H	8.092476	-0.970880	24.053924
C	-3.917374	-1.234721	21.902208	H	7.949240	-2.932503	22.722589
C	-4.953680	-2.355693	22.067561	H	7.252109	-3.463441	21.184982
C	-6.247429	-1.857360	22.708314	H	7.623681	-1.751271	21.445600
O	-7.348634	-2.253489	22.189376	H	5.523790	-3.040032	19.883157
O	-6.169213	-1.122732	23.724069	H	4.196855	-3.488453	16.270117
C	4.563486	-3.548203	17.301856	H	4.328263	-5.692382	17.346615
O	5.663143	-2.627769	17.446576	H	5.514229	-5.081963	18.522323
C	5.119305	-4.952436	17.509452	H	2.240217	-3.391468	15.699406
H	5.925988	-5.134258	16.789259	H	0.823198	-4.157734	16.431048
Cu	0.206864	2.213094	19.959915	H	0.873911	-2.401597	16.224765
H	8.891071	3.392424	20.913367	H	-0.557587	-2.714009	18.118581
H	-4.673317	2.104938	16.938341	H	-4.111740	-1.624660	19.215928
H	-5.531461	3.294705	21.032081	H	-4.318288	-0.479368	21.215256
H	-9.006488	-4.710142	17.956796	H	-3.810346	-0.732051	22.861885
H	-10.071118	-4.017669	23.050776	H	-4.548312	-3.130644	22.734154
H	0.595658	-7.919074	24.825696	H	-5.164119	-2.836627	21.109838
H	-7.746921	-3.426171	30.227401	H	5.309069	-1.715732	17.363750
O	1.958556	-0.531710	21.475030	H	1.452936	0.972195	22.523019
O	0.940443	0.486229	21.841487				

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C	0.705000	7.351000	24.202000	C	-1.888764	2.088111	22.234723
C	1.506532	6.267991	23.555128	N	-1.382613	2.741681	21.193415
O	2.124581	5.418970	24.227367	H	-4.832139	4.908008	20.789019
H	1.306013	7.808676	24.996192	H	-5.231020	4.358284	22.431373
H	-0.177490	6.901019	24.673900	H	-3.740350	2.160487	23.252177
H	0.374334	8.123061	23.503978	H	-2.230128	4.273758	19.936348
N	1.507642	6.257608	22.211023	H	-1.390746	1.323322	22.802478
C	2.285304	5.303825	21.450271	C	-8.635252	-3.716548	17.678760
C	1.774547	5.124746	20.017696	C	-8.367969	-2.877249	18.891727
C	2.538357	3.987872	19.436367	O	-8.665331	-1.690414	18.987762
N	2.119257	2.671737	19.554717	O	-7.746309	-3.565858	19.858414
C	3.832661	3.995336	19.011275	H	-7.689099	-3.858294	17.141435
C	3.152787	1.908084	19.223405	H	-9.344897	-3.211170	17.021549
N	4.220421	2.675676	18.891738	C	-10.869678	-3.422363	22.596998
H	1.076956	7.036164	21.722368	C	-10.838777	-2.040490	23.129717
H	2.245254	4.347526	21.977374	N	-9.679601	-1.290943	23.171608
H	0.700303	4.917290	20.020902	C	-11.819385	-1.250834	23.657941
H	1.932153	6.037393	19.432328	C	-9.933296	-0.098988	23.700612
H	4.513623	4.805257	18.805081	N	-11.227513	-0.060342	23.998861
H	3.172218	0.832345	19.227224	H	-10.725747	-3.425983	21.511229
H	3.337566	5.615667	21.419444	H	-11.831326	-3.888744	22.822603
C	8.975080	3.516775	19.828660	H	-8.728320	-1.620501	22.833433
C	7.924090	2.715572	19.115071	H	-12.870871	-1.432425	23.818110
C	8.245213	1.719348	18.189908	H	-9.223919	0.692415	23.873327
C	6.573678	2.960968	19.352329	C	-0.054972	-7.221704	24.275604
C	7.253019	1.008108	17.524636	C	0.684929	-6.157504	23.543015
C	5.572357	2.278044	18.667962	N	1.690895	-6.413590	22.638707
C	5.907226	1.286393	17.741954	C	0.515285	-4.797255	23.490120
O	4.903931	0.615355	17.094849	C	2.094117	-5.262166	22.079632
H	8.851881	4.584886	19.611777	N	1.395367	-4.248903	22.574638
H	9.979468	3.216609	19.518168	H	-0.649320	-7.815824	23.569721
H	9.286970	1.487745	17.982464	H	-0.741030	-6.758859	24.989911
H	6.283571	3.713212	20.078542	H	2.078234	-7.327171	22.418821
H	7.523239	0.232280	16.812549	H	-0.179664	-4.196219	24.051337
H	-11.698119	0.735070	24.424925	H	2.874654	-5.209601	21.343043
C	-3.912024	1.818460	16.204667	C	-7.097104	-3.032924	29.454796
C	-2.569959	1.840490	16.838881	N	-5.962363	-2.430378	30.124319
N	-1.385609	1.946191	16.144279	C	-5.147971	-1.535238	29.568004
C	-2.192551	1.786327	18.151246	N	-5.308293	-1.164533	28.303782
C	-0.361753	1.975992	17.016540	N	-4.136638	-1.031986	30.291821
N	-0.822233	1.879909	18.256652	H	-6.793933	-3.840065	28.778931
H	-4.156667	0.822610	15.815763	H	-7.656678	-2.273872	28.906249
H	-3.957809	2.529232	15.372435	H	-5.663532	-2.836180	31.005300
H	-1.289143	2.010665	15.134127	H	-6.001530	-1.595346	27.695783
H	-2.822284	1.698202	19.019101	H	-4.832340	-0.328558	27.947152
H	0.669992	2.078858	16.721558	H	-4.220554	-1.047606	31.302805
C	-4.845226	4.042985	21.456869	H	-3.577279	-0.270615	29.887360
C	-3.481798	3.468245	21.564208	Fe	1.620286	-2.212824	21.999795
N	-3.142252	2.499918	22.483808	C	-1.319226	-1.508368	23.565128
C	-2.368273	3.619378	20.783114	C	-0.023360	-2.661512	19.059992

C	4.587829	-2.905099	20.423407	O	-7.924960	1.083998	20.235493
C	3.315098	-1.638716	24.887442	H	-7.574998	1.457075	19.403020
N	1.096906	-1.700192	23.849757	H	-8.094391	0.151862	19.991030
C	-0.170776	-1.460042	24.323662	O	-7.326121	-1.947643	26.124177
C	-0.128127	-1.119797	25.724552	H	-6.977244	-1.669223	25.241910
C	1.193937	-1.135985	26.090153	H	-7.418120	-2.915820	26.032339
C	1.938680	-1.506752	24.914029	O	2.012706	3.950640	28.167590
C	1.788327	-0.824471	27.418529	H	1.677967	3.634541	27.297858
O	-2.823266	-2.394198	17.837439	H	1.240936	3.844935	28.754638
C	-1.301422	-0.803639	26.589345	O	-7.356247	3.013357	25.094490
C	-1.622896	0.704455	26.664888	H	-6.532373	2.497483	24.939180
C	-2.753956	0.943247	27.659581	H	-7.656144	3.240754	24.194564
O	-2.466722	0.899398	28.882082	O	-4.903776	1.438744	24.610294
O	-3.937309	1.107701	27.195431	H	-4.497188	1.288269	25.506340
N	2.170529	-2.780850	20.135395	H	-5.275868	0.571271	24.345172
C	1.337806	-2.872858	19.051582	O	-5.846225	2.515447	28.939071
C	2.088282	-3.183828	17.858022	H	-5.170099	2.077391	28.371776
C	3.400540	-3.278327	18.241576	H	-5.729699	3.460600	28.734913
C	3.436842	-2.996534	19.662172	O	1.056196	3.128059	25.502388
C	1.486471	-3.339397	16.504646	H	1.441663	3.889900	25.009797
N	3.566679	-2.312395	22.561428	H	1.593077	2.369114	25.209715
C	4.647302	-2.571799	21.762665	H	-7.575570	-2.981546	20.671728
C	5.878113	-2.433322	22.504047	H	-1.894267	1.084460	25.676519
C	5.519193	-2.075144	23.782773	H	-0.735696	1.245910	27.005979
C	4.069986	-2.008159	23.793818	H	-1.095836	-1.167069	27.602425
C	7.239276	-2.660251	21.951062	H	-2.184392	-1.351963	26.241341
C	6.348145	-1.830102	24.951198	H	2.554575	-1.556856	27.695045
C	7.581274	-1.304406	24.964041	H	2.266430	0.164518	27.411508
N	-0.314597	-2.143605	21.429558	H	1.025531	-0.820572	28.200873
C	-0.784316	-2.306579	20.159937	H	-2.249396	-1.303612	24.074400
C	-2.195954	-2.019246	20.122684	H	3.843516	-1.412725	25.802025
C	-2.572158	-1.681465	21.411442	H	5.902398	-2.096728	25.908992
C	-1.384999	-1.780093	22.207696	H	8.108711	-1.177960	25.906945
C	-3.091831	-2.024776	18.979978	H	8.085473	-0.967106	24.063962
C	-3.913630	-1.239334	21.893215	H	7.937079	-2.935040	22.746068
C	-4.949810	-2.361372	22.050025	H	7.242640	-3.460203	21.205257
C	-6.243681	-1.862205	22.690763	H	7.621872	-1.749477	21.469757
O	-7.343054	-2.264292	22.175115	H	5.523151	-3.060128	19.910249
O	-6.163588	-1.123085	23.702917	H	4.206420	-3.564396	16.315191
C	4.562456	-3.617868	17.350195	H	4.324697	-5.756537	17.415066
O	5.658509	-2.687556	17.499879	H	5.503530	-5.137616	18.594178
C	5.116357	-5.017349	17.577386	H	2.251108	-3.475758	15.737780
H	5.926375	-5.205075	16.862896	H	0.815344	-4.206389	16.471378
Cu	0.189629	2.226928	20.017583	H	0.897935	-2.454020	16.237264
H	8.891071	3.392424	20.913367	H	-0.555502	-2.758728	18.126237
H	-4.673317	2.104938	16.938341	H	-4.106019	-1.649183	19.201136
H	-5.531461	3.294705	21.032081	H	-4.310030	-0.482251	21.205666
H	-9.006488	-4.710142	17.956796	H	-3.810598	-0.740454	22.854895
H	-10.071118	-4.017669	23.050776	H	-4.545583	-3.139368	22.713521
H	0.595658	-7.919074	24.825696	H	-5.157760	-2.836268	21.088917
H	-7.746921	-3.426171	30.227401	H	5.282598	-1.794051	17.380731
O	1.947606	-0.512918	21.432457	H	1.464932	0.928759	22.549980
O	0.959453	0.476550	21.837056	H	5.248501	0.338293	16.218018

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C	0.705000	7.351000	24.202000	C	-1.865096	2.072114	22.208400
C	1.518954	6.276116	23.553620	N	-1.367903	2.713480	21.153790
O	2.138068	5.428190	24.225783	H	-4.810253	4.894145	20.768572
H	1.311022	7.834445	24.975465	H	-5.189727	4.358494	22.419446
H	-0.156136	6.887483	24.697609	H	-3.706782	2.160156	23.239240
H	0.342794	8.104203	23.498066	H	-2.223119	4.235251	19.888163
N	1.533094	6.270513	22.208857	H	-1.357830	1.316350	22.780620
C	2.316391	5.316121	21.454396	C	-8.631395	-3.722521	17.665922
C	1.791064	5.102952	20.031170	C	-8.361754	-2.871536	18.869918
C	2.554054	3.960511	19.456814	O	-8.652972	-1.682378	18.952586
N	2.134026	2.641142	19.555015	O	-7.745847	-3.554068	19.844851
C	3.850969	3.970096	19.040185	H	-7.685860	-3.874266	17.130355
C	3.170585	1.881853	19.218878	H	-9.339172	-3.222105	17.002968
N	4.239658	2.653069	18.906245	C	-10.873287	-3.422220	22.603538
H	1.104722	7.048584	21.717413	C	-10.839774	-2.039922	23.134920
H	2.297849	4.369674	21.999767	N	-9.683854	-1.284782	23.160584
H	0.717748	4.893556	20.051212	C	-11.817905	-1.252594	23.671785
H	1.937287	6.005375	19.426813	C	-9.937476	-0.092509	23.688763
H	4.533972	4.781838	18.848124	N	-11.228248	-0.058165	24.002317
H	3.188729	0.806043	19.201759	H	-10.739076	-3.426090	21.516430
H	3.363319	5.643337	21.405699	H	-11.832578	-3.889200	22.837854
C	9.007847	3.468551	19.826162	H	-8.732372	-1.612284	22.818059
C	7.946329	2.685645	19.106739	H	-12.866636	-1.438492	23.844134
C	8.258258	1.722442	18.143721	H	-9.229627	0.702773	23.849287
C	6.597635	2.923076	19.362829	C	-0.049243	-7.217256	24.270829
C	7.261723	1.033352	17.463582	C	0.690249	-6.151271	23.536570
C	5.590419	2.261259	18.664361	N	1.704796	-6.404492	22.640917
C	5.917361	1.300881	17.702592	C	0.507337	-4.791937	23.470105
O	4.909335	0.654098	17.042872	C	2.103846	-5.253112	22.077853
H	8.937640	4.531561	19.562856	N	1.389006	-4.240690	22.555914
H	10.006925	3.115643	19.556454	H	-0.643103	-7.811203	23.564343
H	9.297659	1.499847	17.916894	H	-0.737269	-6.753071	24.982079
H	6.311978	3.651199	20.114864	H	2.102694	-7.316248	22.429506
H	7.527317	0.282827	16.722086	H	-0.199569	-4.193333	24.018907
H	-11.697365	0.737559	24.428803	H	2.891774	-5.200835	21.349375
C	-3.913542	1.832578	16.195900	C	-7.104979	-3.018824	29.454124
C	-2.567610	1.853591	16.821450	N	-5.975431	-2.406982	30.124800
N	-1.388162	1.970093	16.120109	C	-5.153834	-1.520335	29.565831
C	-2.182308	1.790158	18.130669	N	-5.302578	-1.160135	28.296263
C	-0.358910	1.999114	16.984192	N	-4.141323	-1.019639	30.289364
N	-0.811583	1.889851	18.227149	H	-6.792799	-3.818564	28.773300
H	-4.154194	0.840933	15.794121	H	-7.675918	-2.264198	28.910723
H	-3.966702	2.554714	15.373927	H	-5.687032	-2.800340	31.014937
H	-1.298542	2.039456	15.110169	H	-6.015529	-1.571090	27.697576
H	-2.805286	1.688868	19.001072	H	-4.831562	-0.319910	27.943299
H	0.670250	2.111183	16.684029	H	-4.222999	-1.037681	31.300398
C	-4.823769	4.032538	21.440861	H	-3.577846	-0.261003	29.884618
C	-3.463171	3.446256	21.533361	Fe	1.603433	-2.221234	21.995236
N	-3.114508	2.489487	22.462620	C	-1.321764	-1.499669	23.572092
C	-2.355859	3.587752	20.741051	C	-0.031530	-2.653057	19.062944

C	4.578930	-2.926504	20.419489	O	-7.986905	1.116709	20.196595
C	3.308924	-1.686225	24.886232	H	-7.580645	1.463079	19.377536
N	1.083251	-1.726398	23.861273	H	-8.119043	0.171299	19.980930
C	-0.174365	-1.466323	24.336413	O	-7.358544	-1.889209	26.127698
C	-0.127667	-1.129445	25.738511	H	-7.003115	-1.624491	25.243443
C	1.195146	-1.161723	26.098765	H	-7.494394	-2.851820	26.033013
C	1.930408	-1.541463	24.915888	O	2.116617	3.934755	28.242847
C	1.800970	-0.864682	27.425574	H	1.769667	3.648575	27.367308
O	-2.838072	-2.364085	17.843230	H	1.353697	3.804474	28.837698
C	-1.297221	-0.804228	26.605651	O	-7.318788	3.035351	25.128921
C	-1.617283	0.704290	26.673082	H	-6.506549	2.510643	24.945228
C	-2.747216	0.948827	27.667290	H	-7.648128	3.271373	24.240714
O	-2.462095	0.896547	28.890574	O	-4.879788	1.449149	24.612913
O	-3.928964	1.126702	27.204212	H	-4.476267	1.301029	25.511504
N	2.159741	-2.774090	20.131787	H	-5.257602	0.583285	24.352173
C	1.329715	-2.875139	19.051749	O	-5.785797	2.568460	29.013136
C	2.078659	-3.204924	17.858047	H	-5.135815	2.117079	28.426364
C	3.389138	-3.298849	18.239242	H	-5.733109	3.500619	28.722815
C	3.427437	-3.007086	19.659614	O	1.105325	3.172012	25.585055
C	1.469419	-3.381728	16.509948	H	1.477986	3.927627	25.073982
N	3.567496	-2.357289	22.562762	H	1.589543	2.398234	25.241866
C	4.645856	-2.605141	21.765230	H	-7.574887	-2.965333	20.653842
C	5.880189	-2.468051	22.505414	H	-1.887637	1.078797	25.682404
C	5.521321	-2.119354	23.785066	H	-0.729081	1.246312	27.011115
C	4.067179	-2.055281	23.795178	H	-1.090461	-1.160785	27.620781
C	7.242426	-2.687470	21.948815	H	-2.182548	-1.353209	26.263690
C	6.347794	-1.871901	24.954589	H	2.507100	-1.648170	27.725266
C	7.581350	-1.346221	24.971666	H	2.353790	0.084416	27.401759
N	-0.310552	-2.114999	21.430497	H	1.035169	-0.784805	28.201279
C	-0.787632	-2.288807	20.163009	H	-2.252420	-1.291553	24.079539
C	-2.202001	-2.009898	20.130937	H	3.836499	-1.467081	25.803502
C	-2.576294	-1.675808	21.421148	H	5.899311	-2.135203	25.912039
C	-1.386656	-1.764832	22.213654	H	8.105273	-1.218969	25.916330
C	-3.104035	-2.016960	18.993947	H	8.089722	-1.010908	24.073260
C	-3.918374	-1.237515	21.905061	H	7.940432	-2.971740	22.740558
C	-4.953343	-2.359851	22.066860	H	7.246589	-3.478823	21.193779
C	-6.251140	-1.854340	22.693833	H	7.626533	-1.771672	21.478448
O	-7.347351	-2.252019	22.166669	H	5.511997	-3.084612	19.903007
O	-6.178078	-1.112834	23.704249	H	4.188566	-3.590572	16.312354
C	4.549594	-3.640611	17.345553	H	4.328221	-5.781219	17.404636
O	5.644498	-2.706381	17.486031	H	5.504313	-5.157151	18.584361
C	5.113742	-5.036140	17.569023	H	2.229120	-3.521862	15.738494
H	5.924279	-5.215003	16.852765	H	0.807424	-4.256522	16.492715
Cu	0.204403	2.187049	19.988614	H	0.868800	-2.506818	16.235023
H	8.891071	3.392424	20.913367	H	-0.568359	-2.755888	18.132146
H	-4.673317	2.104938	16.938341	H	-4.123776	-1.664377	19.227431
H	-5.531461	3.294705	21.032081	H	-4.317914	-0.482268	21.217197
H	-9.006488	-4.710142	17.956796	H	-3.814718	-0.736385	22.865580
H	-10.071118	-4.017669	23.050776	H	-4.551419	-3.129981	22.740597
H	0.595658	-7.919074	24.825696	H	-5.155896	-2.844801	21.109612
H	-7.746921	-3.426171	30.227401	H	5.263624	-1.815870	17.364536
O	2.030174	-0.536090	21.598964	H	1.661069	1.169304	22.297663
O	1.039593	0.515520	21.902754	H	5.271981	0.327617	16.191580

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C	0.705000	7.351000	24.202000	C	-1.865096	2.072114	22.208400
C	1.518954	6.276116	23.553620	N	-1.367903	2.713480	21.153790
O	2.138068	5.428190	24.225783	H	-4.810253	4.894145	20.768572
H	1.311022	7.834445	24.975465	H	-5.189727	4.358494	22.419446
H	-0.156136	6.887483	24.697609	H	-3.706782	2.160156	23.239240
H	0.342794	8.104203	23.498066	H	-2.223119	4.235251	19.888163
N	1.533094	6.270513	22.208857	H	-1.357830	1.316350	22.780620
C	2.316391	5.316121	21.454396	C	-8.631395	-3.722521	17.665922
C	1.791064	5.102952	20.031170	C	-8.361754	-2.871536	18.869918
C	2.554054	3.960511	19.456814	O	-8.652972	-1.682378	18.952586
N	2.134026	2.641142	19.555015	O	-7.745847	-3.554068	19.844851
C	3.850969	3.970096	19.040185	H	-7.685860	-3.874266	17.130355
C	3.170585	1.881853	19.218878	H	-9.339172	-3.222105	17.002968
N	4.239658	2.653069	18.906245	C	-10.873287	-3.422220	22.603538
H	1.104722	7.048584	21.717413	C	-10.839774	-2.039922	23.134920
H	2.297849	4.369674	21.999767	N	-9.683854	-1.284782	23.160584
H	0.717748	4.893556	20.051212	C	-11.817905	-1.252594	23.671785
H	1.937287	6.005375	19.426813	C	-9.937476	-0.092509	23.688763
H	4.533972	4.781838	18.848124	N	-11.228248	-0.058165	24.002317
H	3.188729	0.806043	19.201759	H	-10.739076	-3.426090	21.516430
H	3.363319	5.643337	21.405699	H	-11.832578	-3.889200	22.837854
C	9.007847	3.468551	19.826162	H	-8.732372	-1.612284	22.818059
C	7.946329	2.685645	19.106739	H	-12.866636	-1.438492	23.844134
C	8.258258	1.722442	18.143721	H	-9.229627	0.702773	23.849287
C	6.597635	2.923076	19.362829	C	-0.049243	-7.217256	24.270829
C	7.261723	1.033352	17.463582	C	0.690249	-6.151271	23.536570
C	5.590419	2.261259	18.664361	N	1.704796	-6.404492	22.640917
C	5.917361	1.300881	17.702592	C	0.507337	-4.791937	23.470105
O	4.909335	0.654098	17.042872	C	2.103846	-5.253112	22.077853
H	8.937640	4.531561	19.562856	N	1.389006	-4.240690	22.555914
H	10.006925	3.115643	19.556454	H	-0.643103	-7.811203	23.564343
H	9.297659	1.499847	17.916894	H	-0.737269	-6.753071	24.982079
H	6.311978	3.651199	20.114864	H	2.102694	-7.316248	22.429506
H	7.527317	0.282827	16.722086	H	-0.199569	-4.193333	24.018907
H	-11.697365	0.737559	24.428803	H	2.891774	-5.200835	21.349375
C	-3.913542	1.832578	16.195900	C	-7.104979	-3.018824	29.454124
C	-2.567610	1.853591	16.821450	N	-5.975431	-2.406982	30.124800
N	-1.388162	1.970093	16.120109	C	-5.153834	-1.520335	29.565831
C	-2.182308	1.790158	18.130669	N	-5.302578	-1.160135	28.296263
C	-0.358910	1.999114	16.984192	N	-4.141323	-1.019639	30.289364
N	-0.811583	1.889851	18.227149	H	-6.792799	-3.818564	28.773300
H	-4.154194	0.840933	15.794121	H	-7.675918	-2.264198	28.910723
H	-3.966702	2.554714	15.373927	H	-5.687032	-2.800340	31.014937
H	-1.298542	2.039456	15.110169	H	-6.015529	-1.571090	27.697576
H	-2.805286	1.688868	19.001072	H	-4.831562	-0.319910	27.943299
H	0.670250	2.111183	16.684029	H	-4.222999	-1.037681	31.300398
C	-4.823769	4.032538	21.440861	H	-3.577846	-0.261003	29.884618
C	-3.463171	3.446256	21.533361	Fe	1.603433	-2.221234	21.995236
N	-3.114508	2.489487	22.462620	C	-1.321764	-1.499669	23.572092
C	-2.355859	3.587752	20.741051	C	-0.031530	-2.653057	19.062944

