

Structure of the Cobalt Protoporphyrin Chloride and its Dimer, Observation and DFT Modeling

Aurélien de la Lande*,¹ Minh-Huong Ha-Thi,² Shufeng Chen,^{1‡} Benoît Soep,³ Niloufar
Shafizadeh*²

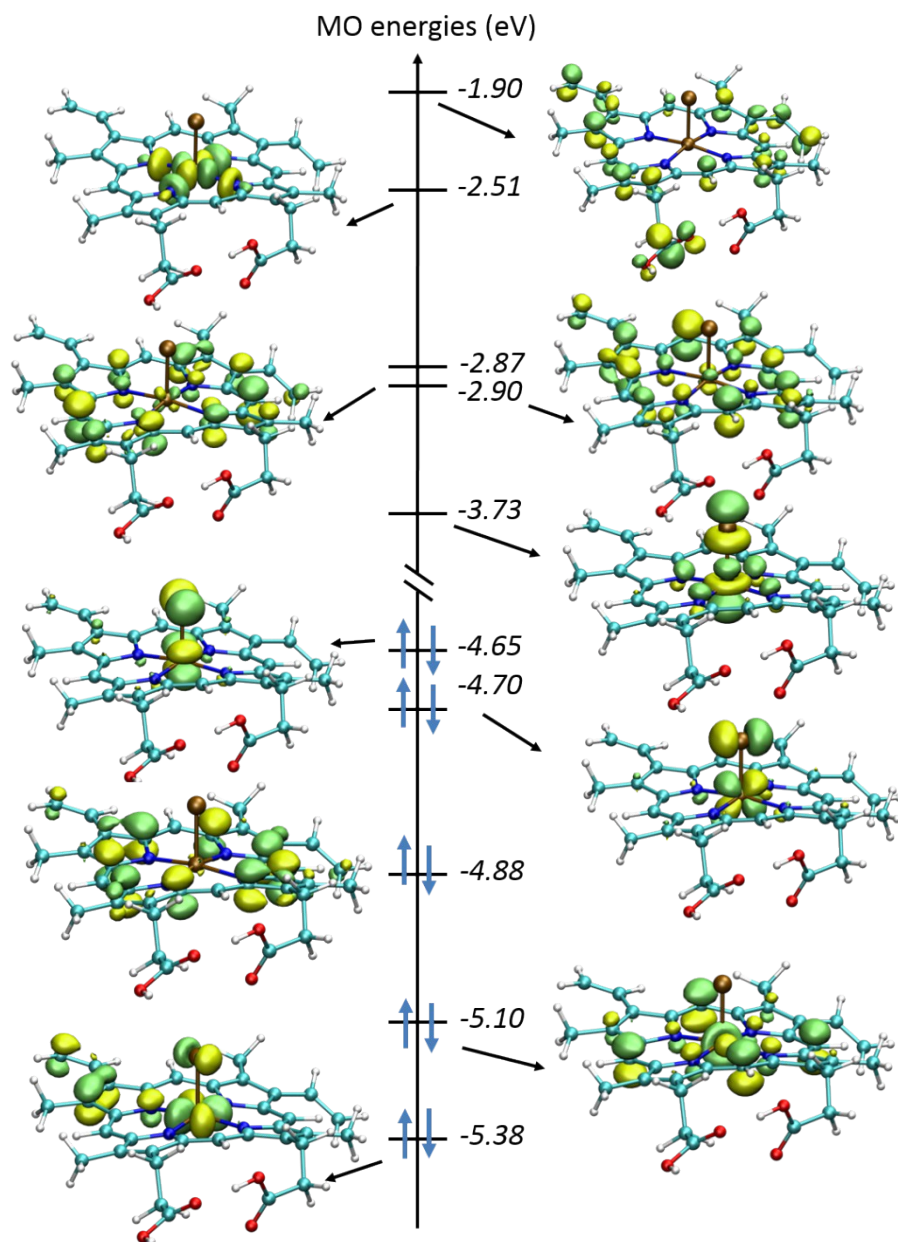
1: Laboratoire de Chimie Physique, CNRS, Université Paris-Sud, Université Paris Saclay, Orsay F-91405, France.

2 ISMO, Univ Paris-Sud ; CNRS UMR 8214, bat 210 Université Paris-Sud, Université Paris Saclay, 91405, Orsay Cedex France

3: Laboratoire Francis Perrin CEA/DSM/IRAMIS/LIDyL – CNRS URA 2453, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France

‡: Present address: School of Chemical and Environment Engineering, Shanghai Institute of Technology, Shanghai 201418, China.

SUPPLEMENTARY MATERIALS



Molecular Orbital diagram showing the highest occupied and lowest molecular orbitals of the monomer [CoPPCl] in the singlet spin state.

OPTIMIZED GEOMETRIES OF MONOMERS IN ANGSTOMS

Singlet state structure s1

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.223409
O	1.129347	0.000000	-0.739310
H	1.915475	0.012974	-0.151321
C	-1.246953	-0.024803	-0.863251
H	-2.130743	-0.058488	-0.198361
H	-1.200400	-0.972064	-1.445879
C	-1.359171	1.158107	-1.867784
C	-1.983280	2.408405	-1.301812
C	-3.324626	2.724778	-1.262153
C	-3.405973	4.059376	-0.702800
C	-4.594688	4.773721	-0.615973
C	-4.651871	6.122761	-0.293403
N	-2.169547	4.531853	-0.350102
N	-3.559841	6.898960	0.000487
C	-1.293627	3.530648	-0.692679
C	0.049480	3.512549	-0.347664
C	0.652208	4.497759	0.423806
N	0.061461	5.678130	0.796088
C	-4.010620	8.197321	-0.055320
C	-3.251580	9.318848	0.256349
C	-1.981853	9.253064	0.812160
N	-1.273237	8.096448	1.007605
C	-0.138011	8.481328	1.677149
C	0.915334	7.635192	2.006647
C	1.002440	6.322773	1.562536
C	-5.423267	8.252314	-0.352208
C	-5.852615	6.936523	-0.420076
C	-0.136494	9.901103	1.952094
C	-1.288854	10.404192	1.367055
C	2.179877	5.502798	1.752702
C	1.974081	4.363881	1.004083
C	-1.810401	11.771439	1.369609
C	-1.076304	12.905957	1.338184
C	-7.230675	6.493607	-0.624990
C	-7.795657	5.374113	-0.116422
C	-6.252205	9.501453	-0.444378
C	0.901858	10.630372	2.758542
C	-4.505556	1.914580	-1.724907
C	3.385477	5.886426	2.570185
C	2.897567	3.182917	0.849717
H	-3.716972	10.306226	0.122179
H	1.758277	8.052853	2.578662
H	-5.533456	4.286707	-0.924688
H	0.647273	2.626789	-0.615553
H	0.022054	12.899664	1.265439
H	-7.247808	4.687169	0.546380
H	-1.569682	13.890423	1.358540
H	-8.852221	5.140576	-0.321923
H	-2.911825	11.868703	1.386575
H	-7.873945	7.175765	-1.212149

H	2.700073	2.659905	-0.105893
H	4.094168	5.040934	2.684439
H	-4.224472	0.869508	-1.966741
H	1.318138	9.980450	3.556743
H	-0.361147	1.382474	-2.293073
H	-7.184838	9.333652	-1.021581
H	-1.983410	0.821518	-2.723149
H	0.466167	11.530449	3.242189
H	3.946566	3.545412	0.803065
H	-5.698406	10.325929	-0.940484
H	-4.950959	2.369663	-2.637506
H	3.085393	6.217057	3.588534
H	-6.546550	9.838145	0.573041
C	2.746355	2.185180	2.024790
C	3.642424	0.980665	1.853247
O	3.622921	0.220253	0.886513
O	4.505102	0.796040	2.869528
H	5.018569	-0.003014	2.651973
H	2.966255	2.680716	2.990882
H	1.707722	1.791946	2.051882
H	3.933371	6.721849	2.079458
H	-5.290571	1.876129	-0.937354
H	1.737540	10.957125	2.102134
Co	-1.685089	6.345977	0.203999
Cl	-1.056479	6.942507	-1.782654

Triplet state structure s1

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C	0.001888	-0.000874	0.000362
O	0.002094	-0.003938	1.223684
O	1.131676	0.002875	-0.738690
H	1.917186	0.008386	-0.149951
C	-1.245108	-0.029799	-0.862952
H	-2.128548	-0.065568	-0.197642
C	-1.360904	1.149396	-1.871797
C	-1.962310	2.411127	-1.308973
C	-3.301345	2.718691	-1.190698
C	-3.361294	4.065901	-0.653423
C	-4.549608	4.744079	-0.405940
C	-4.601437	6.086942	-0.043550
N	-2.106493	4.556518	-0.428796
C	-1.241887	3.554045	-0.773059
C	0.103738	3.522498	-0.428962
C	0.707495	4.496342	0.361875
N	0.140264	5.696872	0.708117
N	-3.499822	6.891654	0.100534
C	1.094699	6.360206	1.439439
C	1.073642	7.720358	1.730541
C	0.065546	8.572388	1.287466
N	-1.090599	8.172139	0.675407
C	-1.823858	9.304317	0.465796
C	-3.171878	9.326575	0.130804
C	-3.967182	8.185059	0.062484
C	-5.407182	8.205689	-0.017780
C	-5.817945	6.877244	-0.013854
C	2.245641	5.518712	1.671075
C	2.020081	4.359547	0.953013

