

# Supporting Information

## An efficient linear scaling procedure for constructing localized orbitals of large molecules based on the one-particle density matrix

Yang Guo<sup>1</sup>, Wei Li<sup>1</sup> and Shuhua Li<sup>1\*</sup>

<sup>1</sup>*School of Chemistry and Chemical Engineering, Key Laboratory of Mesoscopic*

*Chemistry of MOE, Institute of Theoretical and Computational Chemistry, Nanjing*

*University, Nanjing 210093, P. R. China*

### Contents

Cartesian Coordinates:	A . acetyl-(ala) <sub>n</sub> -methylamide
A . acetyl-(ala) <sub>n</sub> -methylamide	1. acetyl-(ala) <sub>9</sub> -methylamide
1. acetyl-(ala) <sub>9</sub> -methylamide	C 4.12520 3.90970 -2.26120
2. acetyl-(ala) <sub>19</sub> -methylamide	N 3.64490 5.28110 -2.26120
3. acetyl-(ala) <sub>29</sub> -methylamide	C 5.64810 3.89760 -2.11420
4. acetyl-(ala) <sub>39</sub> -methylamide	C 3.57020 3.17940 -1.03660
5. acetyl-(ala) <sub>49</sub> -methylamide	O 3.06870 2.06230 -1.15240
6. acetyl-(ala) <sub>59</sub> -methylamide	C -0.51780 3.71760 0.52180
7. acetyl-(ala) <sub>69</sub> -methylamide	C -5.62820 -5.18860 2.38760
8. acetyl-(ala) <sub>79</sub> -methylamide	H 4.33660 6.03070 -2.26120
9. acetyl-(ala) <sub>89</sub> -methylamide	H 3.81100 3.38200 -3.16170
B. Ice-like water clusters	H 6.08920 4.44860 -2.94470
1. (H <sub>2</sub> O) <sub>27</sub>	H 5.93500 4.37680 -1.17820
2. (H <sub>2</sub> O) <sub>64</sub>	H 6.01350 2.87070 -2.11360
3. (H <sub>2</sub> O) <sub>125</sub>	N 0.91240 3.89110 0.71120
4. (H <sub>2</sub> O) <sub>216</sub>	C 3.17510 3.23710 1.37840
5. (H <sub>2</sub> O) <sub>343</sub>	N 3.66430 3.82170 0.14140
6. (H <sub>2</sub> O) <sub>512</sub>	C 3.29000 4.25880 2.51140
C. Protein Molecules	C 1.68480 2.92210 1.23420
1. 1RPB	O 1.24250 1.82990 1.58690
2. 2ETI	C -0.16180 1.32380 -2.43530
3. 1CMR	C -1.08920 4.92730 -0.22060
4. 1CNR	H 4.08930 4.74800 0.18470
5. 2KNZ	H 3.71030 2.31850 1.61890



C	3.62560	9.80910	-0.17880	C	2.40400	6.55470	2.26410
C	-6.90670	-13.06340	3.58120	H	5.93670	6.86520	-1.53540
H	8.48010	12.12210	-2.96180	H	5.90580	4.01890	-1.54790
H	7.95440	9.47340	-3.86230	H	7.72910	5.47670	-0.58600
H	10.23270	10.54010	-3.64540	H	6.63480	5.94640	0.72980
H	10.07840	10.46830	-1.87890	H	7.16420	4.25820	0.58980
H	10.15700	8.96210	-2.81420	N	1.38190	5.22600	-0.22960
N	5.05590	9.98250	0.01060	C	1.71420	4.62370	0.92620
C	7.31850	9.32850	0.67780	O	1.11790	3.64180	1.36560
N	7.80770	9.91320	-0.55930	C	2.11810	1.64420	-2.29710
C	7.43340	10.35030	1.81080	C	0.24460	5.54750	-2.36300
C	5.82820	9.01350	0.53360	H	4.35690	6.40700	0.69690
O	5.38600	7.92130	0.88630	H	3.18300	4.53490	2.49130
C	3.98170	7.41520	-3.13590	H	3.22770	7.04220	2.78570
C	3.05420	11.01870	-0.92120	H	2.06410	7.20120	1.45510
H	8.23270	10.83940	-0.51590	H	1.57690	6.38370	2.95310
H	7.85370	8.41000	0.91830	N	1.75670	2.99330	-1.89600
H	8.47800	10.64120	1.92180	C	0.52750	3.29670	-1.44200
H	6.84190	11.23480	1.57500	O	-0.37130	2.46400	-1.33400
H	7.06750	9.91640	2.74140	C	2.24360	0.27270	1.26740
N	4.12030	8.51620	-2.19780	C	3.61140	1.58730	-2.62510
C	3.37800	8.59700	-1.07900	H	1.90840	6.03830	-0.55120
O	2.53660	7.75440	-0.77090	H	-0.66740	4.82700	-0.52260
C	5.69450	4.85210	-0.87790	H	0.11590	6.60550	-2.13460
C	5.05320	7.52670	-4.22240	H	1.18050	5.41300	-2.90530
H	5.47120	10.87190	-0.26660	H	-0.57950	5.19880	-2.98540
H	3.11800	9.65370	0.77310	N	2.38430	1.08610	0.07150
H	3.24800	11.91800	-0.33650	C	1.90080	0.69130	-1.11990
H	3.53430	11.11810	-1.89460	O	1.31050	-0.37530	-1.28330
H	1.98120	10.89340	-1.06580	C	-1.49410	0.95220	1.67940
N	5.33420	6.04680	-1.62240	C	2.76010	1.04810	2.48100
C	4.24390	6.09500	-2.40860	H	2.46810	3.72070	-1.96700
O	3.47990	5.14200	-2.55370	H	1.51510	1.30900	-3.14100
C	2.89390	5.22140	1.69560	H	3.82430	2.28760	-3.43280
C	6.88990	5.15160	0.02890	H	4.19540	1.86830	-1.74880
H	4.80560	9.24150	-2.40860	H	3.88770	0.57690	-2.92670
H	2.98150	7.38950	-3.56850	N	-0.06350	1.06970	1.45370
H	4.93470	8.47790	-4.74140	C	0.75920	0.00820	1.52730
H	6.04480	7.48960	-3.77160	O	0.36580	-1.12760	1.78820
H	4.95350	6.70280	-4.92900	C	-2.19840	-0.81090	-1.63680
N	3.99600	5.45650	0.77820	C	-2.17350	2.29100	1.38450
C	4.53950	4.46600	0.04840	H	2.86690	1.98080	0.15500
O	4.14820	3.30120	0.10300	H	2.76030	-0.68080	1.15850
C	0.28160	4.75610	-1.05410	H	3.80840	1.30030	2.32110

H	2.18880	1.96800	2.60500	O	-6.15840	-5.97550	0.45000
H	2.65680	0.44200	3.38100	C	-3.05080	-8.66650	1.67790
N	-1.71140	0.08050	-0.59770	C	-2.80830	-6.62010	-2.13050
C	-2.08150	-0.05450	0.68830	H	-3.50450	-2.65160	1.15270
O	-2.85080	-0.93270	1.07540	H	-6.03460	-3.81750	1.73750
C	-0.07780	-3.78880	-0.52450	H	-5.64100	-1.76280	0.32390
C	-1.49160	-0.49720	-2.95700	H	-4.93880	-2.78980	-0.94170
H	0.31240	1.99200	1.23370	H	-6.65400	-2.96550	-0.52110
H	-1.70670	0.61640	2.69440	N	-3.21380	-7.63360	0.66900
H	-1.75270	3.05430	2.03900	C	-4.05480	-7.77900	-0.37050
H	-1.99750	2.57660	0.34750	O	-4.74030	-8.78580	-0.54200
H	-3.24730	2.20810	1.55240	C	-6.44160	-8.04340	3.32590
N	-0.55780	-2.46640	-0.88850	C	-2.14500	-8.15280	2.79890
C	-1.82570	-2.25190	-1.28250	H	-3.55300	-4.64790	-0.77130
O	-2.66330	-3.14910	-1.36290	H	-4.97740	-6.76860	-2.02670
C	-1.95760	-3.90830	2.80030	H	-2.79560	-5.77570	-2.81970
C	1.35040	-3.68760	0.01480	H	-1.97280	-6.52470	-1.43710
H	-1.07020	0.82610	-0.86830	H	-2.70520	-7.55330	-2.68410
H	-3.28100	-0.73980	-1.74160	N	-5.13740	-7.89840	2.70180
H	-1.69140	0.53920	-3.22910	C	-4.40630	-8.96190	2.32300
H	-0.41610	-0.63340	-2.84430	O	-4.78340	-10.12270	2.47520
H	-1.85360	-1.16350	-3.74010	C	-8.21800	-9.10600	0.11390
N	-1.16290	-3.50740	1.65170	C	-7.08220	-6.66570	3.50590
C	-0.93080	-4.33890	0.62040	H	-2.66670	-6.77830	0.76660
O	-1.36900	-5.48720	0.57380	H	-2.65760	-9.58480	1.24170
C	-5.29290	-3.79140	0.93910	H	-1.17610	-7.88480	2.37750
C	-2.16250	-2.70930	3.72830	H	-2.58800	-7.26990	3.25950
H	0.09930	-1.68790	-0.83830	H	-2.01940	-8.92430	3.55850
H	-0.13330	-4.47470	-1.36970	N	-7.38400	-8.44360	1.10240
H	1.99050	-3.25580	-0.75450	C	-7.36520	-8.82730	2.39130
H	1.37070	-3.04510	0.89500	O	-8.04490	-9.75670	2.82370
H	1.71520	-4.67740	0.28940	C	-6.07730	-12.26730	-0.04540
N	-3.96770	-3.50600	1.46220	C	-7.91370	-8.54400	-1.27620
C	-3.35110	-4.32910	2.32910	H	-4.77980	-6.95470	2.55340
O	-3.85780	-5.37240	2.73840	H	-6.36710	-8.57170	4.27640
C	-4.12970	-6.61380	-1.35930	H	-6.43410	-6.05190	4.13140
C	-5.66030	-2.75570	-0.12540	H	-7.20160	-6.18190	2.53650
H	-0.77660	-2.56340	1.64270	H	-8.06120	-6.76910	3.97390
H	-1.49470	-4.74200	3.32820	N	-6.54960	-10.89410	0.00630
H	-1.18930	-2.34360	4.05580	C	-7.85910	-10.59240	0.06370
H	-2.68050	-1.91160	3.19610	O	-8.74360	-11.44700	0.07640
H	-2.75830	-3.00490	4.59190	C	6.15460	13.14350	-2.96180
N	-4.26060	-5.36750	-0.62380	C	-4.55000	-12.29010	0.04290
C	-5.27580	-5.14740	0.23060	H	-6.80100	-7.66590	0.79320

H	-9.27530	-9.00420	0.35840	H	11.90760	14.54140	0.05050
H	-8.11200	-7.47220	-1.27690	H	12.53180	16.77270	1.05400
H	-6.86540	-8.71100	-1.52330	H	10.89570	17.36630	0.70720
H	-8.53700	-9.03780	-2.02160	H	11.12140	16.04780	1.87360
O	5.55930	10.83380	-2.96190	N	8.17410	14.64760	-3.06550
C	-6.58940	-13.02480	1.18130	C	7.43190	14.72840	-1.94680
O	-7.10110	-14.13640	1.05760	O	6.59050	13.88580	-1.63870
H	-7.32470	-14.03670	3.32390	C	9.74830	10.98360	-1.74560
H	-5.85420	-10.14790	-0.00190	C	9.10710	13.65810	-5.09010
H	-6.42860	-12.77120	-0.94580	H	9.52510	17.00330	-1.13440
H	-4.13780	-11.72090	-0.79020	H	7.17190	15.78520	-0.09460
H	-4.22510	-11.83530	0.97860	H	7.30190	18.04940	-1.20430
H	-4.19060	-13.31840	0.00450	H	7.58820	17.24960	-2.76240
N	-6.44690	-12.41200	2.37010	H	6.03510	17.02490	-1.93360
C	6.47630	11.66820	-2.96180	N	9.38810	12.17830	-2.49020
H	5.07210	13.27070	-2.95150	C	8.29780	12.22640	-3.27640
H	6.57600	13.61570	-2.07450	O	7.53380	11.27340	-3.42150
H	6.57590	13.61590	-3.84920	C	6.94780	11.35280	0.82780
H	-6.07130	-13.20590	4.26670	C	10.94380	11.28310	-0.83890
H	-7.66480	-12.45020	4.06840	H	8.85950	15.37300	-3.27640
H	-6.01540	-11.48920	2.41980	H	7.03540	13.52100	-4.43630
3. acetyl-(ala) <sub>29</sub> -methylamide				H	8.98860	14.60930	-5.60910
C	12.32260	16.13250	-3.82960	H	10.09870	13.62100	-4.63930
N	11.84230	17.50390	-3.82960	H	9.00740	12.83420	-5.79670
C	13.84540	16.12040	-3.68260	N	8.04990	11.58790	-0.08950
C	11.76750	15.40230	-2.60500	C	8.59340	10.59750	-0.81940
O	11.26610	14.28520	-2.72080	O	8.20210	9.43270	-0.76480
C	7.67950	15.94050	-1.04660	C	4.33550	10.88760	-1.92190
C	-10.39550	-19.95750	1.49590	C	6.45790	12.68610	1.39630
H	12.53400	18.25350	-3.82960	H	9.99060	12.99660	-2.40320
H	12.00830	15.60490	-4.73010	H	9.95970	10.15030	-2.41570
H	14.28660	16.67150	-4.51310	H	11.78300	11.60820	-1.45380
H	14.13230	16.59970	-2.74660	H	10.68870	12.07780	-0.13800
H	14.21080	15.09350	-3.68200	H	11.21810	10.38970	-0.27790
N	9.10970	16.11400	-0.85720	N	5.43580	11.35740	-1.09740
C	11.37240	15.46000	-0.19000	C	5.76810	10.75510	0.05840
N	11.86160	16.04460	-1.42700	O	5.17180	9.77320	0.49790
C	11.48730	16.48170	0.94310	C	6.17200	7.77570	-3.16480
C	9.88210	15.14500	-0.33410	C	4.29850	11.67900	-3.23080
O	9.43980	14.05280	0.01850	H	8.41080	12.53850	-0.17080
C	8.03560	13.54670	-4.00370	H	7.23690	10.66640	1.62360
C	7.10810	17.15020	-1.78900	H	7.28150	13.17360	1.91790
H	12.28660	16.97080	-1.38370	H	6.11800	13.33270	0.58740
				H	5.63080	12.51520	2.08540

N	5.81060	9.12470	-2.76380	C	5.40430	2.44380	-0.85290
C	4.58140	9.42820	-2.30980	H	2.98370	6.95760	-1.73600
O	3.68260	8.59550	-2.20180	H	0.77290	5.39170	-2.60930
C	6.29750	6.40420	0.39960	H	2.36240	6.67060	-4.09680
C	7.66530	7.71870	-3.49290	H	3.63780	5.49810	-3.71210
H	5.96220	12.16970	-1.41890	H	2.20030	4.96800	-4.60780
H	3.38650	10.95840	-1.39040	N	2.89090	2.62410	0.78400
H	4.16980	12.73700	-3.00230	C	3.12310	1.79250	-0.24740
H	5.23440	11.54440	-3.77300	O	2.68490	0.64420	-0.29390
H	3.47440	11.33020	-3.85310	C	-1.23910	2.34000	0.07140
N	6.43820	7.21750	-0.79630	C	1.89140	3.42220	2.86060
C	5.95470	6.82280	-1.98770	H	4.15320	4.44350	-1.70600
O	5.36440	5.75610	-2.15110	H	3.92050	1.65680	-2.23750
C	2.55980	7.08360	0.81170	H	6.04440	2.87570	-1.62220
C	6.81400	7.17960	1.61320	H	5.42460	3.08630	0.02730
H	6.52200	9.85220	-2.83480	H	5.76910	1.45410	-0.57830
H	5.56900	7.44050	-4.00870	N	0.08620	2.62540	0.59440
H	7.87820	8.41900	-4.30060	C	0.70280	1.80230	1.46130
H	8.24930	7.99970	-2.61650	O	0.19600	0.75900	1.87070
H	7.94160	6.70840	-3.79440	C	-0.07580	-0.48240	-2.22700
N	3.99040	7.20110	0.58590	C	-1.60640	3.37570	-0.99320
C	4.81310	6.13970	0.65950	H	3.27720	3.56800	0.77500
O	4.41970	5.00390	0.92050	H	2.55920	1.38950	2.46040
C	1.85550	5.32060	-2.50460	H	2.86460	3.78790	3.18810
C	1.88040	8.42240	0.51670	H	1.37340	4.21990	2.32830
H	6.92070	8.11230	-0.71280	H	1.29560	3.12650	3.72410
H	6.81420	5.45070	0.29080	N	-0.20670	0.76400	-1.49160
H	7.86230	7.43180	1.45330	C	-1.22190	0.98410	-0.63720
H	6.24270	8.09940	1.73730	O	-2.10450	0.15590	-0.41770
H	6.71070	6.57350	2.51330	C	1.00310	-2.53510	0.81010
N	2.34250	6.21200	-1.46550	C	1.24560	-0.48860	-2.99830
C	1.97240	6.07690	-0.17950	H	0.54940	3.47980	0.28500
O	1.20300	5.19880	0.20760	H	-1.98070	2.31390	0.86970
C	3.97610	2.34270	-1.39220	H	-1.58710	4.36860	-0.54390
C	2.56230	5.63420	-3.82480	H	-0.88490	3.34170	-1.80940
H	4.36630	8.12350	0.36600	H	-2.60010	3.16600	-1.38890
H	2.34720	6.74780	1.82660	N	0.84000	-1.50210	-0.19880
H	2.30120	9.18570	1.17130	C	-0.00100	-1.64760	-1.23830
H	2.05640	8.70800	-0.52030	O	-0.68640	-2.65440	-1.40980
H	0.80660	8.33950	0.68470	C	-2.38770	-1.91200	2.45820
N	3.49610	3.66500	-1.75620	C	1.90890	-2.02140	1.93110
C	2.22820	3.87960	-2.15020	H	0.50090	1.48360	-1.63900
O	1.39060	2.98240	-2.23070	H	-0.92350	-0.63720	-2.89440
C	2.09630	2.22310	1.93250	H	1.25830	0.35570	-3.68740

H	2.08110	-0.39320	-2.30480	O	-4.76900	-8.29600	2.99050
H	1.34870	-1.42190	-3.55190	C	-6.32830	-8.69670	-0.98620
N	-1.08350	-1.76690	1.83400	C	-7.15060	-5.14440	1.34950
C	-0.35240	-2.83040	1.45520	H	-1.96150	-5.35770	1.55200
O	-0.72950	-3.99130	1.60750	H	-2.29910	-7.81980	2.94010
C	-4.16410	-2.97450	-0.75390	H	-1.62460	-5.61670	3.97300
C	-3.02830	-0.53430	2.63810	H	-3.26940	-5.00720	3.70350
H	1.38720	-0.64680	-0.10120	H	-3.00690	-6.35490	4.82800
H	1.39630	-3.45340	0.37400	N	-6.14800	-7.61980	-0.02750
H	2.87780	-1.75340	1.50980	C	-6.84650	-7.56300	1.12050
H	1.46590	-1.13850	2.39170	O	-7.68030	-8.40900	1.43990
H	2.03450	-2.79290	2.69080	C	-4.54510	-11.32240	1.14170
N	-3.33010	-2.31210	0.23460	C	-5.29840	-8.56360	-2.10980
C	-3.31130	-2.69580	1.52360	H	-4.71130	-5.31850	1.90740
O	-3.99100	-3.62530	1.95600	H	-7.02990	-6.55080	3.00640
C	-2.02340	-6.13580	-0.91320	H	-6.92960	-4.26060	1.94800
C	-3.85980	-2.41250	-2.14400	H	-6.70740	-5.02330	0.36110
H	-0.72590	-0.82330	1.68560	H	-8.22900	-5.26110	1.24300
H	-2.31320	-2.44030	3.40860	N	-4.92680	-10.10810	0.44080
H	-2.38020	0.07960	3.26360	C	-6.04590	-10.03560	-0.30180
H	-3.14770	-0.05040	1.66880	O	-6.82020	-10.98120	-0.44070
H	-4.00730	-0.63760	3.10610	C	-7.24340	-11.00330	3.82860
N	-2.49570	-4.76260	-0.86140	C	-3.31430	-11.05080	2.00910
C	-3.80520	-4.46100	-0.80410	H	-5.46710	-6.89260	-0.24670
O	-4.68970	-5.31560	-0.79130	H	-7.34440	-8.70710	-1.38070
C	-2.83800	-6.89310	2.74260	H	-5.43120	-7.59940	-2.60050
C	-0.49620	-6.15860	-0.82480	H	-4.29050	-8.61640	-1.69820
H	-2.74710	-1.53440	-0.07460	H	-5.42960	-9.36950	-2.83190
H	-5.22140	-2.87280	-0.50930	N	-6.17580	-10.75090	2.87570
H	-4.05810	-1.34070	-2.14470	C	-5.66600	-11.72570	2.10180
H	-2.81150	-2.57950	-2.39110	O	-6.06150	-12.88970	2.14290
H	-4.48320	-2.90630	-2.88940	C	-9.96120	-11.38880	1.17020
N	-2.39300	-6.28060	1.50240	C	-7.70390	-9.68210	4.44770
C	-2.53550	-6.89330	0.31360	H	-4.31680	-9.29500	0.52460
O	-3.04720	-8.00490	0.18990	H	-4.36410	-12.13990	0.44390
C	-6.55800	-6.37450	2.03980	H	-2.49740	-10.71460	1.37060
C	-2.67430	-5.90000	3.89500	H	-3.53810	-10.27230	2.73840
H	-1.80030	-4.01650	-0.86960	H	-3.02390	-11.95890	2.53720
H	-2.37470	-6.63980	-1.81360	N	-8.82760	-10.94450	1.96330
H	-0.08390	-5.58940	-1.65800	C	-8.45490	-11.57650	3.09050
H	-0.17120	-5.70380	0.11080	O	-9.03950	-12.56610	3.52840
H	-0.13670	-7.18690	-0.86320	C	-8.19080	-14.47780	-0.21740
N	-5.12070	-6.21240	2.17850	C	-10.04360	-10.56540	-0.11670
C	-4.33440	-7.19750	2.64790	H	-5.81290	-9.80040	2.80390

H	-6.92800	-11.71050	4.59570	O	9.61320	16.96520	-3.82960
H	-6.85820	-9.21140	4.94910	C	-12.11480	-18.37920	0.85210
H	-8.07070	-9.01440	3.66830	O	-12.95980	-19.27030	0.78190
H	-8.50500	-9.86610	5.16350	H	-11.23910	-20.63870	1.38440
N	-8.52910	-13.13730	0.22990	H	-11.32680	-15.31590	1.31190
C	-9.73840	-12.83940	0.73780	H	-13.57800	-16.84960	0.48590
O	-10.63710	-13.67030	0.85980	H	-12.03920	-15.54190	-1.02970
C	-7.93720	-15.93690	3.30520	H	-10.75670	-16.72950	-0.72260
C	-6.71140	-14.53360	-0.60360	H	-12.23020	-17.23070	-1.57540
H	-8.30930	-10.12700	1.64170	N	-10.83400	-18.60930	1.19200
H	-10.88880	-11.32660	1.73920	C	10.53020	17.79960	-3.82960
H	-10.15760	-9.51270	0.14230	H	9.12600	19.40220	-3.81930
H	-9.12980	-10.69100	-0.69740	H	10.62990	19.74720	-2.94220
H	-10.89270	-10.89490	-0.71530	H	10.62980	19.74740	-4.71690
N	-7.83770	-15.09510	2.12500	H	-9.60520	-20.25560	0.80700
C	-8.36840	-15.45830	0.94360	H	-10.01320	-20.00320	2.51560
O	-8.97040	-16.51780	0.77700	H	-10.17110	-17.83540	1.23600
C	-11.65270	-15.25040	3.87630				
C	-7.37050	-15.19400	4.51670	4. acetyl-(ala) <sub>39</sub> -methylamide			
H	-7.81690	-12.41170	0.14950	C	16.28470	22.32110	-4.71850
H	-8.82730	-14.78940	-1.04550	N	15.80440	23.69250	-4.71850
H	-6.52550	-13.81470	-1.40160	C	17.80760	22.30900	-4.57150
H	-6.09290	-14.27690	0.25630	C	15.72970	21.59090	-3.49390
H	-6.45250	-15.53750	-0.94000	O	15.22820	20.47370	-3.60970
N	-10.23110	-15.13410	3.59890	C	11.64170	22.12910	-1.93550
C	-9.41210	-16.20080	3.61520	C	-16.76200	-24.77040	1.18060
O	-9.80160	-17.34080	3.86320	H	16.49610	24.44210	-4.71850
C	-12.49260	-16.92830	0.54740	H	15.97050	21.79340	-5.61900
C	-12.33530	-13.90160	3.64020	H	18.24870	22.86010	-5.40200
H	-7.34730	-14.20500	2.21170	H	18.09450	22.78830	-3.63550
H	-7.43040	-16.88990	3.15350	H	18.17300	21.28210	-4.57090
H	-6.32770	-14.94280	4.32300	N	13.07190	22.30250	-1.74610
H	-7.93150	-14.27480	4.68480	C	15.33460	21.64850	-1.07890
H	-7.44290	-15.82150	5.40500	N	15.82380	22.23310	-2.31590
N	-11.96150	-16.06490	1.58850	C	15.44940	22.67030	0.05410
C	-12.28300	-16.22970	2.88410	C	13.84430	21.33350	-1.22310
O	-13.04190	-17.11350	3.27880	O	13.40200	20.24130	-0.87040
C	10.20850	19.27500	-3.82960	C	11.99770	19.73520	-4.89260
C	-11.83490	-16.58560	-0.79080	C	11.07030	23.33870	-2.67790
H	-9.85870	-14.20840	3.38730	H	16.24880	23.15940	-2.27260
H	-11.82830	-15.61000	4.89010	H	15.86980	20.73000	-0.83840
H	-11.88560	-13.15660	4.29650	H	16.49400	22.96120	0.16510
H	-12.19730	-13.59150	2.60450	H	14.85790	23.55480	-0.18170
H	-13.40230	-13.98360	3.84700				



H	15.08360	22.23640	0.98470	C	10.25970	12.59270	-0.48930
N	12.13630	20.83620	-3.95450	C	11.62750	13.90730	-4.38180
C	11.39410	20.91700	-2.83570	H	9.92440	18.35830	-2.30780
O	10.55270	20.07440	-2.52760	H	7.34870	17.14700	-2.27930
C	13.71050	17.17210	-2.63450	H	8.13200	18.92550	-3.89120
C	13.06920	19.84670	-5.97910	H	9.19650	17.73290	-4.66190
H	13.48730	23.19190	-2.02330	H	7.43660	17.51870	-4.74200
H	11.13410	21.97370	-0.98350	N	10.40040	13.40610	-1.68520
H	11.26410	24.23800	-2.09320	C	9.91690	13.01130	-2.87660
H	11.55040	23.43810	-3.65130	O	9.32660	11.94470	-3.04000
H	9.99720	23.21340	-2.82250	C	6.52200	13.27220	-0.07720
N	13.35020	18.36680	-3.37910	C	10.77620	13.36810	0.72430
C	12.26000	18.41490	-4.16530	H	10.48420	16.04070	-3.72370
O	11.49600	17.46200	-4.31040	H	9.53120	13.62900	-4.89760
C	10.91000	17.54140	-0.06110	H	11.84040	14.60760	-5.18950
C	14.90590	17.47160	-1.72780	H	12.21150	14.18830	-3.50550
H	12.82170	21.56150	-4.16530	H	11.90380	12.89690	-4.68330
H	10.99760	19.70950	-5.32520	N	7.95260	13.38970	-0.30300
H	12.95080	20.79780	-6.49810	C	8.77530	12.32820	-0.22940
H	14.06090	19.80960	-5.52830	O	8.38190	11.19240	0.03160
H	12.96950	19.02280	-6.68560	C	5.81770	11.50910	-3.39350
N	12.01210	17.77650	-0.97840	C	5.84260	14.61100	-0.37220
C	12.55560	16.78600	-1.70830	H	10.88290	14.30080	-1.60170
O	12.16420	15.62120	-1.65370	H	10.77630	11.63920	-0.59820
C	8.29760	17.07610	-2.81080	H	11.82450	13.62030	0.56440
C	10.42010	18.87470	0.50740	H	10.20490	14.28800	0.84830
H	13.95280	19.18520	-3.29210	H	10.67280	12.76200	1.62440
H	13.92180	16.33880	-3.30460	N	6.30460	12.40050	-2.35440
H	15.74520	17.79670	-2.34270	C	5.93460	12.26550	-1.06840
H	14.65090	18.26640	-1.02690	O	5.16520	11.38730	-0.68130
H	15.18020	16.57820	-1.16680	C	7.93820	8.53120	-2.28110
N	9.39800	17.54600	-1.98630	C	6.52450	11.82280	-4.71370
C	9.73030	16.94370	-0.83050	H	8.32850	14.31200	-0.52290
O	9.13400	15.96180	-0.39100	H	6.30940	12.93640	0.93770
C	10.13420	13.96420	-4.05380	H	6.26330	15.37430	0.28240
C	8.26070	17.86750	-4.11970	H	6.01860	14.89660	-1.40920
H	12.37300	18.72700	-1.05970	H	4.76880	14.52810	-0.20420
H	11.19910	16.85490	0.73470	N	7.45830	9.85360	-2.64510
H	11.24370	19.36220	1.02900	C	6.19030	10.06810	-3.03910
H	10.08020	19.52120	-0.30150	O	5.35280	9.17090	-3.11960
H	9.59300	18.70370	1.19650	C	6.05840	8.41170	1.04360
N	9.77280	15.31330	-3.65270	C	9.36650	8.63240	-1.74180
C	8.54360	15.61670	-3.19870	H	6.94590	13.14610	-2.62490
O	7.64480	14.78400	-3.09070	H	4.73510	11.58020	-3.49820

H	6.32460	12.85920	-4.98570	C	3.60980	3.35810	0.56630
H	7.60000	11.68660	-4.60100	O	3.23270	2.19730	0.71860
H	6.16250	11.15650	-5.49670	C	-0.20190	3.21400	-1.64280
N	6.85310	8.81260	-0.10490	C	0.93380	5.65430	1.74920
C	7.08530	7.98110	-1.13630	H	5.34930	5.54170	-0.99010
O	6.64700	6.83270	-1.18280	H	5.35840	2.73520	-0.51490
C	2.72310	8.52860	-0.81750	H	6.84000	4.43520	0.62090
C	5.85360	9.61070	1.97170	H	5.42810	5.05000	1.50280
H	8.11540	10.63210	-2.59490	H	5.99660	3.39570	1.80180
H	7.88270	7.84530	-3.12640	N	0.63210	3.87640	-0.65430
H	10.00660	9.06420	-2.51110	C	0.65090	3.49270	0.63470
H	9.38670	9.27490	-0.86160	O	-0.02890	2.56330	1.06700
H	9.73120	7.64260	-1.46720	C	1.93870	0.05270	-1.80210
N	4.04840	8.81390	-0.29450	C	0.10240	3.77600	-3.03290
C	4.66500	7.99090	0.57240	H	3.23620	5.36530	0.79670
O	4.15820	6.94760	0.98180	H	1.64900	3.74830	2.51970
C	3.88640	5.70620	-3.11600	H	1.58200	6.26810	2.37470
C	2.35580	9.56430	-1.88210	H	0.81450	6.13810	0.77990
H	7.23940	9.75660	-0.11390	H	-0.04510	5.55090	2.21720
H	6.52140	7.57800	1.57150	N	1.46650	1.42590	-1.75030
H	6.82680	9.97640	2.29910	C	0.15700	1.72760	-1.69300
H	5.33550	10.40840	1.43940	O	-0.72750	0.87290	-1.68020
H	5.25780	9.31510	2.83520	C	1.12420	-0.70460	1.85370
N	3.75540	6.95250	-2.38050	C	3.46600	0.02990	-1.71370
C	2.74030	7.17260	-1.52610	H	1.21510	4.65410	-0.96350
O	1.85770	6.34450	-1.30670	H	-1.25920	3.31580	-1.39820
C	4.96530	3.65350	-0.07880	H	-0.09590	4.84780	-3.03360
C	5.20780	5.69990	-3.88720	H	1.15070	3.60900	-3.28000
H	4.51160	9.66840	-0.60400	H	-0.52100	3.28220	-3.77830
H	1.98150	8.50240	-0.01920	N	1.56920	-0.09200	0.61350
H	2.37500	10.55720	-1.43280	C	1.42670	-0.70480	-0.57530
H	3.07730	9.53020	-2.69830	O	0.91500	-1.81640	-0.69900
H	1.36210	9.35450	-2.27780	C	-2.59590	-0.18600	1.15090
N	4.80220	4.68640	-1.08770	C	1.28790	0.28850	3.00610
C	3.96120	4.54100	-2.12720	H	2.16180	2.17210	-1.75850
O	3.27580	3.53420	-2.29870	H	1.58750	-0.45120	-2.70250
C	1.57450	4.27660	1.56920	H	3.87820	0.59910	-2.54690
C	5.87110	4.16720	1.04220	H	3.79100	0.48470	-0.77810
H	4.46310	7.67210	-2.52790	H	3.82540	-0.99840	-1.75220
H	3.03870	5.55140	-3.78340	N	-1.15850	-0.02390	1.28960
H	5.22050	6.54430	-4.57640	C	-0.37220	-1.00900	1.75900
H	6.04330	5.79530	-3.19380	O	-0.80680	-2.10740	2.10160
H	5.31090	4.76660	-4.44080	C	-2.36620	-2.50820	-1.87510
N	2.87870	4.42160	0.94510	C	-3.18840	1.04420	0.46050

