

Supporting information for :

The S₂ to S₃ transition for water oxidation in PSII, revisited

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Structure used in Fig 2:

Mn1	2.9193906020	-1.4738485819	3.9825341119
Mn2	4.5826895172	-1.4861877807	8.5910689182
Mn3	5.2752860959	-1.5042974903	5.4296551351
Mn4	6.6136295738	-0.0062346936	7.3854716020
O5	3.6216224357	-1.2409404138	5.9625148152
O6	5.7873113763	0.2383190330	5.8312073761
O7	5.0735708607	0.2856416265	8.3304580202
O8	6.0208999902	-1.8019682407	7.3566846824
Ca9	3.5215304922	1.2830362152	6.7029448443
C10	0.6675458207#	1.9515082728#	1.7063477712#
H11	1.2251835676#	1.9058029976#	0.7825776899#
H12	-0.3243896157#	2.3686419264#	1.6143240628#
H13	0.4692471165	0.8992471996	1.9498422634
C14	1.4686503770	2.5195836221	2.8939531182
H15	0.7699763700	2.8542874497	3.6725809784
H16	2.0625004549	3.4003131080	2.6244442449
C17	2.4203589741	1.5639935891	3.6535524865
O18	3.2353366622	2.0713051810	4.4614451928
O19	2.2614573916	0.3071761117	3.4516579243
C20	1.0582598993#	1.1829961916#	13.4563132601#
H21	0.3702238917#	0.3601390915#	13.5824630076#
H22	0.7336467781#	2.1291270652#	13.8635786709#
H23	1.9550687323	0.9063826392	14.0307429557
C24	1.4408876838	1.2880372151	11.9657482337
H25	2.2383435593	2.0295817588	11.8316177987
H26	0.5882154879	1.6376952246	11.3712401546
C27	1.9137503829	-0.0718959843	11.4351690792
H28	1.0845713658	-0.7946611659	11.4448578134
H29	2.6790888868	-0.4972543407	12.0974010684
C30	2.4962505102	-0.0905425548	10.0271313267
O31	2.3860817715	0.8470470411	9.2338236463
O32	3.1142541593	-1.2135063696	9.7456539462
C33	2.7844501175#	-7.8608079453#	8.6257439092#
H34	2.4776268182	-8.8291531155	9.0416621883
H35	1.9522180282	-7.4821096359	8.0247958754
C36	4.0184199228	-8.0828536784	7.7463652526
O37	5.1484016583	-8.2675005017	8.2503216207
C38	3.0874058389	-6.9060388384	9.8144367371
H39	3.7874761493	-7.4045343675	10.4956973289
H40	2.1636445932	-6.7249185100	10.3714121288
C41	3.6667690446	-5.5940038275	9.3715244409
N42	4.8371640526	-5.5964099890	8.6260376173
H43	5.3442903685	-6.4588834955	8.4038503443
C44	3.2803262952	-4.2757223275	9.4194322473
H45	2.4339045578	-3.8147795417	9.9029458608
C46	5.0840801167	-4.3550369056	8.1970219770
H47	5.8474280975	-4.0932779934	7.4901767482
N48	4.1775139634	-3.5133052967	8.6805791017
N49	3.8178157755	-7.9513824874	6.4246691399
H50	2.8660350496	-7.7278956144	6.1010279750
C51	4.9172533146#	-7.8463448393#	5.4688658904#
H52	4.6217784186	-8.3779095722	4.5556443456
H53	5.7811975425	-8.3588726801	5.8966953883
C54	5.2813527725	-6.3774065647	5.1307404967
H55	6.1406374935	-6.3852425522	4.4470664528
H56	5.6312835058	-5.8926662446	6.0452635283
C57	4.1253006146	-5.5647001456	4.5183676763
H58	3.1617376616	-5.8533220837	4.9565515293
H59	4.0163870294	-5.7629500648	3.4443354005
C60	4.1853357693	-4.0484280255	4.6591383592
O61	3.1855681962	-3.4270283852	4.1926734867
O62	5.1690863722	-3.4951692361	5.2479863442
C63	9.1595116647#	0.1191580140#	11.4478229114#
H64	9.8026124633	-0.1466766910	10.6022242316
H65	9.7536088501	-0.0099344485	12.3631089826
C66	7.9361419552	-0.7902268824	11.5059081757
H67	7.2408145006	-0.4380677246	12.2740165364
H68	8.2322483881	-1.8055588114	11.8013975170
C69	7.1462007194	-0.9032951521	10.2010015113
O70	7.6161331041	-0.3084275603	9.1794792600
O71	6.1061422638	-1.6235692512	10.2342645471
C72	8.7726327504	1.5964893709	11.3611386921
O73	7.6648516953	2.0127558309	11.7121674557
N74	9.7709827556	2.4266311349	10.9566649375

H75	10.5857734738	2.0185288314	10.5177547123
C76	9.5677774590#	3.8588146781#	10.7651886794#
H77	10.4927928610	4.3882830957	11.0027184585
H78	8.7778238756	4.1713444580	11.4508871160
C79	9.2163689807	4.1639433269	9.2917089992
O80	10.0971406463	4.4355959102	8.4798569451
N81	7.8930545303	4.0775513909	8.9875090020
H82	7.2361112341	3.7007769986	9.6653082608
C83	7.4099175024	4.1351976490	7.6197835478
H84	6.7312425634	4.9816301438	7.4759782718
H85	8.2849292801	4.2665406626	6.9754090778
C86	6.6521679462	2.8580878845	7.2237262501
O87	5.5344030079	2.9431355256	6.6971055341
O88	7.2954268183	1.7645102978	7.4982185664
C89	11.5816617008#	-0.6170834067#	3.4808991646#
H90	12.4441752181#	-1.2180927211#	3.7284029168#
H91	11.8304270752#	0.3821370063#	3.1552080772#
H92	11.1184455804	-1.0965979069	2.6073281384
C93	10.5335787863	-0.4730115378	4.5928538615
H94	9.9288728427	0.4169096325	4.3798024084
H95	10.9978157404	-0.2856716755	5.5674155745
C96	9.5901921727	-1.6757155334	4.6643780227
H97	10.0904176497	-2.5222986772	5.1562205201
H98	9.3336788775	-2.0232039658	3.6592755086
C99	8.2750227454	-1.3720990049	5.3706896159
O100	7.2375142948	-1.8376021909	4.8193075477
O101	8.3151475701	-0.6869300592	6.4472416668
C102	10.8187241880#	4.2285681597#	-0.8150213996#
H103	11.5403644085#	3.4839224127#	-0.5131309584#
H104	11.2010929081#	5.2306259413#	-0.6882232618#
H105	10.6794883404	4.1029232326	-1.8964690970
C106	9.4748431992	3.9860154202	-0.1030764430
H107	9.0102078136	3.0970625807	-0.5546713985
H108	8.7878299426	4.8195324159	-0.3032468728
C109	9.6048283044	3.7815306405	1.4141806375
H110	10.0680909689	4.6705859320	1.8618619113
H111	10.2809129878	2.9406931983	1.6200960854
C112	8.2793753147	3.5430787654	2.1528161472
H113	7.5936934393	4.3830317526	1.9597175788
H114	8.4692048055	3.5135362759	3.2306239434
N115	7.6516767723	2.2705409404	1.7883447067
H116	7.6978044475	1.9766474118	0.8221823638
C117	6.7610095967	1.6019733691	2.5647943893
N118	6.3515961036	2.1364965300	3.7214295809
H119	5.8994447810	1.5452647308	4.4237860845
H120	6.3105351741	3.1328734969	3.8726584687
N121	6.3033678808	0.4122392872	2.1848202743
H122	6.8696564189	-0.3018572279	1.7041240949
H123	5.5861792490	-0.0423698429	2.7752535591
C124	11.8423975860#	-5.3930894542#	7.2492548814#
H125	11.2522023258#	-5.9724612836#	6.5547079597#
H126	12.7964628978#	-5.8524491634#	7.4617421048#
H127	12.0246566922	-4.3993950193	6.8273387487
C128	11.1438578467	-5.3139775152	8.6217008818
H129	11.8237547229	-4.8340543654	9.3404548593
H130	10.9863045883	-6.3353124563	8.9951192076
C131	9.8380033179	-4.5854361423	8.6490095951
N132	8.9729821909	-4.6645927269	9.7370293987
C133	9.2400692874	-3.7105531166	7.7853790691
H134	9.5628850514	-3.3537878411	6.8250233242
C135	7.9076928943	-3.8723339899	9.5341952371
H136	7.0811411303	-3.7041298843	10.2078831030
N137	8.0593398420	-3.2829146534	8.3552755597
H138	7.3347749054	-2.6259455359	7.9262882343
C139	6.0989355780#	-4.2351880402#	-1.2221969304#
H140	5.3833633678#	-4.5684340417#	-1.9592873380#
H141	7.1094170473#	-4.1301812586#	-1.5886719422#
H142	5.7985266320	-3.2110508994	-0.9653142348
C143	5.9903577982	-5.0711859826	0.0705112014
H144	5.9462620587	-6.1440210267	-0.1444026265
H145	6.8721946971	-4.8803626181	0.6946043227
C146	4.7531881911	-4.6410118723	0.8815578960
O147	4.7559852088	-3.4474294085	1.3057764208
O148	3.8107675120	-5.4726701967	1.0641211602
C149	-1.8288750596#	-11.9867171664#	4.2485687038#
H150	-2.3586934181#	-12.7180950354#	3.6563001832#
H151	-2.3284065913#	-11.7832504187#	5.1842337752#
H152	-0.8579059807	-12.4265135155	4.5142707877
C153	-1.6173138759	-10.6702565181	3.4601736551
H154	-2.4981033023	-10.4810567963	2.8301370057
H155	-1.5634860202	-9.8298078160	4.1632016367
C156	-0.3485894031	-10.6773601005	2.5862128074
H157	0.5326938119	-10.57932923670	3.2364321065
H158	-0.2523847093	-11.6603404901	2.1036666828
C159	-0.3092758739	-9.6230341476	1.4631681446
H160	0.6022657625	-9.7603370126	0.8655708350
H161	-1.1487732178	-9.8193005107	0.7814947005
C162	-0.4097225158	-8.1414678574	1.8451044008
H163	-0.5821091204	-7.5485900299	0.9427633808
H164	-1.2405697646	-7.9488171196	2.5296941032
N165	0.8186732597	-7.5615986286	2.4746947382
H166	0.8680647948	-6.5240905546	2.2031981632
H167	0.8222963424	-7.6069990350	3.5112955709

H168	1.7065327269	-7.9571870613	2.0928406465
C169	-1.8652228158#	-2.8063899723#	9.6692394734#
H170	-2.8449961107#	-3.2600297460#	9.6435887468#
H171	-1.9204754843#	-1.8064531627#	10.0735583360#
H172	-1.2272832252	-3.4201294979	10.3179557225
C173	-1.3545494620	-2.7827197178	8.2146022174
H174	-0.2767700701	-2.5824962571	8.2045323606
C175	-2.0494979987	-1.6686781254	7.4172976151
H176	-1.8103824354	-0.6794436217	7.8291550554
H177	-3.1418747721	-1.7886819253	7.4435464932
H178	-1.7415300671	-1.6759464430	6.3658304475
C179	-1.5832492497	-4.1477905039	7.5539836997
H180	-1.0650808914	-4.9509900940	8.0903518253
H181	-1.2187974558	-4.1587914359	6.5236797146
H182	-2.6548350048	-4.3930395004	7.5372216616
C183	0.8676053674	-6.9177848470	5.6013589132
O184	1.1900705943	-1.7433743965	4.6537927504
H185	1.2098401191	-2.5014506569	5.2971719993
O186	4.7521626472	-1.2025253998	3.7732603808
O187	7.1882272525	-2.1836957497	1.8249047979
H188	7.1097341200	-2.1953977675	2.7974005110
H189	6.3342038341	-2.5987703974	1.5367398443
O190	-0.9396618905	1.7663533986	5.2150551695
H191	-1.1128382745	1.0202730011	4.5813559200
H192	-1.6931415103	1.7433030661	5.8245497480
O193	3.0816305694	3.2137591658	8.2600449344
H194	3.9133342482	3.4247824111	8.7243932823
H195	2.5748830825	2.7073464572	8.9251811526
O196	5.3858246479	2.5637794949	10.0175515734
H197	5.3362170210	1.7160337776	9.5228429855
H198	5.9546297986	2.3668809195	10.7856169541
O199	2.7053680549	-1.8510279753	2.2445423991
H200	3.4118157020	-2.4979475412	1.9610368240
H201	1.2178818395	-4.6580573285	6.2550321788
O202	1.0424771934	-5.1789105994	1.3289002136
H203	2.0180465497	-5.0532009790	1.2628158157
H204	0.6627396601	-4.3301184330	1.6656275098
O205	0.1049949365	-2.6852891463	2.1624322141
H206	0.9544922560	-2.2625964326	1.8926836429
H207	0.2435336447	-2.6719611907	3.1315660330
O208	3.3005003859	-8.1191691566	1.22806866053
H209	3.5620593267	-7.1780983559	1.0298588378
H210	4.0710922519	-8.4988484861	1.6746325497
O211	1.3316140561	-3.7304952304	6.5543129392
H212	2.2552289103	-3.6370968111	6.8315368887
H213	9.1115053298	-5.2391183675	10.5581907693
O214	1.2258053261	0.5372511828	6.3888202691
H215	0.4584033902	1.0667233807	6.0560350702
H216	1.1876925086	-0.3024494682	5.8750343749
O217	-1.1321031816	-0.5486857329	3.8544165946
H218	-1.1615245499	-0.8864220715	2.9427156567
H219	-0.2953188007	-0.9412624292	4.2013560727