C	0.092716	10.010267	1.449562
C	-1.081879	10.486403	0.882216
C	-1.589923	11.855001	0.817241
C	-0.844235	12.975946	0.690811
C	-7.207445	6.428358	-0.077804
C	-7.707554	5.292703	0.462265
C	1.161019	10.782421	2.171562
C	-6.305433	9.408609	-0.074683
C	-4.502663	1.880695	-1.533062
C	3.476633	5.906195	2.448333
C	2.935121	3.167718	0.822858
H	-3.667473	10.297172	0.008217
H	0.250432	12.950162	0.578285
H	1.932177	8.158421	2.263139
H	-5.506374	4.235815	-0.605874
H	0.689950	2.627047	-0.685559
H	-8.778889	5.055251	0.367355
H	-7.087092	4.593097	1.042539
H	-1.324737	13.966739	0.664389
C	2.751345	2.186613	2.005948
C	3.636548	0.969781	1.864802
O	3.625084	0.199023	0.906414
O	4.474918	0.785199	2.901007
Co	-1.579123	6.388889	0.011712
H	4.983525	-0.021972	2.702736
H	-2.688612	11.969981	0.862054
H	2.957739	2.690457	2.970415
H	-7.914033	7.123914	-0.570107
H	1.577725	10.191514	3.014156
H	-5.747070	10.365778	-0.037799
H	-4.220894	0.863993	-1.873170
H	2.742428	2.639630	-0.130836
H	4.092513	5.021076	2.709895
H	-0.367229	1.360397	-2.313893
H	-2.003174	0.812725	-2.713536
H	3.988732	3.518628	0.788755
H	-6.899005	9.405676	-1.015978
H	3.207857	6.423387	3.394271
H	-7.024895	9.400267	0.773225
H	-1.197980	-0.978314	-1.443989
H	-5.092018	2.363022	-2.344189
H	0.753801	11.728972	2.585507
H	1.989206	11.031413	1.473432
H	1.708681	1.803612	2.017892
H	4.107870	6.588345	1.836712
H	-5.163947	1.767912	-0.644468
Cl	-1.073866	6.896961	-2.128666

OPTIMIZED GEOMETRIES OF DIMERS IN ANGSTOMS

Structure A

151

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221947
O	1.152273	0.000000	-0.714583
H	1.877720	0.005150	-0.066681
C	-1.232383	-0.013922	-0.882734
C	-2.379445	0.841537	-0.313635

C	-3.625338	0.732004	-1.161199
C	-4.019289	1.555351	-2.188600
C	-5.279114	1.022741	-2.665372
C	-6.092774	1.662735	-3.586461
C	-7.315533	1.168671	-4.025848
N	-7.795296	-0.087066	-3.738573
C	-8.925030	-0.205882	-4.500123
C	-9.646146	-1.381530	-4.654010
C	-9.342506	-2.575152	-4.011746
C	-10.038285	-3.818120	-4.252127
N	-5.636367	-0.114161	-1.980802
C	-4.643518	-0.287178	-1.049929
C	-4.620169	-1.284636	-0.083024
C	-5.525293	-2.337775	-0.039317
N	-6.511550	-2.549092	-0.971089
C	-6.970728	-3.814536	-0.698566
C	-7.853529	-4.533124	-1.494091
C	-8.482118	-4.016826	-2.619416
N	-8.396186	-2.709747	-3.023931
C	-9.472832	-4.744216	-3.396956
C	-9.895978	-6.138054	-3.255106
C	-8.210935	1.906679	-4.884340
C	-9.248353	1.034800	-5.184600
C	-10.406521	1.219293	-6.057417
C	-10.995941	2.382327	-6.418140
C	-6.352953	-4.371287	0.492567
C	-5.437694	-3.427181	0.914559
C	-9.086518	-7.195361	-3.013996
C	-11.144105	-4.069025	-5.241629
C	-7.979464	3.298527	-5.408541
C	-6.633030	-5.747373	1.043668
C	-3.310455	2.793964	-2.678555
C	-4.455952	-3.509268	2.062312
H	-10.489865	-1.398142	-5.352836
H	-10.677715	3.363811	-6.033698
H	-7.992899	-7.092352	-2.932121
H	-5.760281	2.635515	-3.971074
H	-3.802335	-1.265691	0.649676
H	-9.508321	-8.208455	-2.918348
H	-8.121938	-5.558315	-1.190906
H	-11.859353	2.379266	-7.103049
C	-4.828003	-2.615157	3.273155
C	-6.089269	-2.964381	4.034371
O	-6.814695	-2.144612	4.575321
O	-6.320542	-4.296944	4.129065
H	-7.123206	-4.383736	4.672419
H	-10.839466	0.285878	-6.457889
H	-4.914297	-1.553043	2.969798
H	-11.388358	-3.163873	-5.830593
H	-10.973111	-6.336301	-3.416251
H	-6.911206	3.577088	-5.319252
H	-4.322887	-4.557983	2.381926
H	-5.962377	-5.986029	1.888627
H	-2.587189	0.530318	0.729481
H	-8.255207	3.363801	-6.483681
H	-2.214592	2.619174	-2.737075
H	-3.663043	3.096887	-3.685037
H	-3.465349	-3.162879	1.703687
H	-8.579645	4.032878	-4.831306

H	-7.686231	-5.806804	1.391742
H	-6.482033	-6.505058	0.245616
H	-10.847299	-4.872885	-5.951861
H	-3.484824	3.634250	-1.970733
H	-2.056005	1.902820	-0.265498
H	-12.067440	-4.397634	-4.714465
H	-0.966186	0.307330	-1.916580
H	-1.552199	-1.076895	-0.961753
H	-4.005465	-2.678010	4.020993
Co	-6.991411	-1.423684	-2.524445
Cl	-5.474594	-2.406283	-3.836510
Co	-4.692567	-2.521279	-5.985339
N	-5.114717	-0.714584	-6.706463
C	-6.245898	-0.331834	-7.377811
C	-7.281306	-1.173361	-7.754327
C	-7.321576	-2.537928	-7.503325
C	-4.356838	0.428096	-6.631869
C	-3.090810	0.506556	-6.059202
C	-2.426902	-0.569676	-5.491625
N	-2.909291	-1.855775	-5.427912
C	-1.948471	-2.551447	-4.741121
C	-1.977241	-3.914331	-4.476371
C	-3.021703	-4.756432	-4.829037
N	-4.149184	-4.370909	-5.511602
C	-4.897621	-5.517076	-5.618285
C	-6.138289	-5.606448	-6.234915
C	-6.810099	-4.534484	-6.803536
N	-6.357148	-3.240510	-6.824094
C	-8.389142	-3.396626	-7.957287
C	-8.078930	-4.661302	-7.502069
C	-0.827193	-1.706296	-4.381665
C	-1.110332	-0.460414	-4.892186
C	-4.993468	1.547221	-7.281639
C	-6.191208	1.061964	-7.776629
C	-3.046720	-6.168620	-4.509428
C	-4.233001	-6.653281	-5.011850
C	-7.255697	1.766788	-8.494358
C	-7.088442	2.746318	-9.409703
C	-8.833403	-5.879146	-7.817392
C	-9.134716	-6.881156	-6.962830
C	-4.725728	-8.076077	-4.941811
C	-4.483826	2.966455	-7.292794
C	-0.248565	0.777458	-4.869163
C	-9.601998	-3.025319	-8.769729
C	0.409805	-2.134977	-3.628684
C	-2.010270	-6.947812	-3.733563
C	1.530926	-2.576903	-4.589080
C	2.767670	-3.068188	-3.861920
O	2.770887	-3.818867	-2.896898
O	3.913855	-2.596496	-4.409214
H	4.642023	-2.985198	-3.892974
C	-2.034201	-6.672919	-2.197290
C	-3.436606	-6.436568	-1.671446
O	-4.285698	-7.308720	-1.529828
O	-3.644225	-5.144108	-1.375261
H	-4.570936	-5.024111	-1.089591
H	-7.960174	3.219668	-9.889297
H	-1.128555	-4.344317	-3.924300
H	-8.110243	-0.740927	-8.327298

H	-8.281920	1.443677	-8.238705
H	-2.578145	1.480820	-6.071956
H	-6.091042	3.090168	-9.731443
H	-6.609838	-6.593855	-6.319277
H	-8.855651	-6.847654	-5.897031
H	-9.707346	-7.756420	-7.314636
H	-9.235504	-5.947441	-8.847064
H	0.171261	-2.949058	-2.920916
H	-5.721946	-8.200839	-5.408641
H	-3.935157	3.195004	-6.355718
H	-1.409882	-5.788459	-1.953428
H	-4.787688	-8.401421	-3.881286
H	-2.160865	-8.030178	-3.918166
H	-10.521258	-3.459760	-8.320453
H	-5.327037	3.681166	-7.398093
H	-0.990823	-6.702883	-4.106129
H	-4.016512	-8.751807	-5.469282
H	1.179320	-3.432530	-5.205763
H	0.663491	0.631039	-4.258463
H	-0.810118	1.647895	-4.466864
H	0.068173	1.031697	-5.904338
H	-9.511878	-3.439727	-9.800210
H	-9.740095	-1.930234	-8.860881
H	1.811545	-1.749497	-5.274218
H	-3.792310	3.119595	-8.149761
H	-1.616378	-7.556018	-1.669647
H	0.783561	-1.286880	-3.015523