H	2.00070	0.83090	0.66310	H	-4.54280	-3.67760	4.27460
H	1.66310	-1.63120	2.05120	N	-4.56690	-6.94880	-0.65900
H	2.33750	0.57180	3.08410	C	-5.77620	-6.65090	-0.15110
H	0.69280	1.18130	2.81460	O	-6.67490	-7.48180	-0.02910
H	0.95530	-0.16640	3.93910	C	-3.97510	-9.74840	2.41630
N	-2.18580	-1.43120	-0.91640	C	-2.74920	-8.34510	-1.49250
C	-2.88440	-1.37440	0.23150	H	-4.34710	-3.93850	0.75280
O	-3.71810	-2.22040	0.55100	H	-6.92670	-5.13810	0.85030
C	-0.58290	-5.13380	0.25280	H	-6.19540	-3.32420	-0.74670
C	-1.33620	-2.37500	-2.99870	H	-5.16770	-4.50240	-1.58630
H	-0.74910	0.87010	1.01850	H	-6.93050	-4.70640	-1.60430
H	-3.06770	-0.36220	2.11750	N	-3.87550	-8.90660	1.23600
H	-2.96740	1.92790	1.05910	C	-4.40620	-9.26970	0.05470
H	-2.74520	1.16520	-0.52780	O	-5.00820	-10.32930	-0.11190
H	-4.26690	0.92750	0.35410	C	-7.69050	-9.06190	2.98740
N	-0.96460	-3.91960	-0.44820	C	-3.40830	-9.00540	3.62780
C	-2.08380	-3.84710	-1.19070	H	-3.85470	-6.22320	-0.73940
O	-2.85800	-4.79260	-1.32960	H	-4.86520	-8.60090	-1.93450
C	-3.28120	-4.81480	2.93970	H	-2.56340	-7.62620	-2.29050
C	0.64780	-4.86220	1.12020	H	-2.13070	-8.08840	-0.63260
H	-1.50490	-0.70410	-1.13560	H	-2.49030	-9.34900	-1.82890
H	-3.38220	-2.51860	-2.26960	N	-6.26890	-8.94550	2.71000
H	-1.46900	-1.41090	-3.48950	C	-5.44990	-10.01230	2.72630
H	-0.32840	-2.42780	-2.58710	O	-5.83940	-11.15230	2.97430
H	-1.46740	-3.18090	-3.72080	C	-8.53050	-10.73970	-0.34150
N	-2.21360	-4.56240	1.98680	C	-8.37310	-7.71310	2.75130
C	-1.70390	-5.53720	1.21290	H	-3.38510	-8.01640	1.32280
O	-2.09930	-6.70110	1.25400	H	-3.46820	-10.70130	2.26460
C	-5.99900	-5.20030	0.28130	H	-2.36550	-8.75420	3.43410
C	-3.74170	-3.49360	3.55880	H	-3.96930	-8.08620	3.79590
H	-0.35460	-3.10640	-0.36430	H	-3.48070	-9.63290	4.51610
H	-0.40190	-5.95140	-0.44500	N	-7.99930	-9.87640	0.69960
H	1.46480	-4.52610	0.48170	C	-8.32080	-10.04120	1.99520
H	0.42410	-4.08370	1.84950	O	-9.07980	-10.92500	2.38990
H	0.93830	-5.77040	1.64830	C	-6.38570	-13.75380	0.61620
N	-4.86540	-4.75600	1.07430	C	-7.87280	-10.39700	-1.67970
C	-4.49270	-5.38790	2.20160	H	-5.89650	-8.01980	2.49830
O	-5.07740	-6.37760	2.63950	H	-7.86610	-9.42150	4.00120
C	-4.22860	-8.28930	-1.10630	H	-7.92350	-6.96800	3.40760
C	-6.08140	-4.37680	-1.00560	H	-8.23520	-7.40300	1.71550
H	-1.85080	-3.61190	1.91490	H	-9.44020	-7.79510	2.95810
H	-2.96580	-5.52190	3.70680	N	-6.87180	-12.42070	0.30310
H	-2.89610	-3.02290	4.06020	C	-8.15260	-12.19070	-0.03680
H	-4.10850	-2.82580	2.77940	O	-8.99760	-13.08170	-0.10700

C	-8.13810	-13.94620	4.00640	H	-9.20000	-15.67120	-1.62120
C	-4.93740	-13.67260	1.10280	H	-8.32930	-16.45770	-0.28970
H	-7.36460	-9.12730	0.42300	H	-9.11450	-17.45200	-1.53250
H	-9.61590	-10.66100	-0.40300	N	-11.34160	-17.91780	3.93250
H	-8.07700	-9.35330	-1.91860	C	-10.63140	-18.97510	3.50020
H	-6.79450	-10.54090	-1.61160	O	-11.00890	-20.13750	3.63850
H	-8.26800	-11.04220	-2.46430	C	-14.52520	-19.04720	1.43560
N	-7.38550	-13.52090	2.83840	C	-13.24740	-16.69620	4.84010
C	-7.19750	-14.32790	1.77910	H	-8.94020	-16.76210	1.93210
O	-7.64360	-15.47270	1.72130	H	-8.92870	-19.57940	2.33810
C	-11.54120	-13.76820	2.27760	H	-7.39550	-17.91470	3.45750
C	-8.30080	-12.76930	4.97060	H	-8.76930	-17.31510	4.40750
H	-6.20890	-11.64680	0.34710	H	-8.19900	-18.97890	4.64420
H	-6.47720	-14.41850	-0.24280	N	-13.65050	-18.41310	2.40730
H	-4.32470	-13.22500	0.32030	C	-13.58470	-18.82840	3.68490
H	-4.88010	-13.05200	1.99690	O	-14.25270	-19.76500	4.12020
H	-4.56800	-14.67050	1.33900	C	-12.40990	-22.21360	1.11770
N	-10.19540	-13.50190	2.75640	C	-14.27100	-18.45260	0.04900
C	-9.55080	-14.34880	3.57870	H	-10.98460	-16.97250	3.79360
O	-10.04740	-15.39950	3.98170	H	-12.51410	-18.62380	5.53610
C	-10.48220	-16.53870	-0.13170	H	-12.57250	-16.10090	5.45510
C	-11.94300	-12.70490	1.25340	H	-13.40100	-16.18820	3.88810
H	-6.99460	-12.57880	2.83770	H	-14.20840	-16.80650	5.34260
H	-7.66010	-14.79470	4.49580	N	-12.87220	-20.83990	1.22090
H	-7.31380	-12.41630	5.26940	C	-14.17680	-20.53360	1.33560
H	-8.83420	-11.95640	4.47810	O	-15.06490	-21.38420	1.36130
H	-8.86490	-13.08330	5.84880	C	-13.08870	-23.05650	4.78250
N	-10.57800	-15.31020	0.63840	C	-10.88050	-22.24560	1.14700
C	-11.55870	-15.10640	1.53610	H	-13.07530	-17.63080	2.09510
O	-12.43680	-15.93550	1.76890	H	-15.57190	-18.94650	1.72280
C	-9.29980	-18.67030	2.81110	H	-14.46320	-17.38020	0.08190
C	-9.19120	-16.53220	-0.95280	H	-13.23380	-18.61840	-0.24200
H	-9.73960	-12.64230	2.45030	H	-14.92500	-18.92510	-0.68390
H	-12.25200	-13.81040	3.10280	N	-12.68790	-22.41580	3.54140
H	-11.90110	-11.72340	1.72570	C	-12.87900	-22.99850	2.34430
H	-11.25340	-12.72230	0.40960	O	-13.40130	-24.10440	2.21320
H	-12.95230	-12.90030	0.89100	C	-16.82990	-22.50350	4.23520
N	-9.49540	-17.61210	1.83470	C	-12.87570	-22.09280	5.95150
C	-10.37620	-17.72810	0.82490	H	-12.17350	-20.09700	1.20430
O	-11.07330	-18.72720	0.65520	H	-12.79800	-22.69360	0.21940
C	-12.62180	-18.07200	4.60230	H	-10.49720	-21.65800	0.31280
C	-8.34910	-18.18850	3.90890	H	-10.51760	-21.81540	2.08040
H	-9.87250	-14.59050	0.48150	H	-10.52850	-23.27430	1.06980
H	-11.35560	-16.67310	-0.76970	N	-15.38750	-22.35160	4.32280

C	-14.58930	-23.35150	4.73760	N	19.75810	28.44820	-3.14430
O	-15.01670	-24.45600	5.06980	C	19.38370	28.88530	-0.77420
C	14.17070	25.46350	-4.71850	C	17.77860	27.54850	-2.05140
C	-17.44140	-21.25410	3.59820	O	17.33630	26.45630	-1.69880
H	-12.24970	-21.49640	3.59690	C	15.93200	25.95020	-5.72100
H	-12.54790	-23.99020	4.93650	C	15.00460	29.55370	-3.50620
H	-11.82230	-21.81640	5.99620	H	20.18300	29.37440	-3.10090
H	-13.47270	-21.19280	5.80480	H	19.80410	26.94500	-1.66670
H	-13.17500	-22.56890	6.88520	H	20.42830	29.17620	-0.66330
O	13.57540	23.15380	-4.71860	H	18.79220	29.76980	-1.01010
C	-17.15990	-23.66770	3.29890	H	19.01780	28.45140	0.15630
O	-17.98560	-24.51740	3.62930	N	16.07060	27.05120	-4.78280
H	-17.51580	-25.43810	1.59770	C	15.32840	27.13200	-3.66410
H	-14.98370	-21.45310	4.05800	O	14.48690	26.28940	-3.35600
H	-17.26560	-22.70130	5.21450	C	17.64480	23.38710	-3.46290
H	-17.19290	-20.38630	4.20920	C	17.00350	26.06170	-6.80740
H	-17.03560	-21.11090	2.59680	H	17.42150	29.40690	-2.85170
H	-18.52380	-21.36310	3.53020	H	15.06830	28.18870	-1.81190
N	-16.50590	-23.69960	2.12400	H	15.19840	30.45300	-2.92160
C	14.49230	23.98810	-4.71850	H	15.48460	29.65310	-4.47970
H	13.08820	25.59070	-4.70820	H	13.93150	29.42840	-3.65090
H	14.59200	25.93570	-3.83110	N	17.28450	24.58180	-4.20750
H	14.59200	25.93590	-5.60580	C	16.19430	24.62990	-4.99360
H	-17.13300	-24.35830	0.24220	O	15.43030	23.67700	-5.13880
H	-15.84250	-25.32280	0.98660	C	14.84430	23.75640	-0.88950
H	-15.82980	-22.97050	1.89680	C	18.84020	23.68660	-2.55610

5. acetyl-(ala)<sub>49</sub>-methylamide

C	20.21900	28.53610	-5.54690	H	16.88510	27.01280	-7.32640
N	19.73870	29.90750	-5.54690	H	17.99510	26.02460	-6.35660
C	21.74190	28.52400	-5.39980	H	16.90380	25.23780	-7.51400
C	19.66400	27.80590	-4.32230	N	15.94640	23.99150	-1.80680
O	19.16250	26.68870	-4.43810	C	16.48990	23.00100	-2.53660
C	15.57600	28.34410	-2.76380	O	16.09850	21.83620	-2.48210
C	-21.86350	-29.89580	4.56990	C	12.23190	23.29110	-3.63920
H	20.43040	30.65710	-5.54690	C	14.35430	25.08970	-0.32090
H	19.90480	28.00840	-6.44730	H	17.88710	25.40020	-4.12050
H	22.18300	29.07510	-6.23040	H	17.85610	22.55390	-4.13300
H	22.02870	29.00330	-4.46390	H	19.67940	24.01170	-3.17110
H	22.10730	27.49710	-5.39930	H	18.58510	24.48140	-1.85530
N	17.00620	28.51750	-2.57450	H	19.11450	22.79320	-1.99520
C	19.26880	27.86350	-1.90730	N	13.33230	23.76100	-2.81470
				C	13.66460	23.15870	-1.65880
				O	13.06820	22.17680	-1.21940

C	14.06840	20.17920	-4.88210	H	10.19760	21.58930	-0.54600
C	12.19500	24.08250	-4.94810	H	9.95290	21.11160	-2.23760
H	16.30720	24.94200	-1.88810	H	8.70310	20.74310	-1.03260
H	15.13340	23.06990	-0.09370	N	11.39260	16.06860	-3.47350
H	15.17800	25.57720	0.20070	C	10.12460	16.28310	-3.86750
H	14.01450	25.73620	-1.12990	O	9.28710	15.38590	-3.94790
H	13.52730	24.91870	0.36810	C	9.99270	14.62670	0.21520
N	13.70700	21.52830	-4.48110	C	13.30070	14.84740	-2.57020
C	12.47790	21.83170	-4.02710	H	10.88020	19.36110	-3.45330
O	11.57910	20.99900	-3.91910	H	8.66930	17.79520	-4.32660
C	14.19390	18.80770	-1.31770	H	10.25890	19.07420	-5.81410
C	15.56180	20.12230	-5.21010	H	11.53420	17.90160	-5.42930
H	13.85870	24.57330	-3.13620	H	10.09680	17.37150	-6.32510
H	11.28290	23.36200	-3.10770	N	10.78740	15.02760	-0.93330
H	12.06630	25.14050	-4.71960	C	11.01960	14.19610	-1.96470
H	13.13080	23.94800	-5.49030	O	10.58130	13.04780	-2.01120
H	11.37090	23.73380	-5.57040	C	6.65740	14.74360	-1.64590
N	14.33460	19.62110	-2.51350	C	9.78780	15.82570	1.14330
C	13.85120	19.22630	-3.70500	H	12.04970	16.84710	-3.42330
O	13.26090	18.15970	-3.86840	H	11.81700	14.06030	-3.95480
C	10.45620	19.48720	-0.90560	H	13.94080	15.27920	-3.33950
C	14.71050	19.58310	-0.10400	H	13.32100	15.48990	-1.69000
H	14.41850	22.25570	-4.55210	H	13.66550	13.85760	-2.29560
H	13.46550	19.84400	-5.72600	N	7.98270	15.02890	-1.12280
H	15.77470	20.82260	-6.01790	C	8.59920	14.20590	-0.25600
H	16.14580	20.40330	-4.33380	O	8.09250	13.16260	0.15340
H	15.83800	19.11190	-5.51170	C	7.82070	11.92120	-3.94430
N	11.88680	19.60470	-1.13140	C	6.29010	15.77930	-2.71050
C	12.70960	18.54320	-1.05770	H	11.17370	15.97160	-0.94230
O	12.31610	17.40740	-0.79680	H	10.45560	13.79300	0.74310
C	9.75190	17.72410	-4.22180	H	10.76100	16.19140	1.47080
C	9.77690	20.82600	-1.20060	H	9.26980	16.62340	0.61110
H	14.81720	20.51580	-2.43010	H	9.19200	15.53010	2.00680
H	14.71060	17.85420	-1.42650	N	7.68970	13.16750	-3.20890
H	15.75880	19.83530	-0.26400	C	6.67450	13.38760	-2.35450
H	14.13920	20.50300	0.02000	O	5.79200	12.55950	-2.13500
H	14.60710	18.97700	0.79600	C	8.89960	9.86850	-0.90720
N	10.23890	18.61550	-3.18280	C	9.14210	11.91490	-4.71550
C	9.86880	18.48050	-1.89670	H	8.44580	15.88340	-1.43230
O	9.09950	17.60230	-1.50960	H	5.91580	14.71740	-0.84760
C	11.87250	14.74620	-3.10950	H	6.30930	16.77220	-2.26110
C	10.45870	18.03780	-5.54210	H	7.01160	15.74520	-3.52670
H	12.26270	20.52700	-1.35130	H	5.29640	15.56950	-3.10610
H	10.24370	19.15140	0.10930	N	8.73650	10.90140	-1.91610

C	7.89550	10.75600	-2.95560	H	6.09610	8.38710	-2.58690
O	7.21010	9.74920	-3.12710	H	5.52170	5.76380	-3.53090
C	5.50880	10.49160	0.74090	H	7.81250	6.81410	-3.37530
C	9.80540	10.38220	0.21380	H	7.72530	6.69970	-1.60640
H	8.39740	13.88710	-3.35630	H	7.75970	5.21660	-2.58050
H	6.97290	11.76640	-4.61170	N	2.77570	6.19110	0.46120
H	9.15480	12.75930	-5.40470	C	3.56210	5.20600	0.93060
H	9.97750	12.01030	-4.02210	O	3.12750	4.10760	1.27330
H	9.24510	10.98170	-5.26910	C	1.56810	3.70680	-2.70350
N	6.81290	10.63660	0.11670	C	0.74590	7.25920	-0.36780
C	7.54400	9.57310	-0.26210	H	5.93500	7.04590	-0.16530
O	7.16690	8.41230	-0.10980	H	5.59730	4.58380	1.22280
C	3.73230	9.42900	-2.47120	H	6.27180	6.78680	2.25570
C	4.86810	11.86930	0.92080	H	4.62700	7.39630	1.98630
H	9.28360	11.75670	-1.81850	H	4.88960	6.04860	3.11070
H	9.29270	8.95020	-1.34330	N	1.74850	4.78380	-1.74480
H	10.77430	10.65020	-0.20750	C	1.04990	4.84060	-0.59680
H	9.36230	11.26500	0.67450	O	0.21610	3.99460	-0.27740
H	9.93090	9.61070	0.97350	C	3.35130	1.08120	-0.57560
N	4.56640	10.09140	-1.48270	C	2.59800	3.84000	-3.82700
C	4.58520	9.70770	-0.19370	H	3.18520	7.08510	0.19010
O	3.90540	8.77830	0.23870	H	0.86650	5.85280	1.28910
C	5.87300	6.26770	-2.63050	H	0.96680	8.14290	0.23070
C	4.03660	9.99100	-3.86130	H	1.18910	7.38020	-1.35620
H	7.17050	11.58030	-0.03160	H	-0.33260	7.14250	-0.47430
H	5.58330	9.96330	1.69130	N	2.96960	2.29540	-1.27650
H	5.51620	12.48310	1.54630	C	1.85050	2.36790	-2.01900
H	4.74870	12.35310	-0.04850	O	1.07620	1.42240	-2.15800
H	3.88920	11.76590	1.38890	C	0.65300	1.40020	2.11130
N	5.40070	7.64090	-2.57870	C	4.58210	1.35280	0.29180
C	4.09120	7.94260	-2.52140	H	2.42940	5.51090	-1.96390
O	3.20670	7.08790	-2.50860	H	0.55210	3.69640	-3.09800
C	5.05850	5.51040	1.02540	H	2.46520	4.80410	-4.31780
C	7.40030	6.24490	-2.54210	H	3.60590	3.78720	-3.41550
H	5.14940	10.86910	-1.79190	H	2.46690	3.03410	-4.54910
H	2.67500	9.53080	-2.22660	N	1.72070	1.65260	1.15850
H	3.83840	11.06280	-3.86200	C	2.23040	0.67780	0.38450
H	5.08500	9.82400	-4.10840	O	1.83490	-0.48610	0.42560
H	3.41330	9.49720	-4.60670	C	-2.06480	1.01470	-0.54710
N	5.50350	6.12300	-0.21490	C	0.19260	2.72140	2.73040
C	5.36100	5.51020	-1.40370	H	3.57960	3.10860	-1.19270
O	4.84920	4.39860	-1.52740	H	3.53230	0.26360	-1.27330
C	1.33840	6.02900	0.32250	H	5.39910	1.68890	-0.34660
C	5.22220	6.50350	2.17770	H	4.35840	2.13130	1.02110

H	4.87260	0.44460	0.82000	C	-2.45150	-7.53880	-0.21220
N	-0.93120	1.45910	0.24600	C	-3.93850	-4.18200	-2.50810
C	-0.55850	0.82710	1.37320	H	-1.96220	-1.80480	1.67000
O	-1.14310	-0.16250	1.81110	H	-3.93180	-3.20650	3.17280
C	-0.29440	-2.07430	-1.93470	H	-3.98920	-0.75300	2.57930
C	-2.14710	1.83820	-1.83390	H	-4.30090	-1.18790	0.88720
H	2.08350	2.60310	1.08660	H	-5.50590	-1.58010	2.12970
H	0.96840	0.69310	2.87840	N	-2.93750	-6.20570	-0.52530
H	1.03820	3.19210	3.23180	C	-4.21840	-5.97570	-0.86520
H	-0.17430	3.38920	1.95100	O	-5.06330	-6.86670	-0.93540
H	-0.60860	2.53750	3.44620	C	-4.20380	-7.73120	3.17810
N	-0.63270	-0.73380	-1.48740	C	-1.00320	-7.45760	0.27440
C	-1.84190	-0.43590	-0.97950	H	-3.43040	-2.91230	-0.40540
O	-2.74060	-1.26680	-0.85750	H	-5.68160	-4.44600	-1.23140
C	-0.04080	-3.53340	1.58790	H	-4.14280	-3.13830	-2.74700
C	1.18510	-2.13010	-2.32090	H	-2.86030	-4.32590	-2.43990
H	-0.41290	2.27660	-0.07560	H	-4.33370	-4.82720	-3.29270
H	-2.99240	1.07690	0.02190	N	-3.45130	-7.30590	2.01010
H	-2.26110	2.89080	-1.57500	C	-3.26320	-8.11290	0.95070
H	-1.23340	1.71260	-2.41470	O	-3.70930	-9.25770	0.89300
H	-2.99630	1.50860	-2.43260	C	-7.60690	-7.55310	1.44920
N	0.05880	-2.69160	0.40770	C	-4.36650	-6.55430	4.14220
C	-0.47190	-3.05470	-0.77360	H	-2.27460	-5.43180	-0.48130
O	-1.07400	-4.11430	-0.94030	H	-2.54300	-8.20350	-1.07120
C	-3.75620	-2.84680	2.15900	H	-0.39040	-7.01000	-0.50810
C	0.52600	-2.79040	2.79940	H	-0.94580	-6.83700	1.16860
H	0.07960	-0.00820	-1.56780	H	-0.63370	-8.45550	0.51070
H	-0.93090	-2.38580	-2.76280	N	-6.26110	-7.28690	1.92800
H	1.37090	-1.41120	-3.11880	C	-5.61660	-8.13380	2.75040
H	1.80360	-1.87340	-1.46090	O	-6.11320	-9.18450	3.15330
H	1.44400	-3.13400	-2.65730	C	-6.54790	-10.32370	-0.96000
N	-2.33460	-2.73050	1.88160	C	-8.00880	-6.48990	0.42500
C	-1.51560	-3.79730	1.89790	H	-3.06030	-6.36380	2.00930
O	-1.90520	-4.93730	2.14590	H	-3.72580	-8.57970	3.66740
C	-4.59620	-4.52470	-1.16980	H	-3.37950	-6.20130	4.44100
C	-4.43880	-1.49810	1.92290	H	-4.90000	-5.74140	3.64970
H	0.54920	-1.80140	0.49440	H	-4.93060	-6.86830	5.02040
H	0.46600	-4.48630	1.43620	N	-6.64380	-9.09520	-0.19000
H	1.56880	-2.53920	2.60570	C	-7.62440	-8.89130	0.70770
H	-0.03510	-1.87120	2.96750	O	-8.50250	-9.72050	0.94050
H	0.45360	-3.41790	3.68770	C	-5.36550	-12.45530	1.98280
N	-4.06500	-3.66130	-0.12870	C	-5.25690	-10.31720	-1.78110
C	-4.38660	-3.82620	1.16680	H	-5.80530	-6.42730	1.62190
O	-5.14550	-4.71000	1.56160	H	-8.31770	-7.59540	2.27450



H	-7.96690	-5.50840	0.89730	C	-8.94480	-16.78350	1.51600
H	-7.31910	-6.50730	-0.41880	O	-9.46710	-17.88940	1.38490
H	-9.01800	-6.68530	0.06260	C	-12.89570	-16.28850	3.40680
N	-5.56110	-11.39710	1.00630	C	-8.94140	-15.87780	5.12320
C	-6.44190	-11.51310	-0.00350	H	-8.23920	-13.88200	0.37590
O	-7.13900	-12.51220	-0.17310	H	-8.86370	-16.47860	-0.60900
C	-8.68750	-11.85700	3.77390	H	-6.56290	-15.44300	-0.51560
C	-4.41480	-11.97350	3.08050	H	-6.58330	-15.60040	1.25200
H	-5.93820	-8.37540	-0.34680	H	-6.59430	-17.05930	0.24150
H	-7.42130	-10.45810	-1.59810	N	-11.45320	-16.13660	3.49440
H	-5.26580	-9.45620	-2.44950	C	-10.65510	-17.13650	3.90930
H	-4.39510	-10.24270	-1.11810	O	-11.08240	-18.24100	4.24140
H	-5.18020	-11.23700	-2.36080	C	-12.79440	-18.53680	0.31860
N	-7.40730	-11.70280	3.10410	C	-13.50720	-15.03900	2.76980
C	-6.69710	-12.76010	2.67190	H	-8.31540	-15.28140	2.76850
O	-7.07460	-13.92250	2.81010	H	-8.61360	-17.77520	4.10820
C	-10.59100	-12.83220	0.60730	H	-7.88800	-15.60140	5.16780
C	-9.31310	-10.48120	4.01170	H	-9.53840	-14.97780	4.97640
H	-5.00590	-10.54710	1.10370	H	-9.24070	-16.35390	6.05690
H	-4.99440	-13.36440	1.50970	N	-12.57160	-17.48450	1.29570
H	-3.46120	-11.69970	2.62910	C	-13.22560	-17.45270	2.47050
H	-4.83500	-11.10010	3.57910	O	-14.05130	-18.30240	2.80090
H	-4.26470	-12.76390	3.81580	C	-10.94610	-21.22210	2.31220
N	-9.71620	-12.19810	1.57890	C	-11.80730	-18.38090	-0.83990
C	-9.65040	-12.61340	2.85650	H	-11.04940	-15.23810	3.22960
O	-10.31840	-13.55000	3.29180	H	-13.33130	-16.48630	4.38620
C	-8.47560	-15.99860	0.28930	H	-13.25860	-14.17130	3.38080
C	-10.33670	-12.23760	-0.77940	H	-13.10130	-14.89580	1.76840
H	-7.05040	-10.75750	2.96520	H	-14.58960	-15.14810	2.70180
H	-8.57980	-12.40880	4.70770	N	-11.34740	-19.98930	1.65620
H	-8.63820	-9.88590	4.62670	C	-12.49360	-19.89340	0.95900
H	-9.46670	-9.97320	3.05970	O	-13.27790	-20.83170	0.82670
H	-10.27410	-10.59150	4.51420	C	-13.53820	-20.95660	5.10730
N	-8.93790	-14.62480	0.39250	C	-9.68170	-20.97760	3.13830
C	-10.24250	-14.31860	0.50720	H	-11.89550	-16.75540	1.06840
O	-11.13070	-15.16920	0.53290	H	-13.82480	-18.53280	-0.03690
C	-9.15450	-16.84150	3.95410	H	-11.95330	-17.40440	-1.30170
C	-6.94620	-16.03060	0.31860	H	-10.78480	-18.44850	-0.46860
H	-9.14110	-11.41580	1.26670	H	-11.97040	-19.16820	-1.57590
H	-11.63760	-12.73150	0.89450	N	-12.50630	-20.68590	4.12080
H	-10.52890	-11.16520	-0.74640	C	-12.03180	-21.64370	3.30440
H	-9.29950	-12.40340	-1.07040	O	-12.43200	-22.80650	3.33220
H	-10.99080	-12.71010	-1.51220	C	-16.35750	-21.26410	2.54620
N	-8.75360	-16.20080	2.71300	C	-13.96740	-19.64880	5.77550

H	-10.73010	-19.18130	1.73640	H	-13.70440	-25.81100	6.57240
H	-10.79640	-22.02320	1.58840	N	-18.36640	-25.93970	2.92670
H	-8.88770	-20.62970	2.47750	C	-18.63930	-26.13470	4.22920
H	-9.87310	-20.21630	3.89430	O	-19.38750	-27.02440	4.63110
H	-9.37630	-21.89980	3.63270	C	-16.77890	-29.82140	2.68720
N	-15.19200	-20.84460	3.30590	C	-18.33350	-26.40240	0.53230
C	-14.78010	-21.50580	4.40230	H	-16.18630	-24.13760	4.68840
O	-15.35320	-22.50310	4.83800	H	-18.10500	-25.56660	6.23090
C	-14.65850	-24.32630	1.01710	H	-18.17120	-23.09900	5.69980
C	-16.48420	-20.40890	1.28380	H	-18.54960	-23.49090	4.01080
H	-12.14110	-19.73550	4.05820	H	-19.70850	-23.90770	5.28860
H	-13.19780	-21.68380	5.84440	N	-17.26910	-28.47870	2.42550
H	-13.10060	-19.19450	6.25560	C	-18.56060	-28.23450	2.14050
H	-14.35990	-18.96050	5.02720	O	-19.41260	-29.11960	2.08100
H	-14.74170	-19.84660	6.51670	C	-18.40180	-30.08870	6.13640
N	-14.97200	-22.99560	1.50950	C	-15.31270	-29.75890	3.12000
C	-16.15940	-22.70470	2.07040	H	-17.73860	-25.18700	2.64430
O	-17.05740	-23.53410	2.20640	H	-20.02820	-26.68950	1.86790
C	-14.27900	-25.87260	4.49080	H	-18.54090	-25.35220	0.32690
C	-13.19520	-24.37950	0.57340	H	-17.25430	-26.55290	0.55570
H	-14.68180	-20.02190	2.98470	H	-18.76200	-27.02620	-0.25210
H	-17.26240	-21.21150	3.15150	N	-17.69200	-29.63840	4.95110
H	-16.58230	-19.36240	1.57240	C	-17.54890	-30.42010	3.86600
H	-15.59400	-20.52450	0.66570	O	-18.00330	-31.56100	3.79750
H	-17.35740	-20.71980	0.71020	C	18.10490	31.67850	-5.54690
N	-14.21980	-25.00250	3.32850	C	-18.52110	-28.93510	7.13440
C	-14.79720	-25.33410	2.15990	H	-16.60070	-27.70920	2.46300
O	-15.41100	-26.38650	1.99060	H	-16.90680	-30.46440	1.81650
C	-17.96610	-25.18300	5.22010	H	-14.72770	-29.29500	2.32580
C	-13.66240	-25.16220	5.69750	H	-15.21780	-29.16070	4.02610
H	-14.25930	-22.27160	1.41960	H	-14.94010	-30.76390	3.31760
H	-15.32790	-24.61450	0.20660	O	17.50970	29.36880	-5.54690
H	-13.03590	-23.64210	-0.21340	C	-19.83210	-30.47410	5.75330
H	-12.54290	-24.14690	1.41500	O	-20.31880	-31.53210	6.14920
H	-12.95490	-25.37610	0.20300	H	-22.16510	-30.85160	4.99840
N	-16.55550	-25.06650	4.89150	H	-17.29610	-28.69840	4.95840
C	-15.74240	-26.13710	4.85050	H	-17.91020	-30.95120	6.58630
O	-16.12860	-27.28110	5.08540	H	-17.52150	-28.59420	7.40380
C	-18.94170	-26.77470	1.88600	H	-19.06840	-28.10790	6.68260
C	-18.64970	-23.82570	5.04320	H	-19.05310	-29.26800	8.02560
H	-13.72150	-24.11710	3.41810	N	-20.50280	-29.60430	4.97710
H	-13.78370	-26.82390	4.29670	C	18.42660	30.20310	-5.54690
H	-12.62630	-24.91120	5.47030	H	17.02240	31.80570	-5.53660
H	-14.21150	-24.24480	5.90930	H	18.52630	32.15070	-4.65950