Structure used in Fig 3:

Mn1	3.0272218386	-1.4836476192	3.6742911793
Mn2	4.6006557222	-1.4779100989	8.61925550942
Mn3	5.3008039940	-1.5296078587	5.2571033586
Mn4	6.5938269270	-0.0486226414	7.3002445347
O5	3.6026720474	-1.2561899256	5.5802417196
O6	5.7876413736	0.1962520897	5.7392685599
O7	5.0861991044	0.2788432663	8.2802933840
O8	5.9464235148	-1.8211502851	7.2802289928
Ca9	3.3846612275	1.3304473921	6.8840764995
C10	0.6675458165#	1.9515084173#	1.7063477084#
H11	1.2251835742#	1.9058029389#	0.7825776968#
H12	-0.3243896358#	2.3686418809#	1.6143240713#
H13	0.4729291364	0.8917272920	1.9236168459
C14	1.4952507817	2.4904089061	2.8854958620
H15	0.8387109258	2.8533956270	3.6842185085
H16	2.1188204126	3.3482256672	2.6035106111
C17	2.4268785988	1.4840980625	3.6041238205
O18	3.0406290349	1.8814239941	4.6160595476
O19	2.4989278476	0.3047200369	3.1028536200
C20	1.0582598970#	1.1829962110#	13.4563132843#
H21	0.3702238907#	0.3601390909#	13.5824629993#
H22	0.7336467761#	2.1291270612#	13.8635786785#
H23	1.9508247029	0.9064820739	14.0376706895
C24	1.4465897117	1.2921957941	11.9860341927
H25	2.2488725126	2.0281235502	11.8545339857
H26	0.6025788550	1.6378235849	11.3770629440
C27	1.9193045892	-0.0744007283	11.5032458343
H28	1.0746621505	-0.7772933128	11.4437237679
H29	2.6194589135	-0.5163305877	12.2225626827
C30	2.6067904552	-0.0622698005	10.1583837559
O31	2.4726071395	0.8818550023	9.3690658421
O32	3.3153024580	-1.1334873798	9.9547866972
C33	2.7844501128#	-7.8608079441#	8.6257439128#
H34	2.4765599527	-8.8267443210	9.0453674137
H35	1.9469460097	-7.4708220283	8.0414063580
C36	4.0067095334	-8.0832115829	7.7352286779

O37	5.1363386837	-8.2763265637	8.2337620347
C38	3.1254320407	-6.9128911438	9.8107562297
H39	3.8513560335	-7.4195828728	10.4580275456
H40	2.2225505803	-6.7397908643	10.4035895369
C41	3.6843470324	-5.5932567488	9.3624185052
N42	4.7839216249	-5.5774663613	8.5212275678
H43	5.2925263540	-6.4254186791	8.2632429384
C44	3.3235413645	-4.2724540783	9.4910732992
H45	2.5247283705	-3.8258594272	10.0613864554
C46	5.0146556578	-4.3223168689	8.1246168440
H47	5.7258438167	-4.0401600198	7.3714580355
N48	4.1658974487	-3.4905853313	8.7148736897
N49	3.8114778243	-7.9240466791	6.4173398563
H50	2.8597683184	-7.7071475681	6.0895404711
C51	4.9172533283#	-7.8463448436#	5.4688658747#
H52	4.6285743646	-8.4013837173	4.5668743456
H53	5.7731942401	-8.3534406017	5.9181626592
C54	5.2952861876	-6.3950660345	5.0884104844
H55	6.1590158571	-6.4308166640	4.4114190076
H56	5.6397867874	-5.8774305270	5.9866275290
C57	4.1483215660	-5.6061108355	4.4365730030
H58	3.1860149936	-5.8706850139	4.8927769095
H59	4.0380815221	-5.8506860556	3.3721898347
C60	4.2273802902	-4.0889567227	4.5076576509
O61	3.2268065657	-3.4721192042	4.0197495560
O62	5.2083283245	-3.5240540098	5.0781788450
C63	9.1595116866#	0.1191580117#	11.4478229222#
H64	9.8172505654	-0.1350967252	10.6094885811
H65	9.7389396804	-0.0259366426	12.3704000261
C66	7.9396602497	-0.7942075585	11.4731842869
H67	7.2227741365	-0.4409586402	12.2211733583
H68	8.2321682470	-1.8057358626	11.7839070651
C69	7.1801847967	-0.9273594076	10.1529591104
O70	7.6301723836	-0.3291596979	9.1301317684
O71	6.1587422171	-1.6749477279	10.1844356322
C72	8.7835221863	1.5976205621	11.3851516354
O73	7.6903428141	2.0165702725	11.7781169287
N74	9.7698642622	2.4259096616	10.9534140228
H75	10.5706589118	2.0140881199	10.4928239407
C76	9.5677774979#	3.8588146911#	10.7651887005#
H77	10.4973795473	4.3871435541	10.9854261256
H78	8.7889357950	4.1723078129	11.4636640733
C79	9.1921065551	4.1684496360	9.2972750497
O80	10.0540406358	4.5140772942	8.4929388905
N81	7.8795859408	3.9962907388	8.9873634909
H82	7.2352837583	3.5920490342	9.6621914291
C83	7.3836796048	4.0880060940	7.6257722681
H84	6.6876021786	4.9258671688	7.5152482707
H85	8.2518765904	4.2593939905	6.9810238726
C86	6.6463880469	2.8119634079	7.1849111107
O87	5.5325831476	2.8966443276	6.6535992941
O88	7.3014884884	1.7172150335	7.4220540565
C89	11.5816617284#	-0.6170834036#	3.4808991683#
H90	12.4441752209#	-1.2180927203#	3.7284029092#
H91	11.8304270711#	0.3821370059#	3.1552080731#
H92	11.1245070809	-1.0953132814	2.6030622561
C93	10.5280394795	-0.4808774609	4.5826181383
H94	9.8939325473	0.3818175197	4.3440621226
H95	10.9788539492	-0.2557384378	5.5553481656
C96	9.6315174942	-1.7170850500	4.6746521782
H97	10.1559505771	-2.5232771177	5.2057200355
H98	9.4071478987	-2.1044983307	3.6767620392
C99	8.2987303167	-1.4246180177	5.3448263466
O100	7.2766862780	-1.8820266457	4.7634429044
O101	8.3047015554	-0.7464496721	6.4233856566
C102	10.8187241892#	4.2285681673#	-0.8150213986#
H103	11.5403644067#	3.4839224114#	-0.5131309573#
H104	11.2010929108#	5.2306259410#	-0.6882232677#
H105	10.6705784665	4.0999726464	-1.8948289515
C106	9.4844799145	4.0001064630	-0.0856248927
H107	9.0295608829	3.0873792972	-0.4979145011
H108	8.7854219071	4.8161794877	-0.3140172222
C109	9.6350354830	3.8629370957	1.4375919937
H110	10.0723377318	4.7837484696	1.8449488242
H111	10.3386170716	3.0519696408	1.6690404510
C112	8.3222159068	3.6055119813	2.1910926790
H113	7.6196613744	4.4329323567	2.0051501420
H114	8.5230147044	3.5763778403	3.2674857784
N115	7.7237850193	2.3252018957	1.8152152813
H116	7.7937941901	2.0422710657	0.8476177196
C117	6.8113735851	1.6386978045	2.5482133342
N118	6.3381930860	2.1415890376	3.6925662647
H119	5.9106696059	1.5216591434	4.3886159211
H120	6.4007402326	3.1197301895	3.9270671759
N121	6.3774881923	0.4586176927	2.1116024290
H122	6.9702527433	-0.2306524479	1.6318758472
H123	5.6532673064	-0.0343895843	2.6615160308
C124	11.8423976049#	-5.3930894674#	7.2492548871#
H125	11.2522023171#	-5.9724612784#	6.5547079627#
H126	12.7964629013#	-5.8524491602#	7.4617420964#
H127	12.0251146396	-4.4003852903	6.8247856490
C128	11.1339896786	-5.3090028910	8.6173627424
H129	11.7996541683	-4.8067248535	9.3340035721