C	4.578930	-2.926504	20.419489	O	-7.986905	1.116709	20.196595
C	3.308924	-1.686225	24.886232	H	-7.580645	1.463079	19.377536
N	1.083251	-1.726398	23.861273	H	-8.119043	0.171299	19.980930
C	-0.174365	-1.466323	24.336413	O	-7.358544	-1.889209	26.127698
C	-0.127667	-1.129445	25.738511	H	-7.003115	-1.624491	25.243443
C	1.195146	-1.161723	26.098765	H	-7.494394	-2.851820	26.033013
C	1.930408	-1.541463	24.915888	O	2.116617	3.934755	28.242847
C	1.800970	-0.864682	27.425574	H	1.769667	3.648575	27.367308
O	-2.838072	-2.364085	17.843230	H	1.353697	3.804474	28.837698
C	-1.297221	-0.804228	26.605651	O	-7.318788	3.035351	25.128921
C	-1.617283	0.704290	26.673082	H	-6.506549	2.510643	24.945228
C	-2.747216	0.948827	27.667290	H	-7.648128	3.271373	24.240714
O	-2.462095	0.896547	28.890574	O	-4.879788	1.449149	24.612913
O	-3.928964	1.126702	27.204212	H	-4.476267	1.301029	25.511504
N	2.159741	-2.774090	20.131787	H	-5.257602	0.583285	24.352173
C	1.329715	-2.875139	19.051749	O	-5.785797	2.568460	29.013136
C	2.078659	-3.204924	17.858047	H	-5.135815	2.117079	28.426364
C	3.389138	-3.298849	18.239242	H	-5.733109	3.500619	28.722815
C	3.427437	-3.007086	19.659614	O	1.105325	3.172012	25.585055
C	1.469419	-3.381728	16.509948	H	1.477986	3.927627	25.073982
N	3.567496	-2.357289	22.562762	H	1.589543	2.398234	25.241866
C	4.645856	-2.605141	21.765230	H	-7.574887	-2.965333	20.653842
C	5.880189	-2.468051	22.505414	H	-1.887637	1.078797	25.682404
C	5.521321	-2.119354	23.785066	H	-0.729081	1.246312	27.011115
C	4.067179	-2.055281	23.795178	H	-1.090461	-1.160785	27.620781
C	7.242426	-2.687470	21.948815	H	-2.182548	-1.353209	26.263690
C	6.347794	-1.871901	24.954589	H	2.507100	-1.648170	27.725266
C	7.581350	-1.346221	24.971666	H	2.353790	0.084416	27.401759
N	-0.310552	-2.114999	21.430497	H	1.035169	-0.784805	28.201279
C	-0.787632	-2.288807	20.163009	H	-2.252420	-1.291553	24.079539
C	-2.202001	-2.009898	20.130937	H	3.836499	-1.467081	25.803502
C	-2.576294	-1.675808	21.421148	H	5.899311	-2.135203	25.912039
C	-1.386656	-1.764832	22.213654	H	8.105273	-1.218969	25.916330
C	-3.104035	-2.016960	18.993947	H	8.089722	-1.010908	24.073260
C	-3.918374	-1.237515	21.905061	H	7.940432	-2.971740	22.740558
C	-4.953343	-2.359851	22.066860	H	7.246589	-3.478823	21.193779
C	-6.251140	-1.854340	22.693833	H	7.626533	-1.771672	21.478448
O	-7.347351	-2.252019	22.166669	H	5.511997	-3.084612	19.903007
O	-6.178078	-1.112834	23.704249	H	4.188566	-3.590572	16.312354
C	4.549594	-3.640611	17.345553	H	4.328221	-5.781219	17.404636
O	5.644498	-2.706381	17.486031	H	5.504313	-5.157151	18.584361
C	5.113742	-5.036140	17.569023	H	2.229120	-3.521862	15.738494
H	5.924279	-5.215003	16.852765	H	0.807424	-4.256522	16.492715
Cu	0.204403	2.187049	19.988614	H	0.868800	-2.506818	16.235023
H	8.891071	3.392424	20.913367	H	-0.568359	-2.755888	18.132146
H	-4.673317	2.104938	16.938341	H	-4.123776	-1.664377	19.227431
H	-5.531461	3.294705	21.032081	H	-4.317914	-0.482268	21.217197
H	-9.006488	-4.710142	17.956796	H	-3.814718	-0.736385	22.865580
H	-10.071118	-4.017669	23.050776	H	-4.551419	-3.129981	22.740597
H	0.595658	-7.919074	24.825696	H	-5.155896	-2.844801	21.109612
H	-7.746921	-3.426171	30.227401	H	5.263624	-1.815870	17.364536
O	2.030174	-0.536090	21.598964	H	1.661069	1.169304	22.297663
O	1.039593	0.515520	21.902754	H	5.271981	0.327617	16.191580

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C	0.705000	7.351000	24.202000	C	-1.890746	2.076279	22.358396
C	1.507311	6.252938	23.568600	N	-1.341527	2.669935	21.309558
O	2.163644	5.443823	24.255017	H	-4.759987	4.855648	20.693497
H	1.301826	7.809993	24.995959	H	-5.178450	4.421999	22.362306
H	-0.186125	6.910522	24.664512	H	-3.785446	2.190061	23.290537
H	0.388759	8.117276	23.490082	H	-2.139145	4.136679	19.945779
N	1.464214	6.173659	22.226952	H	-1.411209	1.340787	22.979276
C	2.233494	5.185586	21.493293	C	-8.635309	-3.718328	17.673594
C	1.734516	4.971597	20.063357	C	-8.377951	-2.873842	18.885071
C	2.542930	3.863352	19.480053	O	-8.703045	-1.693714	18.983592
N	2.188768	2.529349	19.597455	O	-7.733288	-3.547381	19.846035
C	3.823406	3.939609	19.011843	H	-7.685842	-3.862357	17.142866
C	3.244048	1.824539	19.223777	H	-9.342397	-3.218299	17.009465
N	4.268052	2.641053	18.859524	C	-10.867308	-3.425211	22.589721
H	1.005659	6.918807	21.711774	C	-10.842469	-2.044030	23.124569
H	2.176786	4.242839	22.043197	N	-9.684319	-1.293729	23.175228
H	0.671168	4.716793	20.066108	C	-11.826386	-1.257386	23.651137
H	1.857886	5.887100	19.472126	C	-9.941449	-0.104663	23.708000
H	4.458205	4.783509	18.791648	N	-11.237137	-0.067797	24.000020
H	3.314337	0.750540	19.215910	H	-10.713881	-3.428885	21.505280
H	3.289215	5.486230	21.463843	H	-11.829453	-3.894486	22.807090
C	9.014875	3.518971	19.832608	H	-8.731797	-1.617809	22.827911
C	7.975281	2.729912	19.090535	H	-12.878384	-1.440521	23.805076
C	8.311802	1.731839	18.173945	H	-9.233979	0.687194	23.885512
C	6.620524	2.975730	19.308223	C	-0.040840	-7.228440	24.246297
C	7.329429	1.022374	17.492812	C	0.696646	-6.150400	23.523021
C	5.628557	2.287151	18.616961	N	1.694511	-6.392026	22.606746
C	5.980585	1.300449	17.690452	C	0.521183	-4.786962	23.480153
O	4.989641	0.632753	17.022679	C	2.082466	-5.225376	22.053942
H	8.914687	4.588482	19.613051	N	1.385309	-4.219701	22.560404
H	10.023985	3.202263	19.557463	H	-0.605931	-7.837110	23.528619
H	9.356473	1.496445	17.987250	H	-0.757392	-6.772798	24.934899
H	6.319831	3.725181	20.032975	H	2.084418	-7.301019	22.373118
H	7.610071	0.245069	16.786553	H	-0.171918	-4.193537	24.053290
H	-11.708652	0.726132	24.427192	H	2.856805	-5.161585	21.309820
C	-3.876227	1.840414	16.233394	C	-7.095342	-3.041842	29.451036
C	-2.551038	1.828374	16.909553	N	-5.956993	-2.440013	30.114206
N	-1.358573	1.998425	16.240616	C	-5.152934	-1.535132	29.558397
C	-2.184959	1.665719	18.218239	N	-5.321616	-1.160485	28.296575
C	-0.346012	1.954249	17.128646	N	-4.145600	-1.024151	30.281890
N	-0.815476	1.753860	18.351149	H	-6.796208	-3.854383	28.779867
H	-4.110908	0.860720	15.799252	H	-7.651005	-2.283753	28.897639
H	-3.887274	2.577937	15.423762	H	-5.648656	-2.849860	30.990073
H	5.278023	-1.820880	17.345483	H	-5.999421	-1.608876	27.683527
H	-2.822949	1.509949	19.070988	H	-4.856901	-0.317895	27.942755
H	0.687924	2.084652	16.852046	H	-4.229585	-1.040362	31.292836
C	-4.804656	4.030795	21.409661	H	-3.591278	-0.258366	29.876888
C	-3.455853	3.423808	21.564122	Fe	1.566271	-2.102717	21.963975
N	-3.155828	2.500420	22.541742	C	-1.357097	-1.478241	23.525756
C	-2.308635	3.527024	20.820370	C	-0.057546	-2.587564	19.007464

C	4.544339	-2.803392	20.394945	O	-7.863879	1.058017	20.205073
C	3.268934	-1.532022	24.855393	H	-7.537403	1.422430	19.360336
N	1.055521	-1.619025	23.819269	H	-8.062928	0.129293	19.971146
C	-0.214459	-1.409676	24.292744	O	-7.333673	-1.988311	26.133786
C	-0.181289	-1.087035	25.702622	H	-6.991135	-1.708526	25.249003
C	1.136923	-1.087229	26.069739	H	-7.409968	-2.958259	26.046852
C	1.889643	-1.423259	24.884242	O	1.993471	3.941143	28.201014
C	1.728385	-0.796156	27.407227	H	1.655488	3.655834	27.318945
O	-2.888923	-2.357999	17.798092	H	1.217921	3.820413	28.783178
C	-1.357845	-0.784376	26.570120	O	-7.427234	2.993488	25.103307
C	-1.668271	0.724072	26.665957	H	-6.607520	2.462992	24.960597
C	-2.789610	0.968333	27.666466	H	-7.694680	3.247364	24.201227
O	-2.499041	0.917620	28.888385	O	-5.025693	1.452057	24.668402
O	-3.975878	1.145123	27.211676	H	-4.585045	1.303675	25.549008
N	2.129631	-2.668051	20.088542	H	-5.355196	0.570821	24.394407
C	1.306601	-2.788972	19.001577	O	-5.843966	2.510417	28.941321
C	2.062205	-3.136201	17.818625	H	-5.171031	2.068744	28.369515
C	3.368797	-3.236099	18.214238	H	-5.798798	3.442746	28.652517
C	3.395222	-2.909595	19.629989	O	0.983876	3.230146	25.573474
C	1.468194	-3.327552	16.464729	H	1.405040	3.954225	25.054530
N	3.523667	-2.156251	22.516798	H	1.346647	2.416698	25.175542
C	4.604360	-2.446389	21.729269	H	-7.573126	-2.959699	20.662153
C	5.836176	-2.337064	22.478623	H	-1.938559	1.116964	25.682855
C	5.477933	-1.974384	23.755709	H	-0.773844	1.251809	27.010556
C	4.028693	-1.878890	23.755566	H	-1.158224	-1.163771	27.578730
C	7.196763	-2.609635	21.940391	H	-2.243793	-1.322042	26.211848
C	6.304895	-1.767590	24.933883	H	2.511391	-1.518214	27.662957
C	7.558434	-1.291912	24.968046	H	2.184606	0.202061	27.428946
N	-0.346921	-2.082304	21.378293	H	0.969929	-0.833081	28.192126
C	-0.821632	-2.245273	20.110882	H	-2.293485	-1.294904	24.032734
C	-2.241045	-1.980062	20.079448	H	3.794324	-1.320978	25.775872
C	-2.612948	-1.654046	21.373984	H	5.841159	-2.027455	25.884118
C	-1.420440	-1.739443	22.162769	H	8.078215	-1.199344	25.919556
C	-3.145495	-2.002625	18.951614	H	8.087928	-0.964165	24.080536
C	-3.956897	-1.230919	21.865596	H	7.876406	-2.908418	22.742560
C	-4.971335	-2.368011	22.053466	H	7.181618	-3.410956	21.195660
C	-6.266326	-1.870764	22.690819	H	7.618630	-1.714968	21.461734
O	-7.367607	-2.236877	22.151209	H	5.479984	-2.983586	19.889838
O	-6.188710	-1.158309	23.721970	H	4.178211	-3.617997	16.307024
C	4.529650	-3.633611	17.345604	H	4.266080	-5.766551	17.483534
O	5.645511	-2.718377	17.455630	H	5.439615	-5.119154	18.652806
C	5.063431	-5.029508	17.628260	H	2.238605	-3.437778	15.698542
H	5.879618	-5.253820	16.930534	H	0.832905	-4.222007	16.433834
Cu	0.272938	1.780886	20.182365	H	0.843489	-2.470261	16.187827
H	8.891071	3.392424	20.913367	H	-0.590150	-2.689613	18.074056
H	-4.673317	2.104938	16.938341	H	-4.167470	-1.657061	19.189119
H	-5.531461	3.294705	21.032081	H	-4.377209	-0.490990	21.173768
H	-9.006488	-4.710142	17.956796	H	-3.850387	-0.715049	22.818242
H	-10.071118	-4.017669	23.050776	H	-4.550232	-3.124410	22.731306
H	0.595658	-7.919074	24.825696	H	-5.178092	-2.866962	21.104096
H	-7.746921	-3.426171	30.227401	H	5.366761	0.306263	16.180519
O	1.863857	-0.346497	21.373117	H	-1.252621	2.145511	15.240545
O	0.852090	0.499649	21.675813				

Structure large 62 AF:

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C	0.705000	7.351000	24.202000	C	-1.886056	2.077334	22.352191
C	1.517466	6.254686	23.578737	N	-1.340289	2.656235	21.292641
O	2.176224	5.455193	24.274505	H	-4.752778	4.847035	20.666907
H	1.301758	7.833275	24.982376	H	-5.162403	4.437391	22.343909
H	-0.174391	6.903621	24.680575	H	-3.777207	2.206828	23.289075
H	0.367619	8.099732	23.480433	H	-2.138805	4.109713	19.915341
N	1.481104	6.165919	22.238694	H	-1.404578	1.350086	22.981160
C	2.253252	5.173086	21.513972	C	-8.634714	-3.720815	17.664556
C	1.765707	4.968985	20.075737	C	-8.376212	-2.868725	18.869890
C	2.572576	3.861338	19.487771	O	-8.693063	-1.684404	18.957261
N	2.210399	2.528677	19.592463	O	-7.740958	-3.538755	19.837895
C	3.853260	3.937686	19.019669	H	-7.685363	-3.869099	17.134659
C	3.262113	1.824480	19.211133	H	-9.341415	-3.225666	16.996786
N	4.291653	2.639152	18.854125	C	-10.870276	-3.424061	22.593923
H	1.012413	6.899857	21.716630	C	-10.844980	-2.041321	23.126700
H	2.184529	4.229441	22.059645	N	-9.689855	-1.286515	23.167728
H	0.701765	4.718661	20.070081	C	-11.828554	-1.257282	23.658741
H	1.897767	5.888394	19.494423	C	-9.948156	-0.097502	23.700022
H	4.491944	4.780148	18.806840	N	-11.242588	-0.064621	24.000449
H	3.329096	0.750629	19.191586	H	-10.724345	-3.427496	21.508320
H	3.310356	5.468381	21.495504	H	-11.830766	-3.893357	22.817163
C	9.039887	3.489617	19.833167	H	-8.736398	-1.608292	22.814971
C	7.997852	2.711786	19.082382	H	-12.879200	-1.443562	23.819548
C	8.329821	1.732935	18.143165	H	-9.241874	0.697032	23.873239
C	6.644434	2.955491	19.307301	C	-0.047214	-7.234923	24.247569
C	7.344455	1.035459	17.452860	C	0.685769	-6.162060	23.514263
C	5.649288	2.282369	18.604424	N	1.689698	-6.407441	22.603498
C	5.996304	1.309004	17.662221	C	0.505884	-4.800969	23.459147
O	4.999987	0.645561	16.996533	C	2.074428	-5.242415	22.044576
H	8.972275	4.556932	19.587226	N	1.370705	-4.236188	22.539551
H	10.047242	3.142706	19.586205	H	-0.618912	-7.848659	23.539451
H	9.373588	1.501566	17.946533	H	-0.757445	-6.774733	24.940125
H	6.345819	3.692764	20.045346	H	2.084105	-7.316865	22.379596
H	7.621826	0.269697	16.732123	H	-0.192239	-4.205335	24.024485
H	-11.716402	0.724940	24.430925	H	2.849451	-5.180064	21.301355
C	-3.886323	1.852901	16.216309	C	-7.099428	-3.039406	29.448573
C	-2.557664	1.817112	16.882977	N	-5.961626	-2.435493	30.110940
N	-1.366527	1.992883	16.213553	C	-5.156114	-1.533492	29.553477
C	-2.188079	1.624268	18.186366	N	-5.319737	-1.166455	28.288486
C	-0.351232	1.919733	17.097056	N	-4.148026	-1.021907	30.276616
N	-0.817904	1.697117	18.316604	H	-6.800287	-3.851005	28.776185
H	-4.131671	0.884829	15.761453	H	-7.658635	-2.281953	28.897603
H	-3.900799	2.609691	15.424469	H	-5.659797	-2.836538	30.993118
H	5.270329	-1.833279	17.330329	H	-6.009766	-1.603347	27.681320
H	-2.824842	1.459299	19.038999	H	-4.860567	-0.318851	27.937701
H	0.683085	2.045677	16.819218	H	-4.239249	-1.028855	31.287028
C	-4.797499	4.031532	21.393889	H	-3.596751	-0.253548	29.871483
C	-3.450950	3.419432	21.547338	Fe	1.564977	-2.083119	21.945382
N	-3.148862	2.507957	22.535439	C	-1.371756	-1.448686	23.531454
C	-2.307476	3.509384	20.796461	C	-0.061206	-2.593578	19.022786

C	4.545816	-2.816799	20.392194	O	-7.864648	1.068231	20.191534
C	3.257824	-1.547337	24.848902	H	-7.535531	1.435167	19.347882
N	1.040438	-1.603275	23.813846	H	-8.054924	0.138061	19.955065
C	-0.225892	-1.388052	24.294829	O	-7.347306	-1.960692	26.132513
C	-0.188655	-1.075912	25.706660	H	-7.005930	-1.682477	25.247163
C	1.129635	-1.088006	26.069282	H	-7.450824	-2.927166	26.037151
C	1.877882	-1.422659	24.876952	O	2.056146	3.884812	28.278636
C	1.727462	-0.809900	27.404698	H	1.705964	3.639872	27.389979
O	-2.894956	-2.422451	17.819454	H	1.258362	3.845761	28.844125
C	-1.363081	-0.774043	26.576595	O	-7.440758	3.014452	25.118109
C	-1.676724	0.734807	26.673260	H	-6.618944	2.492521	24.958088
C	-2.793935	0.975779	27.679270	H	-7.714367	3.288939	24.220443
O	-2.498045	0.918734	28.900477	O	-5.026984	1.469339	24.665692
O	-3.981296	1.155691	27.230729	H	-4.593327	1.321216	25.548451
N	2.133762	-2.653844	20.086743	H	-5.356719	0.589126	24.388819
C	1.303941	-2.786996	19.007669	O	-5.789946	2.525235	29.020670
C	2.056024	-3.150094	17.824465	H	-5.139410	2.078845	28.424601
C	3.363738	-3.246099	18.214182	H	-5.794659	3.446218	28.682791
C	3.396858	-2.909220	19.626471	O	1.003362	3.269643	25.635294
C	1.454823	-3.358604	16.475996	H	1.420682	3.993550	25.112291
N	3.521999	-2.180268	22.515317	H	1.347528	2.454949	25.221920
C	4.604884	-2.467911	21.729797	H	-7.580001	-2.946243	20.649236
C	5.834839	-2.361875	22.482284	H	-1.952995	1.126311	25.690910
C	5.470952	-2.003630	23.758679	H	-0.782378	1.265094	27.012679
C	4.020543	-1.902747	23.753955	H	-1.161070	-1.152003	27.585259
C	7.196801	-2.625680	21.943384	H	-2.248941	-1.313274	26.221055
C	6.294892	-1.794000	24.937944	H	2.486638	-1.555995	27.666365
C	7.549981	-1.322664	24.975924	H	2.216192	0.173736	27.421848
N	-0.354438	-2.053161	21.389965	H	0.965625	-0.816714	28.188798
C	-0.825567	-2.241793	20.125586	H	-2.307209	-1.265131	24.038493
C	-2.247111	-1.993147	20.091463	H	3.782037	-1.343085	25.771732
C	-2.623443	-1.647989	21.379354	H	5.826477	-2.046619	25.889685
C	-1.432195	-1.712251	22.169663	H	8.066888	-1.225933	25.927896
C	-3.152704	-2.037138	18.962447	H	8.084134	-1.001754	24.085985
C	-3.969980	-1.223005	21.862291	H	7.876665	-2.928974	22.744096
C	-4.983248	-2.359271	22.058878	H	7.185959	-3.420452	21.191703
C	-6.281405	-1.857564	22.685551	H	7.615981	-1.725225	21.473030
O	-7.376619	-2.222952	22.145876	H	5.481378	-3.003814	19.888862
O	-6.204987	-1.135126	23.716774	H	4.168503	-3.632464	16.304519
C	4.521032	-3.645404	17.341914	H	4.262420	-5.779975	17.482392
O	5.638331	-2.730065	17.448453	H	5.435007	-5.129928	18.650773
C	5.059180	-5.042697	17.626825	H	2.222336	-3.465570	15.706574
H	5.874650	-5.264968	16.928304	H	0.831206	-4.261289	16.456841
Cu	0.249707	1.773242	20.169454	H	0.817935	-2.511456	16.197552
H	8.891071	3.392424	20.913367	H	-0.599366	-2.717439	18.095226
H	-4.673317	2.104938	16.938341	H	-4.172355	-1.680063	19.190311
H	-5.531461	3.294705	21.032081	H	-4.388814	-0.490455	21.161846
H	-9.006488	-4.710142	17.956796	H	-3.866758	-0.697281	22.809911
H	-10.071118	-4.017669	23.050776	H	-4.563297	-3.108660	22.744670
H	0.595658	-7.919074	24.825696	H	-5.188328	-2.867017	21.113501
H	-7.746921	-3.426171	30.227401	H	5.374692	0.321119	16.153093
O	1.834949	-0.346467	21.435885	H	-1.263592	2.164425	15.217275
O	0.966227	0.614055	21.762990				

Cartesian coordinates of the larger models in Table 2 (optimized with OLYP potential):

Structure **11₂_2H¹** (F):

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C	0.705000	7.351000	24.202000	N	-3.081870	2.681618	22.296817
C	1.591682	6.403096	23.446024	C	-2.407379	3.962321	20.668788
O	2.177545	5.471397	24.034855	C	-1.801842	2.383084	22.019717
H	1.297120	7.819415	24.994085	N	-1.356705	3.141818	21.026534
H	-0.095218	6.775043	24.677865	H	-5.009586	4.950550	20.663231
H	0.264531	8.126819	23.569901	H	-5.280354	4.463019	22.352046
N	1.718049	6.605961	22.121699	H	-3.631384	2.275678	23.061874
C	2.578380	5.785208	21.290431	H	-2.326471	4.673031	19.859876
C	2.033620	5.566418	19.869066	H	-1.244438	1.616166	22.528107
C	2.751246	4.401223	19.275846	C	-8.598698	-3.724355	17.702699
N	2.192433	3.131187	19.199650	C	-8.383546	-2.885259	18.928188
C	4.073772	4.311922	18.959109	O	-8.805955	-1.740105	19.057734
C	3.162180	2.304584	18.856258	O	-7.663699	-3.517230	19.865127
N	4.340297	2.977704	18.706840	H	-7.631090	-3.888480	17.213080
H	1.301715	7.440572	21.719233	H	-9.268308	-3.207487	17.013271
H	2.679364	4.823601	21.793942	C	-10.881149	-3.453585	22.582947
H	0.959785	5.361638	19.906131	C	-10.908675	-2.078796	23.128481
H	2.172430	6.466247	19.258567	N	-9.786003	-1.274296	23.188508
H	4.838020	5.067904	18.886204	C	-11.927335	-1.344263	23.661605
H	3.084951	1.242308	18.715731	C	-10.101423	-0.102384	23.734066
H	3.578500	6.233673	21.228053	N	-11.397175	-0.132624	24.023810
C	9.109795	3.273212	19.841044	H	-10.718930	-3.445088	21.499960
C	8.004472	2.565678	19.131938	H	-11.827761	-3.956898	22.792255
C	8.246237	1.414998	18.347451	H	-8.824141	-1.545645	22.861173
C	6.686699	3.043319	19.227760	H	-12.968930	-1.581950	23.814328
C	7.220970	0.766372	17.714960	H	-9.435076	0.723114	23.918891
C	5.636361	2.425859	18.584491	C	-0.095593	-7.282061	24.259330
C	5.852614	1.215696	17.795257	C	0.615096	-6.251253	23.461817
O	4.916948	0.598561	17.218950	N	1.462330	-6.551799	22.419449
H	9.224715	4.285869	19.429695	C	0.585868	-4.883041	23.502323
H	10.058385	2.743145	19.728688	C	1.909670	-5.416740	21.864022
H	9.261807	1.037952	18.255321	N	1.393393	-4.372661	22.502608
H	6.498136	3.911890	19.848098	H	-0.687824	-7.929566	23.602043
H	7.409415	-0.119359	17.114705	H	-0.773670	-6.795109	24.964485
C	-3.923970	1.687118	16.254077	H	1.716733	-7.485054	22.107163
C	-2.567910	1.817033	16.847511	H	0.037830	-4.253575	24.180849
N	-1.400926	1.814903	16.117191	H	2.584406	-5.394034	21.028023
C	-2.159508	1.977460	18.142198	C	-7.155447	-2.898188	29.483273
C	-0.357791	1.989536	16.948427	N	-6.045051	-2.271037	30.177124
N	-0.786854	2.094496	18.199984	C	-5.217634	-1.380857	29.625263
H	-4.176562	0.639069	16.052177	N	-5.382968	-0.979976	28.371527
H	-3.984975	2.237856	15.309087	N	-4.196966	-0.899996	30.348019
H	-1.328060	1.709699	15.108359	H	-6.810436	-3.611943	28.726860
H	-2.771091	2.022146	19.024949	H	-7.788839	-2.138229	29.020215
H	0.663828	2.047399	16.609760	H	-5.730273	-2.702316	31.040485
C	-4.909047	4.130380	21.377790	H	-6.050359	-1.417594	27.740185
C	-3.499838	3.678875	21.443288	H	-4.847132	-0.183598	28.009695