H	18.52620	32.15090	-6.43420
H	-22.53470	-29.11700	4.93190
H	-21.92490	-29.94000	3.48260
H	-20.05420	-28.73960	4.67480

6. acetyl-(ala)<sub>59</sub>-methylamide

C	24.18820	34.73360	-6.34050
N	23.70790	36.10500	-6.34050
C	25.71110	34.72150	-6.19350
C	23.63320	34.00340	-5.11590
O	23.13170	32.88630	-5.23170
C	19.54520	34.54160	-3.55750
C	-23.76000	-37.16360	7.28620
H	24.39960	36.85460	-6.34050
H	23.87400	34.20600	-7.24100
H	26.15220	35.27260	-7.02400
H	25.99790	35.20080	-5.25750
H	26.07650	33.69460	-6.19290
N	20.97540	34.71500	-3.36810
C	23.23800	34.06100	-2.70090
N	23.72730	34.64570	-3.93790
C	23.35290	35.08280	-1.56790
C	21.74780	33.74610	-2.84510
O	21.30550	32.65390	-2.49240
C	19.90120	32.14770	-6.51460
C	18.97380	35.75120	-4.29990
H	24.15220	35.57190	-3.89460
H	23.77330	33.14250	-2.46040
H	24.39750	35.37370	-1.45690
H	22.76140	35.96730	-1.80370
H	22.98700	34.64890	-0.63730
N	20.03980	33.24870	-5.57650
C	19.29760	33.32950	-4.45770
O	18.45610	32.48690	-4.14960
C	21.61400	29.58470	-4.25650
C	20.97270	32.25920	-7.60110
H	21.39070	35.60440	-3.64530
H	19.03750	34.38630	-2.60550
H	19.16760	36.65050	-3.71520
H	19.45380	35.85070	-5.27330
H	17.90070	35.62600	-4.44450
N	21.25370	30.77930	-5.00110

C	20.16350	30.82750	-5.78730
O	19.39950	29.87450	-5.93240
C	18.81350	29.95390	-1.68310
C	22.80940	29.88420	-3.34980
H	20.72510	33.97410	-5.78730
H	18.90110	32.12210	-6.94720
H	20.85430	33.21040	-8.12010
H	21.96430	32.22210	-7.15030
H	20.87300	31.43530	-8.30760
N	19.91560	30.18900	-2.60040
C	20.45910	29.19860	-3.33030
O	20.06770	28.03380	-3.27570
C	16.20110	29.48870	-4.43280
C	18.32350	31.28720	-1.11460
H	21.85630	31.59770	-4.91410
H	21.82530	28.75140	-4.92660
H	23.64860	30.20920	-3.96470
H	22.55430	30.67890	-2.64890
H	23.08370	28.99080	-2.78880
N	17.30150	29.95850	-3.60830
C	17.63380	29.35620	-2.45250
O	17.03740	28.37430	-2.01300
C	18.03760	26.37670	-5.67580
C	16.16420	30.28010	-5.74170
H	20.27640	31.13950	-2.68180
H	19.10260	29.26740	-0.88740
H	19.14720	31.77470	-0.59300
H	17.98360	31.93380	-1.92350
H	17.49650	31.11630	-0.42550
N	17.67620	27.72580	-5.27470
C	16.44710	28.02920	-4.82070
O	15.54820	27.19650	-4.71270
C	18.16310	25.00530	-2.11130
C	19.53100	26.31980	-6.00380
H	17.82790	30.77080	-3.92980
H	15.25210	29.55950	-3.90130
H	16.03550	31.33810	-5.51320
H	17.10000	30.14550	-6.28390
H	15.34010	29.93130	-6.36410
N	18.30380	25.81860	-3.30720
C	17.82030	25.42390	-4.49860
O	17.23010	24.35720	-4.66200
C	14.42540	25.68470	-1.69920
C	18.67970	25.78060	-0.89770

H	18.38760	28.45320	-5.34570	H	17.63470	20.05520	-3.08930
H	17.43470	26.04160	-6.51960	N	11.95190	21.22650	-1.91650
H	19.74380	27.02010	-6.81150	C	12.56840	20.40340	-1.04960
H	20.11490	26.60080	-5.12750	O	12.06170	19.36010	-0.64020
H	19.80720	25.30950	-6.30530	C	11.78990	18.11870	-4.73800
N	15.85600	25.80220	-1.92500	C	10.25930	21.97680	-3.50410
C	16.67880	24.74070	-1.85140	H	15.14290	22.16910	-1.73600
O	16.28530	23.60490	-1.59040	H	14.42480	19.99050	-0.05050
C	13.72110	23.92170	-5.01550	H	14.73020	22.38890	0.67710
C	13.74600	27.02350	-1.99420	H	13.23900	22.82100	-0.18260
H	18.78640	26.71330	-3.22370	H	13.16120	21.72760	1.21320
H	18.67980	24.05170	-2.22020	N	11.65890	19.36510	-4.00250
H	19.72800	26.03290	-1.05760	C	10.64370	19.58520	-3.14810
H	18.10840	26.70050	-0.77370	O	9.76120	18.75700	-2.92870
H	18.57630	25.17460	0.00230	C	12.86880	16.06600	-1.70080
N	14.20810	24.81310	-3.97640	C	13.11130	18.11240	-5.50920
C	13.83800	24.67800	-2.69040	H	12.41500	22.08090	-2.22600
O	13.06870	23.79980	-2.30330	H	9.88500	20.91500	-1.64120
C	15.84170	20.94380	-3.90320	H	10.27850	22.96970	-3.05480
C	14.42790	24.23530	-6.33570	H	10.98080	21.94280	-4.32030
H	16.23190	26.72450	-2.14500	H	9.26550	21.76710	-3.89980
H	14.21280	25.34890	-0.68430	N	12.70570	17.09900	-2.70970
H	14.16680	27.78680	-1.33970	C	11.86470	16.95350	-3.74920
H	13.92210	27.30910	-3.03120	O	11.17920	15.94670	-3.92070
H	12.67230	26.94060	-1.82630	C	9.47800	16.68910	-0.05280
N	15.36180	22.26610	-4.26710	C	13.77450	16.57970	-0.57980
C	14.09380	22.48070	-4.66120	H	12.36660	20.08470	-4.15000
O	13.25630	21.58350	-4.74160	H	10.94210	17.96390	-5.40540
C	13.96190	20.82420	-0.57840	H	13.12400	18.95680	-6.19840
C	17.26990	21.04490	-3.36380	H	13.94670	18.20790	-4.81580
H	14.84940	25.55870	-4.24700	H	13.21430	17.17920	-6.06280
H	12.63850	23.99270	-5.12030	N	10.78210	16.83410	-0.67690
H	14.22810	25.27170	-6.60780	C	11.51320	15.77060	-1.05570
H	15.50340	24.09920	-6.22300	O	11.13610	14.60980	-0.90340
H	14.06600	23.56910	-7.11870	C	7.70150	15.62660	-3.26480
N	14.75660	21.22520	-1.72700	C	8.83730	18.06680	0.12720
C	14.98880	20.39360	-2.75830	H	13.25280	17.95420	-2.61210
O	14.55050	19.24530	-2.80490	H	13.26190	15.14770	-2.13690
C	10.62660	20.94110	-2.43960	H	14.74340	16.84770	-1.00110
C	13.75700	22.02320	0.34970	H	13.33150	17.46260	-0.11920
H	16.01890	23.04460	-4.21690	H	13.90010	15.80820	0.17980
H	15.78620	20.25790	-4.74840	N	8.53560	16.28890	-2.27630
H	17.91000	21.47680	-4.13320	C	8.55440	15.90530	-0.98740
H	17.29020	21.68740	-2.48360	O	7.87460	14.97580	-0.55500

C	9.84220	12.46520	-3.42410	H	4.93600	14.34050	-0.56290
C	8.00580	16.18860	-4.65490	H	5.15820	13.57780	-2.14980
H	11.13970	17.77780	-0.82530	H	3.63660	13.34000	-1.26800
H	9.55250	16.16080	0.89770	N	6.93880	8.49300	-2.07020
H	9.48540	18.68060	0.75270	C	5.81970	8.56550	-2.81270
H	8.71790	18.55060	-0.84210	O	5.04540	7.61990	-2.95160
H	7.85840	17.96340	0.59520	C	4.62220	7.59770	1.31760
N	9.36990	13.83840	-3.37240	C	8.55130	7.55030	-0.50180
C	8.06040	14.14010	-3.31500	H	6.39860	11.70850	-2.75760
O	7.17590	13.28550	-3.30230	H	4.52130	9.89400	-3.89160
C	9.02770	11.70800	0.23170	H	6.43440	11.00160	-5.11150
C	11.36950	12.44240	-3.33580	H	7.57510	9.98470	-4.20920
H	9.11860	17.06670	-2.58550	H	6.43610	9.23160	-5.34280
H	6.64420	15.72830	-3.02020	N	5.68990	7.85010	0.36480
H	7.80760	17.26040	-4.65560	C	6.19960	6.87540	-0.40920
H	9.05420	16.02150	-4.90200	O	5.80410	5.71140	-0.36800
H	7.38250	15.69470	-5.40030	C	1.90440	7.21230	-1.34070
N	9.47270	12.32050	-1.00850	C	4.16180	8.91900	1.93680
C	9.33020	11.70780	-2.19730	H	7.54880	9.30610	-1.98640
O	8.81840	10.59620	-2.32110	H	7.50150	6.46120	-2.06700
C	5.30760	12.22660	-0.47110	H	9.36830	7.88650	-1.14030
C	9.19130	12.70110	1.38400	H	8.32760	8.32880	0.22750
H	10.06530	14.58460	-3.38060	H	8.84180	6.64220	0.02630
H	9.49090	11.96130	-4.32450	N	3.03800	7.65660	-0.54770
H	11.78170	13.01170	-4.16890	C	3.41070	7.02460	0.57960
H	11.69450	12.89730	-2.40010	O	2.82610	6.03500	1.01750
H	11.72890	11.41410	-3.37420	C	3.67480	4.12330	-2.72840
N	6.74490	12.38870	-0.33240	C	1.82200	8.03570	-2.62760
C	7.53130	11.40360	0.13700	H	6.05270	8.80070	0.29290
O	7.09660	10.30510	0.47960	H	4.93760	6.89060	2.08480
C	5.53730	9.90440	-3.49710	H	5.00740	9.38970	2.43820
C	4.71510	13.45670	-1.16150	H	3.79490	9.58670	1.15740
H	9.90410	13.24340	-0.95890	H	3.36060	8.73500	2.65250
H	9.56650	10.78130	0.42910	N	3.33650	5.46370	-2.28110
H	10.24100	12.98430	1.46200	C	2.12730	5.76170	-1.77310
H	8.59620	13.59390	1.19260	O	1.22860	4.93080	-1.65110
H	8.85880	12.24620	2.31710	C	3.92840	2.66420	0.79420
N	5.71770	10.98130	-2.53840	C	5.15430	4.06750	-3.11450
C	5.01910	11.03810	-1.39050	H	3.55630	8.47410	-0.86920
O	4.18530	10.19210	-1.07100	H	0.97680	7.27450	-0.77180
C	7.32050	7.27870	-1.36920	H	1.70810	9.08840	-2.36870
C	6.56720	10.03750	-4.62070	H	2.73580	7.91010	-3.20830
H	7.15440	13.28260	-0.60360	H	0.97290	7.70610	-3.22630
H	4.83570	12.05030	0.49550	N	4.02800	3.50600	-0.38600

C	3.49730	3.14280	-1.56730	H	1.69460	0.76580	-1.27500
O	2.89520	2.08320	-1.73390	H	1.42620	-2.00600	-1.86480
C	0.21300	3.35070	1.36530	H	3.57880	-0.81240	-1.30170
C	4.49510	3.40710	2.00580	H	3.02340	-0.63950	0.37490
H	4.04880	6.18940	-2.36150	H	3.33550	-2.25790	-0.28300
H	3.03830	3.81170	-3.55650	N	-2.29190	-1.08930	1.13440
H	5.34010	4.78640	-3.91250	C	-1.64740	-1.93630	1.95670
H	5.77280	4.32420	-2.25460	O	-2.14400	-2.98690	2.35970
H	5.41320	3.06350	-3.45090	C	-2.57870	-4.12610	-1.75370
N	1.63460	3.46700	1.08800	C	-4.03960	-0.29240	-0.36860
C	2.45360	2.40020	1.10420	H	0.90890	-0.16630	1.21570
O	2.06400	1.26020	1.35230	H	0.24340	-2.38220	2.87380
C	-0.62700	1.67280	-1.96350	H	0.58970	-0.00380	3.64740
C	-0.46970	4.69950	1.12930	H	-0.93080	0.45610	2.85610
H	4.51840	4.39610	-0.29920	H	-0.96140	-0.67080	4.22680
H	4.43520	1.71120	0.64250	N	-2.67460	-2.89760	-0.98360
H	5.53800	3.65830	1.81210	C	-3.65520	-2.69380	-0.08590
H	3.93410	4.32630	2.17390	O	-4.53340	-3.52300	0.14690
H	4.42280	2.77960	2.89410	C	-1.39630	-6.25770	1.18910
N	-0.09580	2.53620	-0.92240	C	-1.28770	-4.11960	-2.57480
C	-0.41740	2.37130	0.37320	H	-1.83610	-0.22970	0.82830
O	-1.17630	1.48750	0.76790	H	-4.34850	-1.39790	1.48080
C	1.51770	-1.34130	-1.00590	H	-3.99770	0.68910	0.10360
C	0.03070	2.01550	-3.30170	H	-3.34990	-0.30980	-1.21250
H	2.00700	4.39270	0.87630	H	-5.04880	-0.48770	-0.73100
H	0.03740	2.99100	2.37920	N	-1.59200	-5.19960	0.21270
H	-0.02000	5.44450	1.78560	C	-2.47280	-5.31560	-0.79720
H	-0.33170	5.00960	0.09350	O	-3.16980	-6.31470	-0.96680
H	-1.53670	4.61750	1.33610	C	-4.71830	-5.65950	2.98030
N	1.03170	-0.00820	-1.31890	C	-0.44560	-5.77590	2.28680
C	-0.24920	0.22190	-1.65880	H	-1.96900	-2.17790	-1.14050
O	-1.09410	-0.66920	-1.72900	H	-3.45210	-4.26050	-2.39170
C	-0.23460	-1.53360	2.38440	H	-1.29660	-3.25870	-3.24320
C	2.96600	-1.26010	-0.51920	H	-0.42590	-4.04510	-1.91170
H	0.53880	3.28520	-1.19900	H	-1.21100	-5.03950	-3.15450
H	-1.71240	1.75150	-2.02500	N	-3.43810	-5.50530	2.31040
H	-0.17360	3.05920	-3.54060	C	-2.72790	-6.56250	1.87820
H	1.10890	1.87160	-3.23360	O	-3.10540	-7.72500	2.01650
H	-0.36450	1.37030	-4.08630	C	-6.62180	-6.63460	-0.18640
N	0.51790	-1.10830	1.21640	C	-5.34400	-4.28370	3.21810
C	0.70600	-1.91540	0.15700	H	-1.03680	-4.34950	0.31010
O	0.25990	-3.06020	0.09930	H	-1.02520	-7.16690	0.71610
C	-3.63780	-1.35560	0.65560	H	0.50800	-5.50220	1.83550
C	-0.39730	-0.35680	3.34860	H	-0.86580	-4.90260	2.78550

H	-0.29550	-6.56640	3.02210	C	-6.97690	-15.02460	1.51860
N	-5.74700	-6.00060	0.78530	C	-7.83810	-12.18340	-1.63360
C	-5.68120	-6.41590	2.06290	H	-7.08020	-9.04060	2.43600
O	-6.34920	-7.35250	2.49820	H	-9.36210	-10.28870	3.59250
C	-4.50640	-9.80100	-0.50430	H	-9.28940	-7.97380	2.58710
C	-6.36750	-6.04010	-1.57300	H	-9.13210	-8.69830	0.97480
H	-3.08120	-4.55990	2.17160	H	-10.62040	-8.95050	1.90820
H	-4.61060	-6.21130	3.91410	N	-7.37820	-13.79180	0.86250
H	-4.66900	-3.68840	3.83310	C	-8.52440	-13.69590	0.16530
H	-5.49750	-3.77560	2.26610	O	-9.30870	-14.63410	0.03310
H	-6.30490	-4.39390	3.72060	C	-9.56900	-14.75910	4.31360
N	-4.96870	-8.42730	-0.40120	C	-5.71250	-14.78010	2.34470
C	-6.27330	-8.12110	-0.28640	H	-7.92630	-10.55790	0.27470
O	-7.16150	-8.97160	-0.26070	H	-9.85560	-12.33530	-0.83050
C	-5.18530	-10.64400	3.16040	H	-7.98410	-11.20690	-2.09530
C	-2.97700	-9.83310	-0.47500	H	-6.81560	-12.25090	-1.26230
H	-5.17190	-5.21820	0.47310	H	-8.00120	-12.97070	-2.36950
H	-7.66840	-6.53400	0.10080	N	-8.53710	-14.48830	3.32710
H	-6.55970	-4.96770	-1.54010	C	-8.06270	-15.44620	2.51070
H	-5.33030	-6.20590	-1.86400	O	-8.46280	-16.60890	2.53860
H	-7.02160	-6.51260	-2.30590	C	-12.38830	-15.06650	1.75250
N	-4.78440	-10.00330	1.91940	C	-9.99820	-13.45130	4.98190
C	-4.97560	-10.58600	0.72230	H	-6.76090	-12.98380	0.94270
O	-5.49790	-11.69180	0.59120	H	-6.82720	-15.82560	0.79470
C	-8.92650	-10.09100	2.61320	H	-4.91850	-14.43220	1.68380
C	-4.97230	-9.68020	4.32950	H	-5.90390	-14.01870	3.10070
H	-4.27000	-7.68440	-0.41780	H	-5.40710	-15.70230	2.83910
H	-4.89460	-10.28110	-1.40260	N	-11.22280	-14.64710	2.51220
H	-2.59370	-9.24550	-1.30920	C	-10.81090	-15.30830	3.60870
H	-2.61410	-9.40290	0.45830	O	-11.38400	-16.30560	4.04440
H	-2.62510	-10.86180	-0.55220	C	-10.68930	-18.12880	0.22340
N	-7.48400	-9.93900	2.70080	C	-12.51500	-14.21140	0.49020
C	-6.68590	-10.93900	3.11560	H	-8.17200	-13.53800	3.26460
O	-7.11330	-12.04350	3.44780	H	-9.22860	-15.48630	5.05070
C	-8.82520	-12.33930	-0.47500	H	-9.13140	-12.99700	5.46190
C	-9.53800	-8.84150	1.97610	H	-10.39070	-12.76290	4.23360
H	-4.34620	-9.08390	1.97490	H	-10.77250	-13.64910	5.72310
H	-4.64450	-11.57770	3.31450	N	-11.00280	-16.79810	0.71580
H	-3.91880	-9.40380	4.37420	C	-12.19020	-16.50710	1.27670
H	-5.56930	-8.78020	4.18280	O	-13.08820	-17.33660	1.41270
H	-5.27160	-10.15630	5.26320	C	-10.30980	-19.67500	3.69720
N	-8.60240	-11.28700	0.50200	C	-9.22600	-18.18200	-0.22030
C	-9.25640	-11.25520	1.67690	H	-10.71260	-13.82440	2.19110
O	-10.08210	-12.10480	2.00730	H	-13.29320	-15.01400	2.35790

H	-12.61320	-13.16490	0.77880	C	-13.57970	-24.22250	3.07240
H	-11.62480	-14.32690	-0.12800	O	-14.03410	-25.36350	3.00390
H	-13.38820	-14.52220	-0.08350	C	-17.89810	-23.65490	3.75010
N	-10.25060	-18.80500	2.53490	C	-14.55190	-22.73760	6.34070
C	-10.82800	-19.13660	1.36620	H	-12.63150	-21.51170	1.66930
O	-11.44180	-20.18890	1.19700	H	-12.93760	-24.26680	1.02280
C	-13.99690	-18.98540	4.42650	H	-10.75850	-23.09750	1.53210
C	-9.69320	-18.96470	4.90390	H	-11.24860	-22.96310	3.23250
H	-10.29010	-16.07400	0.62590	H	-10.97090	-24.56640	2.52390
H	-11.35870	-18.41700	-0.58710	N	-16.53360	-23.40670	4.18340
H	-9.06670	-17.44460	-1.00700	C	-15.86290	-24.27660	4.95970
H	-8.57380	-17.94930	0.62140	O	-16.34960	-25.33450	5.35560
H	-8.98570	-19.17850	-0.59060	C	-16.94710	-26.37040	1.23540
N	-12.58630	-18.86900	4.09790	C	-18.33270	-22.56500	2.76820
C	-11.77320	-19.93960	4.05680	H	-13.32690	-22.50090	4.16470
O	-12.15940	-21.08350	4.29180	H	-13.94110	-24.75370	5.79260
C	-14.97250	-20.57720	1.09230	H	-13.55230	-22.39660	6.61010
C	-14.68050	-17.62810	4.24960	H	-15.09920	-21.91040	5.88890
H	-9.75230	-17.91950	2.62440	H	-15.08390	-23.07040	7.23200
H	-9.81450	-20.62630	3.50310	N	-17.00670	-25.16070	2.03820
H	-8.65710	-18.71370	4.67670	C	-17.95130	-24.97440	2.97740
H	-10.24230	-18.04730	5.11570	O	-18.82460	-25.80500	3.22340
H	-9.73520	-19.61340	5.77880	C	-15.66540	-28.57910	4.07810
N	-14.39720	-19.74210	2.13310	C	-15.68830	-26.34980	0.36590
C	-14.67010	-19.93720	3.43560	H	-16.08500	-22.54200	3.88110
O	-15.41830	-20.82690	3.83740	H	-18.57720	-23.71410	4.60060
C	-12.80970	-23.62380	1.89360	H	-18.26740	-21.59570	3.26230
C	-14.36440	-20.20480	-0.26140	H	-17.67580	-22.56490	1.89840
H	-12.21710	-17.94010	3.89470	H	-19.35610	-22.74670	2.44000
H	-14.13580	-19.36900	5.43720	N	-15.89220	-27.49640	3.13580
H	-14.20200	-16.90150	4.90620	C	-16.81150	-27.58340	2.15790
H	-14.58040	-17.29330	3.21720	O	-17.52010	-28.57480	1.99080
H	-15.73930	-17.71020	4.49490	C	-18.91330	-28.00950	6.00890
N	-13.29990	-22.28120	1.63190	C	-14.67090	-28.12880	5.15000
C	-14.59140	-22.03690	1.34690	H	-16.30370	-24.44070	1.87210
O	-15.44340	-22.92210	1.28740	H	-17.84500	-26.48510	0.62810
C	-14.43260	-23.89120	5.34270	H	-15.71790	-25.47260	-0.28050
C	-11.34350	-23.56130	2.32630	H	-14.80150	-26.29560	0.99720
H	-13.76940	-18.98950	1.85070	H	-15.63890	-27.25550	-0.23850
H	-16.05900	-20.49200	1.07430	N	-17.65870	-27.84480	5.29460
H	-14.57170	-19.15470	-0.46680	C	-16.97150	-28.89450	4.80990
H	-13.28510	-20.35540	-0.23800	O	-17.34990	-30.05820	4.93420
H	-14.79280	-20.82870	-1.04580	C	-20.94150	-28.89780	2.89460
N	-13.72280	-23.44080	4.15750	C	-19.52180	-26.63700	6.30390



H	-15.32890	-26.65150	3.23260	H	-19.40430	-32.55840	8.20120
H	-15.31770	-29.47810	3.56920	N	-22.92040	-33.55640	3.54470
H	-13.73370	-27.84850	4.66930	C	-23.52900	-33.55030	4.74420
H	-15.06690	-27.26600	5.68540	O	-24.34630	-34.40400	5.08510
H	-14.49730	-28.93770	5.85960	C	-21.27830	-37.32530	4.40710
N	-20.02680	-28.29180	3.84720	C	-22.24310	-34.40360	1.36030
C	-19.91470	-28.73860	5.11090	H	-21.31310	-31.36520	5.47320
O	-20.57080	-29.68250	5.54850	H	-23.55620	-32.63070	6.68540
C	-18.85750	-32.06520	2.41900	H	-23.50900	-30.29210	5.73460
C	-20.73700	-28.27060	1.51410	H	-23.41730	-30.97760	4.10030
H	-17.30210	-26.89800	5.16520	H	-24.87030	-31.24580	5.08340
H	-18.77320	-28.58460	6.92420	N	-21.69740	-36.07490	3.79710
H	-18.82060	-26.06020	6.90700	C	-22.86880	-35.95660	3.14680
H	-19.70860	-26.10510	5.37110	O	-23.66280	-36.88760	3.02180
H	-20.46350	-26.75510	6.83990	C	22.07410	37.87600	-6.34050
N	-19.30790	-30.69230	2.57320	C	-19.98190	-37.10710	5.19000
C	-20.60550	-30.38290	2.74510	H	-22.24940	-32.82510	3.30960
O	-21.49670	-31.22970	2.78410	H	-24.22930	-34.56580	2.23590
C	-19.40090	-32.99470	6.08540	H	-22.40120	-33.41540	0.92840
C	-17.32830	-32.10510	2.38900	H	-21.20760	-34.48500	1.69050
H	-19.45960	-27.50470	3.53240	H	-22.43850	-35.17190	0.61220
H	-21.97590	-28.79930	3.22390	O	21.47890	35.56630	-6.34060
H	-20.92170	-27.19840	1.58050	C	-22.32780	-37.76600	5.42950
H	-19.71250	-28.43400	1.17970	O	-22.73300	-38.92730	5.44430
H	-21.42110	-28.72190	0.79550	H	-24.01690	-38.21850	7.18940
N	-19.04410	-32.32560	4.84590	H	-21.07300	-35.27200	3.87330
C	-19.28400	-32.87780	3.64320	H	-21.16070	-38.10900	3.65880
O	-19.81700	-33.97770	3.50530	H	-19.21180	-36.74670	4.50790
C	-23.15710	-32.41100	5.69520	H	-20.14020	-36.36360	5.97110
C	-19.13810	-32.06090	7.26860	H	-19.66310	-38.04250	5.64970
H	-18.60620	-29.95250	2.54800	N	-22.76540	-36.82630	6.28650
H	-19.28230	-32.52130	1.52480	C	22.39580	36.40070	-6.34050
H	-16.97380	-31.49900	1.55530	H	20.99160	38.00330	-6.33020
H	-16.92770	-31.69960	3.31800	H	22.49550	38.34830	-5.45320
H	-16.98530	-33.13320	2.27350	H	22.49540	38.34840	-7.22790
N	-21.71150	-32.26800	5.73130	H	-23.35910	-36.98600	8.28410
C	-20.90380	-33.28150	6.09080	H	-24.65000	-36.55000	7.14700
O	-21.32440	-34.39180	6.41210	H	-22.39760	-35.87650	6.23320
C	-23.18620	-34.58330	2.55160				
C	-23.78550	-31.14350	5.11260				
H	-18.59900	-31.40990	4.90700				
H	-18.85990	-33.93440	6.19590				
H	-18.08220	-31.79060	7.27970				
H	-19.73530	-31.15480	7.16670				
				7. acetyl-(ala) <sub>69</sub> -methylamide			
				C	28.18390	40.91060	-7.16220
				N	27.70360	42.28200	-7.16220
				C	29.70680	40.89850	-7.01520

C	27.62890	40.18030	-5.93760	O	24.06340	34.21070	-4.09740
O	27.12740	39.06320	-6.05340	C	20.19680	35.66560	-5.25450
C	23.54090	40.71850	-4.37920	C	22.31920	37.46420	-1.93630
C	-25.98040	-44.74470	6.11980	H	25.85200	37.77460	-5.73580
H	28.39530	43.03160	-7.16220	H	25.82100	34.92830	-5.74830
H	27.86970	40.38290	-8.06270	H	27.64430	36.38620	-4.78640
H	30.14790	41.44950	-7.84570	H	26.55000	36.85580	-3.47060
H	29.99360	41.37770	-6.07920	H	27.07940	35.16770	-3.61050
H	30.07220	39.87160	-7.01460	N	21.29720	36.13540	-4.43000
N	24.97110	40.89200	-4.18980	C	21.62950	35.53320	-3.27420
C	27.23370	40.23800	-3.52260	O	21.03310	34.55120	-2.83470
N	27.72300	40.82260	-4.75960	C	22.03330	32.55370	-6.49750
C	27.34860	41.25970	-2.38960	C	20.15990	36.45700	-6.56340
C	25.74350	39.92300	-3.66680	H	24.27210	37.31650	-3.50340
O	25.30120	38.83080	-3.31410	H	23.09830	35.44440	-1.70900
C	23.89690	38.32470	-7.33630	H	23.14290	37.95170	-1.41470
C	22.96950	41.92820	-5.12160	H	21.97930	38.11070	-2.74520
H	28.14790	41.74880	-4.71630	H	21.49220	37.29320	-1.24720
H	27.76900	39.31940	-3.28210	N	21.67190	33.90270	-6.09640
H	28.39320	41.55070	-2.27860	C	20.44280	34.20620	-5.64240
H	26.75710	42.14430	-2.62540	O	19.54400	33.37350	-5.53440
H	26.98270	40.82580	-1.45900	C	22.15880	31.18220	-2.93300
N	24.03550	39.42560	-6.39810	C	23.52670	32.49680	-6.82550
C	23.29330	39.50640	-5.27940	H	21.82360	36.94770	-4.75150
O	22.45180	38.66380	-4.97130	H	19.24780	35.73650	-4.72300
C	25.60970	35.76160	-5.07820	H	20.03120	37.51500	-6.33490
C	24.96840	38.43620	-8.42270	H	21.09570	36.32240	-7.10560
H	25.38640	41.78130	-4.46700	H	19.33580	36.10820	-7.18570
H	23.03320	40.56320	-3.42720	N	22.29950	31.99560	-4.12890
H	23.16330	42.82740	-4.53690	C	21.81610	31.60080	-5.32030
H	23.44950	42.02760	-6.09500	O	21.22580	30.53410	-5.48370
H	21.89640	41.80290	-5.26620	C	18.42110	31.86170	-2.52090
N	25.24940	36.95630	-5.82280	C	22.67540	31.95760	-1.71940
C	24.15920	37.00440	-6.60900	H	22.38330	34.63020	-6.16740
O	23.39520	36.05140	-6.75410	H	21.43040	32.21850	-7.34130
C	22.80920	36.13090	-2.50480	H	23.73950	33.19700	-7.63320
C	26.80510	36.06110	-4.17150	H	24.11060	32.77780	-5.94920
H	24.72080	40.15100	-6.60900	H	23.80290	31.48640	-7.12700
H	22.89680	38.29900	-7.76890	N	19.85170	31.97910	-2.74670
H	24.85000	39.38730	-8.94170	C	20.67450	30.91770	-2.67310
H	25.96000	38.39900	-7.97190	O	20.28100	29.78190	-2.41210
H	24.86870	37.61220	-9.12930	C	17.71680	30.09860	-5.83720
N	23.91130	36.36590	-3.42210	C	17.74170	33.20040	-2.81590
C	24.45480	35.37550	-4.15200	H	22.78210	32.89030	-4.04540

H	22.67550	30.22870	-3.04190	N	15.65460	25.54200	-4.82420
H	23.72370	32.20980	-1.87930	C	14.63940	25.76210	-3.96980
H	22.10410	32.87740	-1.59540	O	13.75690	24.93400	-3.75040
H	22.57200	31.35150	-0.81930	C	16.86450	22.24290	-2.52250
N	18.20380	30.99000	-4.79810	C	17.10700	24.28940	-6.33090
C	17.83370	30.85490	-3.51210	H	16.41070	28.25780	-3.04770
O	17.06440	29.97680	-3.12500	H	13.88070	27.09190	-2.46290
C	19.83740	27.12070	-4.72480	H	14.27420	29.14670	-3.87650
C	18.42360	30.41230	-7.15740	H	14.97650	28.11970	-5.14200
H	20.22760	32.90150	-2.96660	H	13.26130	27.94400	-4.72150
H	18.20850	31.52580	-1.50600	N	16.70140	23.27590	-3.53140
H	18.16250	33.96380	-2.16130	C	15.86040	23.13040	-4.57090
H	17.91780	33.48600	-3.85290	O	15.17500	22.12360	-4.74240
H	16.66800	33.11750	-2.64790	C	13.47370	22.86600	-0.87450
N	19.35750	28.44310	-5.08880	C	17.77020	22.75660	-1.40150
C	18.08950	28.65760	-5.48280	H	16.36230	26.26160	-4.97160
O	17.25200	27.76040	-5.56330	H	14.93780	24.14090	-6.22700
C	17.95760	27.00120	-1.40010	H	17.11970	25.13370	-7.02010
C	21.26560	27.22180	-4.18550	H	17.94240	24.38480	-5.63750
H	18.84510	31.73560	-5.06860	H	17.21000	23.35610	-6.88450
H	16.63420	30.16970	-5.94190	N	14.77780	23.01110	-1.49860
H	18.22380	31.44870	-7.42940	C	15.50890	21.94760	-1.87740
H	19.49910	30.27610	-7.04470	O	15.13180	20.78680	-1.72510
H	18.06170	29.74600	-7.94040	C	11.69720	21.80350	-4.08650
N	18.75230	27.40210	-2.54860	C	12.83300	24.24370	-0.69450
C	18.98450	26.57050	-3.58000	H	17.24850	24.13120	-3.43380
O	18.54620	25.42220	-3.62650	H	17.25760	21.32460	-2.95860
C	14.62230	27.11800	-3.26120	H	18.73910	23.02460	-1.82280
C	17.75270	28.20020	-0.47200	H	17.32720	23.63950	-0.94090
H	20.01460	29.22150	-5.03860	H	17.89580	21.98510	-0.64190
H	19.78190	26.43480	-5.57010	N	12.53130	22.46590	-3.09800
H	21.90570	27.65370	-4.95480	C	12.55010	22.08220	-1.80900
H	21.28590	27.86430	-3.30530	O	11.87030	21.15280	-1.37670
H	21.63040	26.23210	-3.91090	C	13.83790	18.64220	-4.24580
N	15.94760	27.40340	-2.73820	C	12.00150	22.36550	-5.47660
C	16.56410	26.58030	-1.87130	H	15.13540	23.95470	-1.64700
O	16.05740	25.53700	-1.46190	H	13.54820	22.33770	0.07600
C	15.78560	24.29560	-5.55970	H	13.48110	24.85760	-0.06900
C	14.25500	28.15380	-4.32580	H	12.71360	24.72760	-1.66380
H	19.13860	28.34600	-2.55760	H	11.85410	24.14040	-0.22650
H	18.42050	26.16750	-0.87220	N	13.36560	20.01540	-4.19400
H	18.72590	28.56590	-0.14450	C	12.05610	20.31700	-4.13670
H	17.23470	28.99790	-1.00430	O	11.17160	19.46240	-4.12390
H	17.15690	27.90450	0.39150	C	13.02340	17.88490	-0.59000