H130	10.9931871906	-6.3284623002	9.0021959947
C131	9.8123048223	-4.6064820535	8.6273222021
N132	8.9287633122	-4.7099637919	9.6990839788
C133	9.2121879005	-3.7361045514	7.7608105351
H134	9.5460563532	-3.3640446727	6.8106337758
C135	7.8510448995	-3.9378038868	9.4852768621
H136	7.0157175753	-3.7821164277	10.1506855422
N137	8.0119279450	-3.3382369874	8.3118996852
H138	7.2953943347	-2.6838905990	7.8808085706
C139	6.0989355787#	-4.2351880641#	-1.2221969393#
H140	5.3833633621#	-4.5684340300#	-1.9592873376#
H141	7.1094170487#	-4.1301812536#	-1.5886719370#
H142	5.7921648842	-3.2306445723	-0.9108025151
C143	6.0548632935	-5.1593704873	0.0132706193
H144	6.0031878642	-6.2141474712	-0.2760801671
H145	6.9649742807	-5.0068913200	0.6066558344
C146	4.8652503075	-4.7766973431	0.8960879862
O147	4.9028537824	-3.6025254552	1.3658397547
O148	3.9234322172	-5.6040455289	1.0888595523
C149	-1.8288749940#	-11.9867172644#	4.2485686955#
H150	-2.3586934525#	-12.7180950344#	3.6563002127#
H151	-2.3284066229#	-11.7832503685#	5.1842337475#
H152	-0.8543224556	-12.4214644667	4.5095185485
C153	-1.6310500286	-10.6619619589	3.4723513567
H154	-2.5422416493	-10.4423240182	2.8972460929
H155	-1.5173408149	-9.8379536830	4.1876748629
C156	-0.4134486296	-10.6759720776	2.5300032506
H157	0.5040911177	-10.5925888015	3.1307656932
H158	-0.3551394507	-11.6550690486	2.0323623207
C159	-0.4246861716	-9.6099814472	1.4163530419
H160	0.4474201182	-9.7572796767	0.7646588175
H161	-1.3065073745	-9.7860422754	0.7835550661
C162	-0.4761816961	-8.1289787112	1.8139056184
H163	-0.6712588076	-7.5275694247	0.9210418910
H164	-1.2765132010	-7.9248278326	2.5308747564
N165	0.7881777194	-7.5854058466	2.4033904786
H166	0.8795854319	-6.5487975044	2.1259919271
H167	0.8134278865	-7.6267470534	3.4424590084
H168	1.6528811973	-8.0190543552	2.0098901189
C169	-1.8652229577#	-2.8063899293#	9.6692394302#
H170	-2.8449969096#	-3.2600297918#	9.6435887901#
H171	-1.9204754493#	-1.8064531710#	10.0735583614#
H172	-1.2361064219	-3.4225041078	10.3236940872
C173	-1.3272230883	-2.7726106774	8.2252238454
H174	-0.2335173390	-2.6527171766	8.2608313649
C175	-1.9228030336	-1.5876247087	7.4504097132
H176	-1.7432566630	-0.6372515295	7.9703621019
H177	-3.0103241884	-1.7023216093	7.3454902590
H178	-1.4916202103	-1.4954028898	6.4482682913
C179	-1.6120639295	-4.0974066449	7.5067187376
H180	-1.1386199075	-4.9457070460	8.0148714154
H181	-1.2419024870	-4.0762596973	6.4786883757
H182	-2.6933557326	-4.2891649046	7.4726799570
C183	0.8190664933	-7.0614303663	5.5658865683
O184	1.2056254718	-1.6910017694	4.1616081735
H185	1.0813360457	-2.4156267690	4.8111413699
O186	4.8932736989	-1.2816824051	3.5604669488
O187	7.2931027136	-2.1674594192	1.7686555394
H188	7.2043449318	-2.1607469539	2.7399134726
H189	6.4592696725	-2.6282509413	1.4983433932
O190	0.9630378325	1.8661328919	7.0150614669
H191	0.4788978513	1.4180498229	6.2726152922
H192	0.7168302838	1.3614070660	7.8064929287
O193	3.3074587182	3.3135168727	8.4912702023
H194	4.1089384460	3.3038395731	9.0540147060
H195	2.6283372527	2.9447239529	9.0820554129
O196	5.4808953657	2.4372684481	10.0645551880
H197	5.4316579772	1.6036472329	9.5436699474
H198	6.0459445023	2.2354549537	10.8351808133
O199	2.8929908035	-1.9142594143	1.9513947582
H200	3.5908292048	-2.6052777709	1.7606263209
H201	0.9042699908	-4.7295061523	6.0275645660
O202	1.1491993096	-5.2058651013	1.3120442076
H203	2.1272978042	-5.1064417355	1.2762209298
H204	0.7685514330	-4.3147255089	1.5433074341
O205	0.2540452721	-2.6586477890	1.7249093191
H206	1.1112513606	-2.3007680619	1.4072261688
H207	0.3499671595	-2.4089517410	2.6716608130
O208	3.3136769786	-8.2265983409	1.2633930361
H209	3.6033726609	-7.2991079724	1.0528110090
H210	3.9997437732	-8.5607362259	1.8602770615
O211	1.3076401575	-3.8382116433	6.1056226126
H212	2.0532887337	-3.8858105188	5.4828965769
H213	9.0636942681	-5.2906027108	10.5165935382
O214	1.9682672978	-0.9167043000	7.3873493196
H215	1.1958282398	-1.3707015539	7.7554419797
H216	2.2801963090	-1.4598882347	6.6322117609
O217	-0.1375794644	0.4444354704	5.0026804743
H218	-0.8802783738	0.5685366403	4.3871607186
H219	0.3750103492	-0.3515542836	4.6741799011

Structure used in Fig 4:

Mn1	2.9719376998	-1.4355953386	3.7671020812
Mn2	4.5203306698	-1.5627566785	8.7122932306
Mn3	5.2452537718	-1.4878341245	5.3593070262
Mn4	6.5512690570	-0.0722443438	7.4076689377
O5	3.5338751108	-1.0611249694	5.6572289140
O6	5.7817002436	0.2158398333	5.8126939212
O7	5.0166801004	0.2308416602	8.3343860768
O8	5.8924067737	-1.8355394023	7.3452801823
Ca9	3.6215080174	1.3712716745	6.6410715767
C10	0.6675457617#	1.9515086227#	1.7063475732#
H11	1.2251835950#	1.9058028567#	0.7825777133#
H12	-0.3243896670#	2.3686418077#	1.6143240750#
H13	0.4737573006	0.8995201806	1.9483565768
C14	1.4805180479	2.5231155451	2.8725520436
H15	0.8056987986	2.8081002258	3.6898169228
H16	2.0352956296	3.4311880053	2.6081105104
C17	2.4835453918	1.5689541915	3.5495459746
O18	3.2570717247	2.0453901088	4.4098842130
O19	2.4199301634	0.3333464319	3.1996274384
C20	1.0582598554#	1.1829962476#	13.4563133666#
H21	0.3702239074#	0.3601390786#	13.5824630085#
H22	0.7336467811#	2.1291270665#	13.8635786702#
H23	1.9541186915	0.9013363490	14.0286475595
C24	1.4331549623	1.2636692165	11.9703959743
H25	2.3291475907	1.8826878172	11.8352356947
H26	0.6353448510	1.7337920563	11.3837601199
C27	1.6924166573	-0.1602751745	11.4542323256
H28	0.7342492303	-0.6746630023	11.2908784579
H29	2.2356773175	-0.7413812918	12.2062626875
C30	2.4781987526	-0.2398598117	10.1610795188
O31	2.2609675296	0.5285216184	9.2079013675
O32	3.3792844858	-1.1734876191	10.1758521697
C33	2.7844500817#	-7.8608080040#	8.6257439553#
H34	2.3663153730	-8.8231035211	8.9487179254
H35	2.0050243704	-7.3492154728	8.0570246178
C36	4.0075059789	-8.1303812672	7.7360641249
O37	5.1295800316	-8.3656473266	8.2377738615
C38	3.1813311927	-7.0569265302	9.8951601375
H39	3.8731355609	-7.6654256208	10.4894701008
H40	2.2901800946	-6.8829827238	10.5057441327
C41	3.8143295165	-5.7377447003	9.5552248940
N42	4.9069262123	-5.7172307278	8.7047285167
H43	5.3754777956	-6.5723572574	8.3947676511
C44	3.5016455845	-4.4126819000	9.7569254506
H45	2.7200915483	-3.9661806312	10.3517589689
C46	5.1699660648	-4.4490230757	8.3635293324
H47	5.8590067890	-4.1594420866	7.5928579470
N48	4.3615331529	-3.6241206387	9.0095993161
N49	3.8166247342	-7.9675145970	6.4182317318
H50	2.8584386987	-7.7979178212	6.0842370644
C51	4.9172533511#	-7.8463448581#	5.4688658318#
H52	4.6347716371	-8.3724400833	4.5486787895
H53	5.7867066667	-8.3511815506	5.8948601839
C54	5.2645987396	-6.3668067102	5.1479603308
H55	6.1345712730	-6.3543789226	4.4780294818
H56	5.5861192712	-5.8814976126	6.0728234969
C57	4.1062104282	-5.5691360724	4.5213089561
H58	3.1536284803	-5.8623789704	4.9752765569
H59	3.9974458044	-5.7873546078	3.4520078672
C60	4.1592834414	-4.0485138785	4.6358286718
O61	3.1758282731	-3.4223539990	4.1231713473
O62	5.1151337054	-3.4822893110	5.2479101006
C63	9.1595117756#	0.1191580412#	11.4478229474#
H64	9.7946612802	-0.1430018458	10.5947503029
H65	9.7648363142	-0.0136219359	12.3554567781
C66	7.9413464117	-0.7879372173	11.5156143199
H67	7.2389911989	-0.4184296245	12.2694913631
H68	8.2339373865	-1.7955892172	11.8380506831
C69	7.1571279453	-0.9380132850	10.2141053114
O70	7.5900279378	-0.3356211342	9.1767544451
O71	6.1517058149	-1.6932578585	10.2629649846
C72	8.7804636823	1.5985210524	11.3750654580
O73	7.6837159230	2.0224326644	11.7528067697
N74	9.7720811165	2.4257443880	10.9507918896
H75	10.5795570201	2.0158783340	10.5001122724
C76	9.567775311#	3.8588146980#	10.7651887465#
H77	10.4931641081	4.3886282926	11.0002538707
H78	8.7806087333	4.1672532558	11.4559602061
C79	9.2077706442	4.1715383585	9.2973768278
O80	10.0743082007	4.5033902477	8.4921400575
N81	7.8925987789	4.0193368177	8.9870737758
H82	7.2503757176	3.6131017563	9.6618406917
C83	7.4133911388	4.0921549412	7.6203459000
H84	6.7304813510	4.9364120205	7.4831401497
H85	8.2893719147	4.2412203880	6.9803981670
C86	6.6641009030	2.8210222194	7.1965858239
O87	5.5875275702	2.9336496563	6.5883421744
O88	7.2520780166	1.7169894689	7.5262843771
C89	11.5816617646#	-0.6170833923#	3.4808991662#

H90	12.4441752188#	-1.2180927251#	3.7284029050#
H91	11.8304270648#	0.3821370057#	3.1552080677#
H92	11.1238578357	-1.0960601822	2.6039594879
C93	10.5214223304	-0.4862440070	4.5912181129
H94	9.9295117076	0.4159328726	4.3938167230
H95	10.9814835472	-0.3263391553	5.5727537995
C96	9.5576505917	-1.6783344701	4.6329243590
H97	10.0514855025	-2.5517161555	5.0840128002
H98	9.2855517426	-1.9849766016	3.6186078978
C99	8.2481381746	-1.4030614339	5.3703688202
O100	7.2075836789	-1.8693949329	4.8177883432
O101	8.2836353057	-0.7555751578	6.4667302234
C102	10.8187242272#	4.2285682079#	-0.8150214087#
H103	11.5403643946#	3.4839224013#	-0.5131309534#
H104	11.2010929240#	5.2306259395#	-0.6882232947#
H105	10.6741116539	4.1022838973	-1.8955266304
C106	9.4833029519	3.9917370508	-0.0906944692
H107	9.0141180849	3.1002746941	-0.5323265024
H108	8.7933012746	4.8238785138	-0.2858886319
C109	9.6391254591	3.7956951433	1.4243295295
H110	10.0940103378	4.6931656962	1.8633998855
H111	10.3315688232	2.9661105617	1.6212038974
C112	8.3284640872	3.5326485363	2.1766337453
H113	7.6312815959	4.3691991012	2.0117966746
H114	8.5330489664	3.4795198911	3.2508690784
N115	7.7133360772	2.2629160809	1.7856926515
H116	7.7525834759	1.9972669944	0.8111994692
C117	6.8223230231	1.5767890715	2.5438909559
N118	6.4150522164	2.0822902922	3.7133699865
H119	5.9757823217	1.4780277988	4.4130218607
H120	6.4000481735	3.0729954536	3.9019375570
N121	6.3631556171	0.3987509598	2.1296557854
H122	6.9363755121	-0.3091995932	1.6494534887
H123	5.6432827964	-0.0672883653	2.7068415095
C124	11.8423976533#	-5.3930895048#	7.2492548963#
H125	11.2522022958#	-5.9724612654#	6.5547079700#
H126	12.7964629093#	-5.8524491526#	7.4617420769#
H127	12.0243550958	-4.3992262568	6.8276528987
C128	11.1473997624	-5.3148350799	8.6219584950
H129	11.8278367795	-4.8339733361	9.3396380055
H130	10.9908739723	-6.3361580706	8.9959649934
C131	9.8423660477	-4.5874919362	8.6487936597
N132	8.9894759557	-4.6498601366	9.7474570527
C133	9.2355116582	-3.7279397876	7.7769059625
H134	9.5511642965	-3.3810670978	6.8104995936
C135	7.9204428859	-3.8652457429	9.5446217594
H136	7.0987695830	-3.6871074170	10.2218109527
N137	8.0604581337	-3.2934413509	8.3546934686
H138	7.3337275147	-2.6603875455	7.9252007430
C139	6.0989356442#	-4.2351880738#	-1.2221969734#
H140	5.3833633461#	-4.5684340249#	-1.9592873244#
H141	7.1094170446#	-4.1301812371#	-1.5886719436#
H142	5.7934826770	-3.2254362510	-0.9246364498
C143	6.0339198523	-5.1370065587	0.0294405594
H144	5.9777434088	-6.1963256803	-0.2417360351
H145	6.9393010046	-4.9840067019	0.6300274478
C146	4.8382432131	-4.7421578646	0.9052811651
O147	4.8684893545	-3.5640677628	1.3699105083
O148	3.9017743975	-5.5751859849	1.1039179631
C149	-1.8288751269#	-11.9867172682#	4.2485686461#
H150	-2.3586934077#	-12.7180950951#	3.6563002476#
H151	-2.3284065653#	-11.7832503397#	5.1842337719#
H152	-0.8577218159	-12.4270703248	4.5131750915
C153	-1.6138315369	-10.6716931730	3.4659738285
H154	-2.5435057309	-10.4085853461	2.9403500694
H155	-1.4199640337	-9.8564275202	4.1742057035
C156	-0.4515332537	-10.7492529253	2.4587136119
H157	0.4995146387	-10.7216641600	3.0093390714
H158	-0.4749130768	-11.7267478746	1.9559470500
C159	-0.4599778207	-9.6775778168	1.3516624368
H160	0.3744872763	-9.8610108675	0.6605994504
H161	-1.3765393321	-9.8017466160	0.7579900462
C162	-0.4183848153	-8.2048689804	1.7741841533
H163	-0.5932438259	-7.5722762385	0.8987603833
H164	-1.1917506639	-7.9689395897	2.5105408410
N165	0.8805944472	-7.7577795095	2.3580689936
H166	0.9637447307	-6.6881534613	2.2866613859
H167	0.9518340585	-7.9585965702	3.3731765284
H168	1.7181746522	-8.1179453131	1.8474487943
C169	-1.8652232051#	-2.8063899173#	9.6692393484#
H170	-2.8449960720#	-3.2600298368#	9.6435888750#
H171	-1.9204753647#	-1.8064531757#	10.0735583848#
H172	-1.2480835132	-3.4134999847	10.3444394391
C173	-1.2882311515	-2.8118474364	8.2426380562
H174	-0.2122361859	-2.5975253455	8.2886923416
C175	-1.9375099568	-1.7182380893	7.3832913572
H176	-1.7780373532	-0.7219545171	7.8152822959
H177	-3.0209077303	-1.8747107757	7.2934430658
H178	-1.5121102421	-1.7217458375	6.3719522197
C179	-1.4809209151	-4.1911574005	7.6003073753
H180	-0.9978726474	-4.9803173047	8.1896636022
H181	-1.0563645835	-4.2242643022	6.5944964140
H182	-2.5492107450	-4.4380823079	7.5314871070