Structure B

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C	-0.008236	0.031923	0.005182
O	0.001288	0.023451	1.354937
O	1.009377	0.030113	-0.673489
H	0.926917	-0.006527	1.682623
C	-1.416421	0.081240	-0.558782
C	-2.369266	-1.028570	-0.040452
C	-2.315501	-2.322674	-0.815272
C	-3.116804	-2.658732	-1.881987
C	-2.829873	-4.048821	-2.168137
C	-3.587802	-4.815972	-3.044080
C	-3.472714	-6.196612	-3.161360
N	-1.817095	-4.529902	-1.377076
N	-2.527763	-6.963107	-2.534547
C	-1.500374	-3.486998	-0.543119
C	-0.444556	-3.485287	0.359594
C	0.461021	-4.528683	0.489155
C	-2.845526	-8.258052	-2.864593
C	-2.093179	-9.372001	-2.516053
C	-0.908188	-9.321568	-1.797437
N	-0.367082	-8.194054	-1.242308
C	0.805526	-8.615526	-0.664912
C	1.688719	-7.792038	0.026839
C	1.445457	-6.453163	0.295070
N	0.339612	-5.751483	-0.113860
C	-3.999765	-8.324302	-3.733241
C	-4.390582	-7.010736	-3.944483
C	2.317146	-5.645488	1.120225
C	1.681789	-4.435247	1.267095

C	1.044259	-10.021690	-0.889608
C	-0.044658	-10.476771	-1.614737
C	-5.532660	-6.490170	-4.694278
C	-6.157681	-7.077747	-5.739788
C	-0.357143	-11.821720	-2.092550
C	0.528550	-12.772291	-2.470060
C	3.617321	-6.117623	1.719099
C	2.179758	-10.818331	-0.299034
C	-4.677182	-9.586085	-4.196211
C	-4.153862	-1.776466	-2.525841
C	2.149761	-3.234572	2.049215
C	3.056410	-2.320469	1.187652
C	3.504545	-1.102001	1.962557
O	2.754916	-0.257780	2.450025
O	4.841240	-1.008869	2.102701
H	5.005167	-0.195518	2.613748
H	2.722010	-3.566743	2.935762
H	3.943243	-2.884104	0.835215
H	1.285538	-2.654717	2.425458
H	2.488845	-1.940568	0.313561
H	-2.428563	-10.347437	-2.891821
H	-4.379760	-4.308794	-3.608451
H	-5.821980	-8.027453	-6.182827
H	1.617064	-12.598919	-2.479250
H	2.624755	-8.234411	0.399239
H	-0.234442	-2.553928	0.912187
H	-1.434475	-12.053627	-2.152162
H	0.179877	-13.759447	-2.812230
H	-7.027760	-6.594532	-6.212000
H	-5.910751	-5.509797	-4.351270
H	-5.781059	-9.447065	-4.194190
H	3.056627	-10.805836	-0.981949
H	-2.167665	-1.227217	1.034023
H	-1.347463	0.058127	-1.661863
H	-3.702399	-0.813134	-2.848165
H	3.420278	-6.956702	2.422008
H	4.296562	-6.486000	0.918234
H	4.142122	-5.301274	2.254613
H	1.879758	-11.874524	-0.134768
H	-3.410279	-0.639354	-0.091422
H	2.490041	-10.389130	0.676162
H	-4.431380	-10.438404	-3.529033
H	-4.363315	-9.848885	-5.229566
H	-4.970652	-1.542192	-1.805790
H	-4.613334	-2.249450	-3.416632
H	-1.827109	1.072452	-0.257393
Co	-1.166340	-6.387897	-1.219710
Cl	-2.749803	-6.699734	0.374794
Co	-3.232564	-7.752884	2.290521
N	-3.711674	-6.031826	3.108716
C	-4.946699	-5.443671	3.205369
C	-2.827890	-5.058679	3.501505
C	-1.470950	-5.262296	3.691986
C	-0.867742	-6.509629	3.600557
N	-1.459844	-7.637603	3.102592
C	-6.123644	-5.976089	2.689131
C	-0.501644	-8.615328	3.202416
C	-0.636229	-9.911425	2.724133
C	-1.738402	-10.365200	2.008923

C	-6.149013	-7.104035	1.875287
N	-5.080302	-7.927281	1.651843
C	-5.507634	-8.826774	0.709972
C	-4.818393	-9.974882	0.341226
C	-3.634391	-10.394548	0.931722
N	-2.854988	-9.612414	1.742331
C	-6.872890	-8.572903	0.312608
C	-7.306660	-7.513807	1.096438
C	-1.822943	-11.669636	1.397589
C	-3.026234	-11.698202	0.717263
C	0.472639	-6.778743	4.070773
C	0.693890	-8.120229	3.849148
C	-4.854765	-4.095687	3.730572
C	-3.508986	-3.826017	3.848328
C	-8.592604	-6.821255	1.092671
C	-9.795169	-7.345063	0.764067
C	-3.515149	-12.841049	-0.047976
C	-4.802570	-13.224479	-0.214504
C	-7.594219	-9.263629	-0.811321
C	-0.807857	-12.773387	1.472455
C	-6.008840	-3.156015	3.968691
C	1.385850	-5.779848	4.731822
C	-2.879422	-2.499555	4.207279
C	1.918525	-8.945313	4.155981
H	-9.928380	-8.401288	0.483462
H	-7.053682	-5.405648	2.823007
C	-2.622601	-2.272706	5.717283
C	-1.240209	-2.694910	6.177303
O	-0.228840	-2.614227	5.486341
O	-1.228445	-3.132525	7.445541
H	-0.309478	-3.376782	7.689499
H	-5.273562	-10.640293	-0.407300
C	1.226197	-5.844672	6.270611
C	2.040449	-4.829606	7.039962
O	1.610083	-4.118714	7.944433
O	3.337504	-4.781178	6.671498
H	3.757800	-4.114836	7.243352
H	0.208112	-10.601854	2.849075
H	-0.856600	-4.409698	4.020412
H	-5.649698	-12.689906	0.240968
H	-10.702398	-6.720628	0.787960
H	-8.557858	-5.762580	1.410465
H	-5.037771	-14.127833	-0.800174
H	-8.279201	-8.553105	-1.325271
H	1.132638	-4.758432	4.394869
H	0.165969	-5.709115	6.551147
H	-3.395041	-2.754434	6.348103
H	2.440677	-5.968307	4.448868
H	-3.550180	-1.695465	3.835072
H	-5.760482	-2.397753	4.739921
H	-1.254977	-13.686955	1.921802
H	-1.918276	-2.385540	3.669339
H	-2.728246	-13.495463	-0.470342
H	2.711130	-8.343482	4.644784
H	-0.437199	-13.030469	0.454355
H	1.654572	-9.784681	4.837554
H	-6.868673	-9.643215	-1.562162
H	-8.198214	-10.117489	-0.433410
H	1.550244	-6.846777	6.632633

H	-2.662304	-1.178352	5.924565
H	0.071287	-12.489822	2.085819
H	2.329865	-9.384559	3.220300
H	-6.254264	-2.626207	3.021630
H	-6.910070	-3.705628	4.312676

Structure C

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C	-0.281369	0.158464	0.391345
O	-0.153893	-0.659070	1.293114
O	0.490378	1.263003	0.305096
H	1.102984	1.236966	1.061040
C	-1.245656	0.037550	-0.767822
C	-2.657597	-0.457146	-0.363839
C	-3.512368	0.591641	0.300121
C	-4.180319	1.623674	-0.322950
C	-4.235117	1.976365	-1.788013
C	-4.928511	2.295405	0.716050
C	-5.835267	3.313265	0.448089
C	-6.688539	3.862880	1.396278
N	-6.669306	3.561030	2.730740
N	-4.681926	1.756089	1.950754
C	-3.838295	0.701223	1.709739
C	-3.315002	-0.127755	2.692376
C	-3.459387	0.107803	4.054488
N	-4.236577	1.095343	4.598843
C	-3.976811	1.044145	5.946995
C	-4.591104	1.823292	6.916017
C	-5.644616	2.692506	6.652894
C	-7.724041	4.259494	3.267222
C	-8.022703	4.310844	4.623127
C	-7.239820	3.741574	5.618343
N	-6.163411	2.926670	5.403720
C	-2.696847	-0.588102	5.071770
C	-2.992029	0.034088	6.261726
C	-6.349191	3.424214	7.676419
C	-7.374676	4.090887	7.024897
C	-8.422149	4.948991	7.570628
C	-8.346764	5.730283	8.672102
C	-6.071038	3.359580	9.157566
C	-2.494800	-0.291791	7.644252
C	-7.750104	4.804088	1.070835
C	-8.422769	5.029667	2.262331
C	-8.010331	5.316934	-0.269428
C	-8.793385	6.359131	-0.635119
C	-9.666464	5.845742	2.483369
C	-1.791643	-1.782648	4.874906
H	-9.211849	6.334836	8.987375
H	-7.431036	5.819867	9.278643
H	-8.889925	6.624497	-1.700577
C	-0.307645	-1.382812	4.841892
C	0.643542	-2.560745	4.912326
O	0.359728	-3.696147	5.265935
O	1.903941	-2.214579	4.554779
H	2.442695	-3.018270	4.658633
H	-9.343416	6.990842	0.075517
H	-7.487459	4.783529	-1.083355
H	-9.361199	4.957848	6.991806