C	15.36520	18.61940	-4.15740	H	11.57080	16.16170	-5.03080
H	13.11430	23.24360	-3.40720	H	10.43180	15.40860	-6.16450
H	10.63990	21.90520	-3.84190	N	9.68560	14.02710	-0.45690
H	11.80330	23.43730	-5.47730	C	10.19530	13.05230	-1.23080
H	13.04990	22.19850	-5.72370	O	9.79980	11.88840	-1.18970
H	11.37820	21.87170	-6.22200	C	5.90010	13.38920	-2.16240
N	13.46840	18.49740	-1.83020	C	8.15750	15.09590	1.11510
C	13.32590	17.88470	-3.01900	H	11.54450	15.48310	-2.80800
O	12.81410	16.77310	-3.14270	H	11.49720	12.63810	-2.88870
C	9.30330	18.40350	-1.29280	H	13.36400	14.06340	-1.96200
C	13.18710	18.87800	0.56240	H	12.32330	14.50570	-0.59420
H	14.06100	20.76150	-4.20220	H	12.83750	12.81910	-0.79540
H	13.48660	18.13820	-5.14620	N	7.03370	13.83350	-1.36930
H	15.77740	19.18860	-4.99060	C	7.40640	13.20150	-0.24210
H	15.69020	19.07420	-3.22180	O	6.82180	12.21190	0.19580
H	15.72460	17.59110	-4.19590	C	7.67050	10.30020	-3.55000
N	10.74060	18.56560	-1.15410	C	5.81770	14.21260	-3.44930
C	11.52700	17.58050	-0.68470	H	10.04840	14.97760	-0.52880
O	11.09230	16.48200	-0.34210	H	8.93330	13.06750	1.26310
C	9.53300	16.08130	-4.31880	H	9.00310	15.56660	1.61650
C	8.71080	19.63360	-1.98320	H	7.79060	15.76370	0.33570
H	13.89980	19.42030	-1.78060	H	7.35630	14.91190	1.83090
H	13.56220	16.95820	-0.39250	N	7.33220	11.64070	-3.10270
H	14.23670	19.16130	0.64040	C	6.12300	11.93860	-2.59480
H	12.59190	19.77080	0.37090	O	5.22430	11.10770	-2.47280
H	12.85450	18.42310	1.49540	C	7.92410	8.84110	-0.02740
N	9.71340	17.15830	-3.36010	C	9.15000	10.24440	-3.93620
C	9.01480	17.21500	-2.21210	H	7.55200	14.65100	-1.69090
O	8.18100	16.36910	-1.89270	H	4.97250	13.45140	-1.59340
C	11.31620	13.45570	-2.19090	H	5.70380	15.26530	-3.19030
C	10.56290	16.21440	-5.44240	H	6.73150	14.08710	-4.03000
H	11.15010	19.45960	-1.42520	H	4.96860	13.88310	-4.04800
H	8.83140	18.22720	-0.32620	N	8.02370	9.68290	-1.20770
H	8.93170	20.51740	-1.38460	C	7.49300	9.31970	-2.38900
H	9.15390	19.75470	-2.97150	O	6.89090	8.26020	-2.55560
H	7.63230	19.51700	-2.08960	C	4.20870	9.52760	0.54370
N	10.93450	14.66990	-2.89190	C	8.49080	9.58400	1.18410
C	9.81540	14.74240	-3.63440	H	8.04450	12.36630	-3.18310
O	9.04110	13.79680	-3.77330	H	7.03400	9.98860	-4.37820
C	8.61790	13.77470	0.49600	H	9.33580	10.96330	-4.73420
C	12.54700	13.72720	-1.32350	H	9.76850	10.50110	-3.07630
H	10.39430	17.88540	-3.57930	H	9.40890	9.24050	-4.27260
H	8.51700	16.07090	-4.71330	N	5.63030	9.64400	0.26630
H	10.43010	17.17860	-5.93320	C	6.44930	8.57720	0.28260

O	6.05970	7.43720	0.53060	H	4.23910	3.79480	2.05210
C	3.36870	7.84980	-2.78520	H	4.58540	6.17310	2.82570
C	3.52600	10.87640	0.30760	H	3.06490	6.63300	2.03440
H	8.51410	10.57300	-1.12090	H	3.03430	5.50610	3.40510
H	8.43090	7.88810	-0.17910	N	1.32110	3.27930	-1.80530
H	9.53370	9.83520	0.99040	C	0.34050	3.48310	-0.90760
H	7.92980	10.50320	1.35220	O	-0.53770	2.65400	-0.67480
H	8.41850	8.95660	2.07240	C	2.59940	-0.08080	0.36740
N	3.89990	8.71310	-1.74410	C	2.70800	2.05730	-3.39650
C	3.57830	8.54830	-0.44850	H	2.15960	5.94720	0.00660
O	2.81940	7.66450	-0.05380	H	-0.35280	4.77910	0.65910
C	5.51340	4.83560	-1.82750	H	-0.00200	6.86600	-0.71800
C	4.02640	8.19240	-4.12340	H	0.64580	5.86720	-2.03410
H	6.00270	10.56960	0.05460	H	-1.05310	5.68920	-1.55270
H	4.03310	9.16800	1.55750	N	2.40370	0.97730	-0.60900
H	3.97570	11.62140	0.96390	C	1.52290	0.86140	-1.61880
H	3.66400	11.18650	-0.72810	O	0.82590	-0.13770	-1.78850
H	2.45900	10.79440	0.51440	C	-0.72260	0.51740	2.15860
N	5.02740	6.16870	-2.14060	C	3.55010	0.40100	1.46520
C	3.74650	6.39880	-2.48050	H	2.02670	3.99900	-1.96220
O	2.90160	5.50770	-2.55070	H	0.54360	1.91640	-3.21340
C	3.76110	4.64330	1.56270	H	2.69910	2.91830	-4.06490
C	6.96170	4.91690	-1.34090	H	3.56980	2.13180	-2.73340
H	4.53450	9.46210	-2.02070	H	2.78470	1.13750	-3.97610
H	2.28330	7.92840	-2.84670	N	0.55760	0.67170	1.48880
H	3.82210	9.23610	-4.36230	C	1.26780	-0.38560	1.05650
H	5.10460	8.04850	-4.05520	O	0.89030	-1.54800	1.19480
H	3.63120	7.54730	-4.90800	C	-2.62610	-0.45770	-1.00810
N	4.51360	5.06860	0.39470	C	-1.34830	1.89330	2.39640
C	4.70170	4.26150	-0.66460	H	2.95890	1.82740	-0.51160
O	4.25560	3.11670	-0.72240	H	2.97050	-0.99000	-0.10560
C	0.35790	4.82130	-0.16610	H	4.50370	0.67480	1.01380
C	3.59840	5.82010	2.52690	H	3.12990	1.27440	1.96380
H	5.69030	6.94270	-2.09660	H	3.70020	-0.38950	2.20050
H	5.42190	4.17090	-2.68650	N	-1.75130	0.17630	-0.03640
H	7.57450	5.36450	-2.12340	C	-1.68550	-0.23890	1.24120
H	7.01910	5.53750	-0.44680	O	-2.35350	-1.17550	1.67650
H	7.33120	3.91900	-1.10470	C	-0.51070	-3.62410	-1.32600
N	1.70380	5.08760	0.31270	C	-2.37180	0.13680	-2.39470
C	2.34830	4.24070	1.13500	H	0.91450	1.61700	1.34990
O	1.85170	3.19000	1.53800	H	-0.61490	-0.03440	3.09240
C	1.41700	2.05080	-2.57540	H	-0.67330	2.48850	3.01140
C	-0.04390	5.88460	-1.19030	H	-1.50180	2.40130	1.44440
H	4.90460	6.01070	0.39400	H	-2.30920	1.78300	2.89890

N	-0.97300	-2.25040	-1.22280	C	-1.71680	-8.60320	1.52300
C	-2.27760	-1.94410	-1.10810	H	-3.93060	-4.38100	-0.54690
O	-3.16580	-2.79470	-1.08240	H	-5.85990	-6.15830	-1.65220
C	-1.18960	-4.46700	2.33880	H	-3.98840	-5.03000	-2.91700
C	1.01870	-3.65610	-1.29670	H	-2.81990	-6.07400	-2.08400
H	-1.17620	0.95870	-0.34860	H	-4.00550	-6.79380	-3.19120
H	-3.67270	-0.35710	-0.72090	N	-4.54140	-8.31140	2.50540
H	-2.56400	1.20920	-2.36180	C	-4.06690	-9.26920	1.68900
H	-1.33460	-0.02900	-2.68570	O	-4.46710	-10.43200	1.71690
H	-3.02590	-0.33570	-3.12750	C	-8.39260	-8.88960	0.93080
N	-0.78870	-3.82630	1.09770	C	-6.00250	-7.27440	4.16020
C	-0.97990	-4.40900	-0.09940	H	-2.76520	-6.80680	0.12100
O	-1.50220	-5.51490	-0.23050	H	-2.83150	-9.64870	-0.02690
C	-4.93080	-3.91400	1.79150	H	-0.92280	-8.25530	0.86210
C	-0.97660	-3.50330	3.50780	H	-1.90820	-7.84180	2.27900
H	-0.27430	-1.50750	-1.23940	H	-1.41140	-9.52540	2.01740
H	-0.89880	-4.10410	-2.22430	N	-7.22710	-8.47020	1.69060
H	1.40200	-3.06860	-2.13090	C	-6.81520	-9.13130	2.78700
H	1.38160	-3.22590	-0.36330	O	-7.38830	-10.12870	3.22270
H	1.37060	-4.68490	-1.37380	C	-6.69360	-11.95180	-0.59830
N	-3.48830	-3.76210	1.87910	C	-8.51930	-8.03450	-0.33150
C	-2.69020	-4.76210	2.29390	H	-4.17620	-7.36110	2.44290
O	-3.11750	-5.86660	2.62610	H	-5.23290	-9.30930	4.22900
C	-4.82950	-6.16230	-1.29670	H	-5.13570	-6.82000	4.64020
C	-5.54230	-2.66460	1.15450	H	-6.39500	-6.58600	3.41190
H	-0.35050	-2.90690	1.15320	H	-6.77680	-7.47210	4.90140
H	-0.64880	-5.40080	2.49280	N	-7.00710	-10.62120	-0.10590
H	0.07690	-3.22690	3.55250	C	-8.19450	-10.33020	0.45500
H	-1.57360	-2.60330	3.36110	O	-9.09250	-11.15960	0.59100
H	-1.27590	-3.97940	4.44150	C	-6.31410	-13.49810	2.87550
N	-4.60670	-5.11010	-0.31970	C	-5.23030	-12.00500	-1.04190
C	-5.26070	-5.07820	0.85520	H	-6.71690	-7.64740	1.36940
O	-6.08640	-5.92790	1.18560	H	-9.29750	-8.83710	1.53620
C	-2.98120	-8.84770	0.69690	H	-8.61750	-6.98800	-0.04290
C	-3.84240	-6.00650	-2.45520	H	-7.62910	-8.15000	-0.94960
H	-3.08450	-2.86370	1.61430	H	-9.39250	-8.34530	-0.90510
H	-5.36640	-4.11180	2.77080	N	-6.25490	-12.62810	1.71320
H	-5.29370	-1.79680	1.76550	C	-6.83230	-12.95970	0.54460
H	-5.13640	-2.52140	0.15310	O	-7.44610	-14.01200	0.37530
H	-6.62470	-2.77360	1.08650	C	-10.00120	-12.80850	3.60480
N	-3.38250	-7.61480	0.04080	C	-5.69750	-12.78770	4.08220
C	-4.52870	-7.51890	-0.65640	H	-6.29440	-9.89710	-0.19570
O	-5.31300	-8.45720	-0.78860	H	-7.36300	-12.24000	-1.40880
C	-5.57330	-8.58210	3.49190	H	-5.07100	-11.26760	-1.82870

H	-4.57810	-11.77240	-0.20030	O	-12.35390	-19.15760	4.53390
H	-4.99000	-13.00160	-1.41230	C	-12.95140	-20.19350	0.41370
N	-8.59060	-12.69200	3.27620	C	-14.33700	-16.38810	1.94650
C	-7.77750	-13.76270	3.23510	H	-9.33120	-16.32390	3.34300
O	-8.16370	-14.90660	3.47010	H	-9.94540	-18.57670	4.97100
C	-10.97680	-14.40030	0.27060	H	-9.55660	-16.21970	5.78840
C	-10.68480	-11.45120	3.42790	H	-11.10350	-15.73340	5.06730
H	-5.75660	-11.74260	1.80270	H	-11.08820	-16.89350	6.41030
H	-5.81880	-14.44940	2.68140	N	-13.01100	-18.98380	1.21650
H	-4.66140	-12.53670	3.85500	C	-13.95560	-18.79750	2.15570
H	-6.24660	-11.87040	4.29400	O	-14.82890	-19.62800	2.40170
H	-5.73950	-13.43650	4.95710	C	-11.66970	-22.40210	3.25640
N	-10.40150	-13.56520	1.31140	C	-11.69260	-20.17280	-0.45580
C	-10.67440	-13.76030	2.61390	H	-12.08930	-16.36510	3.05950
O	-11.42260	-14.65000	3.01570	H	-14.58150	-17.53720	3.77890
C	-8.81400	-17.44690	1.07190	H	-14.27170	-15.41870	2.44060
C	-10.36870	-14.02790	-1.08300	H	-13.68010	-16.38800	1.07670
H	-8.22140	-11.76320	3.07300	H	-15.36040	-16.56980	1.61830
H	-10.14010	-13.19210	4.61550	N	-11.89650	-21.31940	2.31420
H	-10.20630	-10.72460	4.08450	C	-12.81580	-21.40650	1.33620
H	-10.58470	-11.11640	2.39550	O	-13.52440	-22.39790	1.16910
H	-11.74360	-11.53330	3.67330	C	-14.91760	-21.83260	5.18730
N	-9.30420	-16.10430	0.81020	C	-10.67520	-21.95180	4.32830
C	-10.59570	-15.86000	0.52520	H	-12.30800	-18.26370	1.05040
O	-11.44770	-16.74510	0.46570	H	-13.84930	-20.30810	-0.19360
C	-10.43690	-17.71420	4.52100	H	-11.72220	-19.29570	-1.10220
C	-7.34780	-17.38440	1.50460	H	-10.80580	-20.11860	0.17550
H	-9.77370	-12.81260	1.02900	H	-11.64320	-21.07850	-1.06020
H	-12.06330	-14.31500	0.25260	N	-13.66300	-21.66790	4.47290
H	-10.57600	-12.97770	-1.28850	C	-12.97580	-22.71750	3.98820
H	-9.28940	-14.17840	-1.05970	O	-13.35420	-23.88130	4.11250
H	-10.79710	-14.65180	-1.86740	C	-16.94580	-22.72080	2.07290
N	-9.72710	-17.26390	3.33580	C	-15.52610	-20.46010	5.48220
C	-9.58400	-18.04560	2.25070	H	-11.33320	-20.47460	2.41090
O	-10.03840	-19.18650	2.18220	H	-11.32200	-23.30110	2.74750
C	-13.90240	-17.47800	2.92840	H	-9.73800	-21.67150	3.84760
C	-10.55620	-16.56070	5.51900	H	-11.07120	-21.08900	4.86380
H	-8.63580	-15.33470	0.84760	H	-10.50160	-22.76080	5.03790
H	-8.94190	-18.08990	0.20110	N	-16.03110	-22.11490	3.02560
H	-6.76280	-16.92060	0.71040	C	-15.91900	-22.56170	4.28920
H	-7.25290	-16.78620	2.41080	O	-16.57510	-23.50560	4.72680
H	-6.97520	-18.38950	1.70220	C	-14.86180	-25.88830	1.59730
N	-12.53790	-17.22980	3.36170	C	-16.74130	-22.09370	0.69240
C	-11.86720	-18.09970	4.13800	H	-13.30640	-20.72110	4.34350

H	-14.77750	-22.40760	6.10250	N	-17.70170	-29.89800	2.97540
H	-14.82490	-19.88320	6.08530	C	-18.87310	-29.77960	2.32510
H	-15.71290	-19.92810	4.54950	O	-19.66710	-30.71070	2.20010
H	-16.46780	-20.57820	6.01820	C	-19.76480	-30.93940	6.48320
N	-15.31220	-24.51540	1.75150	C	-15.98620	-30.93010	4.36830
C	-16.60980	-24.20600	1.92340	H	-18.25370	-26.64810	2.48790
O	-17.50100	-25.05280	1.96240	H	-20.23360	-28.38880	1.41430
C	-15.40520	-26.81770	5.26370	H	-18.40550	-27.23850	0.10670
C	-13.33260	-25.92820	1.56730	H	-17.21190	-28.30810	0.86880
H	-15.46390	-21.32780	2.71070	H	-18.44280	-28.99490	-0.20950
H	-17.98020	-22.62240	2.40230	N	-18.76970	-30.64940	5.46480
H	-16.92600	-21.02150	0.75880	C	-18.33210	-31.58910	4.60780
H	-15.71680	-22.25710	0.35800	O	-18.73730	-32.75030	4.62260
H	-17.42540	-22.54500	-0.02620	C	-22.68120	-31.17090	4.02500
N	-15.04840	-26.14860	4.02420	C	-20.16080	-29.64650	7.19900
C	-15.28830	-26.70090	2.82150	H	-17.07730	-29.09500	3.05160
O	-15.82130	-27.80080	2.68360	H	-17.16500	-31.93210	2.83710
C	-19.16140	-26.23410	4.87350	H	-15.21610	-30.56980	3.68620
C	-15.14240	-25.88400	6.44690	H	-16.14440	-30.18660	5.14940
H	-14.61050	-23.77560	1.72630	H	-15.66740	-31.86560	4.82800
H	-15.28660	-26.34430	0.70310	N	-21.48530	-30.77560	4.74960
H	-12.97810	-25.32210	0.73360	C	-21.03570	-31.46540	5.81310
H	-12.93200	-25.52270	2.49630	O	-21.59730	-32.47050	6.24600
H	-12.98960	-26.95630	1.45180	C	-21.05890	-34.20250	2.35800
N	-17.71580	-26.09100	4.90960	C	-22.85120	-30.28440	2.78960
C	-16.90810	-27.10460	5.26910	H	-18.40190	-29.69950	5.41150
O	-17.32860	-28.21490	5.59040	H	-19.40060	-31.68610	7.18880
C	-19.19050	-28.40630	1.72990	H	-19.27390	-29.20810	7.65640
C	-19.78980	-24.96650	4.29090	H	-20.57780	-28.93810	6.48320
H	-14.60330	-25.23290	4.08530	H	-20.90740	-29.85880	7.96420
H	-14.86420	-27.75750	5.37430	N	-21.34600	-32.88290	2.89430
H	-14.08650	-25.61370	6.45800	C	-22.50950	-32.60020	3.50700
H	-15.73960	-24.97790	6.34510	O	-23.40630	-33.42860	3.65700
H	-15.40860	-26.38140	7.37950	C	-20.55600	-35.83530	5.77600
N	-18.92470	-27.37940	2.72300	C	-19.61390	-34.25160	1.85750
C	-19.53330	-27.37340	3.92250	H	-20.98310	-29.94760	4.42930
O	-20.35060	-28.22710	4.26340	H	-23.56210	-31.12900	4.66560
C	-17.28250	-31.14840	3.58550	H	-22.93240	-29.24490	3.10720
C	-18.24740	-28.22670	0.53860	H	-21.98580	-30.38890	2.13530
H	-17.31740	-25.18830	4.65150	H	-23.74730	-30.57700	2.24240
H	-19.56050	-26.45380	5.86370	N	-20.53630	-34.93730	4.63380
H	-19.51330	-24.11520	4.91300	C	-21.15960	-35.23740	3.48040
H	-19.42160	-24.80070	3.27860	O	-21.78530	-36.28240	3.30920
H	-20.87460	-25.06880	4.26180	C	-24.20870	-35.14670	6.66230



C	-19.88990	-35.15770	6.97520	H	-21.53010	-39.10660	5.26760
H	-20.63320	-32.16020	2.79480	H	-21.28860	-40.69330	4.51020
H	-21.76030	-34.46760	1.56690	N	-26.77740	-39.54880	6.40880
H	-19.48060	-33.49590	1.08340	C	-26.08250	-40.44060	7.13750
H	-18.92880	-34.04270	2.67900	O	-26.55970	-41.50560	7.52590
H	-19.39350	-35.23990	1.45410	C	-27.31960	-42.43730	3.40750
N	-22.81100	-35.02870	6.28290	C	-28.62450	-38.66430	5.08430
C	-22.00610	-36.10180	6.18480	H	-23.56880	-38.65770	6.28960
O	-22.38940	-37.24940	6.40640	H	-24.13300	-40.94690	7.88450
C	-25.31950	-36.65160	3.33010	H	-23.70020	-38.61250	8.74370
C	-24.89090	-33.78230	6.54470	H	-25.27070	-38.10140	8.09420
H	-20.03000	-34.05660	4.72580	H	-25.21070	-39.29420	9.40700
H	-20.07370	-36.78380	5.54000	N	-27.34180	-41.24740	4.24120
H	-18.86180	-34.90600	6.71470	C	-28.24880	-41.07980	5.22010
H	-20.42530	-34.24320	7.23010	O	-29.11670	-41.91210	5.47900
H	-19.90210	-35.82750	7.83500	C	26.06980	44.05300	-7.16220
N	-24.70030	-35.84500	4.36810	C	-26.09470	-42.40120	2.49130
C	-24.92440	-36.07070	5.67500	H	-26.33580	-38.67900	6.11080
O	-25.66180	-36.96650	6.08340	H	-28.80530	-39.85680	6.89630
C	-23.14480	-39.72700	3.97370	H	-28.53500	-37.70760	5.59900
C	-24.76130	-36.24900	1.96370	H	-28.00120	-38.64590	4.19040
H	-22.44460	-34.09690	6.08850	H	-29.66060	-38.83310	4.79120
H	-24.31110	-35.55430	7.66800	O	25.47460	41.74320	-7.16230
H	-24.38370	-33.07420	7.20010	C	-27.15560	-43.67320	4.29440
H	-24.82830	-33.42270	5.51770	O	-27.87560	-44.65690	4.13040
H	-25.94010	-33.86540	6.82830	H	-26.67630	-45.54090	5.85550
N	-23.63710	-38.37610	3.76370	H	-26.64160	-40.52680	4.06590
C	-24.93720	-38.11890	3.53430	H	-28.24050	-42.53280	2.83240
O	-25.79570	-38.99830	3.48590	H	-26.14400	-41.50830	1.86800
C	-24.63660	-40.07130	7.47480	H	-25.18420	-42.36660	3.08930
C	-21.66280	-39.68190	4.35150	H	-26.07350	-43.29200	1.86360
H	-24.07950	-35.08860	4.08030	N	-26.19930	-43.61450	5.23830
H	-26.40540	-36.56090	3.35570	C	26.39150	42.57760	-7.16220
H	-24.97050	-35.19310	1.79190	H	24.98730	44.18020	-7.15190
H	-23.68280	-36.40500	1.94210	H	26.49120	44.52520	-6.27480
H	-25.22280	-36.85140	1.18130	H	26.49110	44.52540	-8.04950
N	-23.96990	-39.59540	6.27470	H	-24.96060	-45.11240	6.00650
C	-23.87270	-40.35080	5.16610	H	-26.13590	-44.44370	7.15580
O	-24.33570	-41.48760	5.08730	H	-25.62810	-42.77490	5.33400
C	-28.15890	-39.78000	6.02210				
C	-24.71130	-38.94210	8.50450				
H	-22.96350	-37.61080	3.79430				
H	-23.30940	-40.34780	3.09310				
H	-21.10600	-39.20150	3.54700				
				8. acetyl-(ala) <sub>79</sub> -methylamide			
				C	32.16140	47.09480	-8.01730

N	31.68110	48.46620	-8.01730	N	27.88880	42.55010	-4.27720
C	33.68430	47.08260	-7.87030	C	28.43230	41.55970	-5.00710
C	31.60640	46.36450	-6.79270	O	28.04090	40.39490	-4.95250
O	31.10490	45.24740	-6.90850	C	24.17430	41.84980	-6.10960
C	27.51840	46.90270	-5.23430	C	26.29670	43.64830	-2.79140
C	-31.49330	-50.28060	4.48210	H	29.82950	43.95880	-6.59090
H	32.37280	49.21580	-8.01730	H	29.79850	41.11250	-6.60340
H	31.84720	46.56710	-8.91780	H	31.62180	42.57040	-5.64150
H	34.12540	47.63370	-8.70080	H	30.52750	43.04000	-4.32570
H	33.97110	47.56190	-6.93430	H	31.05690	41.35190	-4.46560
H	34.04970	46.05570	-7.86970	N	25.27470	42.31960	-5.28510
N	28.94860	47.07620	-5.04490	C	25.60700	41.71730	-4.12930
C	31.21120	46.42220	-4.37770	O	25.01060	40.73540	-3.68980
N	31.70050	47.00680	-5.61470	C	26.01080	38.73790	-7.35260
C	31.32610	47.44390	-3.24470	C	24.13740	42.64120	-7.41850
C	29.72100	46.10720	-4.52190	H	28.24960	43.50070	-4.35860
O	29.27870	45.01500	-4.16920	H	27.07580	41.62860	-2.56420
C	27.87440	44.50890	-8.19140	H	27.12040	44.13580	-2.26980
C	26.94700	48.11240	-5.97670	H	25.95680	44.29490	-3.60030
H	32.12540	47.93300	-5.57140	H	25.46970	43.47740	-2.10230
H	31.74650	45.50360	-4.13720	N	25.64940	40.08690	-6.95150
H	32.37070	47.73490	-3.13370	C	24.42030	40.39040	-6.49750
H	30.73460	48.32850	-3.48050	O	23.52140	39.55770	-6.38950
H	30.96020	47.01000	-2.31410	C	26.13630	37.36640	-3.78810
N	28.01300	45.60980	-7.25330	C	27.50420	38.68090	-7.68060
C	27.27080	45.69060	-6.13450	H	25.80110	43.13190	-5.60660
O	26.42930	44.84800	-5.82640	H	23.22530	41.92060	-5.57810
C	29.58720	41.94580	-5.93330	H	24.00870	43.69920	-7.19000
C	28.94590	44.62030	-9.27790	H	25.07320	42.50660	-7.96070
H	29.36390	47.96550	-5.32210	H	23.31330	42.29240	-8.04090
H	27.01070	46.74740	-4.28230	N	26.27700	38.17970	-4.98400
H	27.14080	49.01160	-5.39200	C	25.79350	37.78500	-6.17540
H	27.42700	48.21180	-6.95010	O	25.20330	36.71830	-6.33880
H	25.87390	47.98710	-6.12130	C	22.39860	38.04580	-3.37600
N	29.22690	43.14050	-6.67790	C	26.65290	38.14180	-2.57450
C	28.13670	43.18860	-7.46410	H	26.36080	40.81440	-7.02250
O	27.37270	42.23560	-7.60920	H	25.40790	38.40270	-8.19640
C	26.78670	42.31500	-3.35990	H	27.71700	39.38120	-8.48830
C	30.78260	42.24530	-5.02660	H	28.08810	38.96190	-6.80430
H	28.69830	46.33520	-7.46410	H	27.78040	37.67060	-7.98210
H	26.87430	44.48320	-8.62400	N	23.82920	38.16330	-3.60180
H	28.82750	45.57150	-9.79690	C	24.65200	37.10190	-3.52820
H	29.93750	44.58320	-8.82710	O	24.25850	35.96610	-3.26720
H	28.84620	43.79640	-9.98440	C	21.69430	36.28280	-6.69230

C	21.71920	39.38460	-3.67100	H	21.21220	35.18210	-1.85940
H	26.75960	39.07450	-4.90050	H	21.13440	34.08870	-0.46360
H	26.65300	36.41290	-3.89700	N	19.63210	31.72620	-5.67930
H	27.70120	38.39400	-2.73440	C	18.61690	31.94630	-4.82490
H	26.08160	39.06160	-2.45050	O	17.73440	31.11810	-4.60550
H	26.54950	37.53570	-1.67450	C	20.84200	28.42710	-3.37760
N	22.18130	37.17420	-5.65320	C	21.08450	30.47360	-7.18600
C	21.81120	37.03910	-4.36720	H	20.38820	34.44200	-3.90280
O	21.04190	36.16100	-3.98010	H	17.85820	33.27610	-3.31800
C	23.81490	33.30490	-5.58000	H	18.25170	35.33080	-4.73160
C	22.40110	36.59640	-8.01250	H	18.95400	34.30390	-5.99710
H	24.20510	39.08570	-3.82180	H	17.23870	34.12820	-5.57660
H	22.18600	37.71000	-2.36110	N	20.67890	29.46010	-4.38650
H	22.14000	40.14790	-3.01650	C	19.83790	29.31460	-5.42600
H	21.89530	39.67020	-4.70800	O	19.15240	28.30780	-5.59750
H	20.64550	39.30170	-3.50310	C	17.45120	29.05020	-1.72960
N	23.33500	34.62720	-5.94390	C	21.74770	28.94080	-2.25660
C	22.06700	34.84180	-6.33800	H	20.33980	32.44580	-5.82680
O	21.22950	33.94460	-6.41840	H	18.91530	30.32510	-7.08220
C	21.93510	33.18540	-2.25520	H	21.09710	31.31790	-7.87520
C	25.24310	33.40600	-5.04060	H	21.91990	30.56900	-6.49260
H	22.82260	37.91980	-5.92380	H	21.18750	29.54030	-7.73960
H	20.61170	36.35390	-6.79710	N	18.75530	29.19530	-2.35370
H	22.20130	37.63280	-8.28450	C	19.48640	28.13180	-2.73250
H	23.47660	36.46030	-7.89980	O	19.10930	26.97090	-2.58020
H	22.03920	35.93020	-8.79550	C	15.67470	27.98770	-4.94160
N	22.72980	33.58630	-3.40380	C	16.81050	30.42790	-1.54960
C	22.96200	32.75470	-4.43510	H	21.22600	30.31540	-4.28890
O	22.52370	31.60640	-4.48170	H	21.23510	27.50880	-3.81370
C	18.59980	33.30220	-4.11630	H	22.71660	29.20880	-2.67790
C	21.73020	34.38440	-1.32710	H	21.30470	29.82370	-1.79600
H	23.99210	35.40570	-5.89370	H	21.87330	28.16930	-1.49700
H	23.75940	32.61900	-6.42520	N	16.50880	28.65010	-3.95310
H	25.88320	33.83790	-5.81000	C	16.52760	28.26640	-2.66420
H	25.26340	34.04850	-4.16040	O	15.84780	27.33690	-2.23180
H	25.60790	32.41630	-4.76610	C	17.81540	24.82640	-5.10090
N	19.92510	33.58760	-3.59330	C	15.97900	28.54970	-6.33170
C	20.54160	32.76450	-2.72640	H	19.11290	30.13890	-2.50210
O	20.03490	31.72120	-2.31700	H	17.52570	28.52190	-0.77910
C	19.76310	30.47980	-6.41480	H	17.45860	31.04180	-0.92410
C	18.23250	34.33790	-5.18090	H	16.69110	30.91180	-2.51890
H	23.11610	34.53020	-3.41280	H	15.83160	30.32460	-1.08160
H	22.39800	32.35170	-1.72730	N	17.34310	26.19960	-5.04920
H	22.70340	34.75010	-0.99970	C	16.03360	26.50120	-4.99180