Cl183	0.8199073959	-7.4450790818	5.4993788068
O184	1.1496633206	-1.6883792955	4.2562285464
H185	1.0921370926	-2.3087161116	5.0055533508
O186	4.8370553382	-1.2707680984	3.6559610916
O187	7.2596369232	-2.2023016812	1.8145160652
H188	7.1496300927	-2.1913944846	2.7842241550
H189	6.4285861152	-2.6569131050	1.5219485765
O190	1.2122212907	1.2819780583	6.8326837195
H191	0.5625553841	0.9895178407	6.1344625335
H192	1.0302991442	0.7809748925	7.6459540194
O193	3.1966173650	3.0311000363	8.4707104262
H194	3.9572963802	3.1249596325	9.0811823962
H195	2.5649633807	2.4851703458	8.9772892505
O196	5.4017167404	2.3990997054	10.0839000624
H197	5.3580101104	1.5545948367	9.5801756479
H198	5.9982478895	2.2240758371	10.8363501911
O199	2.8477756348	-1.8786471498	2.0443306739
H200	3.5475063799	-2.5618440182	1.8392528722
H201	0.9985713326	-5.1590306354	6.0679380275
O202	1.3438902943	-5.1793050225	2.0962207774
H203	2.2572245657	-5.0762404941	1.7461434735
H204	0.8549261913	-4.3259089708	1.9540727276
O205	0.2245883351	-2.7132964787	1.8160107792
H206	1.0777249185	-2.3243206230	1.5259937659
H207	0.2722791223	-2.4516365085	2.7618624160
O208	3.2971354159	-8.2092881184	0.9353364468
H209	3.5738438840	-7.2564865778	0.8520387857
H210	4.0040425177	-8.6142470385	1.4593748721
O211	1.3748114461	-4.2532133153	6.0759346519
H212	1.7831309938	-4.1729828462	5.1940734823
H213	9.1361455401	-5.2124465924	10.5753916428
O214	2.4394969960	-2.1184297986	7.7023601433
H215	2.1839297129	-3.0283666835	7.4366717093
H216	2.6747512531	-1.6998806214	6.8279013713
O217	-0.3377814085	0.4629460317	4.8256299514
H218	-1.2106100849	0.1097311374	5.0547382459
H219	0.2033647257	-0.3257686062	4.5307963430

Structure used in Fig 5 (the same atoms are frozen):

Mn1	3.0916990000	-1.4644540000	3.7582700000
Mn2	4.4225500000	-1.2965850000	9.1511880000
Mn3	5.3415790000	-1.5469290000	5.3930810000
Mn4	6.6191880000	-0.1220860000	7.4086280000
O5	3.5989050000	-1.1898500000	5.6655650000
O6	5.8295760000	0.1802450000	5.8216430000
O7	5.1444210000	0.2843610000	8.3769150000
O8	6.0205860000	-1.8289240000	7.3046050000
Ca9	3.8143040000	1.3715530000	6.6161370000
C10	0.6675460000	1.9515080000	1.7063480000
H11	1.2251840000	1.9058030000	0.7825780000
H12	-0.3243900000	2.3686420000	1.6143240000
H13	0.4748430000	0.8952810000	1.9404300000
C14	1.4715480000	2.5251930000	2.8780840000
H15	0.7899740000	2.8374120000	3.6803940000
H16	2.0363380000	3.4256200000	2.6066960000
C17	2.4660260000	1.5849970000	3.5929780000
O18	3.1594350000	2.0934070000	4.5064460000
O19	2.4942350000	0.3589240000	3.2308330000
C20	1.0582600000	1.1829960000	13.4563130000
H21	0.3702240000	0.3601390000	13.5824630000
H22	0.7336470000	2.1291270000	13.8635790000
H23	2.0343900000	0.9055190000	13.8681030000
C24	1.0755430000	1.3643610000	11.9216030000
H25	1.8998980000	2.0031940000	11.5880200000
H26	0.1496540000	1.8849440000	11.6452600000
C27	1.1191420000	0.0200210000	11.1720300000
H28	0.5823860000	0.1092620000	10.2162270000
H29	0.6205980000	-0.7723870000	11.7395870000
C30	2.5099380000	-0.4327490000	10.7823170000
O31	3.2497280000	0.4118950000	10.1669370000
O32	2.8971920000	-1.6182570000	10.9348700000
C33	2.7844500000	-7.8608080000	8.6257440000
H34	2.4431740000	-8.8410200000	8.9828500000
H35	1.9642060000	-7.4257830000	8.0464800000
C36	4.0143800000	-8.0647780000	7.7373190000
O37	5.1516070000	-8.1915190000	8.2364110000
C38	3.1212720000	-6.9903730000	9.8736280000
H39	3.8454310000	-7.5441090000	10.4837660000
H40	2.2157320000	-6.8694870000	10.4760610000
C41	3.6767360000	-5.6291180000	9.5467360000
N42	4.7126660000	-5.5201530000	8.6361910000
H43	5.2185230000	-6.3285780000	8.2759930000
C44	3.3860160000	-4.3286520000	9.9016200000
H45	2.6499270000	-3.9375190000	10.5853580000
C46	4.9789480000	-4.2231100000	8.4300530000
H47	5.6234750000	-3.8669040000	7.6517120000
N48	4.2171220000	-3.4623510000	9.2024840000
N49	3.8125020000	-7.9758670000	6.4120960000
H50	2.8522110000	-7.8647600000	6.0553240000

C51	4.9172530000	-7.8463450000	5.4688660000
H52	4.6390370000	-8.3734960000	4.5484840000
H53	5.7884490000	-8.3445130000	5.8991680000
C54	5.2570560000	-6.3687050000	5.1535620000
H55	6.1155930000	-6.3482810000	4.4692070000
H56	5.5923280000	-5.8822900000	6.0736850000
C57	4.0880820000	-5.5755230000	4.5471800000
H58	3.1414870000	-5.8371810000	5.0378060000
H59	3.9441980000	-5.8184170000	3.4872470000
C60	4.1921160000	-4.0568330000	4.6177460000
O61	3.2640460000	-3.4209130000	4.0362190000
O62	5.1482650000	-3.5183410000	5.2579410000
C63	9.1595120000	0.1191580000	11.4478230000
H64	9.7626090000	-0.1396350000	10.5717720000
H65	9.7840190000	-0.0451290000	12.3364210000
C66	7.9230000000	-0.7712580000	11.5357170000
H67	7.2561630000	-0.4298650000	12.3319200000
H68	8.2148890000	-1.7990110000	11.7901970000
C69	7.1070080000	-0.8370230000	10.2492640000
O70	7.6219850000	-0.4035960000	9.1886480000
O71	5.9641120000	-1.4014140000	10.3597670000
C72	8.7904660000	1.6018530000	11.4160170000
O73	7.7086580000	2.0117100000	11.8423370000
N74	9.7693600000	2.4265090000	10.9604200000
H75	10.5576490000	2.0131980000	10.4796360000
C76	9.5677770000	3.8588150000	10.7651890000
H77	10.4702310000	4.3977970000	11.0625750000
H78	8.7334420000	4.1566880000	11.4027830000
C79	9.3090160000	4.1500090000	9.2758270000
O80	10.2433780000	4.3910750000	8.5153890000
N81	8.0075700000	4.0714220000	8.8999620000
H82	7.3036270000	3.7000780000	9.5388710000
C83	7.6129340000	4.0771710000	7.5045480000
H84	6.9909700000	4.9474120000	7.2714540000
H85	8.5300110000	4.1222880000	6.9080760000
C86	6.8131870000	2.8137970000	7.1529540000
O87	5.7120190000	2.9459030000	6.5780620000
O88	7.3655390000	1.7074750000	7.4992100000
C89	11.5816620000	-0.6170840000	3.4808990000
H90	12.4441750000	-1.2180930000	3.7284030000
H91	11.8304270000	0.3821370000	3.1552080000
H92	11.1225310000	-1.0974230000	2.6052580000
C93	10.5291820000	-0.4716040000	4.5824490000
H94	9.8894640000	0.3829580000	4.3294980000
H95	10.9798410000	-0.2284610000	5.5505390000
C96	9.6426650000	-1.7130040000	4.6972520000
H97	10.1883460000	-2.5042980000	5.2279790000
H98	9.4031400000	-2.1072790000	3.7056210000
C99	8.3239140000	-1.4252430000	5.3982480000
O100	7.2911280000	-1.9038780000	4.8394070000
O101	8.3470820000	-0.7393330000	6.4658700000
C102	10.8187240000	4.2285680000	-0.8150210000
H103	11.5403640000	3.4839220000	-0.5131310000
H104	11.2010930000	5.2306260000	-0.6882230000
H105	10.6605360000	4.0997230000	-1.8930330000
C106	9.4990630000	3.9988860000	-0.0643000000
H107	9.0350290000	3.0888330000	-0.4717880000
H108	8.7952820000	4.8171290000	-0.2687000000
C109	9.6963220000	3.8498300000	1.4506670000
H110	10.1292310000	4.7739020000	1.8550100000
H111	10.4210460000	3.0493290000	1.6510470000
C112	8.4139270000	3.5575050000	2.2373460000
H113	7.6891500000	4.3733000000	2.0884620000
H114	8.6468380000	3.5112850000	3.3060760000
N115	7.8277710000	2.2720070000	1.8585770000
H116	7.8386870000	2.0203520000	0.8799410000
C117	6.9781550000	1.5537770000	2.6319140000
N118	6.5853300000	2.0254820000	3.8188530000
H119	6.1997940000	1.3835140000	4.5235780000
H120	6.5722190000	3.0089400000	4.0418170000
N121	6.5389890000	0.3697900000	2.2111920000
H122	7.1052040000	-0.3127960000	1.6936940000
H123	5.8138230000	-0.1130070000	2.7677620000
C124	11.8423980000	-5.3930890000	7.2492550000
H125	11.2522020000	-5.9724610000	6.5547080000
H126	12.7964630000	-5.8524490000	7.4617420000
H127	12.0286400000	-4.4049360000	6.8144700000
C128	11.1319330000	-5.2806700000	8.6126410000
H129	11.7927190000	-4.7447380000	9.3092380000
H130	11.0040320000	-6.2878760000	9.0333410000
C131	9.8055350000	-4.5867740000	8.5991340000
N132	9.0086120000	-4.4967660000	9.7373100000
C133	9.1282530000	-3.8817890000	7.6424350000
H134	9.3746830000	-3.7133950000	6.6107310000
C135	7.9114120000	-3.7673070000	9.4694390000
H136	7.1164010000	-3.5273850000	10.1595780000
N137	7.9744560000	-3.3772020000	8.2041390000
H138	7.2256370000	-2.7308540000	7.7376870000
C139	6.0989350000	-4.2351880000	-1.2221970000
H140	5.3833630000	-4.5684340000	-1.9592870000
H141	7.1094170000	-4.1301810000	-1.5886720000
H142	5.7967000000	-3.2230750000	-0.9292710000
C143	5.9985700000	-5.1396870000	0.0278510000