H	-4.257043	-0.931185	31.359661	H	0.595656	-7.919074	24.825695
H	-3.581124	-0.192514	29.931765	H	-7.746922	-3.426171	30.227401
Fe	1.707292	-2.388360	22.010017	O	1.977227	-0.632320	21.578356
C	-1.214012	-1.540064	23.554265	O	1.412059	2.012895	21.814030
C	0.030559	-2.841736	19.076295	O	-8.469059	1.116294	20.286278
C	4.662182	-3.024649	20.398702	H	-7.955730	1.512253	19.555256
C	3.394478	-1.934194	24.912696	H	-8.476855	0.166136	20.051886
N	1.190186	-1.850272	23.851821	O	-7.302592	-1.732258	26.132055
C	-0.064763	-1.530731	24.313417	H	-6.935748	-1.527240	25.235051
C	-0.014511	-1.194785	25.717913	H	-7.643231	-2.642940	26.040321
C	1.298990	-1.293744	26.095218	O	2.284698	3.681601	27.452882
C	2.030587	-1.711733	24.925355	H	1.854259	3.416615	26.613657
C	1.906921	-1.025154	27.426645	H	1.752023	3.226248	28.133693
O	-2.765305	-2.524450	17.852689	O	-6.750839	3.529677	25.203978
C	-1.180153	-0.840613	26.579814	H	-6.112495	2.816960	24.969364
C	-1.501142	0.668069	26.634780	H	-7.348269	3.572729	24.433107
C	-2.608246	0.922401	27.659822	O	-4.731035	1.491508	24.594534
O	-2.300613	0.809294	28.873861	H	-4.334340	1.341873	25.494519
O	-3.785043	1.181666	27.228548	H	-5.151665	0.639898	24.353078
N	2.242947	-2.891752	20.126209	O	-5.256548	2.846934	29.311168
C	1.396378	-3.024225	19.055370	H	-4.751023	2.330581	28.644645
C	2.140390	-3.327486	17.854615	H	-5.528189	3.644524	28.816514
C	3.462272	-3.361844	18.213621	O	1.051946	3.018729	24.617626
C	3.510410	-3.087220	19.635046	H	1.381735	3.930018	24.423421
C	1.519127	-3.542164	16.517725	H	0.121836	3.157815	24.877818
N	3.638702	-2.562362	22.571515	H	-7.529261	-2.923135	20.680905
C	4.719924	-2.782723	21.758451	H	-1.798445	1.031945	25.647578
C	5.948912	-2.697309	22.509815	H	-0.605756	1.216595	26.946377
C	5.589544	-2.407188	23.806742	H	-0.974670	-1.183922	27.598947
C	4.142382	-2.313476	23.816259	H	-2.069482	-1.389563	26.247511
C	7.310211	-2.902833	21.948437	H	2.502819	-1.878374	27.770592
C	6.413204	-2.234577	24.992030	H	2.573208	-0.154162	27.379249
C	7.660556	-1.744905	25.043721	H	1.142514	-0.821230	28.178709
N	-0.246155	-2.273622	21.434145	H	-2.131870	-1.277033	24.058314
C	-0.724824	-2.460502	20.173086	H	3.924887	-1.754447	25.836784
C	-2.131626	-2.143250	20.135279	H	5.948386	-2.528895	25.932303
C	-2.494674	-1.760107	21.416486	H	8.176483	-1.673701	25.998557
C	-1.301102	-1.856576	22.206599	H	8.188430	-1.383608	24.167077
C	-3.025312	-2.135289	18.990972	H	7.997156	-3.252436	22.723495
C	-3.826929	-1.271447	21.890163	H	7.306171	-3.640296	21.141214
C	-4.913385	-2.349658	22.043274	H	7.710008	-1.962784	21.543888
C	-6.195862	-1.806565	22.687791	H	5.599013	-3.146905	19.879433
O	-7.310504	-2.156521	22.171313	H	4.238785	-3.584490	16.267627
O	-6.078554	-1.083659	23.710450	H	4.484783	-5.785175	17.329159
C	4.622125	-3.635280	17.292580	H	5.668560	-5.132072	18.483448
O	5.672549	-2.656812	17.428621	H	2.270927	-3.706191	15.743831
C	5.245398	-5.011907	17.481243	H	0.857557	-4.416946	16.533328
H	6.041572	-5.150962	16.740532	H	0.916697	-2.675305	16.222102
Cu	0.284816	2.685210	19.898269	H	-0.506566	-2.964409	18.148294
H	8.891071	3.392423	20.913367	H	-4.027946	-1.727106	19.205297
H	-4.673317	2.104939	16.938340	H	-4.185830	-0.501352	21.195521
H	-5.531461	3.294706	21.032081	H	-3.713060	-0.775670	22.852540
H	-9.006489	-4.710140	17.956795	H	-4.540220	-3.143073	22.707161
H	-10.071119	-4.017668	23.050775	H	-5.136900	-2.816852	21.081898

H	5.271681	-1.778835	17.263368
H	1.198802	2.300422	22.728931
H	1.555789	1.032285	21.860234

H	2.407504	-0.648149	20.702275
H	-11.908971	0.633494	24.454781

11₂-2H² (F):

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C	0.705000	7.351000	24.202000
C	1.468291	6.306947	23.442870
O	1.958912	5.322359	24.031514
H	1.315766	7.679594	25.049782
H	-0.204972	6.892972	24.606394
H	0.429701	8.216307	23.594303
N	1.584990	6.487439	22.112403
C	2.375417	5.609911	21.269706
C	1.779288	5.377530	19.867779
C	2.500841	4.214923	19.270862
N	2.068145	2.905546	19.413204
C	3.782810	4.185443	18.803901
C	3.080560	2.114748	19.089891
N	4.152013	2.857566	18.707749
H	1.260910	7.367207	21.721013
H	2.462232	4.658545	21.795006
H	0.705237	5.181369	19.936228
H	1.901975	6.269686	19.243674
H	4.468386	4.981568	18.560989
H	3.090180	1.038710	19.141774
H	3.389129	6.016488	21.158220
C	8.892004	3.608944	19.838825
C	7.845286	2.795806	19.131859
C	8.171103	1.660833	18.385427
C	6.499853	3.143603	19.218993
C	7.192518	0.932215	17.724209
C	5.508169	2.420766	18.557370
C	5.854317	1.309577	17.780373
O	4.951724	0.538312	17.099150
H	8.700633	4.680234	19.716843
H	9.888974	3.387137	19.448303
H	9.207612	1.342885	18.305356
H	6.206169	3.990114	19.829582
H	7.462005	0.066438	17.126347
H	4.200952	1.093440	16.803231
C	-3.816681	1.683655	16.393864
C	-2.522186	1.934273	17.087753
N	-1.345625	2.180244	16.414029
C	-2.168634	1.951958	18.409162
C	-0.348115	2.354976	17.292297
N	-0.818151	2.222161	18.528809
H	-3.987228	0.607635	16.269941
H	-3.799424	2.137564	15.398151
H	-1.240206	2.232803	15.403611

H	-2.796561	1.794121	19.266701
H	0.665631	2.582067	17.010294
C	-4.913335	4.047876	21.542653
C	-3.534922	3.518322	21.664808
N	-3.212788	2.470806	22.499030
C	-2.401407	3.761687	20.938484
C	-1.948649	2.097399	22.258970
N	-1.422919	2.861270	21.307901
H	-4.914571	4.959502	20.940500
H	-5.355856	4.266116	22.518844
H	-3.825448	2.065447	23.229777
H	-2.246945	4.490089	20.157638
H	-1.454801	1.284227	22.760128
C	-8.647646	-3.704268	17.704669
C	-8.393895	-2.886553	18.935897
O	-8.733674	-1.714425	19.066936
O	-7.731059	-3.573077	19.876526
H	-7.698579	-3.820774	17.166312
H	-9.362859	-3.193293	17.057890
C	-10.869841	-3.428690	22.590735
C	-10.854337	-2.051636	23.135887
N	-9.697908	-1.299921	23.217070
C	-11.849292	-1.270175	23.648274
C	-9.968367	-0.113858	23.753080
N	-11.269707	-0.082115	24.017541
H	-10.714895	-3.423464	21.506606
H	-11.829444	-3.904733	22.804091
H	-8.744588	-1.619494	22.888184
H	-12.903419	-1.459162	23.779606
H	-9.267113	0.678410	23.951909
C	-0.083849	-7.351461	24.177968
C	0.631800	-6.292628	23.423359
N	1.598038	-6.557680	22.480537
C	0.523970	-4.927216	23.432440
C	2.032366	-5.397945	21.956500
N	1.397653	-4.378305	22.515011
H	-0.565238	-8.057792	23.491516
H	-0.857136	-6.897244	24.802669
H	1.937645	-7.477610	22.212668
H	-0.122785	-4.320635	24.043797
H	2.787533	-5.348029	21.192841
C	-7.120515	-2.976953	29.464455
N	-6.001002	-2.352233	30.142083
C	-5.182685	-1.466391	29.576212

N	-5.354590	-1.090499	28.316240	H	6.021150	-5.199567	16.876936
N	-4.155315	-0.974450	30.288596	Cu	0.245431	2.448503	20.258015
H	-6.791001	-3.747356	28.758735	H	8.891071	3.392424	20.913367
H	-7.714586	-2.222323	28.946212	H	-4.673317	2.104938	16.938341
H	-5.695163	-2.759364	31.020131	H	-5.531461	3.294705	21.032081
H	-6.040449	-1.531668	27.706653	H	-9.006488	-4.710142	17.956796
H	-4.842954	-0.284936	27.939344	H	-10.071118	-4.017669	23.050776
H	-4.232362	-0.982243	31.300420	H	0.595658	-7.919074	24.825696
H	-3.607531	-0.209092	29.880631	H	-7.746921	-3.426171	30.227401
Fe	1.675896	-2.273626	22.015246	O	1.869701	-0.666111	21.636056
C	-1.279347	-1.593710	23.587796	O	1.322690	1.914348	21.931070
C	0.022962	-2.703117	19.070505	O	-7.914311	1.073878	20.306400
C	4.628060	-2.963532	20.449065	H	-7.687823	1.478437	19.446053
C	3.342291	-1.759152	24.930281	H	-8.094997	0.143849	20.061960
N	1.126108	-1.837052	23.907222	O	-7.361145	-1.882764	26.154286
C	-0.135695	-1.552262	24.357325	H	-6.986563	-1.655536	25.267556
C	-0.096870	-1.173709	25.754342	H	-7.560605	-2.835860	26.077491
C	1.218612	-1.203122	26.127323	O	1.719544	4.393552	27.757360
C	1.964667	-1.618611	24.959852	H	1.547494	4.036532	26.864651
C	1.812336	-0.856410	27.448697	H	1.156072	3.835024	28.329880
O	-2.755684	-2.291649	17.823305	O	-7.343104	2.947049	25.022130
C	-1.272352	-0.812650	26.601892	H	-6.534272	2.411915	24.855385
C	-1.595393	0.697690	26.622102	H	-7.686473	3.130948	24.127735
C	-2.741943	0.967014	27.594216	O	-4.912291	1.333039	24.522244
O	-2.472956	0.976341	28.821509	H	-4.495597	1.212841	25.418673
O	-3.921023	1.097869	27.108008	H	-5.280558	0.454269	24.280353
N	2.214508	-2.847680	20.145094	O	-5.893292	2.654040	28.657672
C	1.384176	-2.923857	19.062712	H	-5.188920	2.177831	28.161502
C	2.140453	-3.228577	17.866168	H	-5.600911	3.586219	28.619492
C	3.450395	-3.321211	18.250393	O	0.933730	2.814677	24.468243
C	3.481330	-3.051248	19.677514	H	1.236045	3.748414	24.334791
C	1.538740	-3.386831	16.511809	H	0.024221	2.903909	24.808803
N	3.605129	-2.438932	22.605201	H	-7.570400	-2.997736	20.699103
C	4.685435	-2.659479	21.797691	H	-1.860333	1.040810	25.618483
C	5.915981	-2.506825	22.541618	H	-0.711228	1.250669	26.955798
C	5.552269	-2.172632	23.824419	H	-1.072582	-1.134194	27.630113
C	4.100239	-2.131348	23.838085	H	-2.157821	-1.370425	26.274569
C	7.281397	-2.695685	21.982446	H	2.639383	-1.524926	27.708395
C	6.377583	-1.921181	24.995922	H	2.205066	0.169656	27.440835
C	7.589779	-1.348686	25.017186	H	1.066450	-0.921468	28.245122
N	-0.284718	-2.228323	21.443738	H	-2.208527	-1.371516	24.092089
C	-0.745958	-2.358607	20.171809	H	3.875607	-1.520862	25.839331
C	-2.158862	-2.062745	20.135283	H	5.946561	-2.224824	25.949642
C	-2.539249	-1.755959	21.431971	H	8.116171	-1.223961	25.960776
C	-1.350402	-1.867270	22.227364	H	8.077127	-0.973026	24.122621
C	-3.043080	-2.011493	18.987655	H	7.992854	-2.937304	22.776100
C	-3.880447	-1.310132	21.918077	H	7.305766	-3.504990	21.246661
C	-4.938651	-2.415674	22.055626	H	7.630319	-1.779761	21.485771
C	-6.223374	-1.907259	22.710871	H	5.567363	-3.096139	19.936308
O	-7.333440	-2.280135	22.200861	H	4.246057	-3.627499	16.324234
O	-6.123383	-1.186466	23.736974	H	4.447851	-5.790119	17.466880
C	4.615189	-3.645783	17.355768	H	5.626311	-5.112768	18.612587
O	5.682125	-2.677700	17.469690	H	2.304623	-3.508975	15.743415
C	5.217528	-5.022531	17.601422	H	0.880592	-4.263787	16.474651

H	0.936886	-2.509674	16.247003
H	-0.503312	-2.782625	18.131448
H	-4.067621	-1.673652	19.222430
H	-4.266180	-0.535839	21.243736
H	-3.772598	-0.832198	22.889758
H	-4.547560	-3.212777	22.704170

H	-5.158552	-2.867949	21.086305
H	5.282667	-1.801196	17.303121
H	1.048621	2.191190	22.851852
H	1.480463	0.921753	21.938181
H	-11.757412	0.703779	24.441132

12_H₂O (F):

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C	0.705000	7.351000	24.202000
C	1.559115	6.364181	23.472315
O	2.105589	5.412670	24.062648
H	1.269780	7.744595	25.056134
H	-0.172652	6.829137	24.601823
H	0.368308	8.181146	23.577431
N	1.696497	6.556154	22.148342
C	2.484480	5.664634	21.321273
C	1.989661	5.576436	19.870699
C	2.684593	4.403342	19.269106
N	2.191771	3.115752	19.422599
C	3.966336	4.336267	18.806077
C	3.178058	2.294790	19.097367
N	4.284477	2.993955	18.706835
H	1.325060	7.408441	21.740688
H	2.424822	4.675631	21.778941
H	0.905675	5.425568	19.855788
H	2.215581	6.497041	19.320667
H	4.683221	5.104883	18.564009
H	3.150795	1.218791	19.152641
H	3.537408	5.977721	21.323464
C	9.046819	3.503146	19.835791
C	7.972784	2.765381	19.090773
C	8.246897	1.654713	18.290528
C	6.643228	3.161927	19.210514
C	7.230912	0.989016	17.617530
C	5.614812	2.507053	18.537147
C	5.908757	1.411377	17.716281
O	4.967967	0.703010	17.019210
H	9.017439	4.574296	19.603303
H	10.039709	3.119654	19.585578
H	9.269518	1.302657	18.181351
H	6.388992	3.995939	19.855843
H	7.457693	0.136648	16.983793
H	4.182219	1.267635	16.868241
C	-3.985539	1.750455	16.165776
C	-2.608159	1.808260	16.709595
N	-1.458008	1.782818	15.952645
C	-2.167593	1.930611	17.997411
C	-0.395468	1.906246	16.776118
N	-0.793879	2.002856	18.034021

H	-4.271339	0.731069	15.878790
H	-4.092905	2.396440	15.287141
H	-1.411231	1.705797	14.940535
H	-2.757284	1.985645	18.896814
H	0.623270	1.930838	16.421280
C	-4.896417	4.094992	21.443295
C	-3.473597	3.668915	21.461905
N	-2.983939	2.726879	22.337865
C	-2.416078	3.964802	20.641961
C	-1.693598	2.477724	22.027461
N	-1.313113	3.206037	20.987387
H	-5.012060	4.976768	20.807492
H	-5.259022	4.340416	22.446924
H	-3.505046	2.315834	23.115515
H	-2.394608	4.652094	19.808703
H	-1.080408	1.771690	22.561362
C	-8.657387	-3.701035	17.695366
C	-8.410974	-2.860146	18.913663
O	-8.783055	-1.697697	19.035293
O	-7.713417	-3.515679	19.853498
H	-7.708043	-3.813169	17.156511
H	-9.378763	-3.205577	17.043265
C	-10.844379	-3.399134	22.585230
C	-10.808866	-2.031616	23.152265
N	-9.646789	-1.287575	23.222569
C	-11.790782	-1.253323	23.695072
C	-9.902489	-0.109366	23.780971
N	-11.198913	-0.073485	24.070699
H	-10.666843	-3.380006	21.504656
H	-11.819564	-3.855346	22.770187
H	-8.690365	-1.603714	22.876050
H	-12.843963	-1.436324	23.842571
H	-9.193608	0.676562	23.978650
C	-0.113759	-7.355729	24.208159
C	0.585119	-6.307632	23.426442
N	1.502237	-6.591307	22.442705
C	0.530951	-4.939358	23.463299
C	1.962688	-5.437343	21.924551
N	1.390835	-4.406512	22.524953
H	-0.626844	-8.063463	23.546644
H	-0.855188	-6.894941	24.865706

H	1.797686	-7.518536	22.150569	C	-6.195786	-1.820144	22.728092
H	-0.070649	-4.320343	24.107414	O	-7.298081	-2.205837	22.202881
H	2.688594	-5.398399	21.132028	O	-6.110573	-1.094273	23.750662
C	-7.125870	-2.939081	29.483877	C	4.617281	-3.590149	17.361204
N	-6.017848	-2.321024	30.186255	O	5.664263	-2.600030	17.480132
C	-5.184183	-1.436961	29.636953	C	5.254036	-4.955492	17.582176
N	-5.345550	-1.043049	28.381983	H	6.063652	-5.098231	16.856673
N	-4.159098	-0.963965	30.359148	Cu	0.222324	2.743189	19.699320
H	-6.783373	-3.679495	28.752124	H	8.891071	3.392424	20.913367
H	-7.731401	-2.176073	28.990469	H	-4.673317	2.104938	16.938341
H	-5.714522	-2.752121	31.054839	H	-5.531461	3.294705	21.032081
H	-6.040618	-1.456790	27.763731	H	-9.006488	-4.710142	17.956796
H	-4.813610	-0.242564	28.016632	H	-10.071118	-4.017669	23.050776
H	-4.225086	-1.000083	31.371114	H	0.595658	-7.919074	24.825696
H	-3.574434	-0.220218	29.955290	H	-7.746921	-3.426171	30.227401
Fe	1.695869	-2.283512	22.041268	O	1.893251	-0.685248	21.667201
C	-1.235052	-1.529798	23.622418	O	2.088084	1.967536	22.950563
C	0.020254	-2.761021	19.123760	O	-8.174595	1.193534	20.315343
C	4.642207	-2.934773	20.459639	H	-7.694438	1.559294	19.545323
C	3.375140	-1.829682	24.972141	H	-8.261123	0.246404	20.084002
N	1.159659	-1.849845	23.944953	O	-7.345312	-1.736910	26.182789
C	-0.093961	-1.535282	24.396609	H	-6.970218	-1.530040	25.290494
C	-0.050789	-1.187780	25.801831	H	-7.590778	-2.679630	26.112460
C	1.260957	-1.262346	26.178340	O	1.953156	4.496527	28.233690
C	1.998894	-1.672831	25.003803	H	1.675015	4.077585	27.386683
C	1.863261	-0.960764	27.507278	H	1.427230	4.015030	28.901667
O	-2.805197	-2.461237	17.914729	O	-7.146928	3.038481	25.245396
C	-1.222097	-0.831969	26.657532	H	-6.347013	2.508876	25.017493
C	-1.526425	0.680316	26.726090	H	-7.506544	3.294621	24.372706
C	-2.663613	0.928735	27.712406	O	-4.777606	1.489457	24.628265
O	-2.388096	0.870479	28.938836	H	-4.378508	1.321561	25.523208
O	-3.841305	1.112729	27.242163	H	-5.157717	0.627935	24.358925
N	2.225287	-2.856914	20.174261	O	-5.703744	2.707724	28.960697
C	1.385983	-2.956071	19.101632	H	-5.055714	2.212082	28.411439
C	2.137159	-3.243187	17.897868	H	-5.548852	3.634295	28.704774
C	3.452833	-3.302780	18.268277	O	1.190197	3.303635	25.629770
C	3.490841	-3.034614	19.695649	H	1.410757	4.102748	25.090980
C	1.526318	-3.405957	16.547744	H	0.215900	3.303423	25.667835
N	3.628308	-2.449303	22.629361	H	-7.552784	-2.928232	20.663113
C	4.705899	-2.650789	21.812694	H	-1.785490	1.059662	25.733457
C	5.940792	-2.510775	22.553345	H	-0.633836	1.207681	27.077576
C	5.581733	-2.208121	23.844867	H	-1.030321	-1.189299	27.675360
C	4.129501	-2.170511	23.865918	H	-2.114480	-1.366246	26.310491
C	7.303660	-2.691305	21.984074	H	2.603107	-1.715511	27.795372
C	6.412523	-1.988268	25.018993	H	2.372507	0.012383	27.491238
C	7.628884	-1.425186	25.049995	H	1.098909	-0.923144	28.287320
N	-0.264367	-2.223254	21.486621	H	-2.155100	-1.265596	24.121511
C	-0.738352	-2.390487	20.224705	H	3.909541	-1.619526	25.886744
C	-2.146638	-2.072009	20.189176	H	5.982343	-2.310862	25.966641
C	-2.506023	-1.703491	21.474838	H	8.158141	-1.325082	25.994924
C	-1.315211	-1.815102	22.264775	H	8.115384	-1.031929	24.162953
C	-3.044866	-2.056428	19.054519	H	8.017963	-2.956565	22.767731
C	-3.839445	-1.231400	21.956635	H	7.320785	-3.482250	21.228335
C	-4.905566	-2.326827	22.087449	H	7.655683	-1.765662	21.508122

H	5.579458	-3.050140	19.938815
H	4.241208	-3.566162	16.332256
H	4.503965	-5.738990	17.429738
H	5.662071	-5.056030	18.592653
H	2.286701	-3.500391	15.769893
H	0.889529	-4.298382	16.507202
H	0.899634	-2.541959	16.298565
H	-0.515420	-2.863326	18.193262
H	-4.038460	-1.628102	19.273825

H	-4.206025	-0.450883	21.278443
H	-3.727582	-0.752285	22.927104
H	-4.522936	-3.124805	22.740258
H	-5.120212	-2.781881	21.118584
H	5.245625	-1.731511	17.319362
H	1.691981	2.096879	23.831984
H	1.900648	1.040818	22.708023
H	-11.669270	0.711736	24.514230

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C	0.705000	7.351000	24.202000
C	1.523937	6.338060	23.461516
O	2.079053	5.396316	24.062366
H	1.283953	7.711526	25.058802
H	-0.192822	6.858137	24.593197
H	0.400171	8.198328	23.583656
N	1.615935	6.490806	22.128694
C	2.411911	5.601270	21.305129
C	1.904072	5.477752	19.860150
C	2.615137	4.314398	19.258185
N	2.114241	3.025161	19.335994
C	3.915265	4.252672	18.849655
C	3.099016	2.210644	18.994169
N	4.226941	2.914063	18.699741
H	1.236959	7.335691	21.712178
H	2.392534	4.620516	21.781254
H	0.822172	5.312884	19.851346
H	2.103571	6.396345	19.297672
H	4.638507	5.030532	18.667641
H	3.063974	1.138068	18.941212
H	3.456112	5.939602	21.287672
C	8.969552	3.513225	19.822732
C	7.907868	2.716186	19.126779
C	8.191759	1.525657	18.433271
C	6.572580	3.124557	19.184160
C	7.189858	0.781962	17.847341
C	5.551207	2.406090	18.581950
C	5.805494	1.159552	17.890568
O	4.883912	0.451336	17.365622
H	8.859178	4.583002	19.610406
H	9.970588	3.197106	19.516349
H	9.221524	1.179639	18.368311
H	6.330107	4.023781	19.739310
H	7.431648	-0.138029	17.321967
H	2.416685	-0.595764	20.792577
C	-3.895956	1.670762	16.303047
C	-2.568568	1.833726	16.948650
N	-1.383257	1.908994	16.253818