O	15.14910	25.64660	-4.97910	H	12.49450	22.25510	-5.56840
C	17.00090	24.06910	-1.44510	H	14.40760	23.36280	-6.78830
C	19.34270	24.80360	-5.01260	H	15.54830	22.34580	-5.88600
H	17.09180	29.42780	-4.26230	H	14.40930	21.59270	-7.01960
H	14.61740	28.08940	-4.69700	N	13.66310	20.21130	-1.31200
H	15.78080	29.62150	-6.33240	C	14.17280	19.23650	-2.08590
H	17.02740	28.38270	-6.57880	O	13.77730	18.07250	-2.04480
H	15.35570	28.05590	-7.07710	C	9.87760	19.57340	-3.01750
N	17.44590	24.68160	-2.68530	C	12.13500	21.28010	0.26000
C	17.30340	24.06890	-3.87410	H	15.52200	21.66720	-3.66320
O	16.79160	22.95730	-3.99790	H	15.47470	18.82230	-3.74380
C	13.28080	24.58770	-2.14790	H	17.34150	20.24760	-2.81710
C	17.16450	25.06220	-0.29270	H	16.30080	20.68990	-1.44930
H	18.03850	26.94570	-5.05740	H	16.81500	19.00330	-1.65050
H	17.46410	24.32240	-6.00130	N	11.01120	20.01770	-2.22450
H	19.75490	25.37280	-5.84570	C	11.38390	19.38570	-1.09720
H	19.66770	25.25840	-4.07690	O	10.79930	18.39610	-0.65930
H	19.70210	23.77530	-5.05100	C	11.64800	16.48440	-4.40510
N	14.71810	24.74980	-2.00920	C	9.79520	20.39680	-4.30440
C	15.50450	23.76470	-1.53980	H	14.02590	21.16180	-1.38390
O	15.06980	22.66620	-1.19720	H	12.91080	19.25170	0.40800
C	13.51050	22.26550	-5.17390	H	12.98060	21.75080	0.76140
C	12.68830	25.81780	-2.83830	H	11.76810	21.94780	-0.51940
H	17.87730	25.60450	-2.63570	H	11.33380	21.09610	0.97580
H	17.53970	23.14240	-1.24770	N	11.30970	17.82490	-3.95790
H	18.21420	25.34550	-0.21480	C	10.10050	18.12280	-3.44990
H	16.56940	25.95500	-0.48420	O	9.20180	17.29190	-3.32790
H	16.83200	24.60730	0.64030	C	11.90160	15.02530	-0.88260
N	13.69090	23.34240	-4.21520	C	13.12750	16.42860	-4.79130
C	12.99230	23.39920	-3.06730	H	11.52950	20.83520	-2.54600
O	12.15850	22.55320	-2.74780	H	8.95000	19.63560	-2.44860
C	15.29370	19.63980	-3.04600	H	9.68130	21.44950	-4.04550
C	14.54040	22.39860	-6.29750	H	10.70900	20.27120	-4.88510
H	15.12760	25.64370	-2.28040	H	8.94610	20.06730	-4.90310
H	12.80890	24.41140	-1.18130	N	12.00120	15.86710	-2.06280
H	12.90920	26.70160	-2.23970	C	11.47050	15.50390	-3.24410
H	13.13140	25.93890	-3.82660	O	10.86840	14.44440	-3.41070
H	11.60980	25.70110	-2.94480	C	8.18620	15.71180	-0.31140
N	14.91200	20.85410	-3.74700	C	12.46830	15.76820	0.32900
C	13.79290	20.92660	-4.48950	H	12.02200	18.55050	-4.03830
O	13.01860	19.98100	-4.62840	H	11.01150	16.17280	-5.23330
C	12.59540	19.95890	-0.35920	H	13.31330	17.14750	-5.58930
C	16.52450	19.91140	-2.17860	H	13.74600	16.68530	-3.93140
H	14.37180	24.06960	-4.43440	H	13.38640	15.42470	-5.12770

N	9.60780	15.82810	-0.58880	C	3.93360	12.06870	-2.04540
C	10.42680	14.76140	-0.57260	H	8.88210	12.19490	-0.46110
O	10.03720	13.62140	-0.32450	H	8.21660	9.97890	1.19700
C	7.34620	14.03400	-3.64030	H	8.56290	12.35730	1.97060
C	7.50350	17.06060	-0.54750	H	7.04240	12.81720	1.17930
H	12.49160	16.75720	-1.97600	H	7.01180	11.69030	2.55000
H	12.40840	14.07230	-1.03430	N	5.29860	9.46350	-2.66040
H	13.51120	16.01940	0.13530	C	4.31800	9.66730	-1.76270
H	11.90730	16.68740	0.49710	O	3.43980	8.83810	-1.52990
H	12.39600	15.14070	1.21730	C	6.57690	6.10340	-0.48770
N	7.87740	14.89730	-2.59920	C	6.68550	8.24150	-4.25160
C	7.55580	14.73250	-1.30360	H	6.13710	12.13140	-0.84850
O	6.79690	13.84870	-0.90890	H	3.62470	10.96330	-0.19600
C	9.49090	11.01980	-2.68270	H	3.97550	13.05020	-1.57310
C	8.00390	14.37660	-4.97850	H	4.62330	12.05140	-2.88930
H	9.98020	16.75380	-0.80050	H	2.92440	11.87340	-2.40780
H	8.01060	15.35220	0.70240	N	6.38120	7.16150	-1.46410
H	7.95320	17.80560	0.10880	C	5.50040	7.04550	-2.47400
H	7.64150	17.37070	-1.58330	O	4.80340	6.04640	-2.64360
H	6.43650	16.97860	-0.34070	C	3.25490	6.70160	1.30350
N	9.00490	12.35290	-2.99570	C	7.52760	6.58520	0.61000
C	7.72400	12.58300	-3.33560	H	6.00420	10.18320	-2.81730
O	6.87910	11.69190	-3.40580	H	4.52110	8.10060	-4.06850
C	7.73860	10.82750	0.70760	H	6.67660	9.10240	-4.92000
C	10.93920	11.10110	-2.19600	H	7.54730	8.31600	-3.58850
H	8.51200	15.64630	-2.87580	H	6.76220	7.32160	-4.83130
H	6.26080	14.11260	-3.70180	N	4.53510	6.85590	0.63360
H	7.79960	15.42030	-5.21740	C	5.24530	5.79860	0.20140
H	9.08210	14.23270	-4.91040	O	4.86780	4.63610	0.33970
H	7.60870	13.73150	-5.76310	C	1.35140	5.72650	-1.86320
N	8.49110	11.25280	-0.46040	C	2.62920	8.07750	1.54130
C	8.67920	10.44570	-1.51980	H	6.93640	8.01160	-1.36670
O	8.23310	9.30090	-1.57750	H	6.94800	5.19420	-0.96070
C	4.33540	11.00550	-1.02120	H	8.48120	6.85890	0.15870
C	7.57590	12.00430	1.67180	H	7.10740	7.45860	1.10870
H	9.66780	13.12690	-2.95180	H	7.67770	5.79470	1.34530
H	9.39940	10.35510	-3.54160	N	2.22620	6.36050	-0.89150
H	11.55200	11.54870	-2.97850	C	2.29200	5.94520	0.38610
H	10.99660	11.72160	-1.30190	O	1.62400	5.00870	0.82140
H	11.30870	10.10320	-1.95980	C	3.46680	2.56010	-2.18110
N	5.68130	11.27180	-0.54240	C	1.60570	6.32100	-3.24980
C	6.32580	10.42490	0.27990	H	4.89200	7.80120	0.49480
O	5.82920	9.37420	0.68290	H	3.36260	6.14980	2.23730
C	5.39450	8.23500	-3.43050	H	3.30420	8.67270	2.15630

H	2.47570	8.58550	0.58930	O	-1.33550	-2.27300	-1.64370
H	1.66830	7.96720	2.04380	C	-1.59580	-2.39790	2.63680
N	3.00450	3.93380	-2.07790	C	2.26070	-2.41900	0.66790
C	1.69980	4.24010	-1.96320	H	0.04690	1.80320	-1.40200
O	0.81170	3.38950	-1.93750	H	-1.88240	0.02590	-2.50730
C	2.78790	1.71710	1.48360	H	-0.01090	1.15420	-3.77210
C	4.99620	2.52800	-2.15180	H	1.15760	0.11020	-2.93910
H	2.80130	7.14290	-1.20370	H	-0.02800	-0.60960	-4.04630
H	0.30480	5.82710	-1.57600	N	-0.56390	-2.12720	1.65030
H	1.41350	7.39340	-3.21690	C	-0.08950	-3.08500	0.83390
H	2.64290	6.15520	-3.54080	O	-0.48960	-4.24780	0.86180
H	0.95160	5.84850	-3.98270	C	-4.41510	-2.70540	0.07570
N	3.18880	2.35790	0.24260	C	-2.02500	-1.09020	3.30510
C	2.99760	1.77510	-0.95450	H	1.21230	-0.62260	-0.73410
O	2.47530	0.66930	-1.08560	H	1.14600	-3.46450	-0.88210
C	-0.95330	2.27010	0.93640	H	3.05470	-2.07110	0.00700
C	3.00090	2.68090	2.65270	H	2.06930	-1.65760	1.42390
H	3.70320	4.67670	-2.09460	H	2.56610	-3.34120	1.16230
H	3.07860	2.08010	-3.07940	N	-3.24960	-2.28600	0.83540
H	5.37950	3.11560	-2.98600	C	-2.83770	-2.94720	1.93190
H	5.35910	2.95820	-1.21850	O	-3.41080	-3.94450	2.36760
H	5.34810	1.49930	-2.22900	C	-2.71610	-5.76770	-1.45340
N	0.48920	2.42210	1.02400	C	-4.54180	-1.85030	-1.18660
C	1.28730	1.42210	1.43880	H	-0.19880	-1.17690	1.58780
O	0.85990	0.31760	1.77100	H	-1.25540	-3.12510	3.37390
C	-0.85200	0.02190	-2.15180	H	-1.15820	-0.63590	3.78510
C	-1.56480	3.51960	0.29930	H	-2.41750	-0.40180	2.55680
H	3.62700	3.27720	0.29810	H	-2.79930	-1.28790	4.04630
H	3.32870	0.78340	1.63770	N	-3.02960	-4.43700	-0.96100
H	4.05440	2.95730	2.69740	C	-4.21700	-4.14600	-0.40010
H	2.40390	3.58090	2.50600	O	-5.11500	-4.97540	-0.26410
H	2.70160	2.20480	3.58640	C	-2.33660	-7.31390	2.02040
N	-0.62920	1.07410	-1.17480	C	-1.25280	-5.82080	-1.89710
C	-1.28320	1.10600	0.00010	H	-2.73940	-1.46320	0.51430
O	-2.10890	0.25630	0.33050	H	-5.32000	-2.65290	0.68110
C	0.99630	-2.66350	-0.15820	H	-4.64000	-0.80380	-0.89800
C	0.13510	0.17770	-3.31040	H	-3.65160	-1.96580	-1.80470
H	0.89300	3.32050	0.75920	H	-5.41500	-2.16110	-1.76030
H	-1.38890	2.07240	1.91570	N	-2.27740	-6.44390	0.85810
H	-1.31620	4.38740	0.91040	C	-2.85480	-6.77550	-0.31060
H	-1.15890	3.66280	-0.70200	O	-3.46860	-7.82780	-0.47980
H	-2.64720	3.41060	0.23140	C	-6.02370	-6.62430	2.74970
N	0.59500	-1.43060	-0.81430	C	-1.72000	-6.60360	3.22710
C	-0.55120	-1.33470	-1.51150	H	-2.31690	-3.71290	-1.05090

H	-3.38550	-6.05580	-2.26390	N	-8.56040	-11.04560	2.50660
H	-1.09350	-5.08350	-2.68380	C	-7.88970	-11.91550	3.28290
H	-0.60060	-5.58820	-1.05540	O	-8.37640	-12.97340	3.67880
H	-1.01250	-6.81740	-2.26740	C	-8.97390	-14.00930	-0.44140
N	-4.61310	-6.50780	2.42110	C	-10.35950	-10.20390	1.09140
C	-3.80000	-7.57850	2.38000	H	-5.35370	-10.13970	2.48790
O	-4.18620	-8.72240	2.61500	H	-5.96790	-12.39260	4.11580
C	-6.99930	-8.21610	-0.58450	H	-5.57910	-10.03550	4.93330
C	-6.70730	-5.26700	2.57280	H	-7.12600	-9.54930	4.21210
H	-1.77910	-5.55840	0.94760	H	-7.11070	-10.70930	5.55520
H	-1.84130	-8.26520	1.82630	N	-9.03350	-12.79960	0.36140
H	-0.68390	-6.35250	2.99990	C	-9.97810	-12.61330	1.30060
H	-2.26910	-5.68620	3.43890	O	-10.85140	-13.44390	1.54660
H	-1.76200	-7.25230	4.10200	C	-7.69220	-16.21790	2.40130
N	-6.42400	-7.38100	0.45630	C	-7.71510	-13.98860	-1.31090
C	-6.69690	-7.57610	1.75880	H	-8.11180	-10.18090	2.20430
O	-7.44510	-8.46580	2.16060	H	-10.60400	-11.35300	2.92380
C	-4.83650	-11.26270	0.21680	H	-10.29420	-9.23450	1.58550
C	-6.39120	-7.84370	-1.93810	H	-9.70260	-10.20380	0.22160
H	-4.24390	-5.57900	2.21790	H	-11.38290	-10.38560	0.76320
H	-6.16260	-7.00790	3.76040	N	-7.91900	-15.13530	1.45900
H	-6.22880	-4.54040	3.22940	C	-8.83830	-15.22230	0.48110
H	-6.60720	-4.93220	1.54040	O	-9.54690	-16.21370	0.31400
H	-7.76610	-5.34910	2.81810	C	-10.94010	-15.64840	4.33220
N	-5.32670	-9.92010	-0.04490	C	-6.69770	-15.76760	3.47320
C	-6.61820	-9.67580	-0.32990	H	-8.33050	-12.07960	0.19530
O	-7.47020	-10.56100	-0.38940	H	-9.87180	-14.12390	-1.04870
C	-6.45940	-11.53000	3.66590	H	-7.74470	-13.11150	-1.95730
C	-3.37030	-11.20020	0.64950	H	-6.82830	-13.93450	-0.67960
H	-5.79620	-6.62840	0.17390	H	-7.66580	-14.89430	-1.91530
H	-8.08580	-8.13090	-0.60250	N	-9.68550	-15.48370	3.61780
H	-6.59860	-6.79350	-2.14360	C	-8.99830	-16.53340	3.13310
H	-5.31190	-7.99430	-1.91480	O	-9.37670	-17.69710	3.25740
H	-6.81960	-8.46760	-2.72250	C	-12.96830	-16.53660	1.21780
N	-5.74960	-11.07970	2.48070	C	-11.54860	-14.27590	4.62710
C	-5.60650	-11.86140	1.39560	H	-7.35570	-14.29040	1.55580
O	-6.06090	-13.00240	1.32710	H	-7.34450	-17.11690	1.89240
C	-9.92490	-11.29380	2.07330	H	-5.76050	-15.48730	2.99250
C	-6.57870	-10.37650	4.66390	H	-7.09370	-14.90480	4.00860
H	-4.65830	-9.15050	-0.00750	H	-6.52410	-16.57660	4.18280
H	-4.96440	-11.90570	-0.65400	N	-12.05360	-15.93070	2.17040
H	-2.78530	-10.73640	-0.14470	C	-11.94150	-16.37750	3.43410
H	-3.27540	-10.60200	1.55570	O	-12.59760	-17.32140	3.87170
H	-2.99770	-12.20530	0.84710	C	-10.88430	-19.70410	0.74220

C	-12.76380	-15.90950	-0.16270	H	-15.44410	-18.61650	2.42350
H	-9.32890	-14.53690	3.48840	H	-16.89710	-18.88460	3.40660
H	-10.80000	-16.22340	5.24740	N	-13.72420	-23.71380	2.12030
H	-10.84740	-13.69900	5.23020	C	-14.89560	-23.59550	1.47000
H	-11.73540	-13.74400	3.69430	O	-15.68960	-24.52650	1.34500
H	-12.49030	-14.39400	5.16310	C	-15.78730	-24.75530	5.62800
N	-11.33470	-18.33120	0.89640	C	-12.00870	-24.74590	3.51320
C	-12.63230	-18.02180	1.06830	H	-14.27630	-20.46390	1.63280
O	-13.52350	-18.86860	1.10730	H	-16.25610	-22.20460	0.55910
C	-11.42770	-20.63350	4.40860	H	-14.42800	-21.05430	-0.74840
C	-9.35510	-19.74400	0.71220	H	-13.23440	-22.12390	0.01370
H	-11.48640	-15.14360	1.85560	H	-14.46530	-22.81070	-1.06460
H	-14.00270	-16.43820	1.54710	N	-14.79220	-24.46520	4.60970
H	-12.94850	-14.83730	-0.09630	C	-14.35460	-25.40490	3.75270
H	-11.73930	-16.07290	-0.49710	O	-14.75980	-26.56610	3.76750
H	-13.44790	-16.36080	-0.88130	C	-18.70380	-24.98670	3.16990
N	-11.07090	-19.96440	3.16910	C	-16.18330	-23.46230	6.34390
C	-11.31080	-20.51670	1.96640	H	-13.09980	-22.91090	2.19650
O	-11.84380	-21.61660	1.82850	H	-13.18750	-25.74790	1.98200
C	-15.18390	-20.04990	4.01840	H	-11.23860	-24.38560	2.83110
C	-11.16490	-19.69980	5.59180	H	-12.16700	-24.00240	4.29430
H	-10.63300	-17.59140	0.87120	H	-11.69000	-25.68140	3.97290
H	-11.30910	-20.16010	-0.15200	N	-17.50780	-24.59140	3.89450
H	-9.00060	-19.13790	-0.12150	C	-17.05820	-25.28120	4.95800
H	-8.95450	-19.33850	1.64120	O	-17.61980	-26.28630	5.39080
H	-9.01210	-20.77210	0.59670	C	-17.08140	-28.01830	1.50290
N	-13.73830	-19.90680	4.05450	C	-18.87370	-24.10020	1.93450
C	-12.93060	-20.92040	4.41400	H	-14.42440	-23.51530	4.55640
O	-13.35120	-22.03070	4.73530	H	-15.42310	-25.50190	6.33370
C	-15.21300	-22.22220	0.87480	H	-15.29640	-23.02390	6.80130
C	-15.81230	-18.78230	3.43580	H	-16.60030	-22.75390	5.62810
H	-10.62580	-19.04880	3.23020	H	-16.92990	-23.67460	7.10910
H	-10.88670	-21.57330	4.51910	N	-17.36850	-26.69870	2.03910
H	-10.10900	-19.42950	5.60290	C	-18.53200	-26.41610	2.65190
H	-11.76210	-18.79370	5.48990	O	-19.42880	-27.24440	2.80190
H	-11.43110	-20.19730	6.52440	C	-16.57850	-29.65110	4.92090
N	-14.94720	-21.19530	1.86790	C	-15.63640	-28.06740	1.00240
C	-15.55580	-21.18920	3.06740	H	-17.00560	-23.76340	3.57420
O	-16.37310	-22.04290	3.40830	H	-19.58460	-24.94480	3.81050
C	-13.30510	-24.96420	2.73030	H	-18.95490	-23.06070	2.25210
C	-14.26990	-22.04250	-0.31650	H	-18.00840	-24.20470	1.28020
H	-13.33990	-19.00410	3.79640	H	-19.76980	-24.39280	1.38730
H	-15.58300	-20.26960	5.00860	N	-16.55880	-28.75310	3.77870
H	-15.53580	-17.93100	4.05780	C	-17.18210	-29.05320	2.62530



O	-17.80780	-30.09820	2.45400	H	-19.33190	-34.16360	2.23800
C	-20.23120	-28.96250	5.80720	H	-17.12850	-33.01730	2.69190
C	-15.91240	-28.97350	6.12010	H	-17.55260	-32.92240	4.41250
H	-16.65570	-25.97600	1.93970	H	-17.31110	-34.50910	3.65500
H	-17.78280	-28.28340	0.71180	N	-22.79990	-33.36460	5.55370
H	-15.50310	-27.31170	0.22830	C	-22.10500	-34.25640	6.28240
H	-14.95130	-27.85850	1.82390	O	-22.58220	-35.32140	6.67070
H	-15.41600	-29.05570	0.59890	C	-23.34210	-36.25310	2.55240
N	-18.83350	-28.84450	5.42780	C	-24.64700	-32.48010	4.22920
C	-18.02860	-29.91760	5.32970	H	-19.59130	-32.47350	5.43450
O	-18.41190	-31.06520	5.55130	H	-20.15550	-34.76270	7.02940
C	-21.34200	-30.46740	2.47500	H	-19.72270	-32.42830	7.88850
C	-20.91340	-27.59810	5.68960	H	-21.29320	-31.91730	7.23910
H	-16.05250	-27.87250	3.87070	H	-21.23330	-33.11000	8.55190
H	-16.09620	-30.59970	4.68490	N	-23.36430	-35.06320	3.38610
H	-14.88430	-28.72180	5.85960	C	-24.27130	-34.89570	4.36500
H	-16.44780	-28.05900	6.37500	O	-25.13920	-35.72790	4.62390
H	-15.92460	-29.64330	6.97990	C	-21.96530	-38.53680	5.28940
N	-20.72280	-29.66080	3.51300	C	-22.11720	-36.21700	1.63620
C	-20.94690	-29.88650	4.81990	H	-22.35830	-32.49490	5.25570
O	-21.68430	-30.78230	5.22820	H	-24.82780	-33.67270	6.04110
C	-19.16730	-33.54280	3.11860	H	-24.55750	-31.52340	4.74390
C	-20.78380	-30.06480	1.10850	H	-24.02370	-32.46170	3.33520
H	-18.46710	-27.91270	5.23340	H	-25.68310	-32.64890	3.93600
H	-20.33360	-29.37010	6.81290	N	-22.22180	-37.43030	4.38320
H	-20.40620	-26.89000	6.34500	C	-23.17810	-37.48900	3.43920
H	-20.85080	-27.23850	4.66260	O	-23.89810	-38.47270	3.27530
H	-21.96260	-27.68120	5.97320	C	-25.13410	-37.99970	7.35630
N	-19.65960	-32.19190	2.90860	C	-20.92820	-38.11760	6.33320
C	-20.95970	-31.93470	2.67920	H	-22.66410	-34.34260	3.21080
O	-21.81830	-32.81410	2.63080	H	-24.26300	-36.34860	1.97720
C	-20.65910	-33.88710	6.61970	H	-22.16650	-35.32410	1.01290
C	-17.68530	-33.49780	3.49640	H	-21.20670	-36.18240	2.23420
H	-20.10200	-28.90440	3.22520	H	-22.09600	-37.10780	1.00850
H	-22.42790	-30.37670	2.50060	N	-23.90670	-37.82340	6.59870
H	-20.99300	-29.00890	0.93680	C	-23.24430	-38.86400	6.06270
H	-19.70530	-30.22080	1.08700	O	-23.62420	-40.02860	6.17300
H	-21.24530	-30.66720	0.32610	C	-27.28440	-38.80180	4.30110
N	-19.99240	-33.41120	5.41960	C	-25.72320	-36.63200	7.70770
C	-19.89520	-34.16670	4.31100	H	-21.65060	-36.59070	4.47880
O	-20.35820	-35.30340	4.23220	H	-21.64230	-39.42460	4.74580
C	-24.18140	-33.59580	5.16690	H	-20.00840	-37.82990	5.82390
C	-20.73380	-32.75790	7.64930	H	-21.29870	-37.26630	6.90420
H	-18.98600	-31.42660	2.93920	H	-20.73220	-38.94450	7.01570

N	-26.33070	-38.22370	5.23250	C	-28.67420	-44.26230	2.68410
C	-26.17300	-38.70190	6.47970	H	-27.57120	-41.33000	6.83120
O	-26.81720	-39.65320	6.91900	H	-29.77360	-42.61440	8.09710
C	-25.23780	-41.96630	3.66920	H	-29.74950	-40.25350	7.20240
C	-27.12910	-38.14190	2.92940	H	-29.72400	-40.89910	5.54950
H	-23.55000	-36.87540	6.47890	H	-31.13990	-41.18450	6.58070
H	-24.96240	-38.59770	8.25130	N	-28.04540	-45.99530	5.05680
H	-24.99630	-36.07340	8.29730	C	-29.24010	-45.85560	4.45480
H	-25.94250	-36.07650	6.79590	O	-30.04340	-46.77970	4.33770
H	-26.64440	-36.75890	8.27620	C	-29.97910	-47.11300	8.61450
N	-25.67420	-40.59550	3.87390	C	-26.28390	-47.06930	6.35760
C	-26.96260	-40.28440	4.10270	H	-28.59750	-42.73200	4.67010
O	-27.85640	-41.12770	4.15510	H	-30.62650	-44.43660	3.63080
C	-25.64620	-42.98290	7.33000	H	-28.84310	-43.26300	2.28270
C	-23.71110	-42.01250	3.57980	H	-27.62730	-44.35650	2.97230
H	-25.77150	-37.43180	4.91550	H	-28.90230	-45.01100	1.92550
H	-28.30490	-38.70670	4.67200	N	-29.02190	-46.80260	7.56620
H	-27.30520	-37.07080	3.02890	C	-28.62260	-47.72310	6.67050
H	-26.11910	-38.30180	2.55230	O	-29.03340	-48.88240	6.67250
H	-27.84260	-38.57230	2.22680	C	-32.98840	-47.27040	6.26470
N	-25.33320	-42.28520	6.09440	C	-30.34040	-45.83610	9.37620
C	-25.62180	-42.80670	4.88870	H	-27.41410	-45.19740	5.12860
O	-26.16590	-43.90040	4.74450	H	-27.52580	-48.02790	4.84860
C	-29.41130	-42.37240	7.09800	H	-25.53840	-46.69600	5.65550
C	-25.33330	-42.07970	8.52470	H	-26.40810	-46.34450	7.16200
H	-24.96990	-39.85860	3.83980	H	-25.95310	-48.01730	6.78190
H	-25.69880	-42.39830	2.78100	N	-31.76360	-46.89860	6.95250
H	-23.38520	-41.38790	2.74820	C	-31.27760	-47.61640	7.98090
H	-23.27310	-41.63190	4.50240	O	-31.82790	-48.62910	8.41030
H	-23.37850	-43.03910	3.42620	C	30.04730	50.23720	-8.01730
N	-27.96460	-42.23700	7.08220	C	-33.20040	-46.35310	5.05870
C	-27.14940	-43.26280	7.38590	H	-28.65120	-45.85350	7.52200
O	-27.56360	-44.37870	7.69590	H	-29.59250	-47.87840	9.28730
C	-29.57220	-44.46670	3.90590	H	-29.43420	-45.41330	9.81000
C	-30.05430	-41.08800	6.57090	H	-30.78030	-45.10850	8.69430
H	-24.88090	-41.37340	6.16070	H	-31.05840	-46.06370	10.16400
H	-25.10660	-43.92760	7.39680	O	29.45200	47.92740	-8.01740
H	-24.27630	-41.81470	8.50200	C	-32.84450	-48.68740	5.70590
H	-25.92880	-41.16860	8.46780	O	-33.73950	-49.51500	5.86990
H	-25.56660	-42.59860	9.45440	H	-32.36440	-50.90090	4.69320
N	-29.26310	-43.46570	4.91280	H	-31.26930	-46.06540	6.63350
C	-29.82550	-43.48630	6.13440	H	-33.84400	-47.24020	6.93940
O	-30.63390	-44.34420	6.48550	H	-33.26360	-45.32130	5.40430
C	-27.61030	-47.26230	5.61980	H	-32.36120	-46.44560	4.36940

H	-34.11830	-46.62800	4.53920
N	-31.70680	-48.96040	5.04240
C	30.36900	48.76180	-8.01730
H	28.96480	50.36440	-8.00700
H	30.46870	50.70940	-7.13000
H	30.46860	50.70960	-8.90470
H	-31.36170	-50.20920	3.40240
H	-30.60190	-50.73030	4.91920
H	-30.99430	-48.23880	4.93350

9. acetyl-(ala)<sub>89</sub>-methylamide

C	36.11240	53.29740	-8.86180
N	35.63210	54.66880	-8.86180
C	37.63530	53.28530	-8.71480
C	35.55740	52.56710	-7.63720
O	35.05590	51.45000	-7.75300
C	31.46940	53.10530	-6.07880
C	-37.65560	-54.89960	6.57930
H	36.32380	55.41840	-8.86180
H	35.79820	52.76970	-9.76230
H	38.07640	53.83630	-9.54530
H	37.92220	53.76450	-7.77880
H	38.00070	52.25830	-8.71420
N	32.89960	53.27880	-5.88940
C	35.16230	52.62480	-5.22220
N	35.65150	53.20940	-6.45920
C	35.27720	53.64650	-4.08920
C	33.67200	52.30980	-5.36640
O	33.22970	51.21760	-5.01370
C	31.82540	50.71150	-9.03590
C	30.89800	54.31500	-6.82120
H	36.07650	54.13560	-6.41590
H	35.69750	51.70620	-4.98170
H	36.32170	53.93750	-3.97820
H	34.68560	54.53110	-4.32500
H	34.91130	53.21260	-3.15860
N	31.96400	51.81240	-8.09780
C	31.22180	51.89320	-6.97900
O	30.38040	51.05060	-6.67090
C	33.53820	48.14840	-6.77780
C	32.89700	50.82290	-10.12240
H	33.31500	54.16810	-6.16660

H	30.96180	52.95000	-5.12680
H	31.09180	55.21420	-6.23650
H	31.37810	54.41440	-7.79460
H	29.82490	54.18970	-6.96580
N	33.17790	49.34310	-7.52240
C	32.08770	49.39120	-8.30860
O	31.32370	48.43820	-8.45370
C	30.73770	48.51760	-4.20440
C	34.73360	48.44790	-5.87110
H	32.64940	52.53780	-8.30860
H	30.82530	50.68580	-9.46850
H	32.77850	51.77410	-10.64140
H	33.88860	50.78580	-9.67160
H	32.79720	49.99900	-10.82890
N	31.83980	48.75270	-5.12170
C	32.38330	47.76230	-5.85160
O	31.99200	46.59750	-5.79700
C	28.12530	48.05240	-6.95410
C	30.24780	49.85090	-3.63590
H	33.78050	50.16140	-7.43540
H	33.74950	47.31510	-7.44790
H	35.57290	48.77300	-6.48600
H	34.47860	49.24260	-5.17020
H	35.00790	47.55450	-5.31010
N	29.22570	48.52220	-6.12960
C	29.55800	47.91990	-4.97380
O	28.96170	46.93800	-4.53430
C	29.96190	44.94050	-8.19710
C	28.08840	48.84380	-8.26300
H	32.20070	49.70330	-5.20310
H	31.02680	47.83120	-3.40870
H	31.07140	50.33840	-3.11430
H	29.90790	50.49750	-4.44480
H	29.42070	49.68000	-2.94680
N	29.60050	46.28950	-7.79600
C	28.37130	46.59300	-7.34200
O	27.47250	45.76030	-7.23400
C	30.08740	43.56900	-4.63260
C	31.45520	44.88350	-8.52510
H	29.75210	49.33450	-6.45110
H	27.17640	48.12320	-6.42260
H	27.95970	49.90180	-8.03450
H	29.02430	48.70920	-8.80520
H	27.26430	48.49500	-8.88540

N	30.22810	44.38230	-5.82850	C	25.68130	40.58700	-2.17160
C	29.74460	43.98760	-7.01990	H	27.94310	41.60830	-6.73820
O	29.15430	42.92090	-7.18330	H	27.71040	38.82160	-7.26970
C	26.34970	44.24840	-4.22050	H	29.83430	40.04050	-6.65440
C	30.60390	44.34440	-3.41900	H	29.21440	40.25110	-5.00490
H	30.31190	47.01700	-7.86700	H	29.55900	38.61890	-5.61060
H	29.35890	44.60530	-9.04090	N	23.87610	39.79020	-4.43780
H	31.66810	45.58380	-9.33280	C	24.49270	38.96710	-3.57090
H	32.03920	45.16450	-7.64880	O	23.98590	37.92380	-3.16150
H	31.73150	43.87320	-8.82660	C	23.71410	36.68240	-7.25930
N	27.78030	44.36590	-4.44630	C	22.18350	40.54060	-6.02540
C	28.60300	43.30450	-4.37270	H	27.06710	40.73280	-4.25730
O	28.20960	42.16870	-4.11170	H	26.34910	38.55430	-2.57180
C	25.64540	42.48540	-7.53680	H	26.65450	40.95270	-1.84420
C	25.67030	45.58720	-4.51550	H	25.16330	41.38470	-2.70390
H	30.71060	45.27710	-5.74500	H	25.08550	40.29130	-1.30810
H	30.60410	42.61550	-4.74150	N	23.58310	37.92880	-6.52380
H	31.65220	44.59660	-3.57890	C	22.56800	38.14890	-5.66940
H	30.03260	45.26420	-3.29500	O	21.68540	37.32070	-5.45000
H	30.50050	43.73830	-2.51900	C	24.79300	34.62970	-4.22210
N	26.13240	43.37680	-6.49770	C	25.03550	36.67620	-8.03050
C	25.76230	43.24170	-5.21170	H	24.33930	40.64460	-4.74730
O	24.99290	42.36360	-4.82460	H	21.80920	39.47870	-4.16250
C	27.76590	39.50750	-6.42450	H	22.20280	41.53340	-5.57610
C	26.35220	42.79900	-8.85700	H	22.90500	40.50650	-6.84160
H	28.15620	45.28830	-4.66630	H	21.18980	40.33080	-6.42110
H	26.13710	43.91260	-3.20560	N	24.62990	35.66270	-5.23100
H	26.09110	46.35050	-3.86100	C	23.78890	35.51720	-6.27050
H	25.84630	45.87280	-5.55250	O	23.10350	34.51040	-6.44200
H	24.59650	45.50430	-4.34760	C	21.40220	35.25280	-2.57410
N	27.28600	40.82980	-6.78840	C	25.69880	35.14340	-3.10110
C	26.01800	41.04440	-7.18250	H	24.29080	38.64840	-6.67130
O	25.18050	40.14720	-7.26290	H	22.86640	36.52770	-7.92670
C	25.88620	39.38800	-3.09970	H	25.04820	37.52050	-8.71970
C	29.19420	39.60860	-5.88510	H	25.87100	36.77160	-7.33710
H	26.77360	44.12240	-6.76830	H	25.13860	35.74290	-8.58410
H	24.56280	42.55650	-7.64160	N	22.70640	35.39790	-3.19820
H	26.15230	43.83550	-9.12900	C	23.43750	34.33440	-3.57700
H	27.42770	42.66290	-8.74430	O	23.06040	33.17350	-3.42470
H	25.99020	42.13280	-9.64000	C	19.62580	34.19030	-5.78610
N	26.68080	39.78890	-4.24830	C	20.76150	36.63050	-2.39410
C	26.91300	38.95730	-5.27960	H	25.17700	36.51800	-5.13340
O	26.47470	37.80900	-5.32620	H	25.18610	33.71140	-4.65820
C	22.55080	39.50480	-4.96080	H	26.66770	35.41140	-3.52240