H144	5.9021040000	-6.1952070000	-0.2472700000
H145	6.9042220000	-5.0229950000	0.6357750000
C146	4.8136860000	-4.6907270000	0.8965650000
O147	4.9068330000	-3.5131430000	1.3515650000
O148	3.8295660000	-5.4654410000	1.0995750000
C149	-1.8288750000	-11.9867170000	4.2485690000
H150	-2.3586930000	-12.7180950000	3.6563000000
H151	-2.3284070000	-11.7832510000	5.1842340000
H152	-0.8540910000	-12.4208340000	4.5101400000
C153	-1.6299660000	-10.6735540000	3.4554040000
H154	-2.5623420000	-10.4346880000	2.9228830000
H155	-1.4526150000	-9.8467160000	4.1538920000
C156	-0.4618480000	-10.7428670000	2.4517950000
H157	0.4842570000	-10.6294390000	2.9994330000
H158	-0.4298670000	-11.7464660000	2.0040290000
C159	-0.5297280000	-9.7418160000	1.2816430000
H160	0.3026020000	-9.9323820000	0.5896210000
H161	-1.4472780000	-9.9433520000	0.7113500000
C162	-0.5517630000	-8.2435050000	1.6052990000
H163	-0.7869160000	-7.6813900000	0.6968020000
H164	-1.3103720000	-7.9992030000	2.3539800000
N165	0.7449030000	-7.6997460000	2.1150310000
H166	0.7861360000	-6.6468900000	1.9886530000
H167	0.8595700000	-7.8553210000	3.1441820000
H168	1.5895270000	-8.0474610000	1.6035830000
C169	-1.8652230000	-2.8063900000	9.6692390000
H170	-2.8449960000	-3.2600300000	9.6435890000
H171	-1.9204760000	-1.8064530000	10.0735590000
H172	-1.2498370000	-3.3996090000	10.3585490000
C173	-1.2634660000	-2.8359550000	8.2537000000
H174	-0.2622160000	-2.3811400000	8.2879600000
C175	-2.1214110000	-2.0214170000	7.2736060000
H176	-2.1830040000	-0.9649890000	7.5697810000
H177	-3.1478900000	-2.4086300000	7.2318990000
H178	-1.7158060000	-2.0857190000	6.2556000000
C179	-1.1098330000	-4.2830530000	7.7635620000
H180	-0.4288170000	-4.8496670000	8.4102400000
H181	-0.7217370000	-4.3250670000	6.7405440000
H182	-2.0785140000	-4.8010580000	7.7681490000
C183	0.8714020000	-7.5684410000	5.2556630000
O184	1.2174790000	-1.7759780000	4.1866690000
H185	0.6763620000	-0.8523180000	4.7871040000
O186	4.9273180000	-1.2808220000	3.6820760000
O187	7.3571280000	-2.2608890000	1.8386280000
H188	7.2441990000	-2.2520040000	2.8074420000
H189	6.5079910000	-2.6725480000	1.5386460000
O190	1.5769050000	0.6915380000	7.2495070000
H191	2.2224860000	-0.5795820000	7.9489440000
O192	3.1824500000	2.6684910000	8.6626050000
H193	3.9311100000	3.1187760000	9.1023790000
H194	3.0222900000	1.9158010000	9.2879430000
O195	5.6524590000	2.6620640000	9.9913030000
H196	5.5526840000	1.7922830000	9.5421040000
H197	6.0378750000	2.4481910000	10.8616560000
O198	2.9591470000	-1.8250330000	2.0218350000
H199	3.6427400000	-2.5231450000	1.7873920000
H200	0.6184830000	-5.2206680000	4.9037410000
O201	1.1002750000	-4.9873690000	1.8478480000
H202	2.0737500000	-4.9356190000	1.6895960000
H203	0.9387150000	-4.7583740000	2.8072380000
O204	0.2877340000	-2.2081560000	1.6628810000
H205	0.3611760000	-3.1839550000	1.5848160000
H206	0.7449530000	-1.9038960000	3.3096240000
O207	3.1983220000	-8.0750490000	0.7818420000
H208	3.4860660000	-7.1201070000	0.7617790000
H209	3.8739890000	-8.5116400000	1.3216110000
O210	0.3327210000	-4.4547510000	4.3650760000
H211	0.8475200000	-3.6622290000	4.6244670000
H212	1.2043510000	-1.9214850000	1.4541480000
H213	9.2070670000	-4.9296720000	10.6296160000
O214	2.8105620000	-1.4129400000	8.0275850000
H215	3.0760800000	-1.5671590000	7.0490970000
H216	1.1304540000	1.3476440000	7.8061340000
O217	0.1405170000	0.0250450000	5.4118090000
H218	-0.6944390000	-0.3431060000	5.7431280000
H219	0.8142110000	0.3436600000	6.3463470000

Structure used in Fig 6 (the same atoms are frozen):

Mn1	3.1264390000	-1.4521340000	3.6070030000
Mn2	4.5245470000	-1.2366030000	8.8440340000
Mn3	5.2984120000	-1.4517440000	5.3077780000
Mn4	6.6613430000	0.0336030000	7.2801830000
O5	3.5107730000	-1.2266690000	5.4171390000
O6	5.7345430000	0.2638770000	5.7089700000
O7	5.3866160000	0.6158100000	8.3011520000
O8	5.8991710000	-1.6856100000	7.2202540000
Ca9	3.6883580000	1.4934750000	6.8532900000
C10	0.6675460000	1.9515080000	1.7063480000
H11	1.2251840000	1.9058030000	0.7825780000

H12	-0.3243900000	2.3686420000	1.6143240000
H13	0.4609530000	0.8932290000	1.9194190000
C14	1.4843230000	2.4743900000	2.9004800000
H15	0.8117570000	2.7626160000	3.7167840000
H16	2.0645000000	3.3730090000	2.6565830000
C17	2.4714440000	1.4920640000	3.5812440000
O18	3.1388540000	1.9000960000	4.5458150000
O19	2.5148680000	0.2951750000	3.0913750000
C20	1.0582600000	1.1829960000	13.4563130000
H21	0.3702240000	0.3601390000	13.5824630000
H22	0.7336470000	2.1291270000	13.8635790000
H23	2.0254270000	0.9033040000	13.8890950000
C24	1.1528740000	1.4189820000	11.9494380000
H25	1.9470540000	2.1386870000	11.7246570000
H26	0.2239510000	1.8860810000	11.6012050000
C27	1.3998680000	0.0998550000	11.1966060000
H28	0.5190570000	-0.1894160000	10.6082530000
H29	1.6089970000	-0.7181300000	11.8921880000
C30	2.5605360000	0.2455730000	10.2466530000
O31	2.5449560000	1.1801650000	9.4184480000
O32	3.5067080000	-0.6129620000	10.4011840000
C33	2.7844500000	-7.8608080000	8.6257440000
H34	2.4565570000	-8.8394910000	8.9990870000
H35	1.9543630000	-7.4375350000	8.0514620000
C36	4.0077400000	-8.0636220000	7.7324300000
O37	5.1426410000	-8.2092160000	8.2275680000
C38	3.1318160000	-6.9671060000	9.8492690000
H39	3.8764520000	-7.4984650000	10.4540210000
H40	2.2380320000	-6.8428200000	10.4682000000
C41	3.6548360000	-5.6133110000	9.4618130000
N42	4.7082300000	-5.5137940000	8.5694180000
H43	5.2426580000	-6.3196120000	8.2511630000
C44	3.2866200000	-4.3081740000	9.7088790000
H45	2.5049680000	-3.9303480000	10.3515290000
C46	4.9019380000	-4.2159800000	8.2735700000
H47	5.5657080000	-3.8606650000	7.5066330000
N48	4.0785190000	-3.4490840000	8.9662550000
N49	3.8070640000	-7.9476020000	6.4076370000
H50	2.8512150000	-7.8656640000	6.0420350000
C51	4.9172530000	-7.8463450000	5.4688660000
H52	4.6320120000	-8.3752920000	4.5519090000
H53	5.7745530000	-8.3612610000	5.9072920000
C54	5.2952760000	-6.3814620000	5.1355670000
H55	6.1618220000	-6.3892890000	4.4620320000
H56	5.6251000000	-5.8814400000	6.0498620000
C57	4.1427490000	-5.5909990000	4.5011640000
H58	3.2032180000	-5.8582710000	5.0018430000
H59	4.0036650000	-5.8620330000	3.4474870000
C60	4.2291930000	-4.0659410000	4.5432550000
O61	3.2712900000	-3.4617680000	3.9491350000
O62	5.1636660000	-3.4964050000	5.1646650000
C63	9.1595120000	0.1191580000	11.4478230000
H64	9.8436150000	-0.1154800000	10.6253260000
H65	9.7046100000	-0.0562840000	12.3854600000
C66	7.9342610000	-0.7901920000	11.4082530000
H67	7.1993020000	-0.4638500000	12.1499400000
H68	8.2170130000	-1.8156560000	11.6826510000
C69	7.2041940000	-0.8645110000	10.0678650000
O70	7.7340940000	-0.3410650000	9.0496200000
O71	6.1108350000	-1.5191340000	10.0895040000
C72	8.7835750000	1.5999160000	11.4140880000
O73	7.6912260000	2.0030470000	11.8191080000
N74	9.7718200000	2.4304800000	10.9850050000
H75	10.5678230000	2.0187380000	10.5152120000
C76	9.5677770000	3.8588150000	10.7651890000
H77	10.4400250000	4.4141860000	11.1182130000
H78	8.6861030000	4.1513520000	11.3381070000
C79	9.4170750000	4.1217190000	9.2508280000
O80	10.4152060000	4.3025360000	8.5556820000
N81	8.1437750000	4.0830740000	8.7838780000
H82	7.3771880000	3.7661140000	9.3842790000
C83	7.8397550000	4.0978040000	7.3617060000
H84	7.2770900000	4.9973910000	7.0914500000
H85	8.7947560000	4.0901470000	6.8276590000
C86	6.9931690000	2.8722450000	6.9676840000
O87	5.8617840000	3.0348600000	6.4808000000
O88	7.5709900000	1.7392490000	7.2012810000
C89	11.5816620000	-0.6170830000	3.4808990000
H90	12.4441750000	-1.2180930000	3.7284030000
H91	11.8304270000	0.3821370000	3.1552080000
H92	11.1464530000	-1.0901160000	2.5882550000
C93	10.5135450000	-0.5291990000	4.5672890000
H94	9.9229620000	0.3808240000	4.4083600000
H95	10.9477200000	-0.4237540000	5.5669870000
C96	9.5592770000	-1.7237750000	4.5139190000
H97	10.0386710000	-2.6252730000	4.9234060000
H98	9.2999090000	-1.9716760000	3.4803950000
C99	8.2669290000	-1.4339470000	5.2531930000
O100	7.2030840000	-1.8514410000	4.7016320000
O101	8.3337890000	-0.7931070000	6.3393950000
C102	10.8187240000	4.2285680000	-0.8150210000
H103	11.5403640000	3.4839220000	-0.5131310000
H104	11.2010930000	5.2306260000	-0.6882230000