H	-5.942707	3.636396	-0.596225
H	-8.860392	4.948777	4.931102
H	-5.568137	2.408546	9.425892
H	-1.945159	0.579973	8.065326
H	-3.624977	1.289810	-2.409362
H	-5.282900	1.921274	-2.157374
H	-9.445260	6.932474	2.411361
H	-1.810362	-1.162653	7.641225
H	-10.113328	5.662107	3.481199
H	-3.864416	3.013472	-1.949261
H	-5.406498	4.196222	9.462415
H	-4.251891	1.717133	7.956123
H	-3.351274	-0.532911	8.310499
H	-7.014116	3.439606	9.739994
H	-2.647602	-0.943661	2.378522
H	-10.427608	5.597332	1.712377
H	-0.076884	-0.740018	5.719764
CO	-5.531546	2.230636	3.662451
H	-1.957929	-2.499141	5.701438
H	-1.298332	1.005041	-1.306676
H	-2.555503	-1.348128	0.286893
H	-0.792500	-0.711197	-1.455888
H	-2.065265	-2.308679	3.940755
H	-3.171150	-0.799532	-1.290058
H	-0.063518	-0.804845	3.929432
CL	-7.077630	0.614831	3.275048
CO	-8.268944	-1.027597	4.279030
N	-7.194020	-1.436093	5.893087
C	-7.307483	-0.887363	7.146004
C	-8.239434	0.077137	7.509059
C	-9.235442	0.546703	6.670090
N	-9.439655	0.135153	5.374661
C	-10.556448	0.821663	4.971015
C	-11.090242	0.795878	3.688862
C	-10.608823	0.002051	2.657817
C	-6.110452	-2.269049	5.982838
C	-5.558394	-2.986604	4.933425
C	-6.085458	-3.026302	3.648809
N	-9.558892	-0.876507	2.772409
C	-9.441599	-1.428660	1.518967
C	-8.434791	-2.299763	1.129107
C	-7.385206	-2.712961	1.938296
N	-7.247918	-2.398734	3.264672
C	-11.104621	1.630513	6.036384
C	-10.256159	1.479468	7.106173
C	-5.488143	-3.773855	2.568374
C	-6.316061	-3.585909	1.472174
C	-6.159820	-4.041778	0.093208
C	-5.398930	-5.060930	-0.369039
C	-5.605780	-2.352422	7.343017
C	-6.365241	-1.457158	8.077365
C	-4.474588	-3.179887	7.761462
C	-4.296280	-3.746691	8.975596
C	-11.199976	-0.030882	1.338825
C	-10.473595	-0.950961	0.620377
C	-6.208020	-1.043993	9.519049
C	-10.352305	2.136378	8.456469
C	-4.178169	-4.516813	2.623248
C	-10.670582	-1.296796	-0.834058

C	-12.334268	0.827917	0.830261
C	-12.365772	2.455194	5.949518
H	-5.368849	-5.281797	-1.448450
H	-3.399155	-4.350445	9.184647
H	-5.038276	-3.655493	9.786375
H	-4.809630	-5.721069	0.281712
C	-12.084444	3.872139	5.388602
C	-13.370759	4.605372	5.077968
O	-13.908680	5.438738	5.791437
O	-13.896612	4.201983	3.897180
H	-14.726094	4.690938	3.766000
C	-13.703553	0.133540	0.977895
C	-14.841612	0.956006	0.401172
O	-14.975283	2.166127	0.511979
O	-15.739590	0.195856	-0.270525
H	-16.430344	0.807070	-0.581580
H	-3.718966	-3.359910	6.979853
H	-4.663192	-3.591639	5.133226
H	-11.961369	1.436423	3.474343
H	-8.449896	-2.645657	0.087757
H	-8.205419	0.478758	8.531741
H	-6.744568	-3.469035	-0.649637
H	-6.444018	0.032802	9.639941
H	-11.716131	-1.625674	-1.021938
H	-10.485636	-0.401799	-1.470586
H	-9.343054	2.336312	8.876200
H	-4.348511	-5.613505	2.605823
H	-10.870577	3.116623	8.388713
H	-3.614202	-4.273893	3.546107
H	-5.173090	-1.224450	9.873994
H	-6.900311	-1.629661	10.162633
H	-9.992217	-2.104378	-1.172822
H	-10.928353	1.489614	9.151847
H	-3.548116	-4.245524	1.747401
H	-12.162222	1.065420	-0.241936
H	-13.698924	-0.865432	0.501986
H	-11.498105	3.777307	4.448781
H	-13.089964	1.936553	5.291364
H	-12.835729	2.535222	6.950665
H	-11.514679	4.464976	6.129677
H	-12.354809	1.799167	1.363689
H	-13.938652	-0.013039	2.054788

Structure D

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C	0.001333	0.007275	-0.002322
O	-0.000279	0.011248	1.233104
O	1.110218	0.006167	-0.737760
H	1.908434	0.038468	-0.149987
C	-1.265254	0.028136	-0.834024
C	-2.324247	-0.994451	-0.363955
C	-3.606385	-0.826814	-1.142473
C	-3.918064	-1.339728	-2.382062
C	-5.236009	-0.831068	-2.699773
C	-5.908242	-1.153318	-3.868228
C	-7.147574	-0.634152	-4.221682
N	-5.736294	-0.031072	-1.698650

C	-4.747647	-0.028807	-0.745140
C	-4.830288	0.620979	0.477522
C	-5.869374	1.468644	0.832599
N	-6.913061	1.827820	0.014921
C	-7.569845	2.813916	0.710799
C	-8.684758	3.501666	0.257381
C	-9.316269	3.245458	-0.950811
N	-8.953796	2.266959	-1.838931
N	-7.855909	0.289878	-3.487704
C	-8.934853	0.599862	-4.277162
C	-9.886148	1.568725	-3.994251
C	-9.872200	2.366706	-2.858853
C	-10.847584	3.405454	-2.609946
C	-10.491149	3.974358	-1.397534
C	-7.815062	-0.971606	-5.459186
C	-8.952951	-0.180848	-5.501196
C	-6.968209	3.050154	2.008169
C	-5.911282	2.172797	2.099315
C	-11.166856	5.015244	-0.625062
C	-11.868647	6.058052	-1.122107
C	-10.020360	-0.136999	-6.500648
C	-9.879199	-0.340838	-7.829280
C	-7.367073	-2.021989	-6.437824
C	-12.039960	3.717885	-3.469191
C	-3.090709	-2.234482	-3.267068
C	-7.457750	4.040074	3.031775
C	-4.982171	1.943480	3.262628
C	-3.803002	2.942462	3.291947
C	-2.816064	2.678579	4.412101
O	-2.383510	3.572304	5.146211
O	-2.454997	1.401110	4.514088
H	-1.770113	1.291712	5.222989
H	-11.965020	6.247483	-2.201932
H	-12.351876	6.778747	-0.444076
H	-10.754931	-0.300706	-8.495900
H	-8.901992	-0.527031	-8.300870
H	-10.673424	1.758597	-4.738222
H	-5.421967	-1.841894	-4.576897
H	-9.080097	4.311516	0.890993
H	-4.001878	0.492284	1.190842
H	-4.590702	0.909656	3.229820
H	-11.032016	0.096386	-6.119295
H	-2.496297	-0.872941	0.723117
H	-11.078089	4.934369	0.475054
H	-4.162366	3.985995	3.391861
H	-2.117155	-2.490050	-2.801081
H	-1.007957	-0.129257	-1.901566
H	-12.893459	4.064254	-2.847211
H	-1.677610	1.054471	-0.733557
H	-6.827481	4.037155	3.944928
H	-8.240512	-2.469695	-6.959110
H	-5.554910	2.035263	4.210137
H	-1.928368	-2.022577	-0.508576
H	-12.372855	2.826373	-4.040687
H	-6.818469	-2.838922	-5.924268
H	-3.227121	2.868847	2.344205
H	-11.788354	4.519668	-4.196041
H	-6.695405	-1.573462	-7.201450
H	-2.885009	-1.734519	-4.238616