H	25.25580	36.02630	-2.64050	O	16.10960	28.75580	-3.59230
H	25.82440	34.37190	-2.34150	C	19.24480	25.84250	-3.89050
N	20.45980	34.85270	-4.79760	C	18.49150	28.60120	-7.14200
C	20.47860	34.46900	-3.50860	H	19.07860	31.84640	-3.12480
O	19.79890	33.53950	-3.07630	H	16.76000	30.61400	-2.02580
C	21.76640	31.02900	-5.94540	H	16.86030	32.90420	-3.08420
C	19.93010	34.75230	-7.17620	H	17.08250	32.14150	-4.67110
H	23.06390	36.34150	-3.34660	H	15.56090	31.90370	-3.78930
H	21.47670	34.72450	-1.62360	N	18.86310	27.05670	-4.59150
H	21.40970	37.24440	-1.76860	C	17.74400	27.12920	-5.33400
H	20.64220	37.11440	-3.36340	O	16.96970	26.18360	-5.47290
H	19.78260	36.52720	-1.92610	C	16.54650	26.16150	-1.20370
N	21.29420	32.40220	-5.89370	C	20.47550	26.11400	-3.02310
C	19.98470	32.70380	-5.83630	H	18.32280	30.27220	-5.27890
O	19.10020	31.84920	-5.82350	H	16.44550	28.45770	-6.41290
C	20.95190	30.27170	-2.28960	H	18.35870	29.56540	-7.63280
C	23.29370	31.00620	-5.85710	H	19.49940	28.54840	-6.73050
H	21.04280	35.63040	-5.10680	H	18.36030	27.79540	-7.86410
H	18.56850	34.29200	-5.54150	N	17.61410	26.41390	-2.15650
H	19.73180	35.82410	-7.17690	C	18.12390	25.43910	-2.93040
H	20.97840	34.58530	-7.42330	O	17.72840	24.27510	-2.88930
H	19.30670	34.25850	-7.92160	C	13.82870	25.77600	-3.86200
N	21.39690	30.88420	-3.52980	C	16.08600	27.48270	-0.58450
C	21.25440	30.27150	-4.71860	H	19.47310	27.86980	-4.50770
O	20.74270	29.15990	-4.84240	H	19.42580	25.02490	-4.58830
C	17.23180	30.79030	-2.99240	H	21.29250	26.45020	-3.66160
C	21.11560	31.26480	-1.13720	H	20.25180	26.89250	-2.29380
H	21.98950	33.14830	-5.90190	H	20.76600	25.20590	-2.49500
H	21.41520	30.52500	-6.84580	N	14.96230	26.22030	-3.06900
H	23.70590	31.57540	-6.69020	C	15.33500	25.58830	-1.94170
H	23.61870	31.46100	-4.92140	O	14.75040	24.59870	-1.50380
H	23.65310	29.97790	-5.89550	C	15.59910	22.68700	-5.24960
N	18.66920	30.95240	-2.85370	C	13.74630	26.59940	-5.14890
C	19.45550	29.96730	-2.38430	H	17.97690	27.36440	-2.22840
O	19.02090	28.86880	-2.04170	H	16.86190	25.45430	-0.43650
C	17.46150	28.46810	-6.01840	H	16.93170	27.95340	-0.08310
C	16.63930	32.02040	-3.68280	H	15.71920	28.15040	-1.36390
H	21.82840	31.80710	-3.48020	H	15.28490	27.29870	0.13130
H	21.49080	29.34500	-2.09220	N	15.26080	24.02750	-4.80240
H	22.16520	31.54810	-1.05930	C	14.05150	24.32540	-4.29440
H	20.52050	32.15760	-1.32870	O	13.15280	23.49450	-4.17240
H	20.78300	30.80990	-0.20420	C	15.85270	21.22790	-1.72710
N	17.64190	29.54500	-5.05970	C	17.07850	22.63120	-5.63580
C	16.94330	29.60180	-3.91180	H	15.48060	27.03780	-3.39050

H	12.90100	25.83820	-3.29310	N	12.44220	17.45540	-1.30490
H	13.63230	27.65210	-4.89000	C	12.63020	16.64830	-2.36430
H	14.66000	26.47380	-5.72960	O	12.18410	15.50350	-2.42200
H	12.89720	26.26990	-5.74760	C	8.28650	17.20810	-1.86570
N	15.95220	22.06970	-2.90730	C	11.52690	18.20690	0.82730
C	15.42150	21.70650	-4.08860	H	13.61880	19.32950	-3.79620
O	14.81950	20.64700	-4.25520	H	13.35050	16.55770	-4.38610
C	12.13720	21.91440	-1.15590	H	15.50300	17.75130	-3.82300
C	16.41940	21.97080	-0.51550	H	14.94770	17.92420	-2.14640
H	15.97300	24.75310	-4.88280	H	15.25970	16.30580	-2.80430
H	14.96250	22.37540	-6.07780	N	9.63230	17.47440	-1.38690
H	17.26440	23.35010	-6.43380	C	10.27690	16.62750	-0.56460
H	17.69700	22.88790	-4.77590	O	9.78030	15.57680	-0.16160
H	17.33740	21.62730	-5.97220	C	9.34560	14.43760	-4.27500
N	13.55880	22.03070	-1.43330	C	7.88470	18.27140	-2.88990
C	14.37780	20.96400	-1.41710	H	12.83310	18.39750	-1.30560
O	13.98830	19.82400	-1.16900	H	12.16760	16.18150	0.35250
C	11.29720	20.23660	-4.48480	H	12.51390	18.55990	1.12610
C	11.45460	23.26320	-1.39200	H	10.99350	19.01980	0.33480
H	16.44260	22.95980	-2.82050	H	10.96280	17.89290	1.70550
H	16.35950	20.27490	-1.87870	N	9.24970	15.66610	-3.50490
H	17.46220	22.22200	-0.70920	C	8.26910	15.86990	-2.60720
H	15.85840	22.89000	-0.34740	O	7.39090	15.04070	-2.37440
H	16.34700	21.34330	0.37280	C	10.52790	12.30600	-1.33220
N	11.82840	21.09990	-3.44370	C	10.63660	14.44410	-5.09610
C	11.50690	20.93510	-2.14810	H	10.08810	18.33400	-1.69300
O	10.74800	20.05130	-1.75340	H	7.57570	17.16590	-1.04050
C	13.44200	17.22240	-3.52720	H	7.92660	19.25280	-2.41760
C	11.95490	20.57920	-5.82300	H	8.57430	18.25400	-3.73380
H	13.93120	22.95640	-1.64500	H	6.87540	18.07600	-3.25230
H	11.96160	21.55480	-0.14210	N	10.33230	13.36410	-2.30860
H	11.90420	24.00820	-0.73570	C	9.45150	13.24810	-3.31850
H	11.59260	23.57330	-2.42780	O	8.75440	12.24900	-3.48810
H	10.38760	23.18120	-1.18520	C	7.20590	12.90420	0.45900
N	12.95590	18.55550	-3.84020	C	11.47860	12.78780	-0.23440
C	11.67510	18.78560	-4.18010	H	9.95520	16.38580	-3.66180
O	10.83010	17.89450	-4.25030	H	8.47210	14.30320	-4.91300
C	11.68960	17.03010	-0.13690	H	10.62770	15.30510	-5.76450
C	14.89030	17.30370	-3.04050	H	11.49840	14.51860	-4.43300
H	12.46310	21.84890	-3.72030	H	10.71320	13.52420	-5.67580
H	10.21190	20.31520	-4.54630	N	8.48610	13.05850	-0.21090
H	11.75070	21.62290	-6.06190	C	9.19630	12.00120	-0.64310
H	13.03320	20.43530	-5.75490	O	8.81880	10.83870	-0.50480
H	11.55970	19.93410	-6.60760	C	5.30250	11.92910	-2.70770

C	6.58030	14.28010	0.69680	H	6.35500	9.78350	1.66150
H	10.88750	14.21420	-2.21120	H	6.65270	8.40740	2.74190
H	10.89900	11.39680	-1.80520	N	3.32180	7.27670	-2.01930
H	12.43220	13.06150	-0.68580	C	2.66780	7.30860	-0.84440
H	11.05840	13.66120	0.26420	O	1.84210	6.45890	-0.51400
H	11.62870	11.99730	0.50080	C	4.94740	3.53910	-1.00270
N	6.17730	12.56310	-1.73600	C	4.08610	6.38030	-4.15490
C	6.24300	12.14780	-0.45840	H	4.84400	9.52310	-0.08530
O	5.57510	11.21130	-0.02310	H	2.56210	8.27500	1.07120
C	7.41780	8.76270	-3.02560	H	2.63480	10.59000	0.06590
C	5.55670	12.52360	-4.09430	H	2.79210	9.86540	-1.54650
H	8.84310	14.00380	-0.34970	H	1.30390	9.61320	-0.61310
H	7.31360	12.35240	1.39280	N	4.54600	4.77200	-1.65880
H	7.25520	14.87530	1.31180	C	3.39980	4.86790	-2.35600
H	6.42680	14.78810	-0.25520	O	2.61560	3.92960	-2.48820
H	5.61930	14.16980	1.19930	C	2.35520	3.80470	1.79230
N	6.95550	10.13640	-2.92240	C	6.21180	3.78360	-0.17660
C	5.65090	10.44270	-2.80770	H	3.99790	8.00580	-2.24650
O	4.76280	9.59210	-2.78200	H	2.06870	6.22850	-3.35180
C	6.73900	7.91980	0.63910	H	3.94010	7.35680	-4.61660
C	8.94720	8.73060	-2.99630	H	5.10860	6.31280	-3.78360
H	6.75240	13.34550	-2.04820	H	3.92300	5.59300	-4.89080
H	4.25580	12.02970	-2.42050	N	3.38720	4.07540	0.80580
H	5.36450	13.59600	-4.06140	C	3.86160	3.11760	-0.01060
H	6.59390	12.35780	-4.38530	O	3.46150	1.95480	0.01730
H	4.90270	12.05110	-4.82720	C	-0.46400	3.49720	-0.76880
N	7.13980	8.56050	-0.60190	C	1.92610	5.11240	2.46060
C	6.94870	7.97770	-1.79900	H	5.16330	5.58000	-1.57860
O	6.42640	6.87190	-1.93010	H	5.09700	2.73810	-1.72660
C	2.99780	8.47280	0.09190	H	7.00570	4.13150	-0.83750
C	6.95200	8.88350	1.80820	H	6.02040	4.54500	0.57940
H	7.65420	10.87930	-2.93910	H	6.51710	2.86140	0.31780
H	7.02970	8.28270	-3.92390	N	0.70140	3.91660	-0.00910
H	9.33060	9.31820	-3.83050	C	1.11330	3.25540	1.08740
H	9.31010	9.16080	-2.06300	O	0.54030	2.25810	1.52310
H	9.29920	7.70190	-3.07350	C	1.23490	0.43490	-2.29790
N	4.44020	8.62470	0.17950	C	-0.59080	4.35230	-2.03110
C	5.23840	7.62470	0.59430	H	3.75230	5.02570	0.74330
O	4.81100	6.52020	0.92650	H	2.69570	3.07750	2.52940
C	3.09900	6.22450	-2.99630	H	2.79280	5.56670	2.94060
C	2.38630	9.72220	-0.54520	H	1.53350	5.80080	1.71230
H	7.57800	9.47980	-0.54640	H	1.15180	4.91470	3.20180
H	7.27980	6.98600	0.79320	N	0.92140	1.76560	-1.80550
H	8.00540	9.15990	1.85290	C	-0.26590	2.05660	-1.24460

O	-1.16390	1.22720	-1.10860	H	-4.13470	-1.92830	-1.44700
C	1.61440	-1.11130	1.17590	H	-2.64750	-0.59090	-2.98810
C	2.69820	0.38180	-2.74150	H	-1.36090	-1.79170	-2.75930
H	1.21170	4.73940	-0.33020	H	-2.86860	-2.26500	-3.56700
H	-1.36890	3.54970	-0.16340	N	-1.79850	-4.87710	1.63620
H	-0.68890	5.39880	-1.74250	C	-1.65550	-5.65880	0.55110
H	0.29950	4.23680	-2.64920	O	-2.10990	-6.79980	0.48260
H	-1.46390	4.04150	-2.60480	C	-5.97390	-5.09120	1.22880
N	1.67360	-0.24130	0.01360	C	-2.62760	-4.17390	3.81940
C	1.09630	-0.57290	-1.15510	H	-0.70720	-2.94790	-0.85200
O	0.48240	-1.62520	-1.32430	H	-1.01330	-5.70310	-1.49850
C	-2.07270	-0.42170	1.90520	H	1.16570	-4.53380	-0.98920
C	2.23100	-0.40100	2.38260	H	0.67560	-4.39940	0.71120
H	1.63410	2.48970	-1.89540	H	0.95340	-6.00270	0.00260
H	0.56560	0.14680	-3.10840	N	-4.60930	-4.84300	1.66210
H	2.85760	1.11910	-3.52830	C	-3.93860	-5.71290	2.43840
H	3.35050	0.61440	-1.89990	O	-4.42540	-6.77080	2.83430
H	2.93850	-0.61480	-3.11190	C	-5.02290	-7.80670	-1.28590
N	-0.66200	-0.30520	1.57660	C	-6.40850	-4.00130	0.24690
C	0.15100	-1.37590	1.53550	H	-1.40260	-3.93710	1.64340
O	-0.23520	-2.51980	1.77050	H	-2.01680	-6.19000	3.27140
C	-3.04830	-2.01350	-1.42900	H	-1.62800	-3.83290	4.08880
C	-2.75630	0.93560	1.72830	H	-3.17490	-3.34670	3.36760
H	2.17190	0.64420	0.10310	H	-3.15960	-4.50670	4.71070
H	2.10980	-2.06260	0.98180	N	-5.08250	-6.59700	-0.48310
H	3.26710	-0.14990	2.15540	C	-6.02700	-6.41070	0.45610
H	1.68200	0.51640	2.59440	O	-6.90030	-7.24130	0.70210
H	2.18910	-1.04970	3.25750	C	-3.74110	-10.01530	1.55680
N	-2.47300	-1.17840	-0.38820	C	-3.76410	-7.78600	-2.15540
C	-2.74580	-1.37350	0.91430	H	-4.16070	-3.97830	1.35980
O	-3.49410	-2.26320	1.31610	H	-6.65290	-5.15040	2.07930
C	-0.88540	-5.06010	-0.62770	H	-6.34320	-3.03190	0.74100
C	-2.44010	-1.64110	-2.78260	H	-5.75160	-4.00120	-0.62290
H	-0.29280	0.62360	1.37340	H	-7.43190	-4.18300	-0.08130
H	-2.21150	-0.80530	2.91590	N	-3.96790	-8.93270	0.61450
H	-2.27780	1.66220	2.38490	C	-4.88720	-9.01970	-0.36340
H	-2.65610	1.27040	0.69590	O	-5.59580	-10.01110	-0.53050
H	-3.81510	0.85350	1.97360	C	-6.98910	-9.44580	3.48770
N	-1.37560	-3.71750	-0.88940	C	-2.74660	-9.56500	2.62870
C	-2.66720	-3.47320	-1.17440	H	-4.37940	-5.87700	-0.64920
O	-3.51920	-4.35840	-1.23390	H	-5.92070	-7.92130	-1.89320
C	-2.50840	-5.32740	2.82140	H	-3.79360	-6.90890	-2.80180
C	0.58080	-4.99760	-0.19500	H	-2.87720	-7.73180	-1.52410
H	-1.84510	-0.42580	-0.67060	H	-3.71470	-8.69170	-2.75980



N	-5.73450	-9.28110	2.77330	C	-11.86120	-12.57970	2.59130
C	-5.04720	-10.33080	2.28860	H	-6.67470	-12.84620	2.38570
O	-5.42570	-11.49450	2.41290	H	-6.93560	-15.37070	3.67460
C	-9.01730	-10.33400	0.37330	H	-6.15800	-13.22690	4.75840
C	-7.59750	-8.07330	3.78260	H	-7.81100	-12.59110	4.64540
H	-3.40470	-8.08780	0.71130	H	-7.48010	-13.99460	5.67990
H	-3.39340	-10.91430	1.04790	N	-10.99620	-14.99270	1.02340
H	-1.80940	-9.28470	2.14800	C	-11.60480	-14.98660	2.22290
H	-3.14270	-8.70220	3.16420	O	-12.42200	-15.84030	2.56380
H	-2.57310	-10.37400	3.33830	C	-9.35400	-18.76160	1.88580
N	-8.10260	-9.72810	1.32590	C	-10.31880	-15.83990	-1.16100
C	-7.99050	-10.17490	2.58960	H	-9.38890	-12.80150	2.95190
O	-8.64660	-11.11880	3.02720	H	-11.63200	-14.06700	4.16410
C	-6.93330	-13.50150	-0.10230	H	-11.58470	-11.72840	3.21330
C	-8.81270	-9.70690	-1.00720	H	-11.49300	-12.41390	1.57900
H	-5.37780	-8.33430	2.64390	H	-12.94600	-12.68200	2.56210
H	-6.84900	-10.02080	4.40290	N	-9.77320	-17.51120	1.27580
H	-6.89640	-7.49640	4.38570	C	-10.94450	-17.39290	0.62550
H	-7.78440	-7.54140	2.84980	O	-11.73850	-18.32390	0.50050
H	-8.53920	-8.19140	4.31860	C	-11.83620	-18.55270	4.78360
N	-7.38360	-12.12860	0.05190	C	-8.05770	-18.54330	2.66870
C	-8.68120	-11.81920	0.22380	H	-10.32520	-14.26130	0.78830
O	-9.57250	-12.66600	0.26280	H	-12.30500	-16.00200	-0.28540
C	-7.47670	-14.43090	3.56410	H	-10.47690	-14.85170	-1.59290
C	-5.40410	-13.54140	-0.13230	H	-9.28330	-15.92130	-0.83080
H	-7.53540	-8.94100	1.01110	H	-10.51420	-16.60810	-1.90910
H	-10.05160	-10.23560	0.70260	N	-10.84110	-18.26260	3.76520
H	-8.99750	-8.63470	-0.94080	C	-10.40350	-19.20230	2.90820
H	-7.78830	-9.87030	-1.34160	O	-10.80880	-20.36350	2.92300
H	-9.49690	-10.15820	-1.72580	C	-14.75270	-18.78410	2.32540
N	-7.11990	-13.76180	2.32460	C	-12.23230	-17.25970	5.49940
C	-7.35970	-14.31410	1.12190	H	-9.14880	-16.70820	1.35200
O	-7.89280	-15.41400	0.98400	H	-9.23650	-19.54530	1.13750
C	-11.23290	-13.84730	3.17390	H	-7.28760	-18.18300	1.98660
C	-7.21390	-13.49720	4.74730	H	-8.21590	-17.79980	3.44980
H	-6.68190	-11.38880	0.02670	H	-7.73890	-19.47880	3.12840
H	-7.35800	-13.95750	-0.99650	N	-13.55680	-18.38880	3.05000
H	-5.04950	-12.93530	-0.96600	C	-13.10720	-19.07860	4.11350
H	-5.00350	-13.13590	0.79670	O	-13.66870	-20.08370	4.54640
H	-5.06110	-14.56950	-0.24780	C	-13.13040	-21.81570	0.65840
N	-9.78730	-13.70420	3.21000	C	-14.92270	-17.89760	1.09000
C	-8.97950	-14.71780	3.56950	H	-10.47330	-17.31270	3.71190
O	-9.40010	-15.82810	3.89080	H	-11.47200	-19.29930	5.48920
C	-11.26190	-16.01960	0.03030	H	-11.34530	-16.82130	5.95680

H	-12.64920	-16.55130	4.78360	O	-17.86720	-26.61150	1.78630
H	-12.97890	-17.47200	6.26460	C	-16.70800	-27.68450	5.77520
N	-13.41750	-20.49610	1.19460	C	-13.73430	-27.29520	2.65190
C	-14.58090	-20.21340	1.80740	H	-16.15100	-22.70180	2.38070
O	-15.47770	-21.04180	1.95740	H	-18.47680	-24.17410	1.65610
C	-12.62740	-23.44850	4.07640	H	-17.04200	-22.80630	0.09230
C	-11.68540	-21.86480	0.15790	H	-15.75430	-24.01820	0.24250
H	-13.05460	-17.56080	2.72970	H	-17.29430	-24.46460	-0.51840
H	-15.63360	-18.74220	2.96600	N	-16.04140	-27.20860	4.57510
H	-15.00390	-16.85810	1.40760	C	-15.94410	-27.96410	3.46650
H	-14.05730	-18.00210	0.43570	O	-16.40720	-29.10080	3.38770
H	-15.81880	-18.19020	0.54280	C	-20.23030	-27.39320	4.32240
N	-12.60770	-22.55050	2.93420	C	-16.78270	-26.55530	6.80480
C	-13.23100	-22.85060	1.78080	H	-15.03490	-25.22400	2.09470
O	-13.85670	-23.89560	1.60950	H	-15.38080	-27.96100	1.39350
C	-16.28010	-22.75990	4.96270	H	-13.17740	-26.81470	1.84740
C	-11.96130	-22.77090	5.27560	H	-13.60160	-26.71980	3.56800
H	-12.70470	-19.77340	1.09520	H	-13.36000	-28.30650	2.81050
H	-13.83170	-22.08080	-0.13270	N	-18.84890	-27.16200	4.70920
H	-11.55200	-21.10910	-0.61620	C	-18.15400	-28.05380	5.43790
H	-11.00020	-21.65590	0.97940	O	-18.63120	-29.11880	5.82620
H	-11.46490	-22.85310	-0.24560	C	-19.39100	-30.05050	1.70790
N	-14.88240	-22.64190	4.58330	C	-20.69590	-26.27750	3.38470
C	-14.07750	-23.71500	4.48520	H	-15.64020	-26.27090	4.59000
O	-14.46080	-24.86260	4.70680	H	-16.20450	-28.56010	6.18490
C	-17.39100	-24.26480	1.63050	H	-15.77170	-26.22570	7.04400
C	-16.96240	-21.39550	4.84510	H	-17.34220	-25.71470	6.39460
H	-12.10140	-21.66980	3.02620	H	-17.28220	-26.90740	7.70740
H	-12.14520	-24.39710	3.84040	N	-19.41320	-28.86060	2.54160
H	-10.93330	-22.51920	5.01510	C	-20.32030	-28.69310	3.52050
H	-12.49680	-21.85640	5.53050	O	-21.18820	-29.52530	3.77940
H	-11.97360	-23.44070	6.13540	C	-18.01430	-32.33420	4.44490
N	-16.77180	-23.45820	2.66850	C	-18.16620	-30.01440	0.79170
C	-16.99590	-23.68390	3.97540	H	-18.40730	-26.29230	4.41120
O	-17.73320	-24.57970	4.38370	H	-20.87680	-27.47000	5.19660
C	-15.21620	-27.34020	2.27410	H	-20.60640	-25.32080	3.89940
C	-16.83280	-23.86220	0.26400	H	-20.07270	-26.25910	2.49070
H	-14.51600	-21.71010	4.38890	H	-21.73210	-26.44630	3.09150
H	-16.38250	-23.16750	5.96840	N	-18.27070	-31.22770	3.53870
H	-16.45520	-20.68740	5.50050	C	-19.22710	-31.28640	2.59470
H	-16.89980	-21.03590	3.81810	O	-19.94710	-32.27010	2.43080
H	-18.01150	-21.47860	5.12870	C	-21.18300	-31.79710	6.51180
N	-15.70850	-25.98930	2.06410	C	-16.97710	-31.91500	5.48870
C	-17.00860	-25.73210	1.83470	H	-18.71300	-28.14000	2.36630

H	-20.31200 -30.14600	1.13270	N	-24.01350 -36.03440	6.23770
H	-18.21540 -29.12150	0.16840	C	-23.19830 -37.06020	6.54140
H	-17.25560 -29.97980	1.38970	O	-23.61260 -38.17610	6.85140
H	-18.14490 -30.90520	0.16400	C	-25.62120 -38.26410	3.06140
N	-19.95570 -31.62080	5.75430	C	-26.10320 -34.88540	5.72640
C	-19.29320 -32.66140	5.21830	H	-20.92990 -35.17080	5.31620
O	-19.67320 -33.82600	5.32850	H	-21.15560 -37.72500	6.55230
C	-23.33330 -32.59920	3.45660	H	-20.32530 -35.61210	7.65750
C	-21.77210 -30.42940	6.86320	H	-21.97780 -34.96600	7.62330
H	-17.69950 -30.38810	3.63430	H	-21.61550 -36.39600	8.60990
H	-17.69120 -33.22200	3.90130	N	-25.31210 -37.26310	4.06830
H	-16.05730 -31.62730	4.97950	C	-25.87440 -37.28370	5.28990
H	-17.34760 -31.06370	6.05970	O	-26.68290 -38.14160	5.64100
H	-16.78110 -32.74190	6.17120	C	-23.65930 -41.05970	4.77530
N	-22.37960 -32.02110	4.38800	C	-24.72320 -38.05970	1.83960
C	-22.22200 -32.49930	5.63520	H	-23.62020 -35.12740	5.98670
O	-22.86620 -33.45060	6.07450	H	-25.82250 -36.41180	7.25260
C	-21.28670 -35.76370	2.82470	H	-25.79850 -34.05090	6.35790
C	-23.17800 -31.93930	2.08490	H	-25.77290 -34.69650	4.70500
H	-19.59890 -30.67280	5.63440	H	-27.18890 -34.98190	5.73620
H	-21.01130 -32.39510	7.40680	N	-24.09440 -39.79270	4.21230
H	-21.04530 -29.87080	7.45280	C	-25.28900 -39.65300	3.61030
H	-21.99140 -29.87390	5.95140	O	-26.09240 -40.57710	3.49320
H	-22.69330 -30.55630	7.43170	C	-26.02810 -40.91040	7.77000
N	-21.72320 -34.39290	3.02940	C	-22.33290 -40.86670	5.51310
C	-23.01150 -34.08180	3.25820	H	-24.64640 -36.52940	3.82560
O	-23.90540 -34.92510	3.31060	H	-26.67540 -38.23400	2.78630
C	-21.69520 -36.78030	6.48550	H	-24.89210 -37.06040	1.43820
C	-19.76000 -35.80990	2.73530	H	-23.67630 -38.15390	2.12790
H	-21.82050 -31.22920	4.07100	H	-24.95120 -38.80840	1.08100
H	-24.35380 -32.50410	3.82750	N	-25.07090 -40.60000	6.72170
H	-23.35420 -30.86820	2.18440	C	-24.67150 -41.52050	5.82600
H	-22.16800 -32.09920	1.70780	O	-25.08240 -42.67980	5.82800
H	-23.89160 -32.36970	1.38230	C	-29.03730 -41.06780	5.42020
N	-21.38210 -36.08260	5.24990	C	-26.38930 -39.63350	8.53170
C	-21.67070 -36.60410	4.04420	H	-23.46310 -38.99480	4.28410
O	-22.21480 -37.69780	3.90000	H	-23.57470 -41.82530	4.00410
C	-25.46020 -36.16980	6.25350	H	-21.58730 -40.49340	4.81100
C	-21.38230 -35.87710	7.68020	H	-22.45700 -40.14190	6.31750
H	-21.01880 -33.65600	2.99530	H	-22.00200 -41.81460	5.93740
H	-21.74780 -36.19570	1.93650	N	-27.81250 -40.69600	6.10800
H	-19.43410 -35.18530	1.90370	C	-27.32650 -41.41380	7.13640
H	-19.32200 -35.42930	3.65790	O	-27.87680 -42.42650	7.56590
H	-19.42740 -36.83650	2.58170	C	-27.49670 -44.06520	3.61910

C	-29.24930	-40.15050	4.21420	H	-31.13850	-43.34560	6.93870
H	-24.70010	-39.65090	6.67750	H	-32.20200	-43.81510	8.27970
H	-25.64140	-41.67580	8.44280	N	-30.04270	-48.25990	5.02040
H	-25.48320	-39.21070	8.96550	C	-31.34910	-47.99110	4.84720
H	-26.82930	-38.90590	7.84980	O	-32.21380	-48.86510	4.81030
H	-27.10740	-39.86110	9.31950	C	-30.90950	-50.04110	8.72460
N	-27.75580	-42.75780	4.19790	C	-28.05480	-49.58900	5.50030
C	-28.89340	-42.48480	4.86140	H	-30.45430	-44.97920	5.43360
O	-29.78850	-43.31240	5.02540	H	-32.81430	-46.42240	4.76280
C	-26.87300	-45.78360	6.97470	H	-31.43250	-45.02330	3.17910
C	-26.07210	-44.10870	3.06270	H	-30.14680	-46.24460	3.25030
H	-27.31820	-39.86280	5.78900	H	-31.71710	-46.66490	2.53830
H	-29.89290	-41.03760	6.09490	N	-30.28640	-49.53890	7.51180
H	-29.31260	-39.11870	4.55980	C	-30.23570	-50.26740	6.38230
H	-28.41010	-40.24300	3.52490	O	-30.70770	-51.39970	6.29360
H	-30.16720	-40.42540	3.69470	C	-34.48290	-49.69770	7.41510
N	-26.89180	-44.85800	5.85470	C	-30.93860	-48.93710	9.78350
C	-27.56030	-45.12680	4.71900	H	-29.36410	-47.49880	5.04380
O	-28.19790	-46.16440	4.54640	H	-29.75180	-50.21610	4.28990
C	-30.48540	-45.10000	8.01640	H	-27.52630	-49.09150	4.68700
C	-26.15790	-45.13870	8.16360	H	-27.88410	-49.03690	6.42440
H	-27.04320	-42.03610	4.08900	H	-27.68040	-50.60570	5.61990
H	-28.22910	-44.30750	2.84920	N	-33.08640	-49.48260	7.75430
H	-25.96410	-43.33480	2.30270	C	-32.36930	-50.39520	8.43390
H	-25.35500	-43.92320	3.86230	O	-32.83730	-51.46720	8.81420
H	-25.87270	-45.08780	2.62720	C	-33.75870	-52.29400	4.70640
N	-29.10250	-44.97930	7.58690	C	-34.97770	-48.55720	6.52330
C	-28.30790	-46.05340	7.43200	H	-29.87970	-48.60380	7.53420
O	-28.68890	-47.20420	7.64010	H	-30.39560	-50.92870	9.09330
C	-31.73070	-46.51750	4.69350	H	-29.91730	-48.61810	9.99190
C	-31.16400	-43.72990	7.95830	H	-31.50860	-48.08400	9.41550
H	-26.37740	-43.98220	5.94870	H	-31.40530	-49.30890	10.69570
H	-26.40540	-46.72840	6.69740	N	-33.74250	-51.12480	5.56910
H	-25.13910	-44.88550	7.87020	C	-34.61060	-50.97710	6.58580
H	-26.67810	-44.22830	8.46100	O	-35.47260	-51.81140	6.85730
H	-26.14110	-45.82940	9.00670	C	-32.29140	-54.65050	7.33240
N	-31.06790	-45.73950	5.72640	C	-32.56950	-52.24110	3.74530
C	-31.24340	-45.99620	7.03500	H	-32.65170	-48.60780	7.46080
O	-31.96960	-46.89830	7.44940	H	-35.09600	-49.79300	8.31120
C	-29.55030	-49.61790	5.17850	H	-34.86320	-47.61390	7.05730
C	-31.22280	-46.08410	3.31690	H	-34.38880	-48.51980	5.60690
H	-28.73860	-44.04470	7.40140	H	-36.02520	-48.71400	6.26590
H	-30.55160	-45.53170	9.01510	N	-32.57610	-53.52090	6.46390
H	-30.62820	-43.04060	8.61080	C	-33.56800	-53.55210	5.55600