H105	10.6699980000	4.0998030000	-1.8948140000
C106	9.4885060000	4.0057810000	-0.0841110000
H107	9.0418510000	3.0827430000	-0.4812850000
H108	8.7835810000	4.8130460000	-0.3253540000
C109	9.6469690000	3.8956300000	1.4385280000
H110	10.0698690000	4.8293650000	1.8308200000
H111	10.3641440000	3.0993600000	1.6786060000
C112	8.3399570000	3.6245630000	2.1927130000
H113	7.6301670000	4.4490390000	2.0213750000
H114	8.5441340000	3.5803040000	3.2675660000
N115	7.7525500000	2.3460350000	1.7974110000
H116	7.7938950000	2.0971390000	0.8191130000
C117	6.8575570000	1.6401520000	2.5306250000
N118	6.4059480000	2.1075120000	3.6929530000
H119	6.0044110000	1.4672340000	4.3932540000
H120	6.4821170000	3.0752480000	3.9659930000
N121	6.4172860000	0.4675720000	2.0693970000
H122	7.0078670000	-0.2060620000	1.5723240000
H123	5.7003960000	-0.0290230000	2.6214030000
C124	11.8423980000	-5.3930890000	7.2492550000
H125	11.2522020000	-5.9724610000	6.5547080000
H126	12.7964630000	-5.8524490000	7.4617420000
H127	12.0392320000	-4.4124760000	6.8012820000
C128	11.1066220000	-5.2515650000	8.5974570000
H129	11.7600150000	-4.7249700000	9.3078000000
H130	10.9490610000	-6.2532540000	9.0205040000
C131	9.7837360000	-4.5429000000	8.5533680000
N132	8.8577790000	-4.6616330000	9.5879570000
C133	9.2139300000	-3.6612080000	7.6752970000
H134	9.5888760000	-3.2666130000	6.7494960000
C135	7.7858940000	-3.8911220000	9.3396270000
H136	6.9237260000	-3.7541820000	9.9733880000
N137	7.9860770000	-3.2781430000	8.1792840000
H138	7.2775740000	-2.6143160000	7.7388540000
C139	6.0989350000	-4.2351880000	-1.2221970000
H140	5.3833630000	-4.5684340000	-1.9592870000
H141	7.1094170000	-4.1301810000	-1.5886720000
H142	5.7919270000	-3.2381360000	-0.8899550000
C143	6.0264560000	-5.2072610000	-0.0187410000
H144	5.9726190000	-6.2479570000	-0.3558340000
H145	6.9230380000	-5.0895790000	0.6014480000
C146	4.8234640000	-4.8437460000	0.8570010000
O147	4.8921520000	-3.7110230000	1.4043110000
O148	3.8378380000	-5.6442300000	0.9764480000
C149	-1.8288750000	-11.9867170000	4.2485690000
H150	-2.3586930000	-12.7180950000	3.6563000000
H151	-2.3284070000	-11.7832500000	5.1842340000
H152	-0.8575010000	-12.4267970000	4.5134930000
C153	-1.6133010000	-10.6921900000	3.4335700000
H154	-2.5561500000	-10.4227580000	2.9349230000
H155	-1.3689640000	-9.8630960000	4.1083030000
C156	-0.4911310000	-10.8405820000	2.3854540000
H157	0.4800380000	-10.7314390000	2.8881640000
H158	-0.5058300000	-11.8644790000	1.9858310000
C159	-0.5756510000	-9.8984980000	1.1690160000
H160	0.2289700000	-10.1426390000	0.4612900000
H161	-1.5155860000	-10.1032190000	0.6378970000
C162	-0.5541750000	-8.3877760000	1.4201280000
H163	-0.7783930000	-7.8600510000	0.4886200000
H164	-1.2990080000	-8.0894070000	2.1631210000
N165	0.7619550000	-7.8604640000	1.8994290000
H166	0.8067040000	-6.8145290000	1.7828570000
H167	0.8978910000	-8.0273200000	2.9236680000
H168	1.5945620000	-8.2081490000	1.3631530000
C169	-1.8652230000	-2.8063900000	9.6692390000
H170	-2.8449960000	-3.2600300000	9.6435890000
H171	-1.9204750000	-1.8064530000	10.0735580000
H172	-1.2550360000	-3.4026830000	10.3610890000
C173	-1.2227720000	-2.7852740000	8.2712830000
H174	-0.2251090000	-2.3313630000	8.3689510000
C175	-2.0363190000	-1.9139460000	7.3023110000
H176	-2.1856650000	-0.9032150000	7.7030750000
H177	-3.0269830000	-2.3498490000	7.1169040000
H178	-1.5234780000	-1.8199860000	6.3370050000
C179	-1.0399360000	-4.2049390000	7.7171080000
H180	-0.4197020000	-4.8144390000	8.3861270000
H181	-0.5580150000	-4.1949340000	6.7329060000
H182	-2.0079510000	-4.7125260000	7.6087240000
C183	0.8633680000	-7.7200000000	5.0469090000
O184	1.1014380000	-1.7905240000	3.8604860000
H185	0.9329270000	-2.5802220000	4.4076020000
O186	4.9122060000	-1.2630520000	3.5359100000
O187	7.2695700000	-2.2023040000	1.7557310000
H188	7.1497170000	-2.1536790000	2.7234730000
H189	6.4552580000	-2.6871160000	1.4827140000
O190	1.2557420000	1.6339220000	6.9978010000
H191	1.1551430000	1.2295780000	7.8782720000
O192	3.4948760000	3.5069830000	8.3626130000
H193	4.3035080000	3.5497570000	8.9167060000
H194	2.8553010000	3.0758390000	8.9609060000
O195	5.7726240000	2.8184140000	9.8861920000
H196	5.7035100000	1.9614260000	9.3876760000
H197	6.1202910000	2.5711290000	10.7640370000

O198	3.0122540000	-1.8487570000	1.7933690000
H199	3.6553090000	-2.5891020000	1.6223040000
H200	0.6815910000	-5.5340430000	4.7411150000
O201	1.1965140000	-5.1100790000	1.6927760000
H202	2.1759890000	-5.1396050000	1.5060240000
H203	1.0947260000	-4.9510680000	2.6678390000
O204	0.6524760000	-2.3772930000	1.5502590000
H205	0.6502070000	-3.3658610000	1.4634350000
H206	0.7054720000	-2.1169420000	2.7000850000
O207	3.1519010000	-8.2113960000	0.4925950000
H208	3.4800400000	-7.2700080000	0.5354600000
H209	3.8427690000	-8.7245180000	0.9374410000
O210	0.7940800000	-4.6282650000	4.3604280000
H211	1.7419700000	-4.4076330000	4.4541010000
H212	1.6832710000	-2.1372070000	1.4411690000
H213	8.9607190000	-5.2522210000	10.4026870000
O214	3.0661030000	-0.9095780000	7.8482980000
H215	3.1033330000	-1.3795370000	6.9799440000
H216	0.7023640000	1.1171560000	6.3589290000
O217	-0.1196910000	0.3418640000	5.0401940000
H218	-1.0433600000	0.0719950000	5.1429140000
H219	0.3370040000	-0.4250610000	4.6040150000

Fully optimized structure for eT (small model, nothing frozen):

Mn1	3.5194270000	-1.3620120000	3.4548930000
Mn2	4.3889190000	-1.2232320000	8.7964620000
Mn3	5.5220360000	-1.5359350000	5.3049820000
Mn4	6.6251660000	-0.0998730000	7.4173610000
O5	3.7420150000	-1.1529790000	5.2695420000
O6	5.9385060000	0.1757790000	5.7306900000
O7	5.1654190000	0.4085630000	8.3314860000
O8	5.7822200000	-1.7328370000	7.2409760000
Ca9	3.7155470000	1.3296850000	6.5820720000
H10	2.5830660000	2.3512510000	2.4761330000
C11	2.9952880000	1.6188710000	3.1972030000
O12	3.2083920000	1.9982760000	4.3584000000
O13	3.2101500000	0.4725640000	2.6815530000
H14	1.4255910000	-0.3753610000	11.2670160000
C15	2.1415540000	-0.0361190000	10.4901580000
O16	1.8593470000	0.9954490000	9.8579050000
O17	3.1746570000	-0.7863020000	10.3925380000
H18	2.8959160000	-6.0001460000	10.5639740000
C19	3.3211290000	-5.2032040000	9.9743710000
N20	4.1048570000	-5.4451710000	8.8591670000
H21	4.3602210000	-6.3510200000	8.4937730000
C22	3.2603520000	-3.8421720000	10.0931350000
H23	2.7697220000	-3.2218460000	10.8261300000
C24	4.4938220000	-4.2546850000	8.3435990000
H25	5.1076670000	-4.1299750000	7.4629210000
N26	3.9900920000	-3.2714490000	9.0717480000
H27	4.3261850000	-5.1827220000	4.3263780000
C28	4.3454640000	-4.0788790000	4.3558640000
O29	3.5674130000	-3.4920130000	3.5520580000
O30	5.1325720000	-3.5634390000	5.1925320000
H31	7.6461370000	-1.2553850000	10.9738470000
C32	7.0128730000	-1.0971840000	10.0875540000
O33	7.5676650000	-0.5105390000	9.1182230000
O34	5.8312790000	-1.5289190000	10.1662880000
H35	7.4647190000	3.6769840000	7.1113900000
C36	6.8339670000	2.7763990000	6.9964760000
O37	5.7253110000	2.8919750000	6.4373600000
O38	7.3795590000	1.7193090000	7.4704890000
H39	9.4117560000	-1.9148520000	5.3621400000
C40	8.4096800000	-1.5742490000	5.6672260000
O41	7.4414500000	-2.0657190000	5.0213230000
O42	8.3681790000	-0.7428650000	6.6105680000
H43	6.2893860000	3.8444020000	2.0555580000
N44	6.3455800000	2.9264140000	1.6383710000
H45	5.9340320000	2.8349200000	0.7210670000
C46	6.3823600000	1.8387430000	2.4543370000
N47	6.4903180000	2.0085460000	3.7680700000
H48	6.4435360000	1.1994040000	4.4131390000
H49	6.1856090000	2.8678710000	4.2119900000
N50	6.4078520000	0.6150510000	1.9270460000
H51	6.3091810000	0.5079510000	0.9274650000
H52	6.0898220000	-0.1885280000	2.5158300000
O53	1.6024560000	-1.5559970000	3.5563630000
H54	1.4568570000	-2.4970910000	3.7551250000
O55	5.3553090000	-1.3385160000	3.4995010000
O56	1.3220550000	1.5483030000	7.0389880000
H57	1.2279460000	1.3936860000	8.0001590000
O58	3.6581600000	2.6811940000	8.6919860000
H59	4.5062060000	2.3447150000	9.0328650000
H60	2.9946620000	2.1872620000	9.2328020000
O61	3.5422870000	-1.8646250000	1.3536300000
H62	3.5722640000	-2.8363470000	1.3899900000
O63	0.9992040000	-1.2189330000	0.9769200000
H64	0.3887020000	-1.9270640000	0.7202060000
H65	1.0076500000	-1.2290470000	1.9766430000

H66	2.6239270000	-1.6177130000	1.0215210000
O67	2.9545530000	-0.9669680000	7.6842840000
H68	3.1463550000	-1.4021010000	6.8208430000
H69	0.8247160000	0.7989600000	6.6171520000
O70	0.4567240000	-0.8127290000	6.0212920000
H71	1.0791710000	-1.2040380000	6.6603670000
H72	0.8631680000	-0.9688000000	5.1342920000

Structure of the large model including Tyr-His for the open cubane:

Mn1	2.8673575059	-1.4699229440	4.0555788403
Mn2	4.5765118204	-1.4914177030	8.5817418925
Mn3	5.2486527916	-1.4416832935	5.4458849834
Mn4	6.5676375121	0.0537876443	7.4032319581
O5	3.6032878053	-1.1778516981	6.0109415244
O6	5.7356104711	0.3079074016	5.8513251664
O7	5.0137758462	0.2974613437	8.3491799489
O8	6.0131766681	-1.7494954934	7.3514366430
Ca9	3.4226936827	1.2981186736	6.7582713101
C10	0.6675456172#	1.9515069323#	1.7063483214#
H11	1.2251836749#	1.9058034500#	0.7825777324#
H12	-0.3243893748#	2.3686424381#	1.6143237842#
H13	0.4665984593	0.9008359137	1.9547732137
C14	1.4870669844	2.5308315181	2.8740901247
H15	0.8151638905	2.9456517818	3.6370542087
H16	2.1258936075	3.3670774654	2.5667733962
C17	2.3946805555	1.5683580369	3.6816971926
O18	3.1623464078	2.0874355079	4.5287963400
O19	2.2528166278	0.3161045296	3.4608144804
C20	1.0582599918#	1.1829959896#	13.4563133369#
H21	0.3702238535#	0.3601391373#	13.5824630990#
H22	0.7336467543#	2.1291271189#	13.8635785272#
H23	1.9506572605	0.9063316468	14.0357574288
C24	1.4469648593	1.2704302586	11.9678509004
H25	2.2601813421	1.9941855668	11.8247833341
H26	0.5987895198	1.6189945528	11.3643521968
C27	1.8997150477	-0.1015244676	11.4547797606
H28	1.0594582153	-0.8106916261	11.4729583660
H29	2.6607205846	-0.5268299985	12.1200682229
C30	2.4729509027	-0.1386432533	10.0445354310
O31	2.3075351444	0.7829011965	9.2307970252
O32	3.1190662656	-1.2328590006	9.7813486834
C33	2.7844501479#	-7.8608080897#	8.6257438687#
H34	2.4683706465	-8.8263630776	9.0399872444
H35	1.9535404344	-7.4740603950	8.0279956272
C36	4.0173385782	-8.0836001166	7.7430521868
O37	5.1499248513	-8.2432481862	8.2505676798
C38	3.1019439196	-6.9099071177	9.8147477392
H39	3.7994868368	-7.4215293221	10.4884144169
H40	2.1835239810	-6.7232217151	10.3789435895
C41	3.6940974961	-5.5991382571	9.3804168037
N42	4.8595605334	-5.599119237	8.6288909817
H43	5.3581629811	-6.4661670510	8.3961809517
C44	3.3238000313	-4.2773724758	9.4536994422
H45	2.4875824363	-3.8188877015	9.9551040752
C46	5.1162385401	-4.3538787285	8.2192808763
H47	5.8803467175	-4.0881513090	7.5140177999
N48	4.2217459674	-3.5118523337	8.7212186597
N49	3.8194857939	-7.9678558253	6.4216340642
H50	2.8671999880	-7.8311539675	6.0623855227
C51	4.9172532358#	-7.8463446973#	5.4688659016#
H52	4.6112758001	-8.3500081785	4.5451031170
H53	5.7816779164	-8.3749092654	5.8756949311
C54	5.2906971741	-6.3707037051	5.1686736462
H55	6.1369757513	-6.3651473873	4.4697957874
H56	5.6579656192	-5.9132649537	6.0905550704
C57	4.1261492362	-5.5444687262	4.5955727846
H58	3.1751317814	-5.8623296216	5.0371380923
H59	4.0094446029	-5.7181821506	3.5163704912
C60	4.1745356059	-4.0343692160	4.7589452128
O61	3.1322641588	-3.4239040603	4.3457434993
O62	5.1731785403	-3.4532528591	5.2755289532
C63	9.1595116146#	0.1191579976#	11.4478228126#
H64	9.8193256287	-0.1559331395	10.6181532850
H65	9.7364452940	0.0042580746	12.3754334218

C66	7.9352852751	-0.7889315452	11.4957424274
H67	7.2462895404	-0.4516926540	12.2762074954
H68	8.2314426262	-1.8099329675	11.7694522952
C69	7.1316803701	-0.8743028526	10.1973310163
O70	7.5835035295	-0.2522267410	9.1821118866
O71	6.0958529091	-1.5994439059	10.2265739784
C72	8.7668911008	1.5938254467	11.3296825420
O73	7.6497430751	2.0145765982	11.6528773598
N74	9.7630192942	2.4225169988	10.9263279077
H75	10.5993981472	2.0189554388	10.5263694619
C76	9.5677770977#	3.8588145838#	10.7651885038#
H77	10.5180456602	4.3674059284	10.9375890465
H78	8.8395926363	4.1795480632	11.5134004081
C79	9.1051724626	4.2044405154	9.3322182815
O80	9.9083774135	4.5256721684	8.4631783626
N81	7.7590154520	4.1095533837	9.1330921561
H82	7.1822052314	3.6859898283	9.8518126552
C83	7.1703439782	4.2164300576	7.8120827187
H84	6.4355134875	5.0264320279	7.7704989745
H85	7.9867998781	4.4441831254	7.1192269412
C86	6.4651765952	2.9234263841	7.3775029334
O87	5.3182390710	2.9814382463	6.9048543035
O88	7.1743310600	1.8543070998	7.5542430469
C89	11.5816614725#	-0.6170833914#	3.4808992123#
H90	12.4441751965#	-1.2180927321#	3.7284029654#
H91	11.8304271141#	0.3821369951#	3.1552080728#
H92	11.1099034113	-1.0978831042	2.6133390167
C93	10.5438456503	-0.4562244540	4.6071907961
H94	9.9884745155	0.4732388850	4.4326667603
H95	11.0247853947	-0.3303266953	5.5837601207
C96	9.5324961740	-1.6040139805	4.6422436298
H97	9.9820438630	-2.5004398241	5.0935674034
H98	9.2538941793	-1.8988029474	3.6260489395
C99	8.2290813998	-1.2781920172	5.3616666044
O100	7.1865032717	-1.7460546200	4.8190535404
O101	8.2723723021	-0.5879050393	6.4363472713
C102	10.8187240085#	4.2285679563#	-0.8150213674#
H103	11.5403644531#	3.4839224590#	-0.5131309518#
H104	11.2010928465#	5.2306259492#	-0.6882231379#
H105	10.6658376814	4.0997417471	-1.8935129700
C106	9.4870083616	3.9981422080	-0.0774760545
H107	9.0140668389	3.0999558411	-0.5016473327
H108	8.7959666847	4.8280361131	-0.2793365358
C109	9.6555261691	3.8263290925	1.4401746981
H110	10.1431663918	4.7186158834	1.8540257871
H111	10.3267222541	2.9817029911	1.6463905568
C112	8.3506269302	3.6253050733	2.2231436278
H113	7.6796704305	4.4803417507	2.0459768419
H114	8.5730315755	3.5945326519	3.2948754267
N115	7.6773782283	2.3690247227	1.8809198136
H116	7.7208919223	2.0508103271	0.9221685206
C117	6.7915839930	1.7285657736	2.6790841206
N118	6.4265764796	2.2772686709	3.8481854755
H119	5.9567939648	1.6952807799	4.5471645050
H120	6.4008179225	3.2767122034	3.9810450906
N121	6.2911365549	0.5494130379	2.3205478692
H122	6.8010837594	-0.1791242240	1.7961408698
H123	5.5643704825	0.1160543031	2.9091378931
C124	11.8423976155#	-5.3930893898#	7.2492548476#
H125	11.2522023327#	-5.9724612982#	6.5547079659#
H126	12.7964628901#	-5.8524491732#	7.4617421180#
H127	12.0283933700	-4.4006114679	6.8258920115
C128	11.1473148486	-5.3101172942	8.6221399990
H129	11.8343503933	-4.8440620790	9.3430061814
H130	10.9723188887	-6.3297020156	8.9917088984
C131	9.8544078187	-4.5603413530	8.6519204731
N132	8.9717626653	-4.6575416395	9.7238978077
C133	9.2841412124	-3.6512277150	7.8048010745
H134	9.6259163522	-3.2700811788	6.8601906715
C135	7.9205446457	-3.8466087575	9.5292954450
H136	7.0834906743	-3.6911618050	10.1924973560
N137	8.0988715697	-3.2258600171	8.3691124307
H138	7.3871012379	-2.5696897353	7.9417826570
C139	6.0989350943#	-4.2351883327#	-1.2221965988#
H140	5.3833635036#	-4.5684339725#	-1.9592875012#

H141	7.1094170603#	-4.1301812350#	-1.5886718992#
H142	5.7971284917	-3.2090354099	-0.9724824956
C143	6.0016752969	-5.0580211463	0.0792499553
H144	5.9801069391	-6.1336147618	-0.1223327371
H145	6.8832788209	-4.8452541402	0.6977676586
C146	4.7635232265	-4.6612083728	0.9076135654
O147	4.7035310816	-3.4575098041	1.3021469238
O148	3.8823215145	-5.5459829271	1.1528788535
C149	-1.8288745197#	-11.9867168076#	4.2485689198#
H150	-2.3586934722#	-12.7180947960#	3.6562999364#
H151	-2.3284067990#	-11.7832505795#	5.1842336993#
H152	-0.8629235557	-12.4344947494	4.5205244024
C153	-1.5915923491	-10.6963205406	3.4260859757
H154	-2.4875232550	-10.4845871544	2.8248158474
H155	-1.4647479455	-9.8407592341	4.1002894004
C156	-0.3555525991	-10.8033818070	2.5053708527
H157	0.5469278748	-10.6094502401	3.1015702936
H158	-0.2637480669	-11.8409976955	2.1548097728
C159	-0.3671097504	-9.9192975283	1.2430083907
H160	0.5054261043	-10.1641027910	0.6211089298
H161	-1.2466603355	-10.1914876520	0.6430221159
C162	-0.4219072736	-8.3979050302	1.4133062755
H163	-0.6329305619	-7.9317574272	0.4467400526
H164	-1.2111155207	-8.0952110099	2.1076226171
N165	0.8451665420	-7.7733374392	1.9042735032
H166	0.8850434353	-6.7550685019	1.5774975193
H167	0.9133712209	-7.7849090814	2.9401754282
H168	1.7194711631	-8.1832973997	1.5040091142
C169	-1.8652235680#	-2.8063900206#	9.6692397071#
H170	-2.8449960614#	-3.2600298660#	9.6435889744#
H171	-1.9204751988#	-1.8064530727#	10.0735581522#
H172	-1.2534929159	-3.3996298837	10.3650580453
C173	-1.2374578662	-2.8369004454	8.2685998294
H174	-1.9042022408	-2.2920836442	7.5825600320
C175	0.1216482952	-2.1349052649	8.2603811993
H176	0.7993698178	-2.5989051015	8.9880698448
H177	0.0355209519	-1.0715172268	8.5097313096
H178	0.6011821709	-2.1972681782	7.2798172638
C179	-1.1175893137	-4.2785779046	7.7576946327
H180	-0.4637592414	-4.8693852520	8.4143950667
H181	-0.6901155311	-4.3107463554	6.7507385079
H182	-2.0932430531	-4.7781896834	7.7277014701
C183	0.9165892455	-7.3954377890	5.0654547571
O184	1.1514295752	-1.6555771676	4.7596501348
H185	0.8648846671	-2.5853224228	4.8895299521
O186	4.6884084989	-1.1868241164	3.7926469040
O187	7.0727286530	-2.0501007819	1.8151421454
H188	7.0011997213	-2.1083883013	2.7858101082
H189	6.2428720029	-2.5008052387	1.5115901812
O190	-1.2185251837	1.0487121854	4.9262983309
H191	-1.2225484019	0.4012847839	4.1646600901
H192	-1.8920311560	0.7028660779	5.5320645260
O193	2.8200962709	3.2506281933	8.5265433895
H194	3.7035954028	3.4222580196	8.9072389121
H195	2.4763030232	2.5227106504	9.0902656371
O196	5.1683482447	2.4386519634	10.1791628584
H197	5.1756484430	1.6329677194	9.6141858234
H198	5.8564779029	2.2668710156	10.8499443491
O199	2.5915796856	-1.9519577060	2.3508114859
H200	3.3433045429	-2.5311472823	2.0349216758
H201	0.3301004606	-5.2585020809	4.6082527232
O202	1.1417884909	-5.4000666242	0.6988476331
H203	2.1066257598	-5.2597911712	0.8456769417
H204	0.7026680712	-4.5619699735	0.9828624950
O205	0.1099468085	-3.0736364781	1.8054165514
H206	0.9736627388	-2.5986952465	1.8900420548
H207	0.0392789207	-3.5289363040	2.6751791341
O208	3.4385763060	-8.2200918843	0.8751272184
H209	3.6848674731	-7.2573737355	0.8392513749
H210	4.0736382105	-8.6043210201	1.4973116264
O211	0.5189889415	-4.3426900165	4.3081573926
H212	1.4934059907	-4.3271836639	4.2331586688
H213	9.0906462870	-5.2590751329	10.5291880747
O214	1.1188347865	0.5584153332	6.3766748396
H215	0.3148478833	0.9055190576	5.9252238963