C	-2.203768	1.944139	18.262501
C	-0.371239	2.073794	17.126137
N	-0.838882	2.100124	18.365855
H	-4.131335	0.613058	16.132842
H	-3.920584	2.182996	15.335984
H	-1.279024	1.858344	15.243801
H	-2.838252	1.930316	19.131199
H	0.657742	2.186002	16.826295
C	-4.948122	4.073587	21.542099
C	-3.544661	3.609223	21.645507
N	-3.164710	2.578189	22.474486
C	-2.430170	3.898743	20.905369
C	-1.881356	2.268915	22.214742
N	-1.400724	3.050081	21.256487
H	-5.001347	4.987761	20.945996
H	-5.393917	4.264220	22.523065
H	-3.750656	2.144337	23.200913
H	-2.321415	4.633699	20.121900
H	-1.347330	1.478099	22.712922
C	-8.657637	-3.703470	17.699725
C	-8.403985	-2.880596	18.927442
O	-8.759350	-1.713489	19.060198
O	-7.721564	-3.558940	19.860824
H	-7.710674	-3.814277	17.156582
H	-9.380736	-3.201276	17.055006
C	-10.852914	-3.403683	22.594222
C	-10.805806	-2.026324	23.137789
N	-9.636122	-1.294820	23.206739
C	-11.783274	-1.225441	23.653776
C	-9.880496	-0.102716	23.740516
N	-11.179909	-0.047183	24.013851
H	-10.697391	-3.402108	21.509981
H	-11.825514	-3.854296	22.805039
H	-8.686076	-1.631852	22.871262
H	-12.840324	-1.391000	23.794136
H	-9.162956	0.676476	23.936853
C	-0.087219	-7.327176	24.203022
C	0.627768	-6.273744	23.442413

N	1.568180	-6.547245	22.476047	C	-2.148747	-2.116264	20.169046
C	0.537766	-4.908318	23.459094	C	-2.516827	-1.777039	21.461995
C	2.006383	-5.396179	21.941050	C	-1.326556	-1.881505	22.250780
N	1.397188	-4.369869	22.519459	C	-3.047649	-2.083224	19.033246
H	-0.600114	-8.015496	23.519985	C	-3.853560	-1.320770	21.946256
H	-0.835959	-6.866863	24.853363	C	-4.910728	-2.425897	22.087348
H	1.881563	-7.472999	22.192138	C	-6.199939	-1.913598	22.725487
H	-0.089119	-4.293382	24.082932	O	-7.305878	-2.279899	22.198550
H	2.744584	-5.352039	21.161106	O	-6.110686	-1.193575	23.751960
C	-7.111136	-2.972902	29.475202	C	4.620465	-3.533985	17.314495
N	-5.987949	-2.369015	30.165303	O	5.676384	-2.568437	17.479011
C	-5.164017	-1.479118	29.611783	C	5.235556	-4.919656	17.472293
N	-5.341777	-1.076107	28.361557	H	6.038936	-5.044844	16.736624
N	-4.130202	-1.008683	30.328836	Cu	0.233974	2.607844	20.101748
H	-6.785998	-3.736545	28.759691	H	8.891071	3.392424	20.913367
H	-7.694815	-2.205213	28.964590	H	-4.673317	2.104938	16.938341
H	-5.675524	-2.805416	31.027076	H	-5.531461	3.294705	21.032081
H	-6.024817	-1.509402	27.743519	H	-9.006488	-4.710142	17.956796
H	-4.814054	-0.277442	27.989139	H	-10.071118	-4.017669	23.050776
H	-4.204155	-1.029844	31.340603	H	0.595658	-7.919074	24.825696
H	-3.574352	-0.245320	29.929752	H	-7.746921	-3.426171	30.227401
Fe	1.695491	-2.377775	22.044818	O	1.936374	-0.599637	21.641347
C	-1.248555	-1.588733	23.606883	O	1.447761	1.992156	22.071391
C	0.026624	-2.758479	19.098071	O	-8.059439	1.143841	20.259036
C	4.645255	-2.997650	20.436557	H	-7.694227	1.501429	19.427307
C	3.370948	-1.817685	24.930063	H	-8.192404	0.199003	20.044749
N	1.157423	-1.840521	23.900191	O	-7.342330	-1.861231	26.173387
C	-0.100225	-1.553838	24.366316	H	-6.971957	-1.636346	25.284420
C	-0.055187	-1.192130	25.769004	H	-7.503112	-2.822298	26.111724
C	1.259642	-1.236677	26.135473	O	1.938193	4.062619	27.736407
C	1.997660	-1.649026	24.958632	H	1.630044	3.691162	26.882762
C	1.864392	-0.902331	27.455068	H	1.222481	3.820261	28.354183
O	-2.792933	-2.414860	17.874047	O	-7.470136	2.704099	24.985898
C	-1.227752	-0.838009	26.624327	H	-6.599116	2.271360	24.851155
C	-1.562420	0.669701	26.645378	H	-7.671508	3.108234	24.127769
C	-2.698817	0.939547	27.628811	O	-4.898649	1.346771	24.562726
O	-2.418969	0.947212	28.854060	H	-4.469959	1.213857	25.450089
O	-3.881719	1.077973	27.153183	H	-5.239491	0.463102	24.305436
N	2.232015	-2.849651	20.155864	O	-5.863588	2.633933	28.684221
C	1.392100	-2.941730	19.076978	H	-5.159122	2.153541	28.190118
C	2.140600	-3.214160	17.867983	H	-5.542277	3.553187	28.698386
C	3.456061	-3.281603	18.233529	O	1.003036	3.005120	24.942888
C	3.496780	-3.047316	19.666632	H	1.292208	3.897937	24.635853
C	1.522078	-3.361227	16.519425	H	0.052680	3.115988	25.133188
N	3.622709	-2.507457	22.604267	H	-7.551035	-2.982817	20.679416
C	4.703840	-2.730138	21.793488	H	-1.837000	1.008505	25.642773
C	5.933925	-2.585586	22.532366	H	-0.677084	1.226651	26.968272
C	5.574243	-2.249473	23.817929	H	-1.020215	-1.157430	27.651790
C	4.123960	-2.201839	23.836419	H	-2.111584	-1.402137	26.302308
C	7.297647	-2.775948	21.967848	H	2.660053	-1.602287	27.726017
C	6.406381	-1.986868	24.981616	H	2.302104	0.103962	27.436383
C	7.619127	-1.414764	24.988027	H	1.115851	-0.922749	28.249901
N	-0.265110	-2.265811	21.470729	H	-2.173263	-1.355411	24.113369
C	-0.737962	-2.417438	20.204073	H	3.906776	-1.594257	25.841448

H	5.979919	-2.276084	25.941770	H	0.909854	-2.485962	16.272618
H	8.150065	-1.273892	25.926934	H	-0.505259	-2.853011	18.163948
H	8.100333	-1.051342	24.085420	H	-4.058809	-1.709898	19.273736
H	8.009225	-3.034465	22.755927	H	-4.233892	-0.546358	21.268076
H	7.314131	-3.574148	21.219955	H	-3.743795	-0.838401	22.915581
H	7.653019	-1.855736	21.484053	H	-4.522914	-3.213562	22.749459
H	5.583541	-3.122995	19.920075	H	-5.122337	-2.892832	21.122932
H	4.241597	-3.459726	16.288339	H	5.282455	-1.670878	17.405507
H	4.473322	-5.685919	17.293788	H	1.152388	2.203681	22.980120
H	5.648700	-5.066539	18.475243	H	1.566637	1.002309	22.042875
H	2.275524	-3.470712	15.737006	H	-11.645287	0.750765	24.439995
H	0.869888	-4.242658	16.481885				

14_H₂O (F):

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C	0.705000	7.351000	24.202000	C	-3.876411	1.594770	16.389568
C	1.460106	6.296620	23.449216	C	-2.568775	1.819478	17.057732
O	2.003886	5.343284	24.041359	N	-1.377355	1.932218	16.378883
H	1.259236	7.598488	25.112017	C	-2.225100	1.940765	18.376943
H	-0.267041	6.939982	24.500963	C	-0.381090	2.126046	17.262029
H	0.534423	8.257172	23.614560	N	-0.866055	2.136238	18.495668
N	1.505412	6.417815	22.109482	H	-4.118191	0.526342	16.340386
C	2.265643	5.489154	21.293526	H	-3.862070	1.986963	15.368056
C	1.802989	5.409726	19.832798	H	-1.261873	1.896336	15.369642
C	2.532363	4.255142	19.231053	H	-2.867623	1.908090	19.239887
N	2.087479	2.951575	19.377952	H	0.647601	2.268979	16.976487
C	3.813502	4.229442	18.762724	C	-4.982056	4.063338	21.591190
C	3.082633	2.166163	19.012410	C	-3.585924	3.594101	21.740677
N	4.169368	2.899589	18.637582	N	-3.241425	2.551262	22.569663
H	1.154711	7.272183	21.687189	C	-2.450125	3.875678	21.030298
H	2.174963	4.504762	21.755224	C	-1.956648	2.228552	22.336482
H	0.719825	5.260379	19.776122	N	-1.440835	3.013201	21.399949
H	2.037949	6.336932	19.298591	H	-5.012529	4.994302	21.019840
H	4.498747	5.027480	18.525666	H	-5.471831	4.220462	22.556213
H	3.093513	1.091359	19.001049	H	-3.854824	2.102060	23.267601
H	3.329575	5.761225	21.312068	H	-2.314228	4.616358	20.256464
C	8.884425	3.610030	19.832984	H	-1.447492	1.424284	22.838613
C	7.846710	2.787218	19.127110	C	-8.638643	-3.698249	17.745037
C	8.161956	1.576469	18.480805	C	-8.405287	-2.922135	19.008928
C	6.507341	3.179695	19.135385	O	-8.855759	-1.798690	19.213983
C	7.184720	0.804047	17.888153	O	-7.636218	-3.584064	19.881439
C	5.509745	2.425824	18.534841	H	-7.682887	-3.803011	17.217323
C	5.794796	1.165035	17.884514	H	-9.346994	-3.166711	17.107355
O	4.894686	0.429612	17.359606	C	-10.860738	-3.407235	22.596803
H	8.678720	4.680240	19.720642	C	-10.853538	-2.026406	23.148733
H	9.885854	3.404392	19.443532	N	-9.703401	-1.281103	23.258082
H	9.195489	1.238493	18.457245	C	-11.846467	-1.208126	23.632093
H	6.236441	4.092803	19.655468	C	-10.029655	-0.080032	23.789195
H	7.452048	-0.128464	17.399429	N	-11.328947	0.008599	24.032757
H	2.344770	-0.591865	20.710322	H	-10.694896	-3.403012	21.513073

H	-11.824899	-3.884630	22.792405	C	4.124302	-2.120346	23.809431
H	-8.763110	-1.600087	22.969788	C	7.308957	-2.641307	21.944903
H	-12.903609	-1.428350	23.717632	C	6.395823	-1.818775	24.952249
H	-9.295825	0.685816	23.991787	C	7.603067	-1.235176	24.960642
C	-0.063386	-7.353595	24.151831	N	-0.247487	-2.254869	21.423419
C	0.655629	-6.282543	23.413632	C	-0.705456	-2.362523	20.146099
N	1.610776	-6.541109	22.456256	C	-2.112514	-2.047633	20.103051
C	0.549717	-4.916528	23.434819	C	-2.494614	-1.750657	21.401801
C	2.040828	-5.382943	21.931574	C	-1.315499	-1.886119	22.201845
N	1.414438	-4.364717	22.507320	C	-2.998350	-1.973575	18.958297
H	-0.509835	-8.065569	23.447587	C	-3.839982	-1.330329	21.889071
H	-0.866515	-6.912784	24.747759	C	-4.846235	-2.480499	22.041321
H	1.942575	-7.460006	22.175901	C	-6.133896	-2.035191	22.736135
H	-0.092332	-4.311132	24.051549	O	-7.242298	-2.398041	22.229162
H	2.785655	-5.328181	21.158406	O	-6.019498	-1.365153	23.799002
C	-7.101527	-3.009732	29.463389	C	4.661525	-3.580568	17.324726
N	-5.956886	-2.429406	30.135967	O	5.718902	-2.609778	17.457405
C	-5.151897	-1.520275	29.588038	C	5.267372	-4.962169	17.544106
N	-5.353281	-1.098467	28.348235	H	6.068484	-5.129048	16.814368
N	-4.115327	-1.048913	30.300921	Cu	0.202159	2.490010	20.234896
H	-6.805792	-3.795260	28.759619	H	8.891071	3.392424	20.913367
H	-7.664830	-2.233530	28.943528	H	-4.673317	2.104938	16.938341
H	-5.638056	-2.868575	30.993747	H	-5.531461	3.294705	21.032081
H	-6.012625	-1.554619	27.719194	H	-9.006488	-4.710142	17.956796
H	-4.836947	-0.290980	27.979943	H	-10.071118	-4.017669	23.050776
H	-4.179235	-1.081831	31.313037	H	0.595658	-7.919074	24.825696
H	-3.568256	-0.278615	29.903114	H	-7.746921	-3.426171	30.227401
Fe	1.695059	-2.369320	22.016712	O	1.944958	-0.589272	21.598703
C	-1.252571	-1.612682	23.562079	O	1.323489	1.897392	22.034297
C	0.068082	-2.685783	19.042254	O	-8.046756	1.066540	20.200612
C	4.664918	-2.993393	20.433524	H	-7.741880	1.349555	19.316940
C	3.367060	-1.714582	24.891471	H	-8.238091	0.116510	20.064407
N	1.155217	-1.818382	23.869318	O	-7.290229	-1.991896	26.180162
C	-0.109733	-1.553772	24.328814	H	-6.918858	-1.783009	25.284422
C	-0.075794	-1.158307	25.721356	H	-7.429951	-2.957816	26.147732
C	1.240979	-1.153221	26.087193	O	1.639146	4.208581	27.819774
C	1.990082	-1.577010	24.921830	H	1.380385	3.792107	26.969990
C	1.821425	-0.756914	27.401448	H	1.055684	3.764799	28.468238
O	-2.732902	-2.273386	17.792907	O	-7.408589	2.908660	24.855352
C	-1.255574	-0.820945	26.575067	H	-6.609317	2.342082	24.761709
C	-1.617294	0.680615	26.602518	H	-7.731504	3.001815	23.939068
C	-2.749108	0.930364	27.596708	O	-4.981570	1.254419	24.546194
O	-2.459360	0.938993	28.819715	H	-4.549612	1.150451	25.434705
O	-3.937138	1.053264	27.130223	H	-5.293770	0.355318	24.300465
N	2.254126	-2.838441	20.132447	O	-6.066096	2.613322	28.408192
C	1.428892	-2.899658	19.039106	H	-5.300363	2.122776	28.029633
C	2.188084	-3.177204	17.838305	H	-5.684130	3.484489	28.631153
C	3.494254	-3.287394	18.224672	O	0.896516	2.987800	24.995886
C	3.521631	-3.055415	19.657950	H	1.193841	3.864910	24.653290
C	1.591205	-3.278375	16.475951	H	-0.065964	3.098573	25.120674
N	3.629357	-2.478279	22.588743	H	-7.488120	-3.039927	20.736350
C	4.715860	-2.692029	21.783544	H	-1.909694	1.016864	25.604713
C	5.943436	-2.490208	22.515053	H	-0.740782	1.254230	26.918378
C	5.575962	-2.128945	23.791220	H	-1.042625	-1.136423	27.602669

H	-2.129787	-1.399478	26.253122
H	2.774388	-1.255191	27.598877
H	2.000849	0.326370	27.434459
H	1.139758	-1.002433	28.221995
H	-2.184825	-1.391490	24.060903
H	3.903452	-1.442079	25.788420
H	5.961058	-2.085174	25.915342
H	8.117714	-1.066811	25.904075
H	8.098428	-0.891831	24.057625
H	8.041809	-2.824020	22.734446
H	7.358103	-3.473020	21.235481
H	7.610479	-1.728477	21.412247
H	5.605955	-3.118371	19.922617
H	4.288935	-3.548797	16.294116

H	4.497551	-5.728576	17.400997
H	5.679766	-5.069470	18.552253
H	2.359515	-3.385259	15.707655
H	0.917076	-4.140752	16.402643
H	1.006809	-2.380905	16.241064
H	-0.451768	-2.744312	18.098185
H	-4.009310	-1.600442	19.198749
H	-4.256510	-0.577326	21.209103
H	-3.742417	-0.837961	22.854946
H	-4.402357	-3.265787	22.670141
H	-5.069124	-2.931796	21.071653
H	5.318143	-1.714926	17.389046
H	1.007320	2.096089	22.938252
H	1.505222	0.905278	21.994968

14_H₂O (AF):

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C	0.705000	7.351000	24.202000
C	1.479104	6.307875	23.454570
O	2.023182	5.357306	24.050623
H	1.267246	7.631137	25.097950
H	-0.247274	6.914481	24.526718
H	0.495731	8.242256	23.604545
N	1.540962	6.440117	22.117088
C	2.310044	5.523140	21.297880
C	1.832531	5.432897	19.842281
C	2.551723	4.272900	19.242021
N	2.087913	2.973127	19.372541
C	3.838569	4.232980	18.792008
C	3.077616	2.176126	19.014592
N	4.178781	2.899660	18.661102
H	1.183937	7.293272	21.697709
H	2.239874	4.539078	21.763082
H	0.748082	5.285179	19.799766
H	2.061277	6.355962	19.298483
H	4.537422	5.022538	18.567970
H	3.073886	1.101581	18.999109
H	3.369563	5.813283	21.305024
C	8.904198	3.581297	19.828015
C	7.857416	2.764686	19.131662
C	8.164509	1.559679	18.468359
C	6.519030	3.161593	19.159654
C	7.180964	0.794485	17.882500
C	5.513619	2.416532	18.561072
C	5.791200	1.158955	17.902463
O	4.883834	0.427742	17.388139
H	8.722475	4.652503	19.685250
H	9.905286	3.343312	19.457087
H	9.198168	1.223480	18.425230
H	6.257890	4.071198	19.689660

H	7.438718	-0.133898	17.380341
H	2.449674	-0.575436	20.786462
C	-3.880744	1.610939	16.368196
C	-2.567601	1.824275	17.028644
N	-1.377405	1.917822	16.344521
C	-2.218090	1.953484	18.345128
C	-0.376441	2.109872	17.222628
N	-0.856992	2.135833	18.457746
H	-4.118664	0.543012	16.293954
H	-3.877916	2.029948	15.357090
H	-1.265904	1.867652	15.335539
H	-2.858720	1.932646	19.209360
H	0.652939	2.238861	16.932436
C	-4.968881	4.064806	21.576366
C	-3.570405	3.595454	21.710419
N	-3.213923	2.553117	22.535475
C	-2.441998	3.881328	20.990183
C	-1.930696	2.233462	22.291060
N	-1.426791	3.019522	21.348626
H	-5.005261	4.991315	20.998262
H	-5.445364	4.232711	22.546509
H	-3.819833	2.105486	23.240263
H	-2.315400	4.623001	20.215716
H	-1.412446	1.433578	22.790731
C	-8.637796	-3.700646	17.737474
C	-8.398923	-2.912933	18.993782
O	-8.824158	-1.775658	19.177281
O	-7.654755	-3.579116	19.883664
H	-7.684224	-3.810970	17.206631
H	-9.345932	-3.172398	17.096765
C	-10.870342	-3.414835	22.603750
C	-10.871356	-2.032747	23.153207
N	-9.727486	-1.276371	23.253313

C	-11.868750	-1.222834	23.641504	N	3.632401	-2.480643	22.585582
C	-10.061933	-0.076825	23.782846	C	4.718761	-2.701983	21.781793
N	-11.360421	0.000413	24.034730	C	5.945822	-2.517771	22.518223
H	-10.714508	-3.411391	21.518449	C	5.577607	-2.163819	23.796487
H	-11.828247	-3.900705	22.809170	C	4.126327	-2.142257	23.811589
H	-8.785794	-1.586494	22.959222	C	7.313020	-2.679885	21.953688
H	-12.922952	-1.453643	23.735466	C	6.400307	-1.866055	24.958516
H	-9.334896	0.697587	23.977039	C	7.603013	-1.273515	24.964844
C	-0.069459	-7.340549	24.170322	N	-0.249974	-2.260526	21.438145
C	0.652606	-6.279802	23.421033	C	-0.709455	-2.378456	20.163031
N	1.601585	-6.547315	22.459957	C	-2.118703	-2.071385	20.119122
C	0.556139	-4.913518	23.439048	C	-2.500767	-1.766602	21.416126
C	2.038621	-5.392047	21.932740	C	-1.319050	-1.892667	22.215013
N	1.421365	-4.368802	22.508756	C	-3.002707	-2.006374	18.973381
H	-0.546711	-8.041653	23.475241	C	-3.845517	-1.340549	21.900994
H	-0.849107	-6.886367	24.787193	C	-4.864966	-2.480217	22.046099
H	1.925454	-7.469115	22.179846	C	-6.151484	-2.018723	22.732786
H	-0.077577	-4.303097	24.059136	O	-7.261493	-2.366052	22.216585
H	2.780349	-5.343025	21.155950	O	-6.034875	-1.351113	23.796393
C	-7.103930	-2.997355	29.468558	C	4.651875	-3.575772	17.314810
N	-5.968258	-2.408142	30.149028	O	5.706834	-2.601387	17.445895
C	-5.156521	-1.506987	29.597334	C	5.268639	-4.954115	17.520910
N	-5.350438	-1.092699	28.354325	H	6.072146	-5.105837	16.790401
N	-4.120071	-1.035827	30.312431	Cu	0.212281	2.546617	20.191742
H	-6.796553	-3.775648	28.761632	H	8.891071	3.392424	20.913367
H	-7.673509	-2.224066	28.951012	H	-4.673317	2.104938	16.938341
H	-5.650362	-2.847789	31.007074	H	-5.531461	3.294705	21.032081
H	-6.008820	-1.551108	27.726273	H	-9.006488	-4.710142	17.956796
H	-4.825561	-0.292698	27.978890	H	-10.071118	-4.017669	23.050776
H	-4.196275	-1.054727	31.324123	H	0.595658	-7.919074	24.825696
H	-3.576823	-0.263215	29.915738	H	-7.746921	-3.426171	30.227401
Fe	1.704518	-2.370691	22.022283	O	1.934477	-0.582223	21.612133
C	-1.254006	-1.616041	23.574869	O	1.381267	1.954754	22.061485
C	0.062273	-2.704253	19.057923	O	-8.000671	1.070666	20.222509
C	4.665385	-2.998206	20.430140	H	-7.750134	1.371581	19.327319
C	3.367568	-1.747920	24.897902	H	-8.194236	0.122324	20.079193
N	1.153026	-1.830117	23.875758	O	-7.292848	-1.980285	26.175481
C	-0.108989	-1.562025	24.338984	H	-6.928558	-1.764232	25.278231
C	-0.071330	-1.176936	25.735238	H	-7.438797	-2.945056	26.130816
C	1.245205	-1.184245	26.099497	O	1.722284	4.170585	27.798303
C	1.990879	-1.603186	24.928956	H	1.451711	3.768344	26.946826
C	1.834989	-0.799313	27.413086	H	1.097780	3.775037	28.438502
O	-2.733179	-2.307367	17.808884	O	-7.384261	2.935166	24.927143
C	-1.248509	-0.832618	26.589489	H	-6.591581	2.364884	24.806671
C	-1.596976	0.672311	26.612081	H	-7.730784	3.040834	24.021178
C	-2.733642	0.934928	27.596856	O	-4.944593	1.278421	24.536268
O	-2.450362	0.965487	28.820921	H	-4.522004	1.160284	25.428763
O	-3.919953	1.044512	27.122249	H	-5.282234	0.388129	24.292510
N	2.253995	-2.842588	20.135792	O	-6.028317	2.609749	28.491689
C	1.424337	-2.910779	19.048167	H	-5.282213	2.129283	28.066217
C	2.178579	-3.190203	17.843589	H	-5.663979	3.504143	28.635782
C	3.487706	-3.292373	18.222566	O	0.921566	2.978913	24.955135
C	3.520155	-3.057778	19.656339	H	1.216645	3.863239	24.635961
C	1.574075	-3.304379	16.485511	H	-0.031469	3.090338	25.118950