O	-34.29920	-54.52810	5.39580	H	-0.79500	9.94090	7.19390
C	-35.37610	-54.14960	9.53140	O	4.50200	10.33620	6.86560
C	-31.21290	-54.26190	8.34570	H	5.29700	9.94090	7.19390
H	-33.04540	-50.40340	5.38480	H	3.70690	9.94090	7.19390
H	-34.70140	-52.37110	4.16480	O	0.00000	18.13420	6.86560
H	-32.63740	-51.33300	3.14620	H	0.79500	17.73890	7.19390
H	-31.63660	-52.22550	4.30870	H	-0.79500	17.73890	7.19390
H	-32.57710	-53.11630	3.09570	O	4.50200	18.13420	6.86560
N	-34.17750	-53.96040	8.73200	H	5.29700	17.73890	7.19390
C	-33.54180	-54.99070	8.14590	H	3.70690	17.73890	7.19390
O	-33.92370	-56.15590	8.24220	O	2.25100	16.95680	10.52960
C	33.99840	56.43980	-8.86180	H	1.45600	17.35210	10.85790
C	-35.94370	-52.78820	9.93820	H	3.04600	17.35210	10.85790
H	-31.99690	-52.68660	6.55800	O	0.00000	12.98210	7.79040
H	-31.99430	-55.52630	6.75550	O	0.00000	10.41190	11.45440
H	-30.31160	-53.96610	7.80880	O	2.25100	9.08310	7.79040
H	-31.55670	-53.42320	8.95100	O	2.25100	14.31090	11.45440
H	-30.99570	-55.10620	8.99990	O	2.25100	14.23520	14.19360
O	33.40310	54.13000	-8.86190	O	2.25100	9.15880	10.52960
C	-36.45160	-54.82520	8.67840	O	0.00000	10.33620	14.19360
O	-37.08390	-55.78400	9.11860	O	0.00000	13.05780	10.52960
H	-38.13980	-55.72620	7.09930	H	0.00000	12.97270	8.74670
H	-33.82030	-53.01150	8.62170	H	0.00000	11.98010	7.46210
H	-35.17370	-54.77010	10.40440	H	0.00000	10.42130	12.41070
H	-35.19180	-52.24760	10.51310	H	0.00000	11.41390	11.12610
H	-36.19440	-52.20950	9.04940	H	2.25100	9.07370	8.74670
H	-36.84330	-52.92470	10.53840	H	2.25100	8.08110	7.46210
N	-36.65400	-54.31590	7.45010	H	2.25100	14.32030	12.41070
C	34.32000	54.96440	-8.86180	H	2.25100	15.31290	11.12610
H	32.91590	56.56700	-8.85150	H	3.04600	13.83990	14.52190
H	34.41980	56.91200	-7.97450	H	1.45600	9.55410	10.85790
H	34.41970	56.91220	-9.74920	H	3.04600	9.55410	10.85790
H	-38.40680	-54.15240	6.32360	H	1.45600	13.83990	14.52190
H	-37.18740	-55.25980	5.66320	H	0.79500	9.94090	14.52190
H	-36.10290	-53.51900	7.13130	H	-0.79500	13.45310	10.85790

## B. Ice-like water clusters

### 1. (H<sub>2</sub>O)<sub>27</sub>

O	2.25100	14.23520	6.86560	O	4.50200	12.98210	7.79040
O	0.00000	10.33620	6.86560	O	4.50200	10.41190	11.45440
H	3.04600	13.83990	7.19390	O	4.50200	10.33620	14.19360
H	1.45600	13.83990	7.19390	O	4.50200	13.05780	10.52960
H	0.79500	9.94090	7.19390	H	4.50200	12.97270	8.74670
				H	4.50200	11.98010	7.46210
				H	4.50200	10.42130	12.41070

H	4.50200	11.41390	11.12610	H	0.00000	19.21190	3.79810
H	5.29700	9.94090	14.52190	O	6.75300	6.51290	4.12640
H	3.70690	13.45310	10.85790	O	6.75300	6.43720	6.86560
H	5.29700	13.45310	10.85790	H	6.75300	6.52230	5.08270
H	3.70690	9.94090	14.52190	H	6.75300	7.51490	3.79810
O	0.00000	18.20990	11.45440	H	7.54800	6.04190	7.19390
O	2.25100	16.88110	7.79040	H	5.95790	6.04190	7.19390
O	0.00000	18.13420	14.19360	O	0.00000	10.41190	4.12640
H	0.00000	18.21930	12.41070	O	2.25100	14.31090	4.12640
H	0.00000	19.21190	11.12610	O	2.25100	14.23520	6.86560
H	2.25100	16.87170	8.74670	O	0.00000	10.33620	6.86560
H	2.25100	15.87910	7.46210	H	0.00000	10.42130	5.08270
H	0.79500	17.73890	14.52190	H	0.00000	11.41390	3.79810
H	-0.79500	17.73890	14.52190	H	2.25100	14.32030	5.08270
O	4.50200	18.20990	11.45440	H	2.25100	15.31290	3.79810
O	4.50200	18.13420	14.19360	H	3.04600	13.83990	7.19390
H	4.50200	18.21930	12.41070	H	1.45600	13.83990	7.19390
H	4.50200	19.21190	11.12610	H	0.79500	9.94090	7.19390
H	5.29700	17.73890	14.52190	H	-0.79500	9.94090	7.19390
H	3.70690	17.73890	14.52190	O	4.50200	10.41190	4.12640
O	0.00000	12.98210	15.11840	O	6.75300	14.31090	4.12640
O	2.25100	9.08310	15.11840	O	6.75300	14.23520	6.86560
H	0.00000	12.97270	16.07470	O	4.50200	10.33620	6.86560
H	0.00000	11.98010	14.79010	H	4.50200	10.42130	5.08270
H	2.25100	9.07370	16.07470	H	4.50200	11.41390	3.79810
H	2.25100	8.08110	14.79010	H	6.75300	14.32030	5.08270
O	4.50200	12.98210	15.11840	H	6.75300	15.31290	3.79810
H	4.50200	12.97270	16.07470	H	7.54800	13.83990	7.19390
H	4.50200	11.98010	14.79010	H	5.95790	13.83990	7.19390
O	2.25100	16.88110	15.11840	H	5.29700	9.94090	7.19390
H	2.25100	16.87170	16.07470	H	3.70690	9.94090	7.19390
H	2.25100	15.87910	14.79010	O	0.00000	18.13420	6.86560
				H	0.79500	17.73890	7.19390
				H	-0.79500	17.73890	7.19390
				O	4.50200	18.20990	4.12640
				O	4.50200	18.13420	6.86560
				H	4.50200	18.21930	5.08270
				H	4.50200	19.21190	3.79810
				H	5.29700	17.73890	7.19390
				H	3.70690	17.73890	7.19390
				O	2.25100	16.95680	10.52960
				H	1.45600	17.35210	10.85790
				H	3.04600	17.35210	10.85790
				O	0.00000	5.18410	7.79040
2. (H <sub>2</sub> O) <sub>64</sub>							
O	2.25100	6.51290	4.12640				
O	2.25100	6.43720	6.86560				
H	2.25100	6.52230	5.08270				
H	2.25100	7.51490	3.79810				
H	3.04600	6.04190	7.19390				
H	1.45600	6.04190	7.19390				
O	0.00000	18.20990	4.12640				
H	0.00000	18.21930	5.08270				

O	2.25100	6.51290	11.45440	H	-0.79500	13.45310	10.85790
O	2.25100	6.43720	14.19360	H	0.79500	13.45310	10.85790
O	0.00000	5.25980	10.52960	H	-0.79500	9.94090	14.52190
H	0.00000	5.17470	8.74670	O	4.50200	12.98210	7.79040
H	0.00000	4.18210	7.46210	O	4.50200	10.41190	11.45440
H	2.25100	6.52230	12.41070	O	6.75300	9.08310	7.79040
H	2.25100	7.51490	11.12610	O	6.75300	14.31090	11.45440
H	3.04600	6.04190	14.52190	O	6.75300	14.23520	14.19360
H	1.45600	6.04190	14.52190	O	6.75300	9.15880	10.52960
H	-0.79500	5.65510	10.85790	O	4.50200	10.33620	14.19360
H	0.79500	5.65510	10.85790	O	4.50200	13.05780	10.52960
O	4.50200	5.18410	7.79040	H	4.50200	12.97270	8.74670
O	6.75300	6.51290	11.45440	H	4.50200	11.98010	7.46210
O	6.75300	6.43720	14.19360	H	4.50200	10.42130	12.41070
O	4.50200	5.25980	10.52960	H	4.50200	11.41390	11.12610
H	4.50200	5.17470	8.74670	H	6.75300	9.07370	8.74670
H	4.50200	4.18210	7.46210	H	6.75300	8.08110	7.46210
H	6.75300	6.52230	12.41070	H	6.75300	14.32030	12.41070
H	6.75300	7.51490	11.12610	H	6.75300	15.31290	11.12610
H	7.54800	6.04190	14.52190	H	7.54800	13.83990	14.52190
H	5.95790	6.04190	14.52190	H	5.95790	9.55410	10.85790
H	3.70690	5.65510	10.85790	H	7.54800	9.55410	10.85790
H	5.29700	5.65510	10.85790	H	5.95790	13.83990	14.52190
O	0.00000	12.98210	7.79040	H	5.29700	9.94090	14.52190
O	0.00000	10.41190	11.45440	H	3.70690	13.45310	10.85790
O	2.25100	9.08310	7.79040	H	5.29700	13.45310	10.85790
O	2.25100	14.31090	11.45440	H	3.70690	9.94090	14.52190
O	2.25100	14.23520	14.19360	O	0.00000	18.20990	11.45440
O	2.25100	9.15880	10.52960	O	2.25100	16.88110	7.79040
O	0.00000	10.33620	14.19360	O	0.00000	18.13420	14.19360
O	0.00000	13.05780	10.52960	H	0.00000	18.21930	12.41070
H	0.00000	12.97270	8.74670	H	0.00000	19.21190	11.12610
H	0.00000	11.98010	7.46210	H	2.25100	16.87170	8.74670
H	0.00000	10.42130	12.41070	H	2.25100	15.87910	7.46210
H	0.00000	11.41390	11.12610	H	0.79500	17.73890	14.52190
H	2.25100	9.07370	8.74670	H	-0.79500	17.73890	14.52190
H	2.25100	8.08110	7.46210	O	4.50200	18.20990	11.45440
H	2.25100	14.32030	12.41070	O	6.75300	16.88110	7.79040
H	2.25100	15.31290	11.12610	O	6.75300	16.95680	10.52960
H	3.04600	13.83990	14.52190	O	4.50200	18.13420	14.19360
H	1.45600	9.55410	10.85790	H	4.50200	18.21930	12.41070
H	3.04600	9.55410	10.85790	H	4.50200	19.21190	11.12610
H	1.45600	13.83990	14.52190	H	6.75300	16.87170	8.74670
H	0.79500	9.94090	14.52190	H	6.75300	15.87910	7.46210

H	5.95790	17.35210	10.85790	H	1.45600	17.35210	18.18590
H	7.54800	17.35210	10.85790	H	3.04600	17.35210	18.18590
H	5.29700	17.73890	14.52190	O	6.75300	16.88110	15.11840
H	3.70690	17.73890	14.52190	O	6.75300	16.95680	17.85760
O	0.00000	5.18410	15.11840	H	6.75300	16.87170	16.07470
O	0.00000	5.25980	17.85760	H	6.75300	15.87910	14.79010
H	0.00000	5.17470	16.07470	H	5.95790	17.35210	18.18590
H	0.00000	4.18210	14.79010	H	7.54800	17.35210	18.18590
H	-0.79500	5.65510	18.18590				
H	0.79500	5.65510	18.18590				
O	4.50200	5.18410	15.11840	3. (H <sub>2</sub> O) <sub>125</sub>			
O	4.50200	5.25980	17.85760	O	2.25100	6.51290	4.12640
H	4.50200	5.17470	16.07470	O	2.25100	6.43720	6.86560
H	4.50200	4.18210	14.79010	O	0.00000	5.25980	3.20160
H	3.70690	5.65510	18.18590	H	2.25100	6.52230	5.08270
H	5.29700	5.65510	18.18590	H	2.25100	7.51490	3.79810
O	0.00000	12.98210	15.11840	H	3.04600	6.04190	7.19390
O	2.25100	9.08310	15.11840	H	1.45600	6.04190	7.19390
O	2.25100	9.15880	17.85760	H	-0.79500	5.65510	3.52990
O	0.00000	13.05780	17.85760	H	0.79500	5.65510	3.52990
H	0.00000	12.97270	16.07470	O	0.00000	18.20990	4.12640
H	0.00000	11.98010	14.79010	O	2.25100	22.10890	4.12640
H	2.25100	9.07370	16.07470	H	0.00000	18.21930	5.08270
H	2.25100	8.08110	14.79010	H	0.00000	19.21190	3.79810
H	1.45600	9.55410	18.18590	H	2.25100	22.11830	5.08270
H	3.04600	9.55410	18.18590	H	2.25100	23.11090	3.79810
H	-0.79500	13.45310	18.18590	H	2.25100	23.11090	3.79810
H	0.79500	13.45310	18.18590	O	6.75300	6.51290	4.12640
O	4.50200	12.98210	15.11840	O	6.75300	6.43720	6.86560
O	6.75300	9.08310	15.11840	O	4.50200	5.25980	3.20160
O	6.75300	9.15880	17.85760	H	6.75300	6.52230	5.08270
O	4.50200	13.05780	17.85760	H	6.75300	7.51490	3.79810
H	4.50200	12.97270	16.07470	H	7.54800	6.04190	7.19390
H	4.50200	11.98010	14.79010	H	5.95790	6.04190	7.19390
H	6.75300	9.07370	16.07470	H	3.70690	5.65510	3.52990
H	6.75300	8.08110	14.79010	H	5.29700	5.65510	3.52990
H	5.95790	9.55410	18.18590	O	9.00400	5.25980	3.20160
H	7.54800	9.55410	18.18590	H	8.20890	5.65510	3.52990
H	3.70690	13.45310	18.18590	H	9.79900	5.65510	3.52990
H	5.29700	13.45310	18.18590	O	0.00000	10.41190	4.12640
O	2.25100	16.88110	15.11840	O	2.25100	14.31090	4.12640
O	2.25100	16.95680	17.85760	O	2.25100	14.23520	6.86560
H	2.25100	16.87170	16.07470	O	2.25100	9.15880	3.20160
H	2.25100	15.87910	14.79010	O	0.00000	10.33620	6.86560



O	0.00000	13.05780	3.20160	H	3.04600	21.63790	7.19390
H	0.00000	10.42130	5.08270	H	1.45600	17.35210	3.52990
H	0.00000	11.41390	3.79810	H	3.04600	17.35210	3.52990
H	2.25100	14.32030	5.08270	H	1.45600	21.63790	7.19390
H	2.25100	15.31290	3.79810	H	0.79500	17.73890	7.19390
H	3.04600	13.83990	7.19390	H	-0.79500	21.25110	3.52990
H	1.45600	9.55410	3.52990	H	0.79500	21.25110	3.52990
H	3.04600	9.55410	3.52990	H	-0.79500	17.73890	7.19390
H	1.45600	13.83990	7.19390	O	4.50200	18.20990	4.12640
H	0.79500	9.94090	7.19390	O	6.75300	22.10890	4.12640
H	-0.79500	13.45310	3.52990	O	6.75300	22.03320	6.86560
H	0.79500	13.45310	3.52990	O	6.75300	16.95680	3.20160
H	-0.79500	9.94090	7.19390	O	4.50200	18.13420	6.86560
O	4.50200	10.41190	4.12640	O	4.50200	20.85580	3.20160
O	6.75300	14.31090	4.12640	H	4.50200	18.21930	5.08270
O	6.75300	14.23520	6.86560	H	4.50200	19.21190	3.79810
O	6.75300	9.15880	3.20160	H	6.75300	22.11830	5.08270
O	4.50200	10.33620	6.86560	H	6.75300	23.11090	3.79810
O	4.50200	13.05780	3.20160	H	7.54800	21.63790	7.19390
H	4.50200	10.42130	5.08270	H	5.95790	17.35210	3.52990
H	4.50200	11.41390	3.79810	H	7.54800	17.35210	3.52990
H	6.75300	14.32030	5.08270	H	5.95790	21.63790	7.19390
H	6.75300	15.31290	3.79810	H	5.29700	17.73890	7.19390
H	7.54800	13.83990	7.19390	H	3.70690	21.25110	3.52990
H	5.95790	9.55410	3.52990	H	5.29700	21.25110	3.52990
H	7.54800	9.55410	3.52990	H	3.70690	17.73890	7.19390
H	5.95790	13.83990	7.19390	O	9.00400	18.20990	4.12640
H	5.29700	9.94090	7.19390	O	9.00400	18.13420	6.86560
H	3.70690	13.45310	3.52990	O	9.00400	20.85580	3.20160
H	5.29700	13.45310	3.52990	H	9.00400	18.21930	5.08270
H	3.70690	9.94090	7.19390	H	9.00400	19.21190	3.79810
O	9.00400	10.41190	4.12640	H	9.79900	17.73890	7.19390
O	9.00400	10.33620	6.86560	H	8.20890	21.25110	3.52990
O	9.00400	13.05780	3.20160	H	9.79900	21.25110	3.52990
H	9.00400	10.42130	5.08270	H	8.20890	17.73890	7.19390
H	9.00400	11.41390	3.79810	O	2.25100	16.95680	10.52960
H	9.79900	9.94090	7.19390	O	0.00000	20.85580	10.52960
H	8.20890	13.45310	3.52990	H	1.45600	17.35210	10.85790
H	9.79900	13.45310	3.52990	H	3.04600	17.35210	10.85790
H	8.20890	9.94090	7.19390	H	-0.79500	21.25110	10.85790
O	2.25100	22.03320	6.86560	H	0.79500	21.25110	10.85790
O	2.25100	16.95680	3.20160	O	4.50200	20.85580	10.52960
O	0.00000	18.13420	6.86560	H	3.70690	21.25110	10.85790
O	0.00000	20.85580	3.20160	H	5.29700	21.25110	10.85790

O	0.00000	5.18410	7.79040	H	2.25100	14.32030	12.41070
O	2.25100	6.51290	11.45440	H	2.25100	15.31290	11.12610
O	2.25100	6.43720	14.19360	H	3.04600	13.83990	14.52190
O	0.00000	5.25980	10.52960	H	1.45600	9.55410	10.85790
H	0.00000	5.17470	8.74670	H	3.04600	9.55410	10.85790
H	0.00000	4.18210	7.46210	H	1.45600	13.83990	14.52190
H	2.25100	6.52230	12.41070	H	0.79500	9.94090	14.52190
H	2.25100	7.51490	11.12610	H	-0.79500	13.45310	10.85790
H	3.04600	6.04190	14.52190	H	0.79500	13.45310	10.85790
H	1.45600	6.04190	14.52190	H	-0.79500	9.94090	14.52190
H	-0.79500	5.65510	10.85790	O	4.50200	12.98210	7.79040
H	0.79500	5.65510	10.85790	O	4.50200	10.41190	11.45440
O	4.50200	5.18410	7.79040	O	6.75300	9.08310	7.79040
O	6.75300	6.51290	11.45440	O	6.75300	14.31090	11.45440
O	6.75300	6.43720	14.19360	O	6.75300	14.23520	14.19360
O	4.50200	5.25980	10.52960	O	6.75300	9.15880	10.52960
H	4.50200	5.17470	8.74670	O	4.50200	10.33620	14.19360
H	4.50200	4.18210	7.46210	O	4.50200	13.05780	10.52960
H	6.75300	6.52230	12.41070	H	4.50200	12.97270	8.74670
H	6.75300	7.51490	11.12610	H	4.50200	11.98010	7.46210
H	7.54800	6.04190	14.52190	H	4.50200	10.42130	12.41070
H	5.95790	6.04190	14.52190	H	4.50200	11.41390	11.12610
H	3.70690	5.65510	10.85790	H	6.75300	9.07370	8.74670
H	5.29700	5.65510	10.85790	H	6.75300	8.08110	7.46210
O	9.00400	5.18410	7.79040	H	6.75300	14.32030	12.41070
O	9.00400	5.25980	10.52960	H	6.75300	15.31290	11.12610
H	9.00400	5.17470	8.74670	H	7.54800	13.83990	14.52190
H	9.00400	4.18210	7.46210	H	5.95790	9.55410	10.85790
H	8.20890	5.65510	10.85790	H	7.54800	9.55410	10.85790
H	9.79900	5.65510	10.85790	H	5.95790	13.83990	14.52190
O	0.00000	12.98210	7.79040	H	5.29700	9.94090	14.52190
O	0.00000	10.41190	11.45440	H	3.70690	13.45310	10.85790
O	2.25100	9.08310	7.79040	H	5.29700	13.45310	10.85790
O	2.25100	14.31090	11.45440	H	3.70690	9.94090	14.52190
O	2.25100	14.23520	14.19360	O	9.00400	12.98210	7.79040
O	2.25100	9.15880	10.52960	O	9.00400	10.41190	11.45440
O	0.00000	10.33620	14.19360	O	9.00400	10.33620	14.19360
O	0.00000	13.05780	10.52960	O	9.00400	13.05780	10.52960
H	0.00000	12.97270	8.74670	H	9.00400	12.97270	8.74670
H	0.00000	11.98010	7.46210	H	9.00400	11.98010	7.46210
H	0.00000	10.42130	12.41070	H	9.00400	10.42130	12.41070
H	0.00000	11.41390	11.12610	H	9.00400	11.41390	11.12610
H	2.25100	9.07370	8.74670	H	9.79900	9.94090	14.52190
H	2.25100	8.08110	7.46210	H	8.20890	13.45310	10.85790

H	9.79900	13.45310	10.85790	O	9.00400	20.85580	10.52960
H	8.20890	9.94090	14.52190	H	9.00400	20.77070	8.74670
O	0.00000	20.78010	7.79040	H	9.00400	19.77810	7.46210
O	0.00000	18.20990	11.45440	H	9.00400	18.21930	12.41070
O	2.25100	16.88110	7.79040	H	9.00400	19.21190	11.12610
O	2.25100	22.10890	11.45440	H	9.79900	17.73890	14.52190
O	2.25100	22.03320	14.19360	H	8.20890	21.25110	10.85790
O	0.00000	18.13420	14.19360	H	9.79900	21.25110	10.85790
H	0.00000	20.77070	8.74670	H	8.20890	17.73890	14.52190
H	0.00000	19.77810	7.46210	O	0.00000	5.18410	15.11840
H	0.00000	18.21930	12.41070	O	2.25100	6.51290	18.78240
H	0.00000	19.21190	11.12610	O	0.00000	5.25980	17.85760
H	2.25100	16.87170	8.74670	H	0.00000	5.17470	16.07470
H	2.25100	15.87910	7.46210	H	0.00000	4.18210	14.79010
H	2.25100	22.11830	12.41070	H	2.25100	6.52230	19.73870
H	2.25100	23.11090	11.12610	H	2.25100	7.51490	18.45410
H	3.04600	21.63790	14.52190	H	-0.79500	5.65510	18.18590
H	1.45600	21.63790	14.52190	H	0.79500	5.65510	18.18590
H	0.79500	17.73890	14.52190	O	4.50200	5.18410	15.11840
H	-0.79500	17.73890	14.52190	O	6.75300	6.51290	18.78240
O	4.50200	20.78010	7.79040	O	4.50200	5.25980	17.85760
O	4.50200	18.20990	11.45440	H	4.50200	5.17470	16.07470
O	6.75300	16.88110	7.79040	H	4.50200	4.18210	14.79010
O	6.75300	22.10890	11.45440	H	6.75300	6.52230	19.73870
O	6.75300	22.03320	14.19360	H	6.75300	7.51490	18.45410
O	6.75300	16.95680	10.52960	H	3.70690	5.65510	18.18590
O	4.50200	18.13420	14.19360	H	5.29700	5.65510	18.18590
H	4.50200	20.77070	8.74670	O	9.00400	5.18410	15.11840
H	4.50200	19.77810	7.46210	O	9.00400	5.25980	17.85760
H	4.50200	18.21930	12.41070	H	9.00400	5.17470	16.07470
H	4.50200	19.21190	11.12610	H	9.00400	4.18210	14.79010
H	6.75300	16.87170	8.74670	H	8.20890	5.65510	18.18590
H	6.75300	15.87910	7.46210	H	9.79900	5.65510	18.18590
H	6.75300	22.11830	12.41070	O	0.00000	12.98210	15.11840
H	6.75300	23.11090	11.12610	O	0.00000	10.41190	18.78240
H	7.54800	21.63790	14.52190	O	2.25100	9.08310	15.11840
H	5.95790	17.35210	10.85790	O	2.25100	14.31090	18.78240
H	7.54800	17.35210	10.85790	O	2.25100	9.15880	17.85760
H	5.95790	21.63790	14.52190	O	0.00000	13.05780	17.85760
H	5.29700	17.73890	14.52190	H	0.00000	12.97270	16.07470
H	3.70690	17.73890	14.52190	H	0.00000	11.98010	14.79010
O	9.00400	20.78010	7.79040	H	0.00000	10.42130	19.73870
O	9.00400	18.20990	11.45440	H	0.00000	11.41390	18.45410
O	9.00400	18.13420	14.19360	H	2.25100	9.07370	16.07470



O	2.25100	1.36080	3.20160	H	7.54800	6.04190	7.19390
O	0.00000	2.53820	6.86560	H	5.95790	1.75610	3.52990
O	0.00000	5.25980	3.20160	H	7.54800	1.75610	3.52990
H	0.00000	5.17470	1.41870	H	5.95790	6.04190	7.19390
H	0.00000	4.18210	0.13410	H	5.29700	2.14290	7.19390
H	0.00000	2.62330	5.08270	H	3.70690	5.65510	3.52990
H	0.00000	3.61590	3.79810	H	5.29700	5.65510	3.52990
H	2.25100	1.27570	1.41870	H	3.70690	2.14290	7.19390
H	2.25100	0.28310	0.13410	O	9.00400	5.18410	0.46240
H	2.25100	6.52230	5.08270	O	9.00400	2.61390	4.12640
H	2.25100	7.51490	3.79810	O	11.25500	1.28510	0.46240
H	3.04600	6.04190	7.19390	O	11.25500	6.51290	4.12640
H	1.45600	1.75610	3.52990	O	11.25500	1.36080	3.20160
H	3.04600	1.75610	3.52990	O	9.00400	2.53820	6.86560
H	1.45600	6.04190	7.19390	O	9.00400	5.25980	3.20160
H	0.79500	2.14290	7.19390	H	9.00400	5.17470	1.41870
H	-0.79500	5.65510	3.52990	H	9.00400	4.18210	0.13410
H	0.79500	5.65510	3.52990	H	9.00400	2.62330	5.08270
H	-0.79500	2.14290	7.19390	H	9.00400	3.61590	3.79810
O	0.00000	18.20990	4.12640	H	11.25500	1.27570	1.41870
O	2.25100	22.10890	4.12640	H	11.25500	0.28310	0.13410
H	0.00000	18.21930	5.08270	H	11.25500	6.52230	5.08270
H	0.00000	19.21190	3.79810	H	11.25500	7.51490	3.79810
H	2.25100	22.11830	5.08270	H	10.45990	1.75610	3.52990
H	2.25100	23.11090	3.79810	H	12.05000	1.75610	3.52990
O	11.25500	6.43720	6.86560	H	9.79900	2.14290	7.19390
H	12.05000	6.04190	7.19390	H	8.20890	5.65510	3.52990
H	10.45990	6.04190	7.19390	H	9.79900	5.65510	3.52990
O	4.50200	5.18410	0.46240	H	8.20890	2.14290	7.19390
O	4.50200	2.61390	4.12640	O	0.00000	12.98210	0.46240
O	6.75300	1.28510	0.46240	O	0.00000	10.41190	4.12640
O	6.75300	6.51290	4.12640	O	2.25100	9.08310	0.46240
O	6.75300	6.43720	6.86560	O	2.25100	14.31090	4.12640
O	6.75300	1.36080	3.20160	O	2.25100	14.23520	6.86560
O	4.50200	2.53820	6.86560	O	2.25100	9.15880	3.20160
O	4.50200	5.25980	3.20160	O	0.00000	10.33620	6.86560
H	4.50200	5.17470	1.41870	O	0.00000	13.05780	3.20160
H	4.50200	4.18210	0.13410	H	0.00000	12.97270	1.41870
H	4.50200	2.62330	5.08270	H	0.00000	11.98010	0.13410
H	4.50200	3.61590	3.79810	H	0.00000	10.42130	5.08270
H	6.75300	1.27570	1.41870	H	0.00000	11.41390	3.79810
H	6.75300	0.28310	0.13410	H	2.25100	9.07370	1.41870
H	6.75300	6.52230	5.08270	H	2.25100	8.08110	0.13410
H	6.75300	7.51490	3.79810	H	2.25100	14.32030	5.08270

H	2.25100	15.31290	3.79810	H	9.00400	11.41390	3.79810
H	3.04600	13.83990	7.19390	H	11.25500	9.07370	1.41870
H	1.45600	9.55410	3.52990	H	11.25500	8.08110	0.13410
H	3.04600	9.55410	3.52990	H	11.25500	14.32030	5.08270
H	1.45600	13.83990	7.19390	H	11.25500	15.31290	3.79810
H	0.79500	9.94090	7.19390	H	12.05000	13.83990	7.19390
H	-0.79500	13.45310	3.52990	H	10.45990	9.55410	3.52990
H	0.79500	13.45310	3.52990	H	12.05000	9.55410	3.52990
H	-0.79500	9.94090	7.19390	H	10.45990	13.83990	7.19390
O	4.50200	12.98210	0.46240	H	9.79900	9.94090	7.19390
O	4.50200	10.41190	4.12640	H	8.20890	13.45310	3.52990
O	6.75300	9.08310	0.46240	H	9.79900	13.45310	3.52990
O	6.75300	14.31090	4.12640	H	8.20890	9.94090	7.19390
O	6.75300	14.23520	6.86560	O	0.00000	20.78010	0.46240
O	6.75300	9.15880	3.20160	O	2.25100	16.88110	0.46240
O	4.50200	10.33620	6.86560	O	2.25100	22.03320	6.86560
O	4.50200	13.05780	3.20160	O	2.25100	16.95680	3.20160
H	4.50200	12.97270	1.41870	O	0.00000	18.13420	6.86560
H	4.50200	11.98010	0.13410	O	0.00000	20.85580	3.20160
H	4.50200	10.42130	5.08270	H	0.00000	20.77070	1.41870
H	4.50200	11.41390	3.79810	H	0.00000	19.77810	0.13410
H	6.75300	9.07370	1.41870	H	2.25100	16.87170	1.41870
H	6.75300	8.08110	0.13410	H	2.25100	15.87910	0.13410
H	6.75300	14.32030	5.08270	H	3.04600	21.63790	7.19390
H	6.75300	15.31290	3.79810	H	1.45600	17.35210	3.52990
H	7.54800	13.83990	7.19390	H	3.04600	17.35210	3.52990
H	5.95790	9.55410	3.52990	H	1.45600	21.63790	7.19390
H	7.54800	9.55410	3.52990	H	0.79500	17.73890	7.19390
H	5.95790	13.83990	7.19390	H	-0.79500	21.25110	3.52990
H	5.29700	9.94090	7.19390	H	0.79500	21.25110	3.52990
H	3.70690	13.45310	3.52990	H	-0.79500	17.73890	7.19390
H	5.29700	13.45310	3.52990	O	4.50200	20.78010	0.46240
H	3.70690	9.94090	7.19390	O	4.50200	18.20990	4.12640
O	9.00400	12.98210	0.46240	O	6.75300	16.88110	0.46240
O	9.00400	10.41190	4.12640	O	6.75300	22.10890	4.12640
O	11.25500	9.08310	0.46240	O	6.75300	22.03320	6.86560
O	11.25500	14.31090	4.12640	O	6.75300	16.95680	3.20160
O	11.25500	14.23520	6.86560	O	4.50200	18.13420	6.86560
O	11.25500	9.15880	3.20160	O	4.50200	20.85580	3.20160
O	9.00400	10.33620	6.86560	H	4.50200	20.77070	1.41870
O	9.00400	13.05780	3.20160	H	4.50200	19.77810	0.13410
H	9.00400	12.97270	1.41870	H	4.50200	18.21930	5.08270
H	9.00400	11.98010	0.13410	H	4.50200	19.21190	3.79810
H	9.00400	10.42130	5.08270	H	6.75300	16.87170	1.41870