H	-7.441997	5.071049	2.614016
H	-8.502428	3.804862	3.333744
H	-3.629804	-3.186307	-3.473315
Co	-7.276997	1.211588	-1.830582
Cl	-6.136989	2.743472	-2.849095
H	1.429182	0.159668	2.400582
O	2.226208	0.263543	2.979525
C	3.333257	0.313509	2.238545
O	3.335241	0.219370	1.007502
C	4.595242	0.499960	3.055618
C	4.817200	-0.636881	4.082749
C	6.014706	-0.381685	4.966551
C	7.336274	-0.687345	4.722294
C	5.980671	0.258434	6.266442
C	4.860728	0.924831	6.750550
C	4.878670	1.682577	7.916070
N	5.917604	1.725215	8.813276
N	7.227242	0.276988	6.842888
C	8.065866	-0.282930	5.909408
C	9.435263	-0.462266	6.054339
C	10.110084	-0.196381	7.239432
N	9.524072	0.223597	8.407763
C	5.484242	2.553096	9.823261
C	6.149180	2.789633	11.019373
C	7.367227	2.201159	11.341783
C	10.484332	0.061827	9.380239
C	10.342743	0.401398	10.721391
C	9.225184	1.059883	11.221256
N	8.115112	1.411432	10.498200
C	11.715415	-0.451919	8.823631
C	11.509592	-0.551030	7.456548
C	7.993379	2.328433	12.641785
C	9.164924	1.588609	12.573314
C	3.783450	2.535587	8.335035
C	4.160822	3.078165	9.544853
C	12.503606	-0.957183	6.467068
C	12.609540	-0.491166	5.200633
C	10.149001	1.290893	13.614705
C	10.497349	2.088600	14.648941
C	12.966800	-0.721656	9.612389
C	7.430188	3.054168	13.831169
C	3.394632	4.039421	10.413473
C	7.932043	-1.332169	3.502569
C	2.522903	2.817729	7.553445
C	1.352768	1.888283	7.951387
C	0.119637	2.108801	7.097180
O	-0.434506	1.194285	6.479620
O	-0.299109	3.373938	7.068361
Co	7.694677	0.901275	8.641356
H	-1.076041	3.460159	6.459518
H	11.938288	0.283104	4.798916
H	13.412464	-0.853796	4.539289
H	11.236505	1.751050	15.392360
H	10.083749	3.100095	14.781693
H	11.191879	0.217861	11.398874
H	10.010806	-0.902858	5.225645
H	5.675117	3.445664	11.764686
H	3.931365	0.893677	6.156707
H	13.267817	-1.676937	6.817540

H	2.230772	3.874464	7.706113
H	1.635768	0.822939	7.848946
H	10.647262	0.306908	13.527352
H	3.915849	-0.758213	4.713472
H	5.450013	0.566748	2.353069
H	13.772600	-1.143989	8.980470
H	2.383278	4.246757	10.008333
H	7.179322	-1.479183	2.701180
H	2.730783	2.703848	6.469818
H	4.962450	-1.597114	3.545224
H	7.667764	2.508607	14.770591
H	6.326638	3.154640	13.763008
H	4.498823	1.468219	3.592005
H	7.864663	4.074146	13.901521
H	1.073971	2.079217	9.010941
H	12.763709	-1.438581	10.437822
H	13.353597	0.218858	10.063764
H	3.940717	5.005049	10.496774
H	8.362334	-2.325412	3.760557
H	8.751575	-0.703584	3.086868
H	3.268924	3.628975	11.440152

Structure E

150

C	-0.000003	-0.000006	0.000005
O	-0.000021	-0.000043	1.223268
O	1.131579	0.000012	-0.736910
H	1.915958	0.038127	-0.148366
C	-1.243506	-0.019194	-0.870008
C	-1.306172	1.128431	-1.917495
C	-1.981904	2.379852	-1.415607
C	-3.318118	2.689108	-1.495028
C	-1.341380	3.527304	-0.808133
C	-0.019041	3.515454	-0.393803
C	0.591010	4.564224	0.275927
N	0.004308	5.772102	0.545228
N	-2.239612	4.537957	-0.573735
C	-3.450573	4.032259	-0.976465
C	-4.676713	4.665564	-0.825855
C	-4.821014	5.937787	-0.288994
N	-3.793468	6.748536	0.112863
C	1.019458	6.533410	1.071547
C	0.924168	7.878161	1.402105
C	-0.259709	8.599474	1.325067
N	-1.475055	8.091289	0.935662
C	-2.362845	9.116565	1.133509
C	-3.741820	9.029808	1.006347
C	-4.406464	7.894573	0.560861
C	-0.358690	9.981834	1.731750
C	-1.698671	10.312404	1.628350
C	-5.845776	7.801979	0.486816
C	-6.114106	6.557896	-0.055626
C	2.247094	5.779055	1.202963
C	1.976871	4.528260	0.695014
C	-2.363420	11.600890	1.825491
C	-2.014216	12.566325	2.705886
C	-7.403400	5.991267	-0.459326
C	-8.566869	6.106337	0.216303

C	0.802164	10.863484	2.105760
C	-4.445077	1.835205	-2.012992
C	-6.815149	8.899366	0.839643
C	2.910797	3.351586	0.551576
C	3.542160	6.310021	1.761558
H	-5.585010	4.129278	-1.139426
H	-4.346275	9.898478	1.305146
C	2.851586	2.434708	1.801471
C	3.776634	1.248169	1.660416
O	3.680388	0.378020	0.796982
O	4.766099	1.217225	2.574128
H	5.292092	0.420534	2.379155
H	1.822636	8.392616	1.777370
H	-1.188097	12.443255	3.425291
H	-8.633732	6.614385	1.192771
H	-9.495594	5.670893	-0.184487
H	-2.574117	13.514017	2.750888
H	0.572790	2.604171	-0.568622
H	-3.232047	11.777357	1.165197
H	-2.136606	0.004323	-0.217468
H	-7.401335	5.449464	-1.423411
H	3.947994	3.716034	0.403438
H	2.644100	2.769420	-0.349796
H	4.287510	5.502433	1.911835
H	-5.125593	2.432325	-2.656806
H	1.725075	10.549184	1.574834
H	3.115997	3.009664	2.710818
H	1.826480	2.022864	1.912917
H	-6.378063	9.899071	0.639288
H	-0.289558	1.377583	-2.274451
H	-7.067695	8.839767	1.920703
H	0.986318	10.804992	3.201825
H	-7.756494	8.801550	0.259816
H	-5.026634	1.427826	-1.155940
H	0.597074	11.922996	1.843478
H	-1.873020	0.773996	-2.802439
H	3.986087	7.062953	1.072957
H	3.379374	6.800813	2.747290
H	-4.064754	0.978386	-2.605273
H	-1.225995	-0.993351	-1.409427
Co	-1.873975	6.290499	0.234917
H	2.514095	3.713803	-3.259697
C	2.945721	4.734271	-3.267327
C	1.852993	5.760981	-3.135573
C	1.970192	7.039863	-2.649963
C	0.462631	5.586263	-3.492959
N	-0.269988	6.704659	-3.197382
C	0.002558	4.466153	-4.166053
C	-1.292653	4.328733	-4.635324
N	-2.296097	5.242661	-4.438888
C	-3.402587	4.650938	-4.997043
C	-4.706695	5.110664	-4.867237
C	-5.032851	6.289430	-4.209905
N	-4.129988	7.198411	-3.727589
C	-4.891981	8.260350	-3.298687
C	-4.392381	9.491760	-2.899591
C	-3.041910	9.763660	-2.735787
N	-2.040837	8.826564	-2.814438
C	0.636644	7.598473	-2.680090

C	0.354283	8.897028	-2.290852
C	-0.909487	9.469112	-2.372132
C	-1.188091	10.836659	-2.011413
C	-2.529721	11.041169	-2.275760
C	-6.307096	7.991246	-3.432669
C	-6.399430	6.743527	-4.025317
C	-3.081010	3.391118	-5.630474
C	-1.744218	3.171103	-5.385451
C	-7.572456	5.934643	-4.347239
C	-8.831674	6.364531	-4.589119
C	-3.239632	12.298607	-2.053697
C	-4.258556	12.788144	-2.796629
C	-0.225761	11.826243	-1.415451
C	-7.418937	8.845810	-2.888689
C	-4.063210	2.501606	-6.347529
C	3.191913	7.731604	-2.097270
C	-0.945557	1.924409	-5.690982
C	3.722758	4.952546	-4.589677
C	4.803651	3.932151	-4.863468
O	4.946501	3.318306	-5.917654
O	5.654849	3.755398	-3.832172
H	6.306436	3.094648	-4.125909
C	0.065942	2.055062	-6.859026
C	1.509847	2.191552	-6.403857
O	1.935206	1.818265	-5.315452
O	2.292350	2.755241	-7.338533
Co	-2.184896	6.989076	-3.524898
H	3.203453	2.825118	-6.980004
H	-5.517659	4.511873	-5.305592
H	1.175090	9.530954	-1.923619
H	0.714996	3.646656	-4.358005
H	-5.105441	10.293287	-2.663871
H	-9.104890	7.431096	-4.601797
H	-4.649524	12.272400	-3.686834
H	-9.636780	5.643268	-4.802686
H	-4.716008	13.758727	-2.543223
H	3.023864	4.942778	-5.445376
H	-7.381321	4.846893	-4.393129
H	-0.175210	2.889586	-7.541699
H	-0.380692	1.625446	-4.786112
H	3.631109	4.806775	-2.399230
H	-2.847661	12.925705	-1.227964
H	4.048745	7.033811	-2.010000
H	-0.685564	12.355796	-0.548958
H	-3.547233	1.765487	-6.998020
H	-4.745805	3.096752	-6.992434
H	-7.029980	9.565535	-2.141300
H	-1.649266	1.097083	-5.909899
H	0.684188	11.327266	-1.025820
H	0.082323	12.571298	-2.178376
H	-7.919496	9.415041	-3.701381
H	-4.678188	1.943130	-5.606811
H	3.487817	8.573539	-2.763260
H	-8.169942	8.198143	-2.381499
H	2.967190	8.144645	-1.089584
H	4.212502	5.952387	-4.553605
H	0.048496	1.125989	-7.472722