H	-7.502121	-3.025918	20.733484
H	-1.878699	1.006888	25.610579
H	-0.716259	1.237544	26.931560
H	-1.037690	-1.150373	27.617015
H	-2.127166	-1.404353	26.267594
H	2.747633	-1.360444	27.634724
H	2.093001	0.268682	27.422348
H	1.128086	-0.974735	28.229399
H	-2.184863	-1.393501	24.075696
H	3.903822	-1.494832	25.801121
H	5.973237	-2.148309	25.920697
H	8.125168	-1.111387	25.905217
H	8.085839	-0.915832	24.060638
H	8.036223	-2.896246	22.744068
H	7.352812	-3.494376	21.224281
H	7.636343	-1.760033	21.446798

H	5.605606	-3.127834	19.918817
H	4.273442	-3.538343	16.286472
H	4.506076	-5.725938	17.369275
H	5.681457	-5.067180	18.528172
H	2.338033	-3.405643	15.712025
H	0.910278	-4.175562	16.420321
H	0.976343	-2.416101	16.249780
H	-0.462939	-2.773891	18.117560
H	-4.016809	-1.639428	19.210726
H	-4.253433	-0.580661	21.223383
H	-3.746954	-0.853845	22.869577
H	-4.434622	-3.270685	22.677550
H	-5.087709	-2.928654	21.075031
H	5.302185	-1.708130	17.383932
H	1.070987	2.153213	22.968627
H	1.534898	0.963854	22.019809

1_H₂O (F):

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C	0.705000	7.351000	24.202000
C	1.533942	6.346130	23.463410
O	2.086256	5.402201	24.063125
H	1.282984	7.724783	25.053912
H	-0.184154	6.848109	24.600060
H	0.386757	8.190930	23.579611
N	1.639897	6.510976	22.132866
C	2.438220	5.625778	21.306888
C	1.914552	5.480656	19.870371
C	2.622675	4.313956	19.269720
N	2.119377	3.023535	19.333320
C	3.924001	4.253255	18.864735
C	3.102471	2.212261	18.980791
N	4.234267	2.915934	18.698754
H	1.258304	7.356252	21.719349
H	2.435544	4.649209	21.792288
H	0.833247	5.311942	19.875917
H	2.103166	6.393711	19.294227
H	4.650050	5.031526	18.696444
H	3.067054	1.140422	18.916680
H	3.477588	5.978518	21.275193
C	8.983464	3.497698	19.822876
C	7.915345	2.711092	19.121402
C	8.194648	1.526202	18.416465
C	6.582778	3.120047	19.184394
C	7.189940	0.787385	17.828047
C	5.557576	2.406322	18.578103
C	5.806284	1.161152	17.884297
O	4.879578	0.449703	17.369315
H	8.899227	4.566591	19.593195

H	9.981432	3.157976	19.531824
H	9.223494	1.179042	18.343951
H	6.339898	4.013516	19.749259
H	7.430276	-0.129187	17.295952
H	2.374133	-0.591761	20.777080
C	-3.877696	1.693635	16.303343
C	-2.527813	1.882559	16.919082
N	-1.369929	1.955257	16.164802
C	-2.192997	1.986119	18.249232
C	-0.392810	2.112973	17.066842
N	-0.829643	2.136164	18.347274
H	-4.102605	0.631839	16.132351
H	-3.927366	2.197948	15.331100
H	-2.822762	1.948379	19.122386
H	0.652096	2.222638	16.809399
C	-4.944024	4.076167	21.534896
C	-3.538132	3.616448	21.631542
N	-3.149522	2.587874	22.460609
C	-2.430630	3.902926	20.880599
C	-1.869321	2.275935	22.187912
N	-1.398601	3.055001	21.223399
H	-5.002384	4.987731	20.934943
H	-5.383990	4.271324	22.517807
H	-3.729045	2.156649	23.191448
H	-2.329483	4.632625	20.091320
H	-1.331129	1.485310	22.681763
C	-8.658079	-3.702652	17.695938
C	-8.391292	-2.877421	18.919928
O	-8.740690	-1.708735	19.053013
O	-7.705282	-3.554959	19.850962

H	-7.717050	-3.813678	17.142519	C	1.389363	-2.940915	19.088221
H	-9.386812	-3.198907	17.058588	C	2.136835	-3.213394	17.877946
C	-10.850066	-3.399522	22.593430	C	3.452716	-3.270680	18.240690
C	-10.798122	-2.023958	23.141843	C	3.494256	-3.035147	19.674742
N	-9.624598	-1.298814	23.212806	C	1.515146	-3.367710	16.531418
C	-11.771479	-1.219141	23.660350	N	3.624148	-2.510203	22.614127
C	-9.862986	-0.106586	23.748433	C	4.704808	-2.729739	21.802255
N	-11.161858	-0.043760	24.022529	C	5.934761	-2.596619	22.543172
H	-10.691760	-3.394442	21.509625	C	5.575130	-2.270460	23.831819
H	-11.824368	-3.847998	22.800773	C	4.125382	-2.217499	23.849154
H	-8.676495	-1.637032	22.871439	C	7.298358	-2.788335	21.978304
H	-12.828891	-1.381540	23.800684	C	6.407498	-2.019639	24.998364
H	-9.140995	0.669002	23.943818	C	7.622260	-1.451827	25.011833
C	-0.090150	-7.323542	24.210188	N	-0.261929	-2.259022	21.480554
C	0.624968	-6.269283	23.448530	C	-0.738084	-2.417659	20.217136
N	1.562372	-6.543763	22.478963	C	-2.147888	-2.115331	20.183085
C	0.537477	-4.903248	23.468774	C	-2.512742	-1.765769	21.474070
C	2.000918	-5.391069	21.946531	C	-1.321160	-1.868772	22.260994
N	1.395169	-4.364995	22.528680	C	-3.044535	-2.092245	19.046117
H	-0.609598	-8.006725	23.527712	C	-3.850161	-1.308777	21.956827
H	-0.832366	-6.862717	24.866773	C	-4.907729	-2.414392	22.092952
H	1.873227	-7.468278	22.193434	C	-6.201484	-1.905697	22.724868
H	-0.087065	-4.289449	24.094422	O	-7.303761	-2.277164	22.193539
H	2.737117	-5.345393	21.164060	O	-6.121380	-1.184293	23.751335
C	-7.112514	-2.969429	29.475855	C	4.617417	-3.513669	17.319882
N	-5.993709	-2.359875	30.168104	O	5.669062	-2.544157	17.486727
C	-5.167409	-1.473129	29.612497	C	5.239356	-4.896995	17.472492
N	-5.342812	-1.075459	28.360264	H	6.044152	-5.016094	16.737298
N	-4.134461	-1.000073	30.328272	Cu	0.204837	2.592783	20.013690
H	-6.783078	-3.731186	28.760568	H	8.891071	3.392425	20.913369
H	-7.700021	-2.204714	28.965060	H	-4.673316	2.104937	16.938340
H	-5.684791	-2.789968	31.034138	H	-5.531461	3.294704	21.032080
H	-6.026056	-1.509525	27.743156	H	-9.006486	-4.710143	17.956795
H	-4.813147	-0.278423	27.986616	H	-10.071118	-4.017670	23.050774
H	-4.205672	-1.022037	31.340096	H	0.595661	-7.919074	24.825698
H	-3.574074	-0.239987	29.924830	H	-7.746923	-3.426172	30.227400
Fe	1.695832	-2.369164	22.055468	O	1.943309	-0.588259	21.651286
C	-1.240911	-1.573511	23.616859	O	1.423657	2.010226	22.039667
C	0.024048	-2.762093	19.110594	O	-8.095502	1.149735	20.250298
C	4.643978	-2.986985	20.442793	H	-7.685475	1.511830	19.440717
C	3.372822	-1.837367	24.945440	H	-8.192504	0.200576	20.034939
N	1.162388	-1.836161	23.911970	O	-7.348334	-1.844878	26.172655
C	-0.093600	-1.544107	24.377895	H	-6.972505	-1.622805	25.284558
C	-0.048828	-1.190982	25.783960	H	-7.517631	-2.804647	26.108404
C	1.263902	-1.249478	26.152488	O	1.985572	4.027082	27.757616
C	2.001266	-1.658397	24.973098	H	1.674323	3.668533	26.899464
C	1.871318	-0.932203	27.475324	H	1.240078	3.835238	28.360675
O	-2.797113	-2.472968	17.900359	O	-7.489762	2.677620	25.000305
C	-1.220552	-0.837653	26.640937	H	-6.609080	2.257352	24.862742
C	-1.556139	0.669887	26.668956	H	-7.648677	3.156723	24.164246
C	-2.693627	0.929274	27.652581	O	-4.904310	1.355683	24.584794
O	-2.419048	0.916914	28.879640	H	-4.478709	1.221865	25.472620
O	-3.875142	1.077491	27.176674	H	-5.244227	0.472312	24.325074
N	2.229751	-2.842081	20.166635	O	-5.816143	2.634183	28.724210

H	-5.120552	2.146999	28.223933	H	7.312107	-3.582521	21.225952
H	-5.524247	3.564659	28.659326	H	7.657603	-1.866932	21.499401
O	1.021189	3.010393	24.961472	H	5.581101	-3.109184	19.924088
H	1.301148	3.905180	24.651112	H	4.237270	-3.438542	16.294167
H	0.070739	3.115628	25.153527	H	4.480407	-5.665642	17.290336
H	-7.538318	-2.979158	20.670445	H	5.652091	-5.046216	18.475266
H	-1.830652	1.014155	25.668401	H	2.266848	-3.476243	15.747148
H	-0.671124	1.225695	26.994929	H	0.866424	-4.251972	16.498193
H	-1.013321	-1.160618	27.666995	H	0.898101	-2.496107	16.283371
H	-2.104859	-1.400121	26.317247	H	-0.511580	-2.860574	18.178628
H	2.631041	-1.668557	27.758566	H	-4.045573	-1.684109	19.271718
H	2.357727	0.052478	27.452163	H	-4.228145	-0.533436	21.278548
H	1.114693	-0.910249	28.263517	H	-3.742934	-0.828186	22.927364
H	-2.164727	-1.332109	24.121300	H	-4.522467	-3.202730	22.756057
H	3.909112	-1.625612	25.859789	H	-5.114977	-2.880965	21.127447
H	5.978817	-2.315221	25.956012	H	5.272220	-1.646485	17.419959
H	8.152955	-1.320899	25.952051	H	1.135565	2.225112	22.949250
H	8.106483	-1.083304	24.112352	H	1.551809	1.020790	22.021511
H	8.008911	-3.054485	22.765211	H	-11.623773	0.755277	24.450696

1_H₂O (AF):

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C	0.705000	7.351000	24.202000	O	4.876429	0.447442	17.367478
C	1.535317	6.346927	23.463929	H	8.904983	4.566771	19.592607
O	2.087023	5.402845	24.063893	H	9.983458	3.156337	19.534175
H	1.282664	7.726476	25.053542	H	9.222650	1.178598	18.343025
H	-0.183199	6.846839	24.600680	H	6.341213	4.012079	19.748590
H	0.385134	8.189819	23.579067	H	7.429372	-0.127937	17.293503
N	1.642161	6.512152	22.133479	H	2.373855	-0.590990	20.778348
C	2.440444	5.627180	21.307105	C	-3.876281	1.695702	16.303820
C	1.914775	5.480601	19.871316	C	-2.525986	1.885341	16.918807
C	2.621341	4.313117	19.269895	N	-1.368192	1.954857	16.163720
N	2.118030	3.022460	19.332227	C	-2.191188	1.990107	18.249604
C	3.922960	4.251314	18.865569	C	-0.391343	2.118083	17.063723
C	3.101787	2.210641	18.979012	N	-0.827241	2.137059	18.346241
N	4.233578	2.914105	18.699062	H	-4.100205	0.634082	16.130704
H	1.260259	7.357328	21.720019	H	-3.925162	2.200254	15.331585
H	2.439690	4.651066	21.793261	H	-2.820822	1.951864	19.122397
H	0.833353	5.313323	19.878206	H	0.652445	2.231181	16.804939
H	2.102955	6.393284	19.294465	C	-4.943235	4.076231	21.534205
H	4.649292	5.029745	18.698603	C	-3.537335	3.615927	21.628668
H	3.066530	1.138907	18.913157	N	-3.147878	2.587886	22.458293
H	3.479433	5.980914	21.273654	C	-2.430595	3.902116	20.876514
C	8.985112	3.497575	19.823219	C	-1.868683	2.274602	22.184608
C	7.916401	2.711431	19.120417	N	-1.398666	3.053344	21.218893
C	8.193835	1.526883	18.415305	H	-5.002426	4.987642	20.934196
C	6.584086	3.118718	19.183206	H	-5.381965	4.271390	22.517655
C	7.188281	0.788482	17.825982	H	-3.726464	2.158375	23.191050
C	5.557859	2.404103	18.577047	H	-2.329776	4.632738	20.088259
C	5.804374	1.159567	17.882286	H	-1.330450	1.484737	22.679149

C	-8.658066	-3.702510	17.695510	C	-2.693887	0.927860	27.653555
C	-8.390516	-2.877234	18.919264	O	-2.418933	0.911899	28.880505
O	-8.739176	-1.708322	19.052222	O	-3.875321	1.078012	27.177767
O	-7.705561	-3.555143	19.850886	N	2.229681	-2.841378	20.167378
H	-7.716943	-3.813539	17.142327	C	1.389321	-2.940313	19.089222
H	-9.386931	-3.198653	17.058280	C	2.136890	-3.212827	17.878589
C	-10.849806	-3.398967	22.593577	C	3.452780	-3.269598	18.241385
C	-10.797484	-2.023502	23.142204	C	3.494201	-3.034387	19.675393
N	-9.623796	-1.298702	23.213472	C	1.515216	-3.368293	16.532449
C	-11.770752	-1.218551	23.660618	N	3.624138	-2.509995	22.614350
C	-9.862023	-0.106390	23.749016	C	4.704779	-2.729819	21.802771
N	-11.160887	-0.043358	24.023234	C	5.934767	-2.597396	22.543803
H	-10.691634	-3.393426	21.509774	C	5.575110	-2.271684	23.832554
H	-11.824316	-3.847032	22.800858	C	4.125358	-2.218202	23.849642
H	-8.675779	-1.636966	22.871851	C	7.298344	-2.789354	21.979078
H	-12.828194	-1.380807	23.800673	C	6.407216	-2.021860	24.999575
H	-9.139796	0.668990	23.944394	C	7.622260	-1.454533	25.013748
C	-0.090557	-7.323179	24.210836	N	-0.262034	-2.258323	21.481806
C	0.624768	-6.268944	23.449154	C	-0.737992	-2.417454	20.218191
N	1.561798	-6.543687	22.479422	C	-2.147983	-2.115240	20.183831
C	0.537819	-4.902798	23.469620	C	-2.512690	-1.765179	21.474894
C	2.000672	-5.391215	21.946929	C	-1.321467	-1.867999	22.261951
N	1.395614	-4.364847	22.529263	C	-3.043947	-2.092913	19.046486
H	-0.610675	-8.006126	23.528630	C	-3.850079	-1.307903	21.957609
H	-0.832073	-6.862314	24.868140	C	-4.907516	-2.413650	22.093351
H	1.872335	-7.468311	22.193838	C	-6.201561	-1.905176	22.724922
H	-0.086528	-4.288643	24.095177	O	-7.303506	-2.277184	22.193611
H	2.736705	-5.345731	21.164263	O	-6.121500	-1.183368	23.751015
C	-7.112352	-2.969161	29.476117	C	4.617532	-3.512111	17.320344
N	-5.993835	-2.359425	30.168696	O	5.668864	-2.542476	17.487215
C	-5.167167	-1.473014	29.612940	C	5.239330	-4.895527	17.471986
N	-5.342315	-1.075806	28.360516	H	6.044141	-5.014359	16.736678
N	-4.134426	-0.999590	30.328729	Cu	0.205629	2.592396	20.012200
H	-6.782449	-3.730769	28.760895	H	8.891071	3.392425	20.913369
H	-7.699992	-2.204600	28.965226	H	-4.673316	2.104937	16.938340
H	-5.685447	-2.789261	31.035059	H	-5.531461	3.294704	21.032080
H	-6.026627	-1.508632	27.743708	H	-9.006486	-4.710143	17.956795
H	-4.812619	-0.278841	27.986929	H	-10.071118	-4.017670	23.050774
H	-4.205948	-1.021305	31.340530	H	0.595661	-7.919074	24.825698
H	-3.573786	-0.239727	29.924996	H	-7.746923	-3.426172	30.227400
Fe	1.695695	-2.368757	22.056140	O	1.942464	-0.587504	21.652233
C	-1.240985	-1.572504	23.617748	O	1.420842	2.011430	22.036690
C	0.024129	-2.761724	19.111692	O	-8.100949	1.150638	20.249692
C	4.643923	-2.986604	20.443384	H	-7.683765	1.511660	19.442899
C	3.372835	-1.838557	24.946150	H	-8.193391	0.200647	20.034454
N	1.162214	-1.836139	23.912839	O	-7.347832	-1.845247	26.173084
C	-0.093587	-1.543682	24.378855	H	-6.975377	-1.620769	25.284166
C	-0.048455	-1.190815	25.784713	H	-7.518903	-2.804580	26.108244
C	1.264126	-1.250143	26.153402	O	1.990160	4.023726	27.758304
C	2.001282	-1.659172	24.973873	H	1.678192	3.665423	26.900305
C	1.871769	-0.934090	27.476449	H	1.242572	3.837120	28.360655
O	-2.796292	-2.474683	17.901131	O	-7.493582	2.672801	25.000139
C	-1.220101	-0.837568	26.641906	H	-6.610703	2.256649	24.863449
C	-1.556137	0.669813	26.670053	H	-7.647893	3.159990	24.167257

O	-4.902673	1.356571	24.581748	H	8.107156	-1.085824	24.114996
H	-4.477177	1.222642	25.469876	H	8.008719	-3.056013	22.765887
H	-5.242703	0.473056	24.322886	H	7.311854	-3.583351	21.226428
O	-5.813245	2.634187	28.725663	H	7.657898	-1.867940	21.500413
H	-5.117321	2.146029	28.227157	H	5.581166	-3.108511	19.924383
H	-5.523972	3.564908	28.656868	H	4.237041	-3.436787	16.294573
O	1.022244	3.010369	24.959757	H	4.480623	-5.664430	17.289543
H	1.300157	3.906905	24.652436	H	5.652182	-5.045216	18.474762
H	0.072394	3.112984	25.155702	H	2.266814	-3.478961	15.748272
H	-7.539716	-2.979513	20.670680	H	0.866212	-4.252414	16.499811
H	-1.830612	1.014773	25.669754	H	0.898402	-2.496680	16.283453
H	-0.671452	1.225621	26.997065	H	-0.511639	-2.860364	18.179848
H	-1.012407	-1.160801	27.667804	H	-4.044992	-1.683814	19.271126
H	-2.104333	-1.400163	26.318181	H	-4.228028	-0.532374	21.279626
H	2.629041	-1.672821	27.760361	H	-3.742600	-0.827831	22.928373
H	2.361295	0.049098	27.453277	H	-4.522396	-3.201937	22.756517
H	1.114632	-0.909714	28.264090	H	-5.114413	-2.880257	21.127870
H	-2.164783	-1.330688	24.122301	H	5.272833	-1.643823	17.421588
H	3.909408	-1.627530	25.860355	H	1.134786	2.227217	22.946892
H	5.978247	-2.317859	25.956711	H	1.552211	1.021934	22.019275
H	8.152545	-1.324780	25.954619	H	-11.622605	0.755744	24.451477

Cartesian coordinates of the larger models in Table 3 (optimized with OLYP potential):

Structure **11₂** (F):

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C	0.705000	7.351000	24.202000	C	8.201394	1.641814	18.331739
C	1.502391	6.329988	23.446286	C	6.551096	3.140326	19.186167
O	2.011958	5.356476	24.037547	C	7.221918	0.899884	17.721720
H	1.308949	7.710732	25.041455	C	5.541813	2.414936	18.548384
H	-0.184923	6.865208	24.617435	C	5.819224	1.214488	17.808561
H	0.394659	8.200039	23.587670	O	4.914992	0.486261	17.275229
N	1.630995	6.522755	22.120241	H	8.792112	4.653242	19.678551
C	2.431951	5.654557	21.276913	H	9.944125	3.315650	19.485575
C	1.838768	5.415958	19.877998	H	9.242934	1.339795	18.231726
C	2.577150	4.256083	19.277468	H	6.272482	4.001895	19.784646
N	2.100954	2.958443	19.367858	H	7.487451	0.019142	17.139803
C	3.860979	4.224558	18.850369	C	-3.838537	1.721451	16.336635
C	3.104179	2.161901	19.006487	C	-2.510479	1.976712	16.978824
N	4.205608	2.891454	18.693115	N	-1.378690	2.268245	16.235611
H	1.275524	7.388852	21.726183	C	-2.162974	1.927774	18.309672
H	2.522546	4.703035	21.800606	C	-0.405498	2.394169	17.144810
H	0.772085	5.192625	19.953517	N	-0.817894	2.190894	18.420186
H	1.943029	6.311572	19.255415	H	-4.012327	0.648267	16.179303
H	4.571456	5.016506	18.653672	H	-3.879451	2.206475	15.355062
H	3.088515	1.087714	18.973623	H	-2.768953	1.714438	19.175904
H	3.441038	6.073230	21.170039	H	0.618443	2.642452	16.901948
C	8.939042	3.576664	19.828917	C	-4.942099	4.069084	21.539604
C	7.889684	2.786758	19.100792	C	-3.548928	3.576207	21.658566

N	-3.198609	2.539131	22.497536	N	1.124996	-1.880878	23.930957
C	-2.430709	3.828048	20.919508	C	-0.132543	-1.574528	24.376142
C	-1.927583	2.196099	22.241082	C	-0.093310	-1.195450	25.773142
N	-1.422294	2.958221	21.277836	C	1.220244	-1.244385	26.150257
H	-4.970251	4.976941	20.932005	C	1.963820	-1.673010	24.985476
H	-5.395417	4.279504	22.512568	C	1.817420	-0.902540	27.471619
H	-3.799124	2.124989	23.225911	O	-2.783809	-2.322556	17.847553
H	-2.300804	4.552979	20.127924	C	-1.268258	-0.827745	26.619125
H	-1.413651	1.395678	22.745253	C	-1.590652	0.682825	26.645612
C	-8.652341	-3.705167	17.697983	C	-2.732102	0.944539	27.624243
C	-8.388269	-2.877950	18.921380	O	-2.461029	0.911740	28.851759
O	-8.714191	-1.700969	19.041563	O	-3.909502	1.113387	27.147375
O	-7.732980	-3.563828	19.868150	N	2.207770	-2.883729	20.164321
H	-7.707704	-3.821785	17.151769	C	1.376784	-2.963406	19.083163
H	-9.373367	-3.198928	17.053850	C	2.136371	-3.237848	17.881274
C	-10.861023	-3.413496	22.594692	C	3.449476	-3.294063	18.258768
C	-10.830335	-2.037771	23.143131	C	3.477301	-3.052598	19.690561
N	-9.666656	-1.297433	23.220874	C	1.530783	-3.404188	16.529108
C	-11.817266	-1.245539	23.654467	N	3.602877	-2.494027	22.629103
C	-9.925028	-0.107494	23.752989	C	4.682725	-2.697717	21.817193
N	-11.225832	-0.062353	24.019839	C	5.913595	-2.552507	22.561561
H	-10.704255	-3.405496	21.510653	C	5.550751	-2.235795	23.849087
H	-11.827748	-3.877323	22.803472	C	4.097999	-2.197625	23.864664
H	-8.714910	-1.624356	22.884984	C	7.278529	-2.728838	21.996244
H	-12.873305	-1.421988	23.788680	C	6.376175	-1.989421	25.021493
H	-9.216656	0.679927	23.947386	C	7.587443	-1.414471	25.047464
C	-0.109651	-7.368064	24.194794	N	-0.286307	-2.257016	21.460959
C	0.593115	-6.317415	23.421331	C	-0.751697	-2.391628	20.190679
N	1.550958	-6.592751	22.473581	C	-2.160027	-2.072870	20.152752
C	0.504687	-4.951719	23.438438	C	-2.532110	-1.747289	21.446558
C	2.000779	-5.436554	21.954714	C	-1.345170	-1.873061	22.242210
N	1.383024	-4.411912	22.522277	C	-3.049499	-2.013266	19.009706
H	-0.604714	-8.083343	23.528073	C	-3.868116	-1.285249	21.930671
H	-0.864470	-6.909938	24.838640	C	-4.930299	-2.387123	22.064187
H	1.878173	-7.516239	22.204096	C	-6.218455	-1.884086	22.713252
H	-0.130917	-4.338084	24.054540	O	-7.324623	-2.267147	22.199953
H	2.752707	-5.390021	21.187339	O	-6.128473	-1.160299	23.737757
C	-7.127509	-2.960597	29.468686	C	4.624478	-3.561812	17.358361
N	-6.019158	-2.322671	30.151926	O	5.677754	-2.590203	17.511675
C	-5.203387	-1.433288	29.584364	C	5.237035	-4.942943	17.563431
N	-5.383000	-1.054012	28.326107	H	6.046107	-5.095349	16.839315
N	-4.177404	-0.938883	30.292597	Cu	0.216580	2.475715	20.109867
H	-6.785434	-3.721108	28.757780	H	8.891071	3.392424	20.913367
H	-7.734165	-2.212602	28.955365	H	-4.673317	2.104938	16.938341
H	-5.702953	-2.737310	31.022717	H	-5.531461	3.294705	21.032081
H	-6.073191	-1.489922	27.718408	H	-9.006488	-4.710142	17.956796
H	-4.865689	-0.252110	27.947390	H	-10.071118	-4.017669	23.050776
H	-4.237069	-0.962061	31.304971	H	0.595658	-7.919074	24.825696
H	-3.609024	-0.189608	29.875717	H	-7.746921	-3.426171	30.227401
Fe	1.672331	-2.320653	22.035632	O	1.885091	-0.720147	21.663732
C	-1.273120	-1.595259	23.601473	O	1.329160	1.896585	21.950875
C	0.013966	-2.750614	19.092065	O	-8.025059	1.128768	20.316136
C	4.624178	-2.970782	20.462194	H	-7.640909	1.531350	19.512931
C	3.339958	-1.828692	24.958860	H	-8.134774	0.192774	20.052697