H216	1.1644300956	-0.3548576591	5.9994556322
O217	-1.0724014624	-1.0361706994	3.3597597485
H218	-0.9595727926	-1.4913445948	2.5020935150
H219	-0.2257093316	-1.2490081191	3.8257511830
C220	-1.7679869892#	8.2624199235#	3.7031819997#
C221	-2.8675444441	7.1922439230	3.8682098021
C222	-2.5134862187	6.1440365748	4.8764056951
C223	-2.7567700994	6.3713119443	6.2603985654
C224	-1.9174305655	4.9286826443	4.4731201594
C225	-2.4236774522	5.4333954686	7.2029663197
C226	-1.5830282950	3.9620131650	5.3892665852
C227	-1.8215618657	4.1794051269	6.7984114663
O228	-1.5113734996	3.2739475276	7.6379443606
H229	-1.5549590912	8.7764870365	4.6457177601
H230	-3.0589199519	6.7219873368	2.8971529131
H231	-3.7962595993	7.6925692483	4.1699599354
H232	-3.2268322955	7.3041692841	6.5620979115
H233	-1.7417871020	4.7529124636	3.4149697605
H234	-2.6269463813	5.6050183493	8.2555714013
H235	-1.1809756252	2.9964628886	5.0953903688
H236	-2.1561200165#	8.9921059994#	2.9823580083#
H237	-0.8314439901#	7.8582950237#	3.3036159992#
C238	-1.2898930032#	3.9433009920#	14.6070429549#
C239	-2.0837260713	4.8099942299	13.6191663663
C240	-1.5800199429	4.6002263695	12.2237351139
N241	-0.2554681717	4.8080517183	11.8445453804
C242	-2.1888454398	4.0878199406	11.1119886727
C243	-0.0778228593	4.4278526481	10.5664856889
N244	-1.2435586981	3.9889072158	10.1111476123
H245	-0.2640182317	4.3174554668	14.7179385811
H246	-2.0277816593	5.8701186189	13.8977415647
H247	-3.1443766519	4.5403630529	13.6317953603
H248	0.4810915068	5.1582666248	12.4436984239
H249	-3.2093897298	3.7714575670	10.9636176256
H250	0.8522726315	4.4440592270	10.0108002433
H251	-1.4107134590	3.6500551732	9.0981359389
H252	-1.7132030020#	3.9091470052#	15.6187189994#
H253	-1.2165709866#	2.9166759922#	14.2394740243#

Structure of the large model including Tyr-His for the closed cubane:

Mn1	2.5739155046	-1.4295117821	3.9125068338
Mn2	4.6316125682	-1.4040385139	8.4784534425
Mn3	5.1951785226	-1.4995252325	5.6476993166
Mn4	6.6006631090	0.1764509588	7.4027084605
O5	3.7876458842	-1.3152849109	6.8820936149
O6	5.6353738479	0.3262836811	5.9305800451
O7	5.0799231324	0.3662469975	8.4052940357
O8	6.1681775116	-1.6778547756	7.4406424457
Ca9	3.3237798322	1.3656988373	6.8380267112
C10	0.6675457163#	1.9515068440#	1.7063484789#
H11	1.2251836192#	1.9058034997#	0.7825776964#
H12	-0.3243893548#	2.3686424770#	1.6143237458#
H13	0.5146813332	0.9161086114	2.0267613625
C14	1.4595829307	2.7050552356	2.8036971212
H15	0.7888074384	3.3220201266	3.4146174981
H16	2.1738737487	3.4172484195	2.3704518420
C17	2.2448727973	1.8567282695	3.8202211093
O18	2.8365182701	2.4705379488	4.7583140046
O19	2.2347292596	0.5977544770	3.6841763122
C20	1.0582599954#	1.1829959908#	13.4563133024#
H21	0.3702238584#	0.3601391333#	13.5824630996#
H22	0.7336467565#	2.1291271171#	13.8635785331#
H23	1.9450009236	0.9070960053	14.0456530305
C24	1.4715606103	1.2667468357	11.9686195009
H25	2.2631727006	2.0165011136	11.8386460731
H26	0.6234821651	1.5873818580	11.3500669451
C27	1.9826691569	-0.0905714042	11.4540533218
H28	1.1717573047	-0.8328418609	11.4670672556
H29	2.7579322139	-0.4869584431	12.1208335880
C30	2.5631223433	-0.1031841201	10.0400165077
O31	2.3808314333	0.8284604426	9.2399141348
O32	3.2388780963	-1.1770459394	9.7613821331
C33	2.7844501730#	-7.8608080679#	8.6257438417#

H34	2.5094637863	-8.8163240547	9.0879411817
H35	1.9374887074	-7.5302816886	8.0172635746
C36	4.0219166963	-8.0691807544	7.7468473612
O37	5.1566368548	-8.2123838666	8.2575519010
C38	3.0702006398	-6.8426716563	9.7759919295
H39	3.7297533542	-7.3307299984	10.5038000189
H40	2.1309949573	-6.6233737639	10.2925486503
C41	3.7047545909	-5.5463581381	9.3395546927
N42	4.9087534150	-5.5743597735	8.6547815347
H43	5.3838297748	-6.4564468714	8.4248503361
C44	3.3789924011	-4.2101269681	9.4167770358
H45	2.5286063695	-3.7347559339	9.8761908370
C46	5.2317547530	-4.3293759784	8.2858432990
H47	6.0350823582	-4.0923381677	7.6161728805
N48	4.3439964727	-3.4612635146	8.7530996906
N49	3.8223582133	-7.9632930223	6.4262352940
H50	2.8680874897	-7.8321040625	6.0691707564
C51	4.9172532185#	-7.8463446898#	5.4688659297#
H52	4.5828162867	-8.3070342642	4.5328635238
H53	5.7644576853	-8.4224836806	5.8483084124
C54	5.3361632885	-6.3795973877	5.2152845627
H55	6.1990015622	-6.3768067605	4.5369852314
H56	5.6898610047	-5.9533864515	6.1575404418
C57	4.1885346574	-5.5358204953	4.6388481945
H58	3.2220201695	-5.9458139050	4.9444045780
H59	4.1755369071	-5.5879343134	3.5404286479
C60	4.1044867580	-4.0573184757	4.9705063576
O61	3.0094120819	-3.4968359408	4.7599299548
O62	5.1444119827	-3.4383552341	5.4358233843
C63	9.1595115851#	0.1191580027#	11.4478227818#
H64	9.8263013569	-0.1576074909	10.6251002400
H65	9.7157273804	-0.0190051815	12.3845243688
C66	7.9097483538	-0.7638827168	11.4669795817
H67	7.2262529849	-0.4288768602	12.2529575875
H68	8.1784705890	-1.7986961204	11.7139295678
C69	7.1189707390	-0.7795251973	10.1551383525
O70	7.6193090065	-0.1401762491	9.1763026370
O71	6.0492864935	-1.4662519193	10.1451938661
C72	8.7817049917	1.5988211184	11.3449018965
O73	7.6768838696	2.0259784242	11.7020772372
N74	9.7676573212	2.4223506879	10.9125351108
H75	10.5926429676	2.0190161897	10.4894685057
C76	9.5677770695#	3.8588145803#	10.7651884793#
H77	10.5240058416	4.3653386328	10.9087571185
H78	8.8658406848	4.1765840783	11.5390173595
C79	9.0617035425	4.2187558784	9.3495756903
O80	9.8418567579	4.5183775477	8.4530858244
N81	7.7054355353	4.1710007766	9.1990140060
H82	7.1405850921	3.7558573689	9.9319871952
C83	7.0735867566	4.3149979477	7.9016205017
H84	6.3159920660	5.1041255983	7.9175294768
H85	7.8619384550	4.5924419440	7.1947937952
C86	6.3915534049	3.0218286003	7.4337771466
O87	5.2240416737	3.0469942760	7.0213467126
O88	7.1523485949	1.9711580832	7.5203485618
C89	11.5816614298#	-0.6170834579#	3.4808991950#
H90	12.4441752089#	-1.2180927075#	3.7284029821#
H91	11.8304271182#	0.3821370013#	3.1552080949#
H92	11.1147719407	-1.0985100666	2.6113120423
C93	10.5448660389	-0.4800818534	4.6233107214
H94	10.1190034623	0.5291822863	4.5980671088
H95	11.0221945851	-0.5666023181	5.6062970001
C96	9.3894597149	-1.4773643603	4.4925128769
H97	9.7032230843	-2.4951614000	4.7721223564
H98	9.0752860811	-1.5649728075	3.4467937452
C99	8.1285360638	-1.1524296829	5.2867022494
O100	7.0659842093	-1.6808325314	4.8359646475
O101	8.2263905809	-0.4157785131	6.3261702674
C102	10.8187240026#	4.2285679404#	-0.8150213857#
H103	11.5403644580#	3.4839224650#	-0.5131309488#
H104	11.2010928395#	5.2306259495#	-0.6882231194#
H105	10.6823481992	4.1039398330	-1.8965683022
C106	9.4674338959	3.9729962086	-0.1100522309
H107	8.9899510363	3.1077846627	-0.5933554190
H108	8.7918179540	4.8225512528	-0.2789678658

C109	9.5882252942	3.7101022914	1.4011393174
H110	10.0946845600	4.5625282440	1.8729349251
H111	10.2274412574	2.8351104661	1.5811667348
C112	8.2605282107	3.5207559729	2.1566249845
H113	7.5886518014	4.3631669486	1.9307564401
H114	8.4616163483	3.5372926483	3.2324964631
N115	7.5884063665	2.2445306922	1.8700407407
H116	7.6330993569	1.8785138720	0.9281213965
C117	6.7045855325	1.6455401722	2.7049335009
N118	6.3454634202	2.2613656067	3.8464499152
H119	5.8744816114	1.7129602056	4.5696515066
H120	6.2995165154	3.2666239871	3.9143907008
N121	6.1988834523	0.4473071421	2.4319700255
H122	6.6800903574	-0.3126718339	1.9166070972
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H125	11.2522023360#	-5.9724613121#	6.5547079747#
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H127	12.0307219876	-4.4007189186	6.8269231921
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C131	9.9015223772	-4.5182617820	8.6745873563
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C133	9.3592671916	-3.5779813127	7.8417434116
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H142	5.7932783203	-3.2156369404	-0.9530861988
C143	6.0257268140	-5.0897611460	0.0619419810
H144	6.0153510620	-6.1597353441	-0.1683212672
H145	6.9127704794	-4.8824056035	0.6744150615
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O148	3.9063940824	-5.6132198951	1.1180289157
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H152	-0.8651499509	-12.4384690515	4.5226089151
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H154	-2.4817295621	-10.4696587031	2.8386819288
H155	-1.4320258812	-9.8476609917	4.1035617293
C156	-0.3598745442	-10.8269441456	2.4935161764
H157	0.5530908404	-10.6533460606	3.0800628928
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C159	-0.3703478951	-9.9355194659	1.2376510698
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C162	-0.4033933164	-8.4155467622	1.4204126858
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H164	-1.1913693213	-8.1073573111	2.1136916069
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H168	1.7388675750	-8.2332018049	1.5212858027
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H174	-1.8602128432	-2.2781365869	7.5842754204
C175	0.1563148070	-2.1696353600	8.2977124995
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H180	-0.4840479164	-4.8922346374	8.4120185408
H181	-0.6872345479	-4.3146771644	6.7517301147
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O184	0.8890023780	-1.6717061234	4.6767916328
H185	0.6601290426	-2.6157714270	4.8198429146
O186	4.4601136760	-1.1256256354	4.1316446022
O187	7.0095677561	-2.1072595956	1.8941570395
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O190	-1.1510039899	1.0238604063	4.8009238395
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H203	2.1103727277	-5.3133280960	0.8024874158
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O205	0.0150181263	-3.1852601187	1.6895913029
H206	0.9032035678	-2.7482889010	1.7704958712
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H213	9.1276372598	-5.2222478351	10.5440318355
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O228	-1.3416784388	3.2995855663	7.6377549032
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C239	-2.0638559961	4.8132684813	13.6063837665
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N241	-0.1870968515	4.8343988149	11.8830686858
C242	-2.0926833338	4.1041439046	11.0905892849
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H245	-0.2622451359	4.3115859328	14.7244385644
H246	-2.0182643402	5.8718917915	13.8924663413
H247	-3.1235208025	4.5401533979	13.5898986660
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