Structure F

C	0.026171	-0.001390	0.013727
O	0.009111	0.009485	1.237005
O	1.178002	-0.020717	-0.692040
H	1.901497	-0.039912	-0.041022
C	-1.192254	0.079531	-0.881746
C	-2.451677	-0.632694	-0.326588
C	-2.470586	-2.117699	-0.598817
C	-2.906829	-2.746239	-1.744545
C	-2.738024	-4.164207	-1.508732
C	-2.999359	-5.121877	-2.479051
C	-2.641392	-6.457453	-2.351591
N	-2.095033	-7.034938	-1.239297
N	-2.213034	-4.414563	-0.266837
C	-2.077614	-3.178405	0.306900
C	-1.722182	-2.942109	1.628176
C	-1.466406	-3.962392	2.534127
N	-1.386064	-5.295547	2.217628
C	-1.122088	-5.914818	3.414881
C	-0.866862	-7.265929	3.580411
C	-0.864311	-8.190201	2.543105
N	-1.200015	-7.910483	1.240979
C	-1.030482	-9.098221	0.576768
C	-1.251652	-9.292819	-0.779738
C	-1.769542	-8.316035	-1.622025
C	-0.461604	-9.563699	2.717445
C	-0.551991	-10.144011	1.462999
C	-2.082046	-8.552345	-3.011529
C	-2.663511	-7.381901	-3.467900
C	-1.053568	-4.968072	4.511688
C	-1.278844	-3.730910	3.953765
C	-0.360511	-11.538956	1.063332
C	0.529087	-12.412058	1.587600
C	-3.272272	-7.109690	-4.769411
C	-2.812311	-7.545541	-5.961147
C	-0.150577	-10.222211	4.036725
C	-3.493614	-2.141403	-2.994818
C	-0.863793	-5.349396	5.956727
C	-1.947830	-9.864164	-3.740499
C	-1.467003	-2.400190	4.648118
C	-0.230456	-1.474095	4.610006
C	0.936575	-1.942909	5.452845
O	0.858799	-2.497207	6.541404
O	2.130528	-1.632158	4.896102
H	2.807327	-1.927786	5.530389
H	-3.412911	-4.787791	-3.443750
H	-1.033894	-10.278604	-1.210615
H	-1.872960	-8.114641	-6.057957
H	-0.604311	-7.618821	4.590936
H	1.246898	-12.123474	2.373334
H	-1.675352	-1.898813	1.968610
H	-3.356950	-7.325502	-6.893188
H	0.581083	-13.450082	1.222801
H	-1.787056	-2.558069	5.693870
H	-1.024574	-11.879362	0.249688
H	-4.208197	-6.518894	-4.737142
H	-0.919631	-4.465987	6.619744
H	-2.546078	-0.425666	0.753528

H	-0.934230	-0.289275	-1.895089
H	0.109358	-1.276417	3.574124
H	-4.415587	-2.686318	-3.286811
H	-0.707264	-9.735609	4.863955
H	-2.305574	-1.873850	4.145263
H	-2.032063	-10.719751	-3.038914
H	-0.956931	-9.919721	-4.241194
H	-1.631451	-6.101901	6.244509
H	-2.764015	-2.209183	-3.832492
H	-0.422709	-11.298496	4.020968
H	0.141151	-5.802715	6.099047
H	0.936728	-10.143417	4.256902
H	-2.737629	-9.958626	-4.515413
H	-0.519907	-0.492514	5.047281
H	-1.405128	1.170102	-0.971724
H	-3.337508	-0.164386	-0.805375
H	-3.747474	-1.072376	-2.846983
Co	-1.739197	-6.170277	0.498614
O	-4.956229	-1.135409	3.684916
C	-6.143719	-1.234392	3.388624
O	-7.114662	-1.356665	4.306176
H	-6.703675	-1.379196	5.199983
C	-6.684381	-1.224746	1.967568
C	-5.692363	-1.815597	0.930012
C	-5.998145	-3.222270	0.471151
C	-6.634215	-3.599354	-0.686646
C	-5.578319	-4.447480	1.114455
C	-5.099029	-4.480815	2.415151
C	-4.906130	-5.658363	3.120927
N	-4.949910	-6.917172	2.582563
N	-5.853648	-5.545649	0.344270
C	-6.488174	-5.039621	-0.763102
C	-6.844891	-5.784065	-1.878449
C	-6.486187	-7.116350	-2.048146
N	-5.875348	-7.901124	-1.105075
C	-4.656046	-7.760000	3.629068
C	-4.414364	-9.120980	3.515394
C	-4.443698	-9.814455	2.310970
N	-4.870307	-9.286450	1.114279
C	-4.789926	-10.322922	0.217497
C	-5.134168	-10.239902	-1.122523
C	-5.668141	-9.109980	-1.727495
C	-4.052625	-11.196728	2.171155
C	-4.285738	-11.530447	0.850782
C	-6.143036	-9.097514	-3.091981
C	-6.675512	-7.834042	-3.296643
C	-4.511468	-7.030581	4.867887
C	-4.638833	-5.698962	4.539648
C	-7.223469	-7.231023	-4.511943
C	-7.785725	-7.865471	-5.565614
C	-4.024627	-12.849168	0.277204
C	-4.762815	-13.487635	-0.658968
C	-3.452767	-12.086795	3.224009
C	-5.939466	-10.190281	-4.108900
C	-4.508285	-4.505685	5.451436
C	-7.276980	-2.677208	-1.691912
C	-4.197896	-7.649592	6.204322
H	-7.371470	-5.270905	-2.693916
H	-4.129014	-9.680710	4.416493

H	-7.929816	-8.956133	-5.598510
H	-4.974358	-11.134976	-1.739411
H	-4.983687	-3.524205	2.949201
C	-5.813151	-4.296869	6.269862
C	-5.661417	-3.137701	7.223487
O	-5.997375	-1.976409	7.000641
O	-5.058893	-3.480601	8.380138
Co	-5.360074	-7.415760	0.727919
H	-4.972266	-2.662256	8.900348
H	-5.676928	-13.060673	-1.098092
H	-8.141261	-7.292518	-6.436600
H	-4.473449	-14.496857	-0.995046
H	-6.650610	-4.078940	5.582460
H	-7.154807	-6.129305	-4.551398
H	-7.664434	-1.734362	1.948262
H	-4.290132	-3.588589	4.869214
H	-7.679040	-3.219527	-2.569266
H	-3.647875	-4.660736	6.134925
H	-4.078564	-6.886442	6.999685
H	-2.445022	-12.433685	2.899370
H	-3.169195	-13.397431	0.719850
H	-4.677455	-1.809993	1.375801
H	-3.323217	-11.558065	4.189427
H	-6.885196	-10.744152	-4.289231
H	-5.641933	-1.164754	0.032536
H	-5.174589	-10.916195	-3.765904
H	-8.113562	-2.124436	-1.212904
H	-5.017879	-8.339081	6.509112
H	-6.034258	-5.218533	6.848714
H	-4.092738	-12.979429	3.397668
H	-5.599661	-9.746691	-5.071204
H	-3.259182	-8.243171	6.144045
H	-6.876285	-0.151964	1.736369
H	-6.547652	-1.921619	-2.062821

Structure G

150

C	0.000030	0.000393	-0.000109
O	0.000091	0.000485	1.222299
O	1.148023	0.000186	-0.719050
H	1.872535	-0.004903	-0.068197
C	-1.233860	-0.032239	-0.882293
C	-2.413062	0.773600	-0.301794
C	-3.660795	0.629499	-1.135373
C	-4.635244	-0.337904	-1.034836
C	-4.716059	-1.497996	-0.076148
C	-4.073178	1.498619	-2.221160
C	-3.291630	2.548337	-2.683156
C	-3.616603	3.332909	-3.783512
N	-4.781012	3.242795	-4.502566
C	-4.653039	4.176983	-5.501576
C	-5.603925	4.460641	-6.474035
C	-6.861637	3.863335	-6.531410
N	-7.310916	2.895359	-5.656209
N	-5.277616	1.113322	-2.749534
C	-5.640062	0.010655	-2.019099
C	-6.851370	-0.661203	-2.134828
C	-7.873332	-0.266326	-2.990551