O	-7.391955	-1.832009	26.146533	H	-2.198642	-1.347155	24.099638
H	-7.005001	-1.610915	25.263130	H	3.873289	-1.596738	25.869752
H	-7.587133	-2.786140	26.073484	H	5.944988	-2.298317	25.973525
O	1.811202	4.423625	27.724785	H	8.111667	-1.292562	25.992666
H	1.612190	4.083467	26.830967	H	8.075682	-1.033344	24.155735
H	1.216924	3.896692	28.296161	H	7.993967	-2.978012	22.784047
O	-7.362265	2.917475	25.058617	H	7.302871	-3.528537	21.250002
H	-6.539554	2.399764	24.894227	H	7.622795	-1.805926	21.509178
H	-7.640693	3.192964	24.164708	H	5.563130	-3.078420	19.943092
O	-4.934068	1.371685	24.566453	H	4.256533	-3.515689	16.326621
H	-4.504168	1.244061	25.454510	H	4.473571	-5.712456	17.404324
H	-5.283297	0.488226	24.314845	H	5.640835	-5.059736	18.574198
O	-5.761578	2.700782	28.812463	H	2.293598	-3.542285	15.760472
H	-5.111326	2.200996	28.266283	H	0.865832	-4.276344	16.503091
H	-5.601734	3.629443	28.547186	H	0.935138	-2.525110	16.255860
O	0.941840	2.861305	24.602644	H	-0.510428	-2.829093	18.151966
H	1.226195	3.785371	24.402321	H	-4.061119	-1.640423	19.247523
H	0.021285	2.955239	24.909246	H	-4.244203	-0.507303	21.255331
H	-7.564769	-2.984122	20.684940	H	-3.757873	-0.806961	22.902055
H	-1.857023	1.032684	25.645046	H	-4.542656	-3.184870	22.714275
H	-0.705559	1.233691	26.980931	H	-5.146157	-2.840234	21.094305
H	-1.072222	-1.152120	27.646956	H	5.286233	-1.693763	17.406885
H	-2.155304	-1.381565	26.288857	H	1.064480	2.161340	22.863345
H	2.591637	-1.620045	27.762183	H	1.477995	0.915199	21.971205
H	2.281494	0.092501	27.442654	H	-11.701683	0.734089	24.437804
H	1.058193	-0.891804	28.257267				

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C	0.705000	7.351000	24.202000	C	9.004158	3.542572	19.834308
C	1.539485	6.367659	23.443017	C	7.935967	2.779268	19.108264
O	2.066618	5.387712	24.005995	C	8.216887	1.647473	18.340019
H	1.270850	7.691755	25.076038	C	6.603673	3.167455	19.221982
H	-0.195079	6.843366	24.567427	C	7.205090	0.954495	17.688833
H	0.406626	8.214446	23.602951	C	5.580140	2.481906	18.573837
N	1.685639	6.590147	22.124636	C	5.879708	1.367570	17.781819
C	2.480744	5.712735	21.290627	O	4.940175	0.632057	17.111376
C	1.955240	5.567569	19.854927	H	8.919891	4.617362	19.637775
C	2.646233	4.375923	19.285470	H	10.002791	3.210282	19.538672
N	2.175295	3.089777	19.515055	H	9.242295	1.301444	18.237733
C	3.913459	4.301007	18.787004	H	6.343536	4.017244	19.843988
C	3.162204	2.265520	19.195965	H	7.438032	0.088416	17.076352
N	4.245417	2.959569	18.739596	H	4.159033	1.193654	16.927928
H	1.322693	7.453694	21.732466	C	-3.963412	1.715478	16.202291
H	2.471837	4.734171	21.774279	C	-2.599343	1.805461	16.776311
H	0.871534	5.413408	19.866131	N	-1.436396	1.788156	16.041088
H	2.166488	6.467664	19.266582	C	-2.184559	1.942265	18.071832
H	4.613596	5.065958	18.490170	C	-0.389734	1.928525	16.882014
H	3.148510	1.192235	19.295211	N	-0.812399	2.026996	18.132628
H	3.522898	6.058891	21.261303	H	-4.237219	0.681133	15.960401

H	-4.049681	2.315257	15.289549	H	-3.563913	-0.240154	29.931122
H	-1.369616	1.705127	15.030489	Fe	1.696253	-2.282989	22.025429
H	-2.790516	1.996984	18.960717	C	-1.242018	-1.552942	23.602065
H	0.634385	1.964988	16.545590	C	0.031082	-2.743712	19.097901
C	-4.898276	4.066828	21.496510	C	4.647578	-2.945621	20.451313
C	-3.481120	3.622582	21.545587	C	3.370605	-1.814184	24.953864
N	-3.029404	2.643854	22.401643	N	1.154877	-1.850977	23.926348
C	-2.395494	3.934871	20.769923	C	-0.101522	-1.544413	24.377141
C	-1.733347	2.388117	22.121155	C	-0.060669	-1.186431	25.780176
N	-1.312468	3.149086	21.119441	C	1.252403	-1.249113	26.157308
H	-4.980657	4.975904	20.894810	C	1.993902	-1.663185	24.984659
H	-5.290688	4.275730	22.497058	C	1.850345	-0.928759	27.483492
H	-3.578413	2.216057	23.152594	O	-2.797357	-2.454727	17.885045
H	-2.340492	4.651883	19.963660	C	-1.233513	-0.831641	26.634256
H	-1.148310	1.647371	22.642124	C	-1.545781	0.679659	26.698665
C	-8.643461	-3.701866	17.711446	C	-2.684629	0.922655	27.687274
C	-8.413709	-2.876911	18.944437	O	-2.408246	0.858738	28.911503
O	-8.813691	-1.725478	19.087827	O	-3.861887	1.107892	27.217871
O	-7.699044	-3.531016	19.870571	N	2.230956	-2.854307	20.156708
H	-7.684964	-3.818602	17.190316	C	1.396405	-2.942884	19.080436
H	-9.348971	-3.194414	17.051263	C	2.151604	-3.231317	17.877937
C	-10.855933	-3.411861	22.587313	C	3.464200	-3.306342	18.255786
C	-10.830488	-2.042244	23.150722	C	3.497542	-3.041177	19.684157
N	-9.671263	-1.295437	23.231564	C	1.547123	-3.379460	16.523379
C	-11.818695	-1.263752	23.681431	N	3.631441	-2.447873	22.616001
C	-9.933394	-0.115490	23.786640	C	4.709846	-2.653367	21.802811
N	-11.232572	-0.081687	24.062669	C	5.944002	-2.503368	22.543880
H	-10.685912	-3.394696	21.505407	C	5.582378	-2.193161	23.833293
H	-11.823979	-3.879141	22.781120	C	4.129249	-2.161332	23.852173
H	-8.717406	-1.611238	22.893531	C	7.308458	-2.676440	21.976965
H	-12.873018	-1.450769	23.816175	C	6.409947	-1.951791	25.005463
H	-9.226264	0.669941	23.991690	C	7.622049	-1.377710	25.033062
C	-0.096036	-7.364108	24.180919	N	-0.262728	-2.229754	21.464059
C	0.614704	-6.315606	23.409699	C	-0.733433	-2.388786	20.199622
N	1.546571	-6.595843	22.437907	C	-2.145840	-2.084309	20.165129
C	0.551047	-4.947634	23.441388	C	-2.511969	-1.733158	21.454574
C	2.004087	-5.439295	21.921394	C	-1.318923	-1.838212	22.244554
N	1.417035	-4.410952	22.511676	C	-3.043415	-2.067995	19.029552
H	-0.585033	-8.080118	23.510427	C	-3.849984	-1.275204	21.939970
H	-0.860202	-6.903925	24.812427	C	-4.915714	-2.374632	22.070161
H	1.851103	-7.521592	22.151288	C	-6.201345	-1.872247	22.730040
H	-0.062276	-4.330234	24.076228	O	-7.311522	-2.233855	22.206692
H	2.739301	-5.397498	21.137296	O	-6.101961	-1.170235	23.768036
C	-7.120914	-2.947165	29.482540	C	4.630152	-3.607167	17.355059
N	-6.004357	-2.341196	30.181362	O	5.683245	-2.622619	17.470468
C	-5.173723	-1.457200	29.626017	C	5.258345	-4.974505	17.587858
N	-5.349296	-1.058569	28.373534	H	6.066578	-5.129162	16.863131
N	-4.139469	-0.988099	30.340058	Cu	0.212199	2.718559	19.809154
H	-6.788012	-3.692785	28.751857	H	8.891071	3.392424	20.913367
H	-7.717769	-2.178044	28.989300	H	-4.673317	2.104938	16.938341
H	-5.692098	-2.781493	31.041311	H	-5.531461	3.294705	21.032081
H	-6.039964	-1.484393	27.758964	H	-9.006488	-4.710142	17.956796
H	-4.822413	-0.258057	28.003374	H	-10.071118	-4.017669	23.050776
H	-4.205423	-1.014196	31.352085	H	0.595658	-7.919074	24.825696

H	-7.746921	-3.426171	30.227401	H	-2.123666	-1.371970	26.290457
O	1.898355	-0.688209	21.646451	H	2.642357	-1.635512	27.752512
O	-8.140411	1.157678	20.282771	H	2.292272	0.077305	27.476815
H	-7.681867	1.503282	19.491038	H	1.095132	-0.953930	28.273512
H	-8.250730	0.208874	20.068374	H	-2.165181	-1.297062	24.101167
O	-7.363599	-1.822995	26.187852	H	3.903598	-1.596384	25.868543
H	-6.981779	-1.613045	25.299613	H	5.980493	-2.264811	25.956797
H	-7.572579	-2.774847	26.123579	H	8.147917	-1.261853	25.978022
O	1.834810	4.446188	28.118711	H	8.109492	-0.992218	24.142918
H	1.547801	4.037961	27.264515	H	8.024144	-2.931924	22.762640
H	1.352545	3.920420	28.785544	H	7.332619	-3.470866	21.225092
O	-7.299785	2.932093	25.124371	H	7.653656	-1.750528	21.496516
H	-6.466727	2.432926	24.950356	H	5.585242	-3.066349	19.933020
H	-7.606825	3.175756	24.229736	H	4.257673	-3.588345	16.324675
O	-4.837906	1.423437	24.611723	H	4.503670	-5.755130	17.443606
H	-4.431229	1.276331	25.506551	H	5.667032	-5.067566	18.598837
H	-5.196578	0.549259	24.351108	H	2.311524	-3.481136	15.750208
O	-5.774208	2.667272	28.890035	H	0.897987	-4.262511	16.473445
H	-5.102234	2.183965	28.358179	H	0.935260	-2.504677	16.273918
H	-5.625177	3.599505	28.638757	H	-0.500341	-2.835260	18.163006
O	1.114160	3.324406	25.575641	H	-4.043194	-1.656895	19.253862
H	1.345627	4.107870	25.018060	H	-4.222692	-0.492794	21.266796
H	0.144395	3.249508	25.500065	H	-3.739739	-0.800511	22.913203
H	-7.549390	-2.951602	20.692549	H	-4.526884	-3.178088	22.712807
H	-1.808433	1.056144	25.706179	H	-5.138791	-2.820736	21.098543
H	-0.656939	1.213350	27.049516	H	5.264976	-1.750297	17.331082
H	-1.039024	-1.182310	27.654028	H	-11.715198	0.697106	24.500583

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C	0.705000	7.351000	24.202000	H	3.478454	6.005336	21.279650
C	1.536162	6.357263	23.463600	C	8.981140	3.500602	19.823830
O	2.096487	5.410489	24.049822	C	7.910236	2.714041	19.133663
H	1.277009	7.718861	25.064177	C	8.189113	1.526409	18.427009
H	-0.185790	6.846130	24.597005	C	6.577207	3.123777	19.214505
H	0.389275	8.197543	23.590128	C	7.183422	0.782237	17.856640
N	1.637371	6.532199	22.134055	C	5.546819	2.399176	18.638149
C	2.439903	5.650338	21.315797	C	5.796981	1.154518	17.936406
C	1.913683	5.488719	19.884742	O	4.868942	0.448396	17.431200
C	2.620116	4.308948	19.316388	H	8.890050	4.569316	19.596403
N	2.121783	3.016101	19.446958	H	9.977685	3.161184	19.529159
C	3.911194	4.238793	18.892015	H	9.219610	1.188078	18.341084
C	3.105094	2.196687	19.106815	H	6.344957	4.022432	19.775701
N	4.224962	2.896377	18.772197	H	7.416867	-0.132633	17.319174
H	1.249266	7.375161	21.721574	H	2.355053	-0.549879	20.818781
H	2.443757	4.677608	21.810979	C	-3.938804	1.681089	16.252537
H	0.831789	5.320786	19.896662	C	-2.595245	1.823850	16.860563
H	2.106142	6.389160	19.290764	N	-1.420227	1.884281	16.148833
H	4.631104	5.011794	18.678143	C	-2.215492	1.941145	18.168443
H	3.069089	1.123668	19.071537	C	-0.395986	2.047194	17.007321

N	-0.849735	2.086654	18.251813	H	-4.808477	-0.276742	27.997600
H	-4.190818	0.629872	16.067912	H	-4.197558	-1.026870	31.349155
H	-3.999091	2.222365	15.302815	H	-3.568973	-0.243773	29.935388
H	-1.331050	1.829031	15.138022	Fe	1.688535	-2.340758	22.046476
H	-2.839556	1.941344	19.046131	C	-1.250024	-1.576976	23.613247
H	0.631639	2.146859	16.696944	C	0.019685	-2.750521	19.103968
C	-4.907160	4.044727	21.547837	C	4.643677	-2.967728	20.434597
C	-3.500458	3.571996	21.628789	C	3.369200	-1.832400	24.937288
N	-3.090726	2.557543	22.466543	N	1.153779	-1.836275	23.906576
C	-2.395512	3.875086	20.879051	C	-0.101906	-1.546535	24.373667
C	-1.802313	2.268912	22.199483	C	-0.054492	-1.194336	25.778734
N	-1.343105	3.045456	21.224321	C	1.261345	-1.250039	26.145500
H	-4.953282	4.971988	20.970491	C	1.996114	-1.659105	24.966245
H	-5.333144	4.230527	22.538737	C	1.870635	-0.920782	27.463634
H	-3.664665	2.128607	23.205603	O	-2.794983	-2.407973	17.880782
H	-2.305295	4.610181	20.093453	C	-1.223042	-0.840581	26.637642
H	-1.245534	1.499957	22.710106	C	-1.557153	0.667319	26.662390
C	-8.656636	-3.699312	17.702876	C	-2.693259	0.930727	27.646770
C	-8.388285	-2.877200	18.928810	O	-2.415294	0.921852	28.872954
O	-8.734367	-1.707471	19.062609	O	-3.875529	1.078330	27.172060
O	-7.705623	-3.557284	19.860474	N	2.226516	-2.820883	20.159553
H	-7.715191	-3.808646	17.149539	C	1.386119	-2.925150	19.081686
H	-9.384003	-3.191478	17.067081	C	2.135039	-3.202952	17.874357
C	-10.852672	-3.399085	22.598877	C	3.450386	-3.263543	18.238389
C	-10.803108	-2.023755	23.148117	C	3.492508	-3.019273	19.669417
N	-9.631714	-1.295336	23.221369	C	1.515633	-3.360253	16.526602
C	-11.779523	-1.221514	23.664595	N	3.623596	-2.474555	22.598715
C	-9.874356	-0.103649	23.757107	C	4.705087	-2.700977	21.790564
N	-11.173940	-0.045213	24.029129	C	5.934737	-2.577158	22.535445
H	-10.699448	-3.391889	21.514279	C	5.573772	-2.254772	23.823894
H	-11.825288	-3.849804	22.809237	C	4.123828	-2.196999	23.837761
H	-8.682552	-1.631779	22.882382	C	7.298223	-2.776804	21.972404
H	-12.836619	-1.386722	23.804147	C	6.404202	-2.009685	24.993198
H	-9.154454	0.673235	23.954675	C	7.616955	-1.437485	25.010179
C	-0.085215	-7.317683	24.209267	N	-0.270328	-2.257548	21.475333
C	0.634117	-6.266628	23.448659	C	-0.744111	-2.410730	20.210103
N	1.573202	-6.540902	22.481209	C	-2.156039	-2.112624	20.176984
C	0.550304	-4.898272	23.470194	C	-2.521380	-1.770021	21.469976
C	2.018593	-5.387067	21.953849	C	-1.329402	-1.871787	22.256711
N	1.414571	-4.361866	22.536289	C	-3.052586	-2.078023	19.040205
H	-0.608148	-7.998309	23.526684	C	-3.856925	-1.314220	21.956494
H	-0.825635	-6.854386	24.866333	C	-4.914769	-2.419000	22.092522
H	1.882786	-7.465703	22.195585	C	-6.204136	-1.905416	22.728501
H	-0.074394	-4.285704	24.095465	O	-7.308943	-2.274018	22.200841
H	2.756834	-5.342089	21.173295	O	-6.116587	-1.182053	23.752944
C	-7.108763	-2.967515	29.481257	C	4.615638	-3.519231	17.319563
N	-5.989417	-2.361349	30.176078	O	5.676184	-2.558953	17.486212
C	-5.162006	-1.474840	29.621876	C	5.227218	-4.906635	17.472974
N	-5.338186	-1.073762	28.370669	H	6.032197	-5.029189	16.738519
N	-4.127007	-1.005195	30.337240	Cu	0.177435	2.696953	19.917884
H	-6.778956	-3.726466	28.763303	H	8.891071	3.392425	20.913369
H	-7.694339	-2.199763	28.972683	H	-4.673316	2.104937	16.938340
H	-5.681356	-2.793194	31.041651	H	-5.531461	3.294704	21.032080
H	-6.023672	-1.504579	27.753757	H	-9.006486	-4.710143	17.956795

H	-10.071118	-4.017670	23.050774	H	-1.012505	-1.161696	27.663633
H	0.595661	-7.919074	24.825698	H	-2.107582	-1.403730	26.316215
H	-7.746923	-3.426172	30.227400	H	2.640521	-1.646245	27.747259
O	1.867765	-0.564886	21.664470	H	2.345543	0.069424	27.431628
O	-8.043051	1.143842	20.262243	H	1.117311	-0.902375	28.254873
H	-7.687566	1.502642	19.425888	H	-2.174374	-1.341853	24.119574
H	-8.176811	0.198364	20.049521	H	3.904070	-1.627639	25.853650
O	-7.339697	-1.851839	26.178857	H	5.976134	-2.312163	25.948714
H	-6.968140	-1.628946	25.289183	H	8.146874	-1.310372	25.951507
H	-7.512607	-2.810999	26.113630	H	8.100264	-1.063128	24.112835
O	1.965466	4.028858	27.743775	H	8.006915	-3.043327	22.760719
H	1.614086	3.686533	26.888274	H	7.309222	-3.573671	21.222722
H	1.241943	3.835315	28.371187	H	7.662273	-1.858836	21.490684
O	-7.483569	2.692024	25.009192	H	5.579745	-3.099702	19.915628
H	-6.608450	2.266913	24.862639	H	4.237931	-3.439867	16.293237
H	-7.662897	3.143706	24.162305	H	4.464822	-5.671415	17.289499
O	-4.875276	1.361528	24.563680	H	5.638684	-5.057548	18.476080
H	-4.472592	1.223062	25.461740	H	2.269822	-3.464556	15.744134
H	-5.219560	0.480819	24.300062	H	0.871633	-4.247774	16.491798
O	-5.825382	2.641053	28.698617	H	0.895496	-2.491069	16.278633
H	-5.126953	2.145660	28.211030	H	-0.514016	-2.851521	18.171184
H	-5.505585	3.563643	28.665982	H	-4.064337	-1.705606	19.278524
O	1.036199	3.093235	25.158305	H	-4.236519	-0.536036	21.282594
H	1.294181	3.932005	24.703643	H	-3.746131	-0.837320	22.928212
H	0.061509	3.105065	25.141650	H	-4.529484	-3.209128	22.753337
H	-7.541153	-2.981919	20.681253	H	-5.125154	-2.883452	21.126812
H	-1.832301	1.008583	25.660983	H	5.283273	-1.660875	17.420643
H	-0.671363	1.223174	26.985613	H	-11.639562	0.750800	24.458715

13 (AF):

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C	0.705000	7.351000	24.202000	H	3.078801	1.121294	19.093556
C	1.540416	6.357861	23.461683	H	3.493542	6.032509	21.262263
O	2.093447	5.406160	24.047409	C	8.987932	3.491773	19.821805
H	1.279879	7.727328	25.056178	C	7.917115	2.706254	19.135588
H	-0.179854	6.840443	24.600348	C	8.194916	1.520692	18.424551
H	0.380726	8.191389	23.584414	C	6.582403	3.118908	19.225313
N	1.656040	6.541460	22.134937	C	7.187350	0.778770	17.857450
C	2.460371	5.664070	21.313324	C	5.552589	2.399686	18.649945
C	1.917825	5.486746	19.889581	C	5.801990	1.157271	17.941870
C	2.625101	4.307064	19.321811	O	4.873666	0.457248	17.435749
N	2.128093	3.014697	19.450815	H	8.896961	4.559276	19.588414
C	3.917622	4.238139	18.900904	H	9.983957	3.147877	19.532058
C	3.112760	2.194395	19.118001	H	9.224981	1.183916	18.333149
N	4.232059	2.896311	18.786537	H	6.353932	4.015510	19.790776
H	1.273199	7.387730	21.724871	H	7.415842	-0.135094	17.316597
H	2.482292	4.695027	21.815254	H	2.289928	-0.549019	20.787124
H	0.837847	5.310735	19.917463	C	-3.947019	1.691195	16.235589
H	2.095506	6.384706	19.287231	C	-2.596572	1.825891	16.830228
H	4.637438	5.011003	18.686890	N	-1.425967	1.881978	16.110333

C	-2.206679	1.940856	18.134705	H	-5.685634	-2.787896	31.046302
C	-0.394834	2.039676	16.962019	H	-6.017720	-1.508829	27.753889
N	-0.840189	2.080361	18.208925	H	-4.803526	-0.280385	27.997138
H	-4.201054	0.642755	16.037919	H	-4.201184	-1.020905	31.352695
H	-4.020533	2.246477	15.294993	H	-3.566657	-0.242857	29.936842
H	-1.343696	1.828507	15.098870	Fe	1.688744	-2.336839	22.050280
H	-2.823932	1.943669	19.017048	C	-1.246292	-1.569865	23.617355
H	0.630980	2.135016	16.644405	C	0.016955	-2.745177	19.106881
C	-4.899294	4.038381	21.543347	C	4.639707	-2.956612	20.434113
C	-3.493034	3.563102	21.608993	C	3.369011	-1.839238	24.944322
N	-3.074382	2.552837	22.446491	N	1.156615	-1.831451	23.911025
C	-2.394928	3.866679	20.849442	C	-0.098455	-1.540617	24.378228
C	-1.787356	2.265902	22.170324	C	-0.051921	-1.193823	25.785905
N	-1.338166	3.042585	21.190526	C	1.261023	-1.256121	26.154184
H	-4.948348	4.969298	20.972370	C	1.996890	-1.662487	24.973621
H	-5.314217	4.219289	22.539861	C	1.871725	-0.937852	27.474923
H	-3.643137	2.123678	23.188745	O	-2.802531	-2.411922	17.886565
H	-2.312748	4.600622	20.061739	C	-1.221318	-0.839793	26.645156
H	-1.225325	1.498040	22.677058	C	-1.553063	0.668249	26.672163
C	-8.658548	-3.700440	17.701809	C	-2.691963	0.930712	27.653466
C	-8.389073	-2.876973	18.926646	O	-2.418244	0.920405	28.880754
O	-8.725569	-1.703897	19.055593	O	-3.872460	1.078534	27.175059
O	-7.714860	-3.559711	19.862585	N	2.224396	-2.810087	20.160396
H	-7.717385	-3.809396	17.148074	C	1.383255	-2.917040	19.083013
H	-9.386979	-3.194178	17.066074	C	2.129886	-3.195393	17.873615
C	-10.851163	-3.395057	22.600373	C	3.445875	-3.254931	18.236916
C	-10.799716	-2.021264	23.154180	C	3.488398	-3.008680	19.669086
N	-9.626955	-1.294969	23.227314	C	1.508896	-3.356842	16.527663
C	-11.774474	-1.217853	23.672818	N	3.622020	-2.472642	22.603366
C	-9.867120	-0.103462	23.764145	C	4.702220	-2.695232	21.792731
N	-11.166321	-0.042510	24.037160	C	5.933033	-2.574575	22.536793
H	-10.696477	-3.383661	21.516046	C	5.572515	-2.258035	23.826220
H	-11.825220	-3.844293	22.807342	C	4.123807	-2.199700	23.843290
H	-8.679254	-1.632020	22.884367	C	7.296022	-2.774541	21.972519
H	-12.832117	-1.380505	23.811397	C	6.406846	-2.019634	24.997918
H	-9.146099	0.672513	23.961758	C	7.620179	-1.451224	25.014774
C	-0.084678	-7.316325	24.210211	N	-0.269845	-2.251723	21.478219
C	0.635389	-6.264365	23.449056	C	-0.745703	-2.405453	20.214894
N	1.572691	-6.538805	22.479388	C	-2.157285	-2.106304	20.181179
C	0.550582	-4.897837	23.470294	C	-2.520852	-1.762120	21.475863
C	2.013187	-5.383909	21.949980	C	-1.327956	-1.864679	22.260933
N	1.410257	-4.358171	22.533481	C	-3.055941	-2.073582	19.049060
H	-0.611084	-7.994606	23.528181	C	-3.855740	-1.305130	21.962521
H	-0.822347	-6.850901	24.868846	C	-4.914721	-2.409032	22.097191
H	1.883553	-7.463097	22.193855	C	-6.206761	-1.898239	22.729094
H	-0.072016	-4.284467	24.098327	O	-7.308213	-2.279484	22.202699
H	2.750276	-5.337399	21.168079	O	-6.126475	-1.167485	23.748486
C	-7.107896	-2.965917	29.481800	C	4.608393	-3.511635	17.315961
N	-5.991322	-2.357485	30.179169	O	5.669729	-2.551337	17.480364
C	-5.161345	-1.473393	29.624273	C	5.220849	-4.898609	17.467912
N	-5.332774	-1.077535	28.370739	H	6.025969	-5.020654	16.733463
N	-4.128509	-1.001237	30.340866	Cu	0.184566	2.671685	19.887121
H	-6.774797	-3.724619	28.765024	H	8.891071	3.392425	20.913369
H	-7.693570	-2.199521	28.971317	H	-4.673316	2.104937	16.938340

H	-5.531461	3.294704	21.032080	H	-0.667468	1.221837	26.999611
H	-9.006486	-4.710143	17.956795	H	-1.012045	-1.162973	27.670774
H	-10.071118	-4.017670	23.050774	H	-2.106913	-1.400599	26.322520
H	0.595661	-7.919074	24.825698	H	2.626068	-1.678391	27.761062
H	-7.746923	-3.426172	30.227400	H	2.366069	0.042528	27.444974
O	1.876015	-0.558123	21.671716	H	1.116581	-0.904942	28.263749
O	-8.048397	1.150406	20.275525	H	-2.170663	-1.333007	24.123366
H	-7.689004	1.514550	19.443179	H	3.904490	-1.639056	25.861866
H	-8.172493	0.204542	20.058513	H	5.977164	-2.325490	25.951896
O	-7.337260	-1.842785	26.181190	H	8.152868	-1.328348	25.955979
H	-6.969667	-1.615414	25.291342	H	8.103199	-1.072926	24.118296
H	-7.511194	-2.801426	26.113582	H	8.004270	-3.045283	22.759939
O	1.991442	3.987030	27.792144	H	7.305412	-3.569246	21.220534
H	1.611051	3.668013	26.937942	H	7.662857	-1.856260	21.493501
H	1.256759	3.853180	28.422469	H	5.575883	-3.086076	19.915018
O	-7.487332	2.666245	25.011276	H	4.229160	-3.432183	16.290144
H	-6.600984	2.264700	24.863590	H	4.457997	-5.662471	17.282939
H	-7.652098	3.164433	24.187776	H	5.631602	-5.050834	18.471075
O	-4.854528	1.367141	24.561343	H	2.261128	-3.458939	15.742942
H	-4.444305	1.231802	25.456392	H	0.868431	-4.247181	16.494686
H	-5.211941	0.488454	24.309159	H	0.883689	-2.491401	16.279143
O	-5.794722	2.649160	28.736949	H	-0.517916	-2.845369	18.174970
H	-5.109397	2.149489	28.234631	H	-4.065353	-1.696440	19.285973
H	-5.499585	3.576610	28.652783	H	-4.235382	-0.526405	21.289182
O	1.054420	3.121695	25.215122	H	-3.744775	-0.829236	22.934716
H	1.308821	3.962727	24.764030	H	-4.530294	-3.199546	22.758010
H	0.081804	3.099488	25.153551	H	-5.123487	-2.872494	21.130719
H	-7.545512	-2.982993	20.681225	H	5.274170	-1.655445	17.416249
H	-1.824874	1.012326	25.670642	H	-11.628359	0.756028	24.466273

14 (F):

203

C	0.705000	7.351000	24.202000	H	4.600782	4.993189	18.662047
C	1.516105	6.333702	23.466355	H	3.099684	1.088902	19.103504
O	2.037013	5.364226	24.051837	H	3.471850	5.974685	21.266084
H	1.269513	7.683872	25.081247	C	8.963142	3.541888	19.826075
H	-0.215131	6.876191	24.564078	C	7.906766	2.742141	19.128563
H	0.437800	8.215840	23.591568	C	8.198114	1.555614	18.427450
N	1.645695	6.516163	22.140250	C	6.569276	3.134474	19.207335
C	2.433842	5.621281	21.321254	C	7.198924	0.792709	17.866691
C	1.887988	5.442166	19.898714	C	5.548672	2.391297	18.638585
C	2.603789	4.269954	19.324502	C	5.808821	1.140877	17.956949
N	2.122885	2.971990	19.462163	O	4.883655	0.407036	17.480181
C	3.892605	4.213454	18.889678	H	8.831933	4.613688	19.636851
C	3.115236	2.162324	19.121245	H	9.965571	3.247045	19.504114
N	4.222651	2.874512	18.779869	H	9.232412	1.230079	18.337812
H	1.288574	7.373850	21.730783	H	6.322805	4.031703	19.764355
H	2.442279	4.655167	21.829060	H	7.444643	-0.122759	17.335736
H	0.809399	5.258574	19.931268	H	2.167351	-0.535251	20.742342
H	2.056000	6.342444	19.297110	C	-3.966344	1.684170	16.220122

C	-2.604667	1.806667	16.790959	H	-6.789144	-3.750302	28.760246
N	-1.442907	1.858087	16.056555	H	-7.676635	-2.206873	28.965392
C	-2.197479	1.914339	18.090408	H	-5.661874	-2.838510	31.025138
C	-0.400388	2.007988	16.896454	H	-6.001978	-1.522516	27.748447
N	-0.829724	2.046354	18.149501	H	-4.800074	-0.284697	28.008597
H	-4.235348	0.638135	16.029667	H	-4.191329	-1.061110	31.351887
H	-4.053557	2.239179	15.280548	H	-3.557412	-0.272687	29.946142
H	-1.373566	1.809696	15.043817	Fe	1.688937	-2.316630	22.044056
H	-2.804492	1.917952	18.979653	C	-1.250302	-1.576546	23.607384
H	0.621631	2.099976	16.565311	C	0.023230	-2.699036	19.085642
C	-4.887228	4.027268	21.545640	C	4.639973	-2.911546	20.437806
C	-3.483454	3.542490	21.586609	C	3.365529	-1.798836	24.946367
N	-3.057109	2.533489	22.421297	N	1.154359	-1.819271	23.909719
C	-2.394910	3.837607	20.810023	C	-0.105720	-1.541561	24.372851
C	-1.776050	2.238213	22.126963	C	-0.065683	-1.190460	25.777631
N	-1.337514	3.009207	21.138199	C	1.249169	-1.235238	26.149083
H	-4.937276	4.967665	20.990587	C	1.991525	-1.637519	24.973653
H	-5.286706	4.194859	22.550300	C	1.848065	-0.900400	27.471125
H	-3.619045	2.106144	23.167607	O	-2.788556	-2.342033	17.865387
H	-2.320106	4.568183	20.018619	C	-1.239309	-0.840708	26.632772
H	-1.211010	1.469409	22.628654	C	-1.565770	0.668804	26.667799
C	-8.641626	-3.700642	17.722551	C	-2.701115	0.934668	27.654530
C	-8.395762	-2.890605	18.963472	O	-2.418555	0.934801	28.880106
O	-8.767257	-1.728692	19.104978	O	-3.883240	1.076117	27.181056
O	-7.704042	-3.566685	19.887540	N	2.223094	-2.772747	20.152041
H	-7.688671	-3.815130	17.190927	C	1.389559	-2.871551	19.067932
H	-9.351045	-3.182800	17.074681	C	2.144645	-3.135431	17.863017
C	-10.874440	-3.406011	22.621122	C	3.458707	-3.199976	18.235510
C	-10.863872	-2.026474	23.179645	C	3.492501	-2.964613	19.667575
N	-9.717165	-1.272531	23.266574	C	1.533322	-3.279071	16.510833
C	-11.852070	-1.217306	23.687284	N	3.618221	-2.450164	22.611966
C	-10.041303	-0.075627	23.806952	C	4.699236	-2.654212	21.796312
N	-11.335452	0.003243	24.079586	C	5.929859	-2.513829	22.535954
H	-10.736625	-3.396023	21.533351	C	5.570385	-2.197095	23.826472
H	-11.830864	-3.889990	22.837900	C	4.120108	-2.159977	23.846638
H	-8.778893	-1.581230	22.954273	C	7.292873	-2.693701	21.966927
H	-12.905288	-1.445549	23.796086	C	6.402695	-1.945080	24.992566
H	-9.308866	0.696055	23.991982	C	7.615193	-1.371917	25.005703
C	-0.059874	-7.318953	24.178974	N	-0.265396	-2.240300	21.465439
C	0.673994	-6.261415	23.436480	C	-0.738998	-2.373059	20.195718
N	1.617844	-6.525402	22.469934	C	-2.147474	-2.065797	20.163960
C	0.581270	-4.895119	23.463167	C	-2.513687	-1.741433	21.460410
C	2.053577	-5.367274	21.945829	C	-1.324233	-1.858893	22.249324
N	1.440951	-4.347185	22.530594	C	-3.043606	-2.015552	19.025867
H	-0.556818	-8.001484	23.479439	C	-3.851040	-1.301542	21.950430
H	-0.825608	-6.856047	24.806724	C	-4.890446	-2.424224	22.067634
H	1.939167	-7.446344	22.184241	C	-6.184708	-1.946127	22.724683
H	-0.048439	-4.287775	24.090205	O	-7.284157	-2.330351	22.210100
H	2.792187	-5.315102	21.165858	O	-6.088042	-1.234557	23.760181
C	-7.103799	-2.982776	29.475681	C	4.627273	-3.450589	17.320047
N	-5.973077	-2.394395	30.166857	O	5.686629	-2.493625	17.494279
C	-5.147428	-1.502271	29.619917	C	5.235484	-4.839905	17.471643
N	-5.324307	-1.089339	28.373436	H	6.043170	-4.961321	16.739963
N	-4.110390	-1.041169	30.340477	Cu	0.181050	2.635174	19.831509

H	8.891071	3.392424	20.913367
H	-4.673317	2.104938	16.938341
H	-5.531461	3.294705	21.032081
H	-9.006488	-4.710142	17.956796
H	-10.071118	-4.017669	23.050776
H	0.595658	-7.919074	24.825696
H	-7.746921	-3.426171	30.227401
O	1.888223	-0.546118	21.677259
O	-7.977212	1.082723	20.312742
H	-7.782556	1.457655	19.431741
H	-8.149959	0.141651	20.107613
O	-7.282446	-1.894108	26.181582
H	-6.943548	-1.668152	25.277377
H	-7.487617	-2.845756	26.113136
O	1.840277	4.144871	28.002844
H	1.506073	3.800912	27.138637
H	1.145263	3.871490	28.631609
O	-7.294934	2.962045	25.077781
H	-6.493764	2.420590	24.895721
H	-7.687459	3.094916	24.194796
O	-4.852191	1.348117	24.562626
H	-4.451309	1.209348	25.460959
H	-5.222266	0.475166	24.309437
O	-5.942720	2.612611	28.696887
H	-5.223811	2.151362	28.209076
H	-5.672373	3.551291	28.654965
O	1.010641	3.211755	25.436174
H	1.273726	4.019705	24.930989
H	0.040620	3.181141	25.356144
H	-7.536012	-2.999414	20.722854

H	-1.838186	1.017666	25.667947
H	-0.677250	1.217158	26.995066
H	-1.035121	-1.171648	27.657091
H	-2.124256	-1.397168	26.301959
H	2.655072	-1.590089	27.737874
H	2.270367	0.113471	27.456715
H	1.098509	-0.936990	28.265373
H	-2.177972	-1.350054	24.111984
H	3.900069	-1.583406	25.860389
H	5.977659	-2.246017	25.949790
H	8.147269	-1.244893	25.945792
H	8.096740	-0.996844	24.107726
H	8.008563	-2.950911	22.751858
H	7.311617	-3.489777	21.216656
H	7.641370	-1.770077	21.484743
H	5.577507	-3.029460	19.918777
H	4.252140	-3.368659	16.292788
H	4.472542	-5.602927	17.283229
H	5.642968	-4.994037	18.475950
H	2.291404	-3.378356	15.731663
H	0.887486	-4.164666	16.463945
H	0.916412	-2.406224	16.267156
H	-0.508678	-2.782694	18.150489
H	-4.051291	-1.634196	19.266999
H	-4.240235	-0.519761	21.286457
H	-3.750269	-0.837648	22.929295
H	-4.485623	-3.223009	22.705862
H	-5.099912	-2.866925	21.091488
H	5.298358	-1.590460	17.444750

14 (AF):

203

C	0.705000	7.351000	24.202000
C	1.531118	6.344955	23.465370
O	2.051436	5.374659	24.049555
H	1.277814	7.712564	25.063120
H	-0.193788	6.855581	24.587181
H	0.404752	8.199770	23.583235
N	1.677630	6.544546	22.143260
C	2.476474	5.666985	21.317268
C	1.900455	5.452820	19.910136
C	2.622759	4.286924	19.332558
N	2.135920	2.985225	19.430454
C	3.918134	4.237348	18.921428
C	3.129555	2.181158	19.086884
N	4.245944	2.899894	18.781465
H	1.317190	7.404348	21.741120
H	2.529896	4.708880	21.837489

H	0.827522	5.247282	19.972832
H	2.033854	6.347619	19.291927
H	4.631650	5.020232	18.724509
H	3.110499	1.108127	19.050928
H	3.499425	6.056232	21.231650
C	8.990298	3.519734	19.824607
C	7.927111	2.735160	19.128037
C	8.213308	1.543892	18.425867
C	6.593677	3.147294	19.211072
C	7.212235	0.795184	17.861042
C	5.567173	2.419181	18.641197
C	5.825602	1.170914	17.943722
O	4.900227	0.465323	17.444611
H	8.884405	4.590687	19.615634
H	9.990198	3.194205	19.527155
H	9.245028	1.210348	18.343149

H	6.362292	4.043490	19.775177	N	-5.978686	-2.383135	30.169021
H	7.444118	-0.122158	17.327861	C	-5.154498	-1.490973	29.618566
H	2.100222	-0.511595	20.737379	N	-5.336538	-1.081089	28.371289
C	-3.977604	1.705342	16.195223	N	-4.118678	-1.024468	30.335276
C	-2.607114	1.807012	16.749613	H	-6.788817	-3.739379	28.759087
N	-1.450611	1.838896	16.005351	H	-7.684462	-2.201452	28.970317
C	-2.187643	1.918176	18.044289	H	-5.663320	-2.828161	31.025226
C	-0.399013	1.984470	16.834654	H	-6.009152	-1.522566	27.746618
N	-0.817675	2.035858	18.091184	H	-4.811028	-0.279217	28.002917
H	-4.252115	0.667194	15.972785	H	-4.193514	-1.045244	31.347056
H	-4.077699	2.292953	15.276673	H	-3.557354	-0.263334	29.932475
H	-1.390864	1.786622	14.992053	Fe	1.680935	-2.312402	22.049016
H	-2.787933	1.931482	18.937396	C	-1.246006	-1.559924	23.613870
H	0.621245	2.061497	16.494019	C	0.019483	-2.704178	19.094693
C	-4.875498	4.025645	21.530449	C	4.635874	-2.900585	20.440565
C	-3.473470	3.534955	21.546151	C	3.361118	-1.826247	24.960972
N	-3.036074	2.524304	22.373819	N	1.155531	-1.818060	23.916133
C	-2.397386	3.827090	20.751621	C	-0.102239	-1.531923	24.379535
C	-1.760868	2.225988	22.059834	C	-0.063797	-1.192046	25.790849
N	-1.336958	2.995919	21.063832	C	1.246001	-1.255946	26.165615
H	-4.932306	4.964714	20.973879	C	1.989578	-1.654117	24.984755
H	-5.254154	4.197977	22.542513	C	1.848152	-0.946696	27.492917
H	-3.586439	2.100897	23.130640	O	-2.796551	-2.358821	17.877301
H	-2.334347	4.556888	19.958313	C	-1.238237	-0.841587	26.645155
H	-1.190802	1.452038	22.548291	C	-1.556976	0.668994	26.693508
C	-8.636659	-3.705135	17.716732	C	-2.699241	0.926310	27.672513
C	-8.385940	-2.885287	18.950400	O	-2.428378	0.895114	28.901167
O	-8.733202	-1.713972	19.073121	O	-3.875945	1.091626	27.193448
O	-7.718336	-3.564356	19.890320	N	2.220672	-2.764589	20.156636
H	-7.684187	-3.826659	17.185593	C	1.386846	-2.870447	19.073774
H	-9.342587	-3.187347	17.064935	C	2.139456	-3.135627	17.866053
C	-10.879383	-3.409170	22.627364	C	3.453723	-3.192809	18.235236
C	-10.873375	-2.031775	23.189637	C	3.488631	-2.953490	19.669660
N	-9.732690	-1.269240	23.273807	C	1.523720	-3.287237	16.516180
C	-11.867763	-1.230012	23.699139	N	3.615741	-2.447342	22.617534
C	-10.065943	-0.074552	23.815287	C	4.696034	-2.652348	21.802151
N	-11.360641	-0.006185	24.089903	C	5.926790	-2.527033	22.543920
H	-10.746711	-3.395074	21.539023	C	5.567249	-2.222478	23.838334
H	-11.832576	-3.898195	22.846934	C	4.117990	-2.178039	23.856550
H	-8.791324	-1.571597	22.963078	C	7.290817	-2.708859	21.976158
H	-12.919064	-1.467103	23.807966	C	6.399858	-1.984657	25.007523
H	-9.339560	0.703462	23.999688	C	7.614690	-1.416652	25.028581
C	-0.065997	-7.314988	24.190721	N	-0.267184	-2.235901	21.471434
C	0.666080	-6.259484	23.443759	C	-0.743068	-2.376608	20.204932
N	1.603988	-6.525888	22.472326	C	-2.151980	-2.070413	20.172989
C	0.580244	-4.892538	23.473686	C	-2.515088	-1.737324	21.469875
C	2.041045	-5.366073	21.948647	C	-1.325329	-1.849833	22.255754
N	1.437039	-4.344693	22.538470	C	-3.047704	-2.024036	19.037721
H	-0.575649	-7.993337	23.496115	C	-3.852936	-1.296357	21.958610
H	-0.821054	-6.849999	24.829925	C	-4.893462	-2.418320	22.076432
H	1.921952	-7.447276	22.185170	C	-6.188723	-1.939872	22.731447
H	-0.044795	-4.283838	24.104260	O	-7.288455	-2.316596	22.211215
H	2.776097	-5.314128	21.165032	O	-6.092678	-1.233954	23.771153
C	-7.106910	-2.975883	29.477454	C	4.616665	-3.452020	17.315925

O	5.684207	-2.498770	17.481534	H	0.075556	3.212321	25.450687
C	5.221675	-4.842541	17.465157	H	-7.545356	-2.990270	20.718862
H	6.028905	-4.964810	16.732975	H	-1.817123	1.032318	25.695334
Cu	0.188315	2.639948	19.760147	H	-0.668824	1.207195	27.038935
H	8.891071	3.392424	20.913367	H	-1.040661	-1.181845	27.667685
H	-4.673317	2.104938	16.938341	H	-2.125997	-1.389846	26.307533
H	-5.531461	3.294705	21.032081	H	2.610571	-1.681447	27.773306
H	-9.006488	-4.710142	17.956796	H	2.330216	0.040408	27.479015
H	-10.071118	-4.017669	23.050776	H	1.088706	-0.933639	28.278590
H	0.595658	-7.919074	24.825696	H	-2.171863	-1.321520	24.116386
H	-7.746921	-3.426171	30.227401	H	3.894420	-1.627867	25.879868
O	1.881814	-0.524210	21.687895	H	5.971833	-2.291506	25.961728
O	-7.942573	1.082147	20.339186	H	8.145015	-1.299001	25.970959
H	-7.782066	1.467673	19.455444	H	8.099947	-1.036665	24.134685
H	-8.117714	0.142674	20.128625	H	8.003248	-2.978680	22.760006
O	-7.296823	-1.877028	26.188455	H	7.306779	-3.497785	21.218107
H	-6.944245	-1.662665	25.286277	H	7.647382	-1.783187	21.503551
H	-7.552987	-2.816565	26.114786	H	5.573729	-3.020331	19.921987
O	1.916222	4.157663	28.133249	H	4.239090	-3.368637	16.289913
H	1.559364	3.847176	27.265013	H	4.456215	-5.602380	17.274411
H	1.197060	3.936561	28.756774	H	5.628096	-5.000071	18.469343
O	-7.218243	2.988875	25.114742	H	2.278981	-3.376975	15.732831
H	-6.432484	2.434130	24.905189	H	0.886922	-4.179696	16.471552
H	-7.649545	3.112321	24.247582	H	0.895498	-2.421933	16.274395
O	-4.821907	1.354866	24.552505	H	-0.514180	-2.794969	18.161161
H	-4.422875	1.222115	25.451840	H	-4.053926	-1.637153	19.277058
H	-5.206096	0.484417	24.312375	H	-4.242035	-0.515141	21.293746
O	-5.822682	2.636954	28.793475	H	-3.751927	-0.831872	22.937168
H	-5.134899	2.153529	28.281020	H	-4.488503	-3.216540	22.715403
H	-5.654097	3.570029	28.570245	H	-5.102324	-2.861678	21.100377
O	1.041811	3.290614	25.557654	H	5.295121	-1.600224	17.416347
H	1.287887	4.080020	25.014812				

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C	0.705000	7.351000	24.202000	H	1.329157	7.432945	21.744175
C	1.546971	6.362511	23.461181	H	2.584592	4.756981	21.834061
O	2.075687	5.394252	24.041724	H	0.862905	5.284631	19.977623
H	1.286801	7.745202	25.043431	H	2.067761	6.378915	19.283648
H	-0.165180	6.831073	24.619130	H	4.675018	5.019570	18.753339
H	0.359779	8.180322	23.580628	H	3.090825	1.131126	19.038087
N	1.701477	6.576741	22.142856	H	3.529747	6.120819	21.226202
C	2.513881	5.713840	21.313417	C	9.020432	3.471092	19.825344
C	1.935779	5.488737	19.909068	C	7.944357	2.701581	19.122322
C	2.649135	4.313334	19.338003	C	8.212220	1.527699	18.392697
N	2.142093	3.021333	19.427604	C	6.613690	3.112234	19.220781
C	3.948799	4.245341	18.938435	C	7.196980	0.795785	17.818645
C	3.129236	2.203090	19.087275	C	5.576406	2.400859	18.638915
N	4.258452	2.903489	18.798368	C	5.813974	1.166127	17.920988