C	-8.646787	2.745191	-5.943103
C	-9.477440	1.788685	-5.373032
C	-9.072372	0.860581	-4.421017
N	-7.826219	0.802657	-3.842603
C	-2.721594	4.332269	-4.339754
C	-3.382624	4.871250	-5.422370
C	-2.922712	5.947901	-6.368154
C	-9.171719	-0.920776	-3.030718
C	-9.934305	-0.199212	-3.934159
C	-9.506059	-2.135880	-2.289271
C	-10.725851	-2.484575	-1.821345
C	-11.331120	-0.485201	-4.408131
C	-1.327010	4.662746	-3.868160
C	-9.063469	3.644969	-7.003362
C	-7.917783	4.312604	-7.405957
C	-10.386825	3.831881	-7.599950
C	-11.578695	3.784755	-6.962291
C	-7.822414	5.338346	-8.499816
H	-12.513558	3.957998	-7.518851
H	-11.609514	-1.836754	-1.928665
H	-11.664437	3.617457	-5.878334
H	-10.869199	-3.439956	-1.292892
C	-1.249248	5.797253	-2.815725
C	-1.316737	5.335251	-1.373218
O	-0.856881	4.273748	-0.960156
O	-1.889368	6.244346	-0.571294
H	-1.850427	5.910250	0.349542
H	-5.376271	5.237725	-7.218192
H	-10.511327	1.728723	-5.743817
H	-10.390803	4.095963	-8.675582
H	-8.664462	-2.827343	-2.095313
H	-7.030947	-1.518242	-1.469344
H	-2.354876	2.774397	-2.147938
H	-1.941718	6.370525	-6.071481
H	-8.215498	4.931742	-9.458563
H	-6.777917	5.661584	-8.688194
H	-4.894956	-2.449366	-0.624244
H	-3.785174	-1.614715	0.514476
H	-3.655381	6.785371	-6.392197
H	-8.420687	6.241051	-8.250644
H	-11.540769	-1.576647	-4.388349
H	-2.825690	5.545141	-7.401499
H	-5.557686	-1.349628	0.636440
H	-11.486063	-0.121092	-5.445359
H	-12.073379	0.021071	-3.753023
H	-0.251584	6.287460	-2.900726
H	-0.962920	0.319154	-1.897374
H	-2.118520	1.841098	-0.240334
H	-0.722146	4.968756	-4.747284
H	-2.011450	6.578858	-2.998873
H	-1.521520	-1.103382	-0.966849
H	-0.835093	3.758275	-3.460530
H	-2.612401	0.444564	0.736195
Co	-6.332430	2.066095	-4.131206
H	-7.368363	4.938570	-4.455500
O	-7.922684	5.442678	-3.824621
C	-8.066296	4.701310	-2.717651
O	-7.505022	3.621999	-2.548617
C	-9.011538	5.336792	-1.719153

C	-8.999642	4.694095	-0.312200
C	-7.758376	5.005963	0.484877
C	-6.700179	4.175511	0.780032
C	-6.494763	2.738192	0.418674
C	-5.750484	4.989183	1.518897
C	-4.503536	4.520430	1.906393
C	-3.519160	5.340653	2.452536
N	-3.661756	6.681386	2.720739
C	-2.405577	7.114710	3.062452
C	-2.085642	8.393254	3.505430
C	-3.040081	9.367353	3.773562
N	-4.389909	9.242302	3.532495
C	-4.946693	10.405481	3.994798
C	-6.280527	10.776156	3.863573
C	-7.211822	10.017871	3.168114
N	-6.960567	8.816272	2.549568
C	-8.117340	8.510538	1.877036
C	-8.354797	7.338911	1.169411
C	-7.451468	6.284579	1.104091
N	-6.213020	6.272926	1.696136
C	-2.728790	10.626323	4.417731
C	-3.940874	11.282320	4.573110
C	-4.232275	12.548339	5.242317
C	-3.448392	13.649781	5.235629
C	-1.365579	11.052625	4.892247
C	-2.157822	4.895756	2.660890
C	-1.435228	6.035492	2.995831
C	-0.011663	6.155426	3.314216
C	0.980540	5.442002	2.736603
C	-1.679404	3.472802	2.584671
C	-9.126869	9.535352	2.070159
C	-8.566010	10.468998	2.914796
C	-9.178523	11.731736	3.460285
C	-10.511150	9.541602	1.475755
H	-3.746522	14.554416	5.788443
H	2.026918	5.582218	3.049076
H	0.789572	4.720056	1.927762
H	-2.502793	13.696324	4.672971
C	-11.552423	8.892507	2.413102
C	-12.932833	8.827993	1.786838
O	-13.173788	8.454089	0.647979
O	-13.910174	9.226879	2.634900
Co	-5.309239	7.754345	2.626401
H	-14.747774	9.132235	2.148241
H	-9.321952	7.232828	0.652403
H	-6.600262	11.744620	4.282422
H	0.261030	6.900518	4.085271
H	-1.030221	8.636435	3.697065
H	-4.242972	3.468554	1.707091
H	-5.193199	12.601428	5.790311
H	-6.305145	2.125909	1.329983
H	-5.628391	2.617285	-0.266976
H	-10.247084	11.828905	3.178634
H	-2.479053	2.761552	2.873875
H	-0.776589	10.180866	5.247062
H	-0.807281	11.535874	4.061758
H	-9.116567	11.749866	4.570816
H	-8.641146	12.626290	3.072244
H	-1.351401	3.232466	1.554318

H	-1.447638	11.774619	5.731333
H	-0.820779	3.318192	3.272960
H	-7.373794	2.322202	-0.111866
H	-10.817636	10.588987	1.268710
H	-11.609937	9.431264	3.380373
H	-9.899252	5.060251	0.230817
H	-8.790750	6.422040	-1.679121
H	-10.034342	5.255758	-2.149018
H	-9.118160	3.598393	-0.423141
H	-11.256903	7.842316	2.622861
H	-10.525005	9.021318	0.497132

Structure H
150

C	-0.001560	0.004359	0.000218
O	-0.001633	0.011333	1.229965
O	1.113109	0.001417	-0.743004
C	-1.272660	0.037242	-0.817942
C	-1.428028	-1.146644	-1.813836
C	-1.525619	-2.498522	-1.152171
C	-0.534634	-3.435313	-0.964063
C	-1.178890	-4.572215	-0.332658
C	-0.485811	-5.731214	-0.014544
C	-1.084001	-6.859273	0.536740
N	-2.522753	-4.356808	-0.145275
C	-2.740814	-3.088970	-0.617575
C	-3.958076	-2.421038	-0.586295
C	-5.133177	-2.976497	-0.101025
N	-5.273310	-4.251364	0.380887
C	-6.615830	-4.393384	0.624956
C	-7.230494	-5.524646	1.143360
C	-6.539559	-6.674615	1.503229
N	-5.191827	-6.867449	1.368165
C	-4.955123	-8.118270	1.889973
C	-3.719737	-8.750538	1.941931
C	-2.544103	-8.204160	1.441931
N	-2.416057	-6.952174	0.890421
C	-0.356897	-8.064043	0.862191
C	-1.277862	-8.913820	1.460282
C	-1.096885	-10.286020	1.929634
C	0.035832	-10.798491	2.462084
C	-6.405153	-2.276237	-0.130141
C	-7.347002	-3.182989	0.301282
C	-6.171923	-8.730014	2.384813
C	-7.185639	-7.822464	2.118772
C	-8.606838	-7.896200	2.448563
C	-9.359898	-9.018815	2.485158
C	1.075800	-8.352191	0.503098
C	-6.267561	-10.052424	3.093009
C	-8.833568	-2.996689	0.444454
C	0.917197	-3.385754	-1.346983
C	-6.621258	-0.848268	-0.558925
H	1.888077	0.030704	-0.141357
H	-10.423584	-8.968982	2.766282
H	0.076678	-11.855227	2.769889
C	-6.998279	-0.736303	-2.052634
C	-7.102809	0.705396	-2.512880
O	-6.287975	1.583870	-2.269365

O	-8.214631	0.939637	-3.249520
H	-8.179236	1.878092	-3.505215
H	-8.957815	-10.009085	2.222774
H	0.939739	-10.194400	2.629609
H	1.186890	-9.422303	0.218010
H	-1.257534	0.976747	-1.412743
H	-0.593459	-1.134455	-2.542803
H	-2.126816	0.073758	-0.117012
H	-2.354947	-0.958584	-2.398114
H	-3.676601	-9.747451	2.406410
H	-8.324043	-5.503859	1.281628
H	-3.994016	-1.382890	-0.953675
H	-9.105998	-6.936103	2.681099
H	0.601543	-5.758652	-0.188453
H	-1.975062	-10.953914	1.841464
H	-9.384076	-3.767650	-0.139858
H	1.560390	-3.485403	-0.440898
H	1.402026	-7.732850	-0.356646
H	-6.465849	-10.867415	2.363139
H	1.161894	-4.218754	-2.042973
H	-5.327914	-10.291421	3.632661
H	1.181913	-2.434313	-1.844859
H	-9.139994	-3.091047	1.510654
H	-9.163370	-2.000857	0.083361
H	-7.095556	-10.041498	3.834756
H	1.748816	-8.157290	1.363169
H	-5.717543	-0.238393	-0.362924
H	-7.433083	-0.397958	0.051079
H	-7.949327	-1.265485	-2.265656
H	-6.201408	-1.204784	-2.669311
Co	-3.841048	-5.577700	0.685452
O	-3.260851	-4.491301	3.144861
C	-2.367080	-4.747367	3.941525
O	-1.349978	-5.584325	3.660718
H	-1.477444	-5.925392	2.750106
C	-2.338378	-4.207094	5.357334
C	-0.976170	-3.685878	5.887414
C	-0.571204	-2.336060	5.351925
C	-0.985058	-1.101680	5.804018
C	-0.265227	-0.124460	5.009960
C	-0.440504	1.245002	5.157025
C	0.170249	2.190686	4.340328
N	1.066450	1.918114	3.338033
C	1.318823	3.124572	2.737222
C	2.276444	3.345828	1.756689
C	3.104363	2.359750	1.230486
N	3.058052	1.022016	1.555698
C	4.062913	0.439896	0.818358
C	4.347217	-0.921653	0.790581
C	3.630153	-1.872866	1.507514
N	2.546195	-1.615249	2.310415
C	2.116004	-2.845172	2.732723
C	1.075064	-3.073269	3.622238
C	0.395982	-2.070422	4.300962
N	0.576042	-0.726161	4.110088
C	4.152734	2.639449	0.272868
C	4.760748	1.421043	0.005194
C	5.914192	1.119857	-0.840874
C	6.251255	1.739556	-1.994267

C	2.934934	-3.909889	2.186177
C	3.916809	-3.291595	1.442377
C	-1.968607	-0.775170	6.895062
C	4.515854	4.000314	-0.251919
C	5.075168	-3.911189	0.709649
C	-0.136663	3.601803	4.407801
C	0.542716	4.195050	3.356655
C	0.479970	5.609623	2.998965
C	0.571614	6.147872	1.760130
C	-1.077612	4.232709	5.392645
C	2.787795	-5.377983	2.480731
H	5.642641	2.544476	-2.434462
H	7.155868	1.439995	-2.546221
C	3.578306	-5.771141	3.749148
C	3.440355	-7.234645	4.122940
O	3.433042	-8.175119	3.340153
O	3.339889	-7.413858	5.460151
Co	1.742401	0.142306	2.766735
H	3.275791	-8.375029	5.603108
H	0.491503	7.237705	1.622793
H	0.686778	5.537495	0.851422
H	-0.182979	-4.434550	5.700430
H	-3.114388	-3.419790	5.430259
H	-2.645827	-5.059652	6.003993
H	-1.071206	-3.610789	6.993929
H	0.789119	-4.117408	3.823682
H	5.166403	-1.270189	0.143775
H	0.284975	6.300666	3.840469
H	-1.141611	1.602515	5.928197
H	6.558219	0.288108	-0.497598
H	2.416726	4.380792	1.412164
H	4.316135	4.787848	0.504700
H	5.138193	-5.006426	0.874965
H	-0.827827	3.933653	6.433953
H	-1.500222	-0.120961	7.663452
H	-2.850169	-0.238852	6.476330
H	6.036787	-3.461958	1.044768
H	-1.052509	5.340230	5.341661
H	-2.341926	-1.684973	7.407794
H	4.986741	-3.739764	-0.387659
H	5.591335	4.047151	-0.524828
H	3.914167	4.232809	-1.157450
H	-2.125310	3.918907	5.185763
H	1.718694	-5.637927	2.626574
H	3.272810	-5.148351	4.612640
H	4.662778	-5.596662	3.575195
H	3.135275	-5.977917	1.618773

Structure I

C	0.001324	0.033521	0.042383
O	0.010087	0.005462	1.277101
O	1.106183	0.031988	-0.701528
C	-1.278713	0.098867	-0.764788
H	1.910556	0.024114	-0.121325
C	-1.322162	-0.879763	-1.960656
C	-2.580641	-0.722945	-2.774534
C	-3.803836	-1.323037	-2.575005
C	-4.206802	-2.283919	-1.489585

C	-2.734387	0.124008	-3.942496
C	-1.750901	1.006589	-4.365012
C	-1.912479	1.874322	-5.436555
N	-3.004020	1.917031	-6.269059
C	-2.695946	2.876941	-7.205481
C	-3.490695	3.245537	-8.280737
C	-4.723848	2.666632	-8.555119
N	-3.993511	0.015348	-4.480960
C	-4.656371	-0.861089	-3.655262
C	-5.971028	-1.278699	-3.801391
C	-6.782947	-0.886147	-4.856744
N	-6.393818	-0.087135	-5.903166
C	-7.437349	-0.129603	-6.799429
C	-7.509394	0.569915	-7.997049
C	-6.520752	1.438659	-8.436810
N	-5.339159	1.699754	-7.792448
C	-0.899482	2.831520	-5.837172
C	-1.387253	3.454634	-6.964678
C	-0.736270	4.533279	-7.788908
C	-5.511608	3.010665	-9.721424
C	-6.655385	2.231313	-9.648754
C	-7.760925	2.106943	-10.598680
C	-8.263761	3.091013	-11.377445
C	-5.098968	3.958805	-10.813089
C	0.410667	3.086545	-5.135682
C	-8.130017	-1.407274	-5.065395
C	-8.514084	-0.966168	-6.320083
C	-8.928048	-2.240599	-4.168529
C	-8.974583	-2.152832	-2.819039
C	-9.803910	-1.217146	-7.051417
H	-9.628162	-2.823810	-2.239498
H	-9.089178	2.885402	-12.076806
H	-8.406357	-1.395943	-2.256926
H	-7.893021	4.126847	-11.333456
C	1.556428	2.219158	-5.711567
C	2.843340	2.367354	-4.924879
O	3.398562	1.412426	-4.372259
O	3.306298	3.615883	-4.875873
H	4.128214	3.649718	-4.321525
H	-8.420645	0.463550	-8.605873
H	-3.124992	4.030701	-8.960582
H	-9.590484	-2.977214	-4.661274
H	-6.389958	-1.988684	-3.071083
H	-8.224120	1.104698	-10.668250
H	-5.109371	-1.915130	-0.952603
H	-10.475646	-1.892195	-6.485401
H	-3.994505	3.988716	-10.922986
H	0.296961	4.744558	-7.446960
H	-5.454180	4.986331	-10.585034
H	-0.684213	4.235213	-8.859939
H	-0.796630	1.027799	-3.813455
H	-3.400738	-2.421510	-0.740289
H	-10.352508	-0.263660	-7.217618
H	-1.322195	5.476858	-7.724314
H	-9.607382	-1.675641	-8.045381
H	-4.451936	-3.279291	-1.922491
H	-5.531325	3.647495	-11.788105
H	1.753658	2.521541	-6.763060
H	-2.123784	-0.079646	-0.071105

H	-1.257512	-1.920532	-1.578678
H	-1.356749	1.143691	-1.137340
H	1.285694	1.146062	-5.695843
H	0.298418	2.876129	-4.051792
H	0.671703	4.158996	-5.219651
H	-0.433604	-0.724514	-2.602693
CO	-4.682549	0.885236	-6.111055
H	1.437071	0.128639	2.428605
O	2.237435	0.262504	2.999667
C	3.337067	0.263748	2.250806
O	3.332348	0.097721	1.026362
C	4.605110	0.501710	3.045093
C	5.689277	-0.565697	2.772112
C	6.978303	-0.224840	3.477018
C	7.316059	-0.479760	4.787667
C	6.513208	-1.192093	5.841964
C	8.646162	0.067272	4.970936
C	9.338839	-0.036405	6.168399
C	10.617593	0.470535	6.362432
N	9.113584	0.660928	3.821289
C	8.108784	0.479997	2.901869
C	8.138425	0.913208	1.582515
C	9.199183	1.616255	1.027535
N	11.359871	1.150233	5.424231
C	12.524114	1.481880	6.069943
C	13.579453	2.202749	5.526728
C	13.583235	2.687247	4.225046
N	10.335898	2.002507	1.696331
C	11.050869	2.734900	0.778812
C	12.297554	3.303732	0.993843
C	12.997225	3.186253	2.187322
N	12.567846	2.526361	3.309405
C	11.325568	0.343604	7.620140
C	12.533838	0.996296	7.439602
C	13.660466	1.138822	8.363618
C	13.562062	1.374539	9.690171
C	10.830487	-0.415699	8.819215
C	9.198915	2.093158	-0.343900
C	10.356523	2.823896	-0.491465
C	10.852329	3.558219	-1.707778
C	8.137119	1.826252	-1.378349
C	14.688702	3.444045	3.673560
C	14.311923	3.775020	2.382134
C	15.065724	4.484010	1.347664
C	15.850625	5.565010	1.549168
C	15.987676	3.720746	4.379051
H	15.961312	6.033711	2.540055
H	16.401059	6.024647	0.712779
H	12.591638	1.520036	10.191235
H	14.464969	1.443379	10.317689
C	7.065751	2.938478	-1.419311
C	5.981438	2.725654	-2.456562
O	5.543229	3.647186	-3.153193
O	5.539318	1.472594	-2.530065
CO	10.844628	1.585369	3.562319
H	4.804467	1.407889	-3.193253
H	12.748769	3.894216	0.179127
H	14.966764	4.099023	0.313964
H	14.672042	1.051384	7.923009

H	14.447951	2.427154	6.166779
H	8.847373	-0.542924	7.015751
H	7.261099	0.705708	0.946838
H	10.357970	-1.374845	8.515199
H	16.336317	2.822798	4.933296
H	10.105985	3.554178	-2.529131
H	6.372231	-0.546854	6.737498
H	7.031242	-2.122661	6.166273
H	10.077629	0.184732	9.375773
H	11.786648	3.092708	-2.094449
H	5.506988	-1.479081	5.473537
H	15.862184	4.553148	5.105736
H	11.074551	4.621288	-1.465399
H	16.780724	4.004175	3.656518
H	11.664127	-0.653208	9.512942
H	4.981501	1.496158	2.727236
H	8.615119	1.753961	-2.378230
H	7.520226	3.929793	-1.613703
H	5.322389	-1.553207	3.125949
H	4.359733	0.551913	4.125712
H	5.845565	-0.661994	1.680168
H	6.544385	2.992737	-0.439016
H	7.653323	0.848303	-1.192904