O	4.878335	0.461455	17.420789	H	-0.046903	-4.279005	24.143660
H	8.972142	4.536525	19.569578	H	2.715527	-5.326043	21.154637
H	10.013651	3.093810	19.567763	C	-7.111013	-2.957351	29.484838
H	9.240203	1.186812	18.289332	N	-6.002739	-2.340912	30.188350
H	6.384687	3.997887	19.803345	C	-5.167423	-1.460491	29.633831
H	7.424157	-0.110237	17.263750	N	-5.328495	-1.073645	28.375630
H	2.165613	-0.523335	20.790774	N	-4.141246	-0.983720	30.353909
C	-3.972363	1.725199	16.187301	H	-6.769561	-3.712403	28.767937
C	-2.584000	1.889378	16.697284	H	-7.701951	-2.195164	28.974267
N	-1.467530	1.970362	15.891915	H	-5.698352	-2.771579	31.055779
C	-2.192742	1.985470	18.017298	H	-6.022335	-1.494503	27.761055
C	-0.455499	2.123490	16.758212	H	-4.804369	-0.271487	28.006863
N	-0.836051	2.135862	18.058114	H	-4.211994	-1.008268	31.365449
H	-4.218317	0.673423	15.986785	H	-3.563286	-0.237620	29.944574
H	-4.118173	2.284583	15.256175	Fe	1.686839	-2.328051	22.078209
H	-2.787701	1.939941	18.915923	C	-1.233020	-1.544402	23.648404
H	0.577675	2.246932	16.459215	C	0.009555	-2.745959	19.138876
C	-4.885513	4.036760	21.528192	C	4.635750	-2.919339	20.458730
C	-3.474477	3.569631	21.548879	C	3.374046	-1.883896	24.990618
N	-3.019858	2.571403	22.382760	N	1.166764	-1.836214	23.947061
C	-2.402492	3.874047	20.753471	C	-0.086473	-1.531768	24.411370
C	-1.738586	2.293058	22.068622	C	-0.041165	-1.200362	25.822851
N	-1.327694	3.064726	21.068839	C	1.268492	-1.288423	26.197272
H	-4.956548	4.971074	20.964931	C	2.003850	-1.691605	25.015549
H	-5.270722	4.209542	22.538100	C	1.877854	-1.005305	27.526856
H	-3.562660	2.147951	23.142220	O	-2.819931	-2.481160	17.944707
H	-2.352088	4.598420	19.954516	C	-1.210944	-0.843578	26.679568
H	-1.156174	1.532577	22.564012	C	-1.536295	0.665619	26.715009
C	-8.666011	-3.700866	17.692645	C	-2.678618	0.920058	27.693365
C	-8.396431	-2.869219	18.911425	O	-2.411925	0.868253	28.921698
O	-8.742750	-1.699119	19.036603	O	-3.853096	1.102185	27.214058
O	-7.712944	-3.543430	19.848069	N	2.219169	-2.782704	20.186825
H	-7.728032	-3.805458	17.132768	C	1.377464	-2.901295	19.110941
H	-9.402035	-3.202540	17.059299	C	2.124882	-3.166881	17.900002
C	-10.842361	-3.382328	22.601711	C	3.442663	-3.204848	18.259286
C	-10.777368	-2.011418	23.162582	C	3.485223	-2.964652	19.692329
N	-9.599680	-1.293241	23.229064	C	1.503186	-3.341107	16.556124
C	-11.742790	-1.204174	23.693330	N	3.620441	-2.481545	22.640521
C	-9.827044	-0.104053	23.775990	C	4.698844	-2.688925	21.822930
N	-11.123632	-0.035398	24.060225	C	5.930813	-2.589170	22.566944
H	-10.684716	-3.366903	21.517778	C	5.574764	-2.298279	23.864969
H	-11.822411	-3.821015	22.803101	C	4.125680	-2.235019	23.884198
H	-8.651765	-1.635160	22.879884	C	7.292124	-2.782165	21.996568
H	-12.800500	-1.359862	23.838757	C	6.410077	-2.085891	25.037059
H	-9.098546	0.664743	23.975263	C	7.628712	-1.526716	25.064312
C	-0.088533	-7.310804	24.221348	N	-0.267756	-2.243960	21.509711
C	0.630022	-6.258257	23.460154	C	-0.749674	-2.407337	20.249108
N	1.547415	-6.530981	22.471475	C	-2.158579	-2.101430	20.220047
C	0.560385	-4.891310	23.499654	C	-2.514280	-1.741148	21.510712
C	1.991323	-5.374320	21.948460	C	-1.320246	-1.843722	22.293375
N	1.408920	-4.349526	22.554128	C	-3.058913	-2.083668	19.086706
H	-0.624831	-7.982267	23.540275	C	-3.849422	-1.284422	21.996395
H	-0.817430	-6.845254	24.889651	C	-4.904526	-2.392989	22.120823
H	1.848670	-7.454585	22.173619	C	-6.200407	-1.890046	22.749271

O	-7.299033	-2.261127	22.208400	H	1.347326	3.981626	24.858906
O	-6.124278	-1.173880	23.778808	H	0.156948	3.078788	25.273139
C	4.605959	-3.442141	17.333574	H	-7.544436	-2.964847	20.662457
O	5.665346	-2.485008	17.513052	H	-1.800296	1.020703	25.715084
C	5.218802	-4.831704	17.464516	H	-0.651472	1.212903	27.055644
H	6.023386	-4.942964	16.727680	H	-1.008614	-1.174078	27.703995
Cu	0.168892	2.672567	19.684043	H	-2.098286	-1.397963	26.350069
H	8.891071	3.392425	20.913369	H	2.567316	-1.800582	27.831649
H	-4.673316	2.104937	16.938340	H	2.447832	-0.066680	27.500371
H	-5.531461	3.294704	21.032080	H	1.113201	-0.907013	28.300735
H	-9.006486	-4.710143	17.956795	H	-2.153869	-1.293249	24.153901
H	-10.071118	-4.017670	23.050774	H	3.908594	-1.701126	25.912042
H	0.595661	-7.919074	24.825698	H	5.980822	-2.404841	25.986713
H	-7.746923	-3.426172	30.227400	H	8.161588	-1.425613	26.007245
O	1.879399	-0.547074	21.723011	H	8.114199	-1.136440	24.174936
O	-8.160115	1.168636	20.248599	H	8.001889	-3.067302	22.777367
H	-7.667618	1.506824	19.475679	H	7.297762	-3.564502	21.231570
H	-8.245777	0.214857	20.049438	H	7.659198	-1.856779	21.531464
O	-7.343428	-1.816338	26.207645	H	5.571725	-3.035192	19.935924
H	-6.975986	-1.603462	25.313916	H	4.225201	-3.348681	16.309301
H	-7.560536	-2.766142	26.140321	H	4.456396	-5.593716	17.270003
O	2.091127	3.860108	27.955269	H	5.630629	-4.998213	18.465195
H	1.711531	3.601363	27.078619	H	2.257204	-3.447185	15.773674
H	1.294152	3.918069	28.524914	H	0.866802	-4.234682	16.531272
O	-7.504048	2.645568	25.008103	H	0.873188	-2.480364	16.301921
H	-6.608728	2.259533	24.872657	H	-0.528955	-2.851261	18.209476
H	-7.617557	3.228950	24.233595	H	-4.054269	-1.660090	19.309119
O	-4.835874	1.397101	24.591324	H	-4.226453	-0.503028	21.324241
H	-4.430549	1.264450	25.488328	H	-3.742350	-0.812921	22.971115
H	-5.191306	0.517640	24.344441	H	-4.519996	-3.183556	22.781650
O	-5.689386	2.682860	28.859601	H	-5.106473	-2.854878	21.152142
H	-5.043894	2.164250	28.324252	H	5.276656	-1.584116	17.444564
H	-5.497521	3.605895	28.594703	H	-11.577548	0.763213	24.497490
O	1.127736	3.145909	25.340521				

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C	0.705000	7.351000	24.202000	N	4.256810	2.902738	18.797554
C	1.546853	6.362223	23.461409	H	1.327069	7.430607	21.743397
O	2.075932	5.394275	24.042235	H	2.578899	4.753340	21.833770
H	1.286505	7.744666	25.043818	H	0.861590	5.284073	19.976249
H	-0.165845	6.831580	24.618469	H	2.069131	6.377564	19.284615
H	0.361069	8.180675	23.580441	H	4.671954	5.018704	18.750594
N	1.699526	6.574810	22.142814	H	3.090128	1.129640	19.041349
C	2.511306	5.710598	21.314120	H	3.528256	6.115163	21.228744
C	1.934766	5.487125	19.909106	C	9.018654	3.471614	19.824354
C	2.647237	4.311431	19.337809	C	7.942391	2.701282	19.123242
N	2.140997	3.019104	19.428116	C	8.210658	1.527249	18.393771
C	3.946481	4.244319	18.936851	C	6.611737	3.112231	19.222187
C	3.128346	2.201719	19.089160	C	7.195794	0.794861	17.820293

C	5.574561	2.400729	18.640128	H	-0.818230	-6.846725	24.887126
C	5.812666	1.165906	17.921725	H	1.850246	-7.455728	22.173550
O	4.877117	0.462634	17.420275	H	-0.046708	-4.279937	24.141890
H	8.968397	4.537031	19.568861	H	2.716766	-5.326612	21.154076
H	10.011696	3.095485	19.564557	C	-7.110632	-2.958304	29.484591
H	9.238822	1.187052	18.290407	N	-6.001718	-2.342528	30.187652
H	6.383585	3.998244	19.804469	C	-5.167055	-1.461474	29.633268
H	7.422974	-0.111370	17.265805	N	-5.329242	-1.073575	28.375585
H	2.172882	-0.525162	20.789874	N	-4.140305	-0.985095	30.352968
C	-3.970753	1.724648	16.189878	H	-6.770184	-3.713685	28.767561
C	-2.582987	1.889194	16.700846	H	-7.701514	-2.195863	28.974398
N	-1.466151	1.965877	15.896652	H	-5.697109	-2.773375	31.054919
C	-2.192186	1.986137	18.023361	H	-6.022363	-1.495198	27.760718
C	-0.456524	2.125070	16.765453	H	-4.804996	-0.271383	28.006742
N	-0.836681	2.134167	18.066905	H	-4.210715	-1.009768	31.364493
H	-4.216072	0.672142	15.991787	H	-3.563456	-0.238100	29.944004
H	-4.113744	2.279955	15.255952	Fe	1.687591	-2.329078	22.077250
H	-2.787733	1.942507	18.921390	C	-1.233206	-1.544555	23.647011
H	0.576572	2.251345	16.467005	C	0.011141	-2.745363	19.137911
C	-4.885942	4.037154	21.528445	C	4.636391	-2.922547	20.457621
C	-3.475012	3.570107	21.552128	C	3.373554	-1.880440	24.987993
N	-3.022796	2.571473	22.386750	N	1.166275	-1.835299	23.945355
C	-2.401267	3.874290	20.758795	C	-0.086804	-1.531208	24.410021
C	-1.740879	2.293459	22.075382	C	-0.041746	-1.198952	25.821581
N	-1.327926	3.063885	21.075973	C	1.267798	-1.285898	26.195455
H	-4.955607	4.970800	20.964013	C	2.003268	-1.689069	25.013307
H	-5.272392	4.211543	22.537602	C	1.877453	-1.000952	27.524548
H	-3.566793	2.147205	23.145094	O	-2.820732	-2.484714	17.943677
H	-2.348719	4.598772	19.960039	C	-1.211732	-0.842720	26.678479
H	-1.158863	1.533396	22.571716	C	-1.538341	0.666195	26.713578
C	-8.665672	-3.700558	17.692854	C	-2.680674	0.921011	27.691761
C	-8.395472	-2.868989	18.911544	O	-2.414004	0.870484	28.920132
O	-8.740068	-1.698264	19.035956	O	-3.855441	1.102155	27.212515
O	-7.712839	-3.543559	19.848360	N	2.220587	-2.783824	20.185724
H	-7.727712	-3.805264	17.132893	C	1.379093	-2.900546	19.109827
H	-9.401237	-3.201372	17.059654	C	2.126055	-3.166504	17.898269
C	-10.841789	-3.382218	22.600711	C	3.443546	-3.206363	18.257619
C	-10.777279	-2.011326	23.161641	C	3.486068	-2.967096	19.691039
N	-9.599474	-1.293473	23.229817	C	1.504092	-3.340201	16.554267
C	-11.743068	-1.203985	23.691530	N	3.621379	-2.481162	22.638754
C	-9.827227	-0.104241	23.776533	C	4.699622	-2.690487	21.821738
N	-11.124059	-0.035461	24.059534	C	5.931249	-2.589981	22.565816
H	-10.682739	-3.366953	21.516976	C	5.574968	-2.296524	23.863251
H	-11.822239	-3.820615	22.800848	C	4.125946	-2.232654	23.882089
H	-8.651609	-1.635355	22.881149	C	7.292506	-2.785045	21.995972
H	-12.800927	-1.359536	23.835969	C	6.410254	-2.082282	25.035001
H	-9.098756	0.664420	23.976489	C	7.628837	-1.522885	25.061743
C	-0.088423	-7.311991	24.219633	N	-0.267500	-2.244439	21.508779
C	0.630303	-6.259419	23.458676	C	-0.748767	-2.407600	20.248137
N	1.548788	-6.532111	22.470939	C	-2.158244	-2.103208	20.218747
C	0.560759	-4.892489	23.498165	C	-2.514319	-1.742288	21.509341
C	1.992623	-5.375297	21.948012	C	-1.320268	-1.844361	22.291926
N	1.409649	-4.350647	22.553169	C	-3.059018	-2.086847	19.085903
H	-0.623318	-7.984619	23.538685	C	-3.849604	-1.285201	21.994950

C	-4.904816	-2.393504	22.121537	O	1.127001	3.143596	25.331473
C	-6.202022	-1.891027	22.748252	H	1.346391	3.980410	24.853981
O	-7.299796	-2.263882	22.207028	H	0.156565	3.075582	25.266703
O	-6.129312	-1.172893	23.776712	H	-7.542751	-2.964318	20.662055
C	4.606864	-3.444411	17.332306	H	-1.802461	1.020640	25.713485
O	5.666944	-2.487758	17.512504	H	-0.653497	1.213733	27.053759
C	5.219794	-4.833984	17.462765	H	-1.009137	-1.172757	27.703035
H	6.025344	-4.944497	16.726836	H	-2.098886	-1.397750	26.349495
Cu	0.168889	2.667439	19.694660	H	2.569617	-1.793921	27.828919
H	8.891071	3.392425	20.913369	H	2.444543	-0.060719	27.497613
H	-4.673316	2.104937	16.938340	H	1.113339	-0.904926	28.299209
H	-5.531461	3.294704	21.032080	H	-2.154184	-1.293440	24.152246
H	-9.006486	-4.710143	17.956795	H	3.907925	-1.696860	25.909390
H	-10.071118	-4.017670	23.050774	H	5.981062	-2.399951	25.985145
H	0.595661	-7.919074	24.825698	H	8.161774	-1.420424	26.004443
H	-7.746923	-3.426172	30.227400	H	8.114204	-1.133703	24.171773
O	1.879951	-0.547455	21.720464	H	8.002038	-3.069308	22.777277
O	-8.157876	1.167434	20.250949	H	7.297360	-3.569066	21.232706
H	-7.666658	1.508667	19.478539	H	7.660413	-1.860907	21.529063
H	-8.241674	0.213983	20.049267	H	5.572286	-3.039221	19.934948
O	-7.344432	-1.818810	26.206670	H	4.226672	-3.350213	16.307862
H	-6.976378	-1.605486	25.313268	H	4.457838	-5.596078	17.266894
H	-7.560813	-2.768853	26.139140	H	5.630592	-5.001398	18.463733
O	2.086380	3.863932	27.946046	H	2.257936	-3.445614	15.771489
H	1.709697	3.602750	27.070245	H	0.866873	-4.233292	16.529157
H	1.294370	3.916662	28.515792	H	0.874645	-2.479224	16.299791
O	-7.504593	2.644521	25.007579	H	-0.527355	-2.851341	18.208487
H	-6.609515	2.258051	24.873014	H	-4.054464	-1.663370	19.308427
H	-7.619229	3.225216	24.231195	H	-4.227199	-0.504811	21.322002
O	-4.840342	1.397047	24.590524	H	-3.742033	-0.812211	22.968856
H	-4.428934	1.263333	25.484576	H	-4.519565	-3.183082	22.783172
H	-5.190627	0.516136	24.341156	H	-5.106349	-2.856948	21.153474
O	-5.693393	2.682394	28.855732	H	5.277985	-1.587003	17.445914
H	-5.046903	2.162974	28.322394	H	-11.578165	0.763161	24.496632
H	-5.499754	3.603720	28.594672				

2H:

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C	0.705000	7.351000	24.202000	C	3.158498	2.024800	19.296914
C	1.523664	6.316956	23.490690	N	4.205287	2.756277	18.809944
O	2.112236	5.408539	24.109892	H	1.173142	7.226177	21.702099
H	1.253798	7.691500	25.085720	H	2.354606	4.529139	21.878546
H	-0.227055	6.885735	24.545148	H	0.751139	5.079061	19.964944
H	0.455666	8.207586	23.570929	H	1.983204	6.179096	19.319836
N	1.578355	6.409828	22.149933	H	4.484577	4.871243	18.529597
C	2.361941	5.486308	21.353662	H	3.190563	0.953042	19.406172
C	1.825549	5.283783	19.931430	H	3.404620	5.827067	21.300145
C	2.561612	4.113579	19.372945	C	8.942209	3.577206	19.836058
N	2.146039	2.813173	19.626182	C	7.903731	2.753503	19.133364
C	3.820355	4.083843	18.849440	C	8.230811	1.636937	18.360937

C	6.555636	3.069875	19.268725	C	2.017996	-5.509614	21.904094
C	7.246577	0.893806	17.723556	N	1.409917	-4.478038	22.468915
C	5.558532	2.336743	18.630500	H	-0.554824	-8.169831	23.497944
C	5.903079	1.241805	17.830663	H	-0.894687	-6.959460	24.755709
O	4.997088	0.472116	17.152991	H	1.876037	-7.590155	22.163449
H	8.766132	4.646621	19.675529	H	-0.101115	-4.377747	23.998894
H	9.948982	3.331781	19.487603	H	2.772179	-5.469346	21.135853
H	9.270654	1.343022	18.242323	C	-7.105379	-2.983128	29.474462
H	6.259355	3.903541	19.896202	N	-5.984787	-2.379459	30.163454
H	7.515978	0.042402	17.105608	C	-5.168918	-1.477281	29.616662
H	4.168761	0.977398	17.023957	N	-5.349041	-1.071636	28.366650
C	-3.963357	1.730552	16.194626	N	-4.146511	-0.992292	30.339153
C	-2.608121	1.753882	16.794654	H	-6.782404	-3.756225	28.767690
N	-1.432581	1.710479	16.081356	H	-7.682763	-2.217216	28.953369
C	-2.214223	1.836095	18.101049	H	-5.669094	-2.815982	31.025722
C	-0.397430	1.783162	16.945530	H	-6.008239	-1.525468	27.737298
N	-0.841290	1.863099	18.190062	H	-4.834298	-0.259732	28.005689
H	-4.261775	0.717241	15.899041	H	-4.224471	-1.017886	31.350315
H	-4.018981	2.375815	15.310959	H	-3.584089	-0.231671	29.937118
H	-1.348695	1.656098	15.070063	Fe	1.704897	-2.361267	22.033552
H	-2.834195	1.889522	18.980218	C	-1.234904	-1.397229	23.552886
H	0.633536	1.789488	16.628826	C	0.090393	-2.440883	18.998275
C	-4.889164	4.040141	21.524607	C	4.703773	-2.793992	20.396519
C	-3.488286	3.550715	21.601685	C	3.404705	-1.531105	24.893280
N	-3.074065	2.587769	22.493577	N	1.170247	-1.622532	23.898299
C	-2.389567	3.798998	20.821417	C	-0.099641	-1.366584	24.348996
C	-1.786541	2.279804	22.228929	C	-0.059060	-1.024397	25.761731
N	-1.335124	2.990393	21.203604	C	1.258880	-1.044392	26.133890
H	-4.929801	4.960147	20.935298	C	2.017499	-1.415701	24.951294
H	-5.301262	4.246738	22.517489	C	1.836966	-0.731507	27.472130
H	-3.644946	2.190842	23.246186	O	-2.770758	-2.248568	17.794372
H	-2.307518	4.485222	19.991290	C	-1.234756	-0.716530	26.630062
H	-1.226933	1.543592	22.781441	C	-1.571442	0.787224	26.737924
C	-8.630676	-3.707456	17.714194	C	-2.723327	0.984419	27.719358
C	-8.398150	-2.888612	18.950295	O	-2.455425	0.915040	28.946927
O	-8.814741	-1.744287	19.104806	O	-3.902253	1.139054	27.243401
O	-7.666283	-3.537647	19.865444	N	2.299540	-2.600487	20.049250
H	-7.672406	-3.835109	17.195735	C	1.458305	-2.679688	18.972881
H	-9.329955	-3.192019	17.053606	C	2.210153	-3.043082	17.784472
C	-10.855180	-3.407470	22.593786	C	3.516198	-3.183408	18.176208
C	-10.821559	-2.042515	23.165512	C	3.563115	-2.870328	19.599882
N	-9.657899	-1.301333	23.248947	C	1.607225	-3.219421	16.431646
C	-11.804165	-1.264900	23.706324	N	3.714923	-2.167978	22.550962
C	-9.911652	-0.125698	23.815820	C	4.790016	-2.443284	21.748019
N	-11.209111	-0.090613	24.096355	C	6.012840	-2.310106	22.501722
H	-10.689442	-3.384517	21.511546	C	5.646087	-1.944439	23.785858
H	-11.824653	-3.871060	22.789808	C	4.196492	-1.875278	23.794004
H	-8.709340	-1.616683	22.907583	C	7.381168	-2.559862	21.971286
H	-12.858525	-1.448762	23.844941	C	6.476499	-1.701234	24.954099
H	-9.200865	0.655911	24.024704	C	7.723196	-1.205588	24.980263
C	-0.105292	-7.415750	24.153614	N	-0.252418	-1.943738	21.368638
C	0.598010	-6.373727	23.370238	C	-0.708135	-2.101207	20.096601
N	1.557686	-6.661419	22.427369	C	-2.132444	-1.855035	20.071583
C	0.525932	-5.006367	23.385994	C	-2.514311	-1.553677	21.379720

C	-1.323860	-1.630346	22.169795	H	-5.744410	3.594772	28.695193
C	-3.033391	-1.879116	18.944166	O	1.310134	3.318944	25.764297
C	-3.873996	-1.171471	21.871082	H	1.492972	4.088935	25.171758
C	-4.876123	-2.328588	22.026873	H	0.373913	3.105166	25.596365
C	-6.170112	-1.885360	22.716206	H	-7.518634	-2.959829	20.691176
O	-7.280614	-2.233195	22.186597	H	-1.829898	1.190545	25.754647
O	-6.070151	-1.229898	23.786378	H	-0.695328	1.322436	27.117067
C	4.656264	-3.603915	17.293643	H	-1.033985	-1.092305	27.639995
O	5.761226	-2.671348	17.345509	H	-2.117388	-1.260041	26.271719
C	5.209740	-4.986970	17.613449	H	2.737076	-1.321205	27.672166
H	6.006646	-5.232942	16.901341	H	2.114274	0.329110	27.542296
Cu	0.172683	2.433547	19.910874	H	1.118985	-0.938312	28.271620
H	8.891071	3.392424	20.913367	H	-2.169261	-1.193809	24.058129
H	-4.673317	2.104938	16.938341	H	3.934469	-1.307723	25.809130
H	-5.531461	3.294705	21.032081	H	6.016957	-1.944250	25.912294
H	-9.006488	-4.710142	17.956796	H	8.240410	-1.083595	25.929510
H	-10.071118	-4.017669	23.050776	H	8.249803	-0.889398	24.085269
H	0.595658	-7.919074	24.825696	H	8.066989	-2.831851	22.778013
H	-7.746921	-3.426171	30.227401	H	7.381411	-3.372526	21.238189
O	-8.057885	1.099309	20.234414	H	7.783730	-1.664302	21.477873
H	-7.637384	1.418352	19.412207	H	5.641739	-2.983326	19.896908
H	-8.196540	0.148606	20.049285	H	4.282731	-3.632457	16.263493
O	-7.318333	-1.954202	26.169235	H	4.413402	-5.733201	17.518227
H	-6.943579	-1.708940	25.285923	H	5.615022	-5.037942	18.628720
H	-7.405053	-2.925784	26.112272	H	2.368693	-3.355207	15.660619
O	1.566566	4.666653	28.312449	H	0.945712	-4.095143	16.406652
H	1.443847	4.184334	27.458983	H	1.004941	-2.346177	16.155539
H	1.100940	4.096893	28.955387	H	-0.437060	-2.524193	18.059305
O	-7.341898	2.898649	25.091737	H	-4.056043	-1.529936	19.172906
H	-6.510711	2.385877	24.948080	H	-4.302643	-0.420491	21.195621
H	-7.614181	3.145924	24.186908	H	-3.778664	-0.680303	22.838119
O	-4.898252	1.391502	24.659712	H	-4.431564	-3.108183	22.662110
H	-4.481914	1.265983	25.554391	H	-5.095968	-2.785869	21.059503
H	-5.231735	0.505411	24.406605	H	5.376947	-1.780049	17.233542
O	-5.909561	2.650909	28.895905	H	-11.685235	0.691740	24.540924
H	-5.216210	2.190603	28.371383				