H	6.75300	15.87910	0.13410	O	4.50200	20.85580	10.52960
H	6.75300	22.11830	5.08270	H	3.70690	21.25110	10.85790
H	6.75300	23.11090	3.79810	H	5.29700	21.25110	10.85790
H	7.54800	21.63790	7.19390	O	0.00000	5.18410	7.79040
H	5.95790	17.35210	3.52990	O	0.00000	2.61390	11.45440
H	7.54800	17.35210	3.52990	O	2.25100	1.28510	7.79040
H	5.95790	21.63790	7.19390	O	2.25100	6.51290	11.45440
H	5.29700	17.73890	7.19390	O	2.25100	6.43720	14.19360
H	3.70690	21.25110	3.52990	O	2.25100	1.36080	10.52960
H	5.29700	21.25110	3.52990	O	0.00000	2.53820	14.19360
H	3.70690	17.73890	7.19390	O	0.00000	5.25980	10.52960
O	9.00400	20.78010	0.46240	H	0.00000	5.17470	8.74670
O	9.00400	18.20990	4.12640	H	0.00000	4.18210	7.46210
O	11.25500	16.88110	0.46240	H	0.00000	2.62330	12.41070
O	11.25500	22.10890	4.12640	H	0.00000	3.61590	11.12610
O	11.25500	22.03320	6.86560	H	2.25100	1.27570	8.74670
O	11.25500	16.95680	3.20160	H	2.25100	0.28310	7.46210
O	9.00400	18.13420	6.86560	H	2.25100	6.52230	12.41070
O	9.00400	20.85580	3.20160	H	2.25100	7.51490	11.12610
H	9.00400	20.77070	1.41870	H	3.04600	6.04190	14.52190
H	9.00400	19.77810	0.13410	H	1.45600	1.75610	10.85790
H	9.00400	18.21930	5.08270	H	3.04600	1.75610	10.85790
H	9.00400	19.21190	3.79810	H	1.45600	6.04190	14.52190
H	11.25500	16.87170	1.41870	H	0.79500	2.14290	14.52190
H	11.25500	15.87910	0.13410	H	-0.79500	5.65510	10.85790
H	11.25500	22.11830	5.08270	H	0.79500	5.65510	10.85790
H	11.25500	23.11090	3.79810	H	-0.79500	2.14290	14.52190
H	12.05000	21.63790	7.19390	O	4.50200	5.18410	7.79040
H	10.45990	17.35210	3.52990	O	4.50200	2.61390	11.45440
H	12.05000	17.35210	3.52990	O	6.75300	1.28510	7.79040
H	10.45990	21.63790	7.19390	O	6.75300	6.51290	11.45440
H	9.79900	17.73890	7.19390	O	6.75300	6.43720	14.19360
H	8.20890	21.25110	3.52990	O	6.75300	1.36080	10.52960
H	9.79900	21.25110	3.52990	O	4.50200	2.53820	14.19360
H	8.20890	17.73890	7.19390	O	4.50200	5.25980	10.52960
O	11.25500	16.95680	10.52960	H	4.50200	5.17470	8.74670
H	10.45990	17.35210	10.85790	H	4.50200	4.18210	7.46210
H	12.05000	17.35210	10.85790	H	4.50200	2.62330	12.41070
O	2.25100	16.95680	10.52960	H	4.50200	3.61590	11.12610
O	0.00000	20.85580	10.52960	H	6.75300	1.27570	8.74670
H	1.45600	17.35210	10.85790	H	6.75300	0.28310	7.46210
H	3.04600	17.35210	10.85790	H	6.75300	6.52230	12.41070
H	-0.79500	21.25110	10.85790	H	6.75300	7.51490	11.12610
H	0.79500	21.25110	10.85790	H	7.54800	6.04190	14.52190

H	5.95790	1.75610	10.85790	H	2.25100	8.08110	7.46210
H	7.54800	1.75610	10.85790	H	2.25100	14.32030	12.41070
H	5.95790	6.04190	14.52190	H	2.25100	15.31290	11.12610
H	5.29700	2.14290	14.52190	H	3.04600	13.83990	14.52190
H	3.70690	5.65510	10.85790	H	1.45600	9.55410	10.85790
H	5.29700	5.65510	10.85790	H	3.04600	9.55410	10.85790
H	3.70690	2.14290	14.52190	H	1.45600	13.83990	14.52190
O	9.00400	5.18410	7.79040	H	0.79500	9.94090	14.52190
O	9.00400	2.61390	11.45440	H	-0.79500	13.45310	10.85790
O	11.25500	1.28510	7.79040	H	0.79500	13.45310	10.85790
O	11.25500	6.51290	11.45440	H	-0.79500	9.94090	14.52190
O	11.25500	6.43720	14.19360	O	4.50200	12.98210	7.79040
O	11.25500	1.36080	10.52960	O	4.50200	10.41190	11.45440
O	9.00400	2.53820	14.19360	O	6.75300	9.08310	7.79040
O	9.00400	5.25980	10.52960	O	6.75300	14.31090	11.45440
H	9.00400	5.17470	8.74670	O	6.75300	14.23520	14.19360
H	9.00400	4.18210	7.46210	O	6.75300	9.15880	10.52960
H	9.00400	2.62330	12.41070	O	4.50200	10.33620	14.19360
H	9.00400	3.61590	11.12610	O	4.50200	13.05780	10.52960
H	11.25500	1.27570	8.74670	H	4.50200	12.97270	8.74670
H	11.25500	0.28310	7.46210	H	4.50200	11.98010	7.46210
H	11.25500	6.52230	12.41070	H	4.50200	10.42130	12.41070
H	11.25500	7.51490	11.12610	H	4.50200	11.41390	11.12610
H	12.05000	6.04190	14.52190	H	6.75300	9.07370	8.74670
H	10.45990	1.75610	10.85790	H	6.75300	8.08110	7.46210
H	12.05000	1.75610	10.85790	H	6.75300	14.32030	12.41070
H	10.45990	6.04190	14.52190	H	6.75300	15.31290	11.12610
H	9.79900	2.14290	14.52190	H	7.54800	13.83990	14.52190
H	8.20890	5.65510	10.85790	H	5.95790	9.55410	10.85790
H	9.79900	5.65510	10.85790	H	7.54800	9.55410	10.85790
H	8.20890	2.14290	14.52190	H	5.95790	13.83990	14.52190
O	0.00000	12.98210	7.79040	H	5.29700	9.94090	14.52190
O	0.00000	10.41190	11.45440	H	3.70690	13.45310	10.85790
O	2.25100	9.08310	7.79040	H	5.29700	13.45310	10.85790
O	2.25100	14.31090	11.45440	H	3.70690	9.94090	14.52190
O	2.25100	14.23520	14.19360	O	9.00400	12.98210	7.79040
O	2.25100	9.15880	10.52960	O	9.00400	10.41190	11.45440
O	0.00000	10.33620	14.19360	O	11.25500	9.08310	7.79040
O	0.00000	13.05780	10.52960	O	11.25500	14.31090	11.45440
H	0.00000	12.97270	8.74670	O	11.25500	14.23520	14.19360
H	0.00000	11.98010	7.46210	O	11.25500	9.15880	10.52960
H	0.00000	10.42130	12.41070	O	9.00400	10.33620	14.19360
H	0.00000	11.41390	11.12610	O	9.00400	13.05780	10.52960
H	2.25100	9.07370	8.74670	H	9.00400	12.97270	8.74670



H	9.00400	11.98010	7.46210	H	6.75300	16.87170	8.74670
H	9.00400	10.42130	12.41070	H	6.75300	15.87910	7.46210
H	9.00400	11.41390	11.12610	H	6.75300	22.11830	12.41070
H	11.25500	9.07370	8.74670	H	6.75300	23.11090	11.12610
H	11.25500	8.08110	7.46210	H	7.54800	21.63790	14.52190
H	11.25500	14.32030	12.41070	H	5.95790	17.35210	10.85790
H	11.25500	15.31290	11.12610	H	7.54800	17.35210	10.85790
H	12.05000	13.83990	14.52190	H	5.95790	21.63790	14.52190
H	10.45990	9.55410	10.85790	H	5.29700	17.73890	14.52190
H	12.05000	9.55410	10.85790	H	3.70690	17.73890	14.52190
H	10.45990	13.83990	14.52190	O	9.00400	20.78010	7.79040
H	9.79900	9.94090	14.52190	O	9.00400	18.20990	11.45440
H	8.20890	13.45310	10.85790	O	11.25500	16.88110	7.79040
H	9.79900	13.45310	10.85790	O	11.25500	22.10890	11.45440
H	8.20890	9.94090	14.52190	O	11.25500	22.03320	14.19360
O	0.00000	20.78010	7.79040	O	9.00400	18.13420	14.19360
O	0.00000	18.20990	11.45440	O	9.00400	20.85580	10.52960
O	2.25100	16.88110	7.79040	H	9.00400	20.77070	8.74670
O	2.25100	22.10890	11.45440	H	9.00400	19.77810	7.46210
O	2.25100	22.03320	14.19360	H	9.00400	18.21930	12.41070
O	0.00000	18.13420	14.19360	H	9.00400	19.21190	11.12610
H	0.00000	20.77070	8.74670	H	11.25500	16.87170	8.74670
H	0.00000	19.77810	7.46210	H	11.25500	15.87910	7.46210
H	0.00000	18.21930	12.41070	H	11.25500	22.11830	12.41070
H	0.00000	19.21190	11.12610	H	11.25500	23.11090	11.12610
H	2.25100	16.87170	8.74670	H	12.05000	21.63790	14.52190
H	2.25100	15.87910	7.46210	H	10.45990	21.63790	14.52190
H	2.25100	22.11830	12.41070	H	9.79900	17.73890	14.52190
H	2.25100	23.11090	11.12610	H	8.20890	21.25110	10.85790
H	3.04600	21.63790	14.52190	H	9.79900	21.25110	10.85790
H	1.45600	21.63790	14.52190	H	8.20890	17.73890	14.52190
H	0.79500	17.73890	14.52190	O	0.00000	5.18410	15.11840
H	-0.79500	17.73890	14.52190	O	0.00000	2.61390	18.78240
O	4.50200	20.78010	7.79040	O	2.25100	1.28510	15.11840
O	4.50200	18.20990	11.45440	O	2.25100	6.51290	18.78240
O	6.75300	16.88110	7.79040	O	2.25100	6.43720	21.52160
O	6.75300	22.10890	11.45440	O	2.25100	1.36080	17.85760
O	6.75300	22.03320	14.19360	O	0.00000	2.53820	21.52160
O	6.75300	16.95680	10.52960	O	0.00000	5.25980	17.85760
O	4.50200	18.13420	14.19360	H	0.00000	5.17470	16.07470
H	4.50200	20.77070	8.74670	H	0.00000	4.18210	14.79010
H	4.50200	19.77810	7.46210	H	0.00000	2.62330	19.73870
H	4.50200	18.21930	12.41070	H	0.00000	3.61590	18.45410
H	4.50200	19.21190	11.12610	H	2.25100	1.27570	16.07470

H	2.25100	0.28310	14.79010	H	9.00400	4.18210	14.79010
H	2.25100	6.52230	19.73870	H	9.00400	2.62330	19.73870
H	2.25100	7.51490	18.45410	H	9.00400	3.61590	18.45410
H	3.04600	6.04190	21.84990	H	11.25500	1.27570	16.07470
H	1.45600	1.75610	18.18590	H	11.25500	0.28310	14.79010
H	3.04600	1.75610	18.18590	H	11.25500	6.52230	19.73870
H	1.45600	6.04190	21.84990	H	11.25500	7.51490	18.45410
H	0.79500	2.14290	21.84990	H	12.05000	6.04190	21.84990
H	-0.79500	5.65510	18.18590	H	10.45990	1.75610	18.18590
H	0.79500	5.65510	18.18590	H	12.05000	1.75610	18.18590
H	-0.79500	2.14290	21.84990	H	10.45990	6.04190	21.84990
O	4.50200	5.18410	15.11840	H	9.79900	2.14290	21.84990
O	4.50200	2.61390	18.78240	H	8.20890	5.65510	18.18590
O	6.75300	1.28510	15.11840	H	9.79900	5.65510	18.18590
O	6.75300	6.51290	18.78240	H	8.20890	2.14290	21.84990
O	6.75300	6.43720	21.52160	O	0.00000	12.98210	15.11840
O	6.75300	1.36080	17.85760	O	0.00000	10.41190	18.78240
O	4.50200	2.53820	21.52160	O	2.25100	9.08310	15.11840
O	4.50200	5.25980	17.85760	O	2.25100	14.31090	18.78240
H	4.50200	5.17470	16.07470	O	2.25100	14.23520	21.52160
H	4.50200	4.18210	14.79010	O	2.25100	9.15880	17.85760
H	4.50200	2.62330	19.73870	O	0.00000	10.33620	21.52160
H	4.50200	3.61590	18.45410	O	0.00000	13.05780	17.85760
H	6.75300	1.27570	16.07470	H	0.00000	12.97270	16.07470
H	6.75300	0.28310	14.79010	H	0.00000	11.98010	14.79010
H	6.75300	6.52230	19.73870	H	0.00000	10.42130	19.73870
H	6.75300	7.51490	18.45410	H	0.00000	11.41390	18.45410
H	7.54800	6.04190	21.84990	H	2.25100	9.07370	16.07470
H	5.95790	1.75610	18.18590	H	2.25100	8.08110	14.79010
H	7.54800	1.75610	18.18590	H	2.25100	14.32030	19.73870
H	5.95790	6.04190	21.84990	H	2.25100	15.31290	18.45410
H	5.29700	2.14290	21.84990	H	3.04600	13.83990	21.84990
H	3.70690	5.65510	18.18590	H	1.45600	9.55410	18.18590
H	5.29700	5.65510	18.18590	H	3.04600	9.55410	18.18590
H	3.70690	2.14290	21.84990	H	1.45600	13.83990	21.84990
O	9.00400	5.18410	15.11840	H	0.79500	9.94090	21.84990
O	9.00400	2.61390	18.78240	H	-0.79500	13.45310	18.18590
O	11.25500	1.28510	15.11840	H	0.79500	13.45310	18.18590
O	11.25500	6.51290	18.78240	H	-0.79500	9.94090	21.84990
O	11.25500	6.43720	21.52160	O	4.50200	12.98210	15.11840
O	11.25500	1.36080	17.85760	O	4.50200	10.41190	18.78240
O	9.00400	2.53820	21.52160	O	6.75300	9.08310	15.11840
O	9.00400	5.25980	17.85760	O	6.75300	14.31090	18.78240
H	9.00400	5.17470	16.07470	O	6.75300	14.23520	21.52160

O	6.75300	9.15880	17.85760	O	0.00000	18.20990	18.78240
O	4.50200	10.33620	21.52160	O	2.25100	16.88110	15.11840
O	4.50200	13.05780	17.85760	O	2.25100	22.10890	18.78240
H	4.50200	12.97270	16.07470	O	2.25100	22.03320	21.52160
H	4.50200	11.98010	14.79010	O	2.25100	16.95680	17.85760
H	4.50200	10.42130	19.73870	O	0.00000	18.13420	21.52160
H	4.50200	11.41390	18.45410	O	0.00000	20.85580	17.85760
H	6.75300	9.07370	16.07470	H	0.00000	20.77070	16.07470
H	6.75300	8.08110	14.79010	H	0.00000	19.77810	14.79010
H	6.75300	14.32030	19.73870	H	0.00000	18.21930	19.73870
H	6.75300	15.31290	18.45410	H	0.00000	19.21190	18.45410
H	7.54800	13.83990	21.84990	H	2.25100	16.87170	16.07470
H	5.95790	9.55410	18.18590	H	2.25100	15.87910	14.79010
H	7.54800	9.55410	18.18590	H	2.25100	22.11830	19.73870
H	5.95790	13.83990	21.84990	H	2.25100	23.11090	18.45410
H	5.29700	9.94090	21.84990	H	3.04600	21.63790	21.84990
H	3.70690	13.45310	18.18590	H	1.45600	17.35210	18.18590
H	5.29700	13.45310	18.18590	H	3.04600	17.35210	18.18590
H	3.70690	9.94090	21.84990	H	1.45600	21.63790	21.84990
O	9.00400	12.98210	15.11840	H	0.79500	17.73890	21.84990
O	9.00400	10.41190	18.78240	H	-0.79500	21.25110	18.18590
O	11.25500	9.08310	15.11840	H	0.79500	21.25110	18.18590
O	11.25500	14.31090	18.78240	H	-0.79500	17.73890	21.84990
O	11.25500	14.23520	21.52160	O	4.50200	20.78010	15.11840
O	11.25500	9.15880	17.85760	O	4.50200	18.20990	18.78240
O	9.00400	10.33620	21.52160	O	6.75300	16.88110	15.11840
O	9.00400	13.05780	17.85760	O	6.75300	22.10890	18.78240
H	9.00400	12.97270	16.07470	O	6.75300	22.03320	21.52160
H	9.00400	11.98010	14.79010	O	6.75300	16.95680	17.85760
H	9.00400	10.42130	19.73870	O	4.50200	18.13420	21.52160
H	9.00400	11.41390	18.45410	O	4.50200	20.85580	17.85760
H	11.25500	9.07370	16.07470	H	4.50200	20.77070	16.07470
H	11.25500	8.08110	14.79010	H	4.50200	19.77810	14.79010
H	11.25500	14.32030	19.73870	H	4.50200	18.21930	19.73870
H	11.25500	15.31290	18.45410	H	4.50200	19.21190	18.45410
H	12.05000	13.83990	21.84990	H	6.75300	16.87170	16.07470
H	10.45990	9.55410	18.18590	H	6.75300	15.87910	14.79010
H	12.05000	9.55410	18.18590	H	6.75300	22.11830	19.73870
H	10.45990	13.83990	21.84990	H	6.75300	23.11090	18.45410
H	9.79900	9.94090	21.84990	H	7.54800	21.63790	21.84990
H	8.20890	13.45310	18.18590	H	5.95790	17.35210	18.18590
H	9.79900	13.45310	18.18590	H	7.54800	17.35210	18.18590
H	8.20890	9.94090	21.84990	H	5.95790	21.63790	21.84990
O	0.00000	20.78010	15.11840	H	5.29700	17.73890	21.84990

H	3.70690	21.25110	18.18590	H	2.25100	29.91630	5.08270
H	5.29700	21.25110	18.18590	H	2.25100	30.90890	3.79810
H	3.70690	17.73890	21.84990	O	6.75300	6.51290	4.12640
O	9.00400	20.78010	15.11840	O	6.75300	6.43720	6.86560
O	9.00400	18.20990	18.78240	O	4.50200	5.25980	3.20160
O	11.25500	16.88110	15.11840	H	6.75300	6.52230	5.08270
O	11.25500	22.10890	18.78240	H	6.75300	7.51490	3.79810
O	11.25500	22.03320	21.52160	H	7.54800	6.04190	7.19390
O	11.25500	16.95680	17.85760	H	5.95790	6.04190	7.19390
O	9.00400	18.13420	21.52160	H	3.70690	5.65510	3.52990
O	9.00400	20.85580	17.85760	H	5.29700	5.65510	3.52990
H	9.00400	20.77070	16.07470	O	11.25500	6.51290	4.12640
H	9.00400	19.77810	14.79010	O	11.25500	6.43720	6.86560
H	9.00400	18.21930	19.73870	O	9.00400	5.25980	3.20160
H	9.00400	19.21190	18.45410	H	11.25500	6.52230	5.08270
H	11.25500	16.87170	16.07470	H	11.25500	7.51490	3.79810
H	11.25500	15.87910	14.79010	H	12.05000	6.04190	7.19390
H	11.25500	22.11830	19.73870	H	10.45990	6.04190	7.19390
H	11.25500	23.11090	18.45410	H	8.20890	5.65510	3.52990
H	12.05000	21.63790	21.84990	H	9.79900	5.65510	3.52990
H	10.45990	17.35210	18.18590	O	13.50600	5.25980	3.20160
H	12.05000	17.35210	18.18590	H	12.71090	5.65510	3.52990
H	10.45990	21.63790	21.84990	H	14.30100	5.65510	3.52990
H	9.79900	17.73890	21.84990	O	0.00000	10.41190	4.12640
H	8.20890	21.25110	18.18590	O	2.25100	14.31090	4.12640
H	9.79900	21.25110	18.18590	O	2.25100	14.23520	6.86560
H	8.20890	17.73890	21.84990	O	2.25100	9.15880	3.20160
				O	0.00000	10.33620	6.86560
				O	0.00000	13.05780	3.20160
				H	0.00000	10.42130	5.08270
				H	0.00000	11.41390	3.79810
				H	2.25100	14.32030	5.08270
				H	2.25100	15.31290	3.79810
				H	3.04610	13.83990	7.19390
				H	1.45590	9.55410	3.52990
				H	3.04610	9.55410	3.52990
				H	1.45590	13.83990	7.19390
				H	0.79510	9.94090	7.19390
				H	-0.79500	13.45310	3.52990
				H	0.79510	13.45310	3.52990
				H	-0.79500	9.94090	7.19390
				O	4.50200	10.41190	4.12640
				O	6.75300	14.31090	4.12640
				O	6.75300	14.23520	6.86560
5. (H <sub>2</sub> O) <sub>343</sub>							
O	2.25100	6.51290	4.12640				
O	2.25100	6.43720	6.86560				
O	0.00000	5.25980	3.20160				
H	2.25100	6.52230	5.08270				
H	2.25100	7.51490	3.79810				
H	3.04610	6.04190	7.19390				
H	1.45590	6.04190	7.19390				
H	-0.79500	5.65510	3.52990				
H	0.79510	5.65510	3.52990				
O	0.00000	26.00790	4.12640				
O	2.25100	29.90690	4.12640				
H	0.00000	26.01730	5.08270				
H	0.00000	27.00990	3.79810				

O	6.75300	9.15880	3.20160	O	2.25100	22.03320	6.86560
O	4.50200	10.33620	6.86560	O	2.25100	16.95680	3.20160
O	4.50200	13.05780	3.20160	O	0.00000	18.13420	6.86560
H	4.50200	10.42130	5.08270	O	0.00000	20.85580	3.20160
H	4.50200	11.41390	3.79810	H	0.00000	18.21930	5.08270
H	6.75300	14.32030	5.08270	H	0.00000	19.21190	3.79810
H	6.75300	15.31290	3.79810	H	2.25100	22.11830	5.08270
H	7.54800	13.83990	7.19390	H	2.25100	23.11090	3.79810
H	5.95790	9.55410	3.52990	H	3.04610	21.63790	7.19390
H	7.54800	9.55410	3.52990	H	1.45590	17.35210	3.52990
H	5.95790	13.83990	7.19390	H	3.04610	17.35210	3.52990
H	5.29700	9.94090	7.19390	H	1.45590	21.63790	7.19390
H	3.70690	13.45310	3.52990	H	0.79510	17.73890	7.19390
H	5.29700	13.45310	3.52990	H	-0.79500	21.25110	3.52990
H	3.70690	9.94090	7.19390	H	0.79510	21.25110	3.52990
O	9.00400	10.41190	4.12640	H	-0.79500	17.73890	7.19390
O	11.25500	14.31090	4.12640	O	4.50200	18.20990	4.12640
O	11.25500	14.23520	6.86560	O	6.75300	22.10890	4.12640
O	11.25500	9.15880	3.20160	O	6.75300	22.03320	6.86560
O	9.00400	10.33620	6.86560	O	6.75300	16.95680	3.20160
O	9.00400	13.05780	3.20160	O	4.50200	18.13420	6.86560
H	9.00400	10.42130	5.08270	O	4.50200	20.85580	3.20160
H	9.00400	11.41390	3.79810	H	4.50200	18.21930	5.08270
H	11.25500	14.32030	5.08270	H	4.50200	19.21190	3.79810
H	11.25500	15.31290	3.79810	H	6.75300	22.11830	5.08270
H	12.05000	13.83990	7.19390	H	6.75300	23.11090	3.79810
H	10.45990	9.55410	3.52990	H	7.54800	21.63790	7.19390
H	12.05000	9.55410	3.52990	H	5.95790	17.35210	3.52990
H	10.45990	13.83990	7.19390	H	7.54800	17.35210	3.52990
H	9.79900	9.94090	7.19390	H	5.95790	21.63790	7.19390
H	8.20890	13.45310	3.52990	H	5.29700	17.73890	7.19390
H	9.79900	13.45310	3.52990	H	3.70690	21.25110	3.52990
H	8.20890	9.94090	7.19390	H	5.29700	21.25110	3.52990
O	13.50600	10.41190	4.12640	H	3.70690	17.73890	7.19390
O	13.50600	10.33620	6.86560	O	9.00400	18.20990	4.12640
O	13.50600	13.05780	3.20160	O	11.25500	22.10890	4.12640
H	13.50600	10.42130	5.08270	O	11.25500	22.03320	6.86560
H	13.50600	11.41390	3.79810	O	11.25500	16.95680	3.20160
H	14.30100	9.94090	7.19390	O	9.00400	18.13420	6.86560
H	12.71090	13.45310	3.52990	O	9.00400	20.85580	3.20160
H	14.30100	13.45310	3.52990	H	9.00400	18.21930	5.08270
H	12.71090	9.94090	7.19390	H	9.00400	19.21190	3.79810
O	0.00000	18.20990	4.12640	H	11.25500	22.11830	5.08270
O	2.25100	22.10890	4.12640	H	11.25500	23.11090	3.79810

H	12.05000	21.63790	7.19390	H	3.70690	29.04910	3.52990
H	10.45990	17.35210	3.52990	H	5.29700	29.04910	3.52990
H	12.05000	17.35210	3.52990	H	3.70690	25.53690	7.19390
H	10.45990	21.63790	7.19390	O	9.00400	26.00790	4.12640
H	9.79900	17.73890	7.19390	O	11.25500	29.90690	4.12640
H	8.20890	21.25110	3.52990	O	11.25500	29.83120	6.86560
H	9.79900	21.25110	3.52990	O	11.25500	24.75480	3.20160
H	8.20890	17.73890	7.19390	O	9.00400	25.93230	6.86560
O	13.50600	18.20990	4.12640	O	9.00400	28.65380	3.20160
O	13.50600	18.13420	6.86560	H	9.00400	26.01730	5.08270
O	13.50600	20.85580	3.20160	H	9.00400	27.00990	3.79810
H	13.50600	18.21930	5.08270	H	11.25500	29.91630	5.08270
H	13.50600	19.21190	3.79810	H	11.25500	30.90890	3.79810
H	14.30100	17.73890	7.19390	H	12.05000	29.43590	7.19390
H	12.71090	21.25110	3.52990	H	10.45990	25.15010	3.52990
H	14.30100	21.25110	3.52990	H	12.05000	25.15010	3.52990
H	12.71090	17.73890	7.19390	H	10.45990	29.43590	7.19390
O	2.25100	29.83120	6.86560	H	9.79900	25.53690	7.19390
O	2.25100	24.75480	3.20160	H	8.20890	29.04910	3.52990
O	0.00000	25.93230	6.86560	H	9.79900	29.04910	3.52990
O	0.00000	28.65380	3.20160	H	8.20890	25.53690	7.19390
H	3.04610	29.43590	7.19390	O	13.50600	26.00790	4.12640
H	1.45590	25.15010	3.52990	O	13.50600	25.93230	6.86560
H	3.04610	25.15010	3.52990	O	13.50600	28.65380	3.20160
H	1.45590	29.43590	7.19390	H	13.50600	26.01730	5.08270
H	0.79510	25.53690	7.19390	H	13.50600	27.00990	3.79810
H	-0.79500	29.04910	3.52990	H	14.30100	25.53690	7.19390
H	0.79510	29.04910	3.52990	H	12.71090	29.04910	3.52990
H	-0.79500	25.53690	7.19390	H	14.30100	29.04910	3.52990
O	4.50200	26.00790	4.12640	H	12.71090	25.53690	7.19390
O	6.75300	29.90690	4.12640	O	2.25100	24.75480	10.52960
O	6.75300	29.83120	6.86560	O	0.00000	28.65380	10.52960
O	6.75300	24.75480	3.20160	H	3.04610	25.15010	10.85790
O	4.50200	25.93230	6.86560	H	-0.79500	29.04910	10.85790
O	4.50200	28.65380	3.20160	H	0.79510	29.04910	10.85790
H	4.50200	26.01730	5.08270	O	4.50200	28.65380	10.52960
H	4.50200	27.00990	3.79810	H	5.29700	29.04910	10.85790
H	6.75300	29.91630	5.08270	O	0.00000	5.18410	7.79040
H	6.75300	30.90890	3.79810	O	2.25100	6.51290	11.45440
H	7.54800	29.43590	7.19390	O	2.25100	6.43720	14.19360
H	5.95790	25.15010	3.52990	O	0.00000	5.25980	10.52960
H	7.54800	25.15010	3.52990	H	0.00000	5.17470	8.74670
H	5.95790	29.43590	7.19390	H	0.00000	4.18210	7.46210
H	5.29700	25.53690	7.19390	H	2.25100	6.52230	12.41070

H	2.25100	7.51490	11.12610	H	0.00000	11.98010	7.46210
H	3.04610	6.04190	14.52190	H	0.00000	10.42130	12.41070
H	1.45590	6.04190	14.52190	H	0.00000	11.41390	11.12610
H	-0.79500	5.65510	10.85790	H	2.25100	9.07370	8.74670
H	0.79510	5.65510	10.85790	H	2.25100	8.08110	7.46210
O	4.50200	5.18410	7.79040	H	2.25100	14.32030	12.41070
O	6.75300	6.51290	11.45440	H	2.25100	15.31290	11.12610
O	6.75300	6.43720	14.19360	H	3.04610	13.83990	14.52190
O	4.50200	5.25980	10.52960	H	1.45590	9.55410	10.85790
H	4.50200	5.17470	8.74670	H	3.04610	9.55410	10.85790
H	4.50200	4.18210	7.46210	H	1.45590	13.83990	14.52190
H	6.75300	6.52230	12.41070	H	0.79510	9.94090	14.52190
H	6.75300	7.51490	11.12610	H	-0.79500	13.45310	10.85790
H	7.54800	6.04190	14.52190	H	0.79510	13.45310	10.85790
H	5.95790	6.04190	14.52190	H	-0.79500	9.94090	14.52190
H	3.70690	5.65510	10.85790	O	4.50200	12.98210	7.79040
H	5.29700	5.65510	10.85790	O	4.50200	10.41190	11.45440
O	9.00400	5.18410	7.79040	O	6.75300	9.08310	7.79040
O	11.25500	6.51290	11.45440	O	6.75300	14.31090	11.45440
O	11.25500	6.43720	14.19360	O	6.75300	14.23520	14.19360
O	9.00400	5.25980	10.52960	O	6.75300	9.15880	10.52960
H	9.00400	5.17470	8.74670	O	4.50200	10.33620	14.19360
H	9.00400	4.18210	7.46210	O	4.50200	13.05780	10.52960
H	11.25500	6.52230	12.41070	H	4.50200	12.97270	8.74670
H	11.25500	7.51490	11.12610	H	4.50200	11.98010	7.46210
H	12.05000	6.04190	14.52190	H	4.50200	10.42130	12.41070
H	10.45990	6.04190	14.52190	H	4.50200	11.41390	11.12610
H	8.20890	5.65510	10.85790	H	6.75300	9.07370	8.74670
H	9.79900	5.65510	10.85790	H	6.75300	8.08110	7.46210
O	13.50600	5.18410	7.79040	H	6.75300	14.32030	12.41070
O	13.50600	5.25980	10.52960	H	6.75300	15.31290	11.12610
H	13.50600	5.17470	8.74670	H	7.54800	13.83990	14.52190
H	13.50600	4.18210	7.46210	H	5.95790	9.55410	10.85790
H	12.71090	5.65510	10.85790	H	7.54800	9.55410	10.85790
H	14.30100	5.65510	10.85790	H	5.95790	13.83990	14.52190
O	0.00000	12.98210	7.79040	H	5.29700	9.94090	14.52190
O	0.00000	10.41190	11.45440	H	3.70690	13.45310	10.85790
O	2.25100	9.08310	7.79040	H	5.29700	13.45310	10.85790
O	2.25100	14.31090	11.45440	H	3.70690	9.94090	14.52190
O	2.25100	14.23520	14.19360	O	9.00400	12.98210	7.79040
O	2.25100	9.15880	10.52960	O	9.00400	10.41190	11.45440
O	0.00000	10.33620	14.19360	O	11.25500	9.08310	7.79040
O	0.00000	13.05780	10.52960	O	11.25500	14.31090	11.45440
H	0.00000	12.97270	8.74670	O	11.25500	14.23520	14.19360

O	11.25500	9.15880	10.52960	H	2.25100	15.87910	7.46210
O	9.00400	10.33620	14.19360	H	2.25100	22.11830	12.41070
O	9.00400	13.05780	10.52960	H	2.25100	23.11090	11.12610
H	9.00400	12.97270	8.74670	H	3.04610	21.63790	14.52190
H	9.00400	11.98010	7.46210	H	1.45590	17.35210	10.85790
H	9.00400	10.42130	12.41070	H	3.04610	17.35210	10.85790
H	9.00400	11.41390	11.12610	H	1.45590	21.63790	14.52190
H	11.25500	9.07370	8.74670	H	0.79510	17.73890	14.52190
H	11.25500	8.08110	7.46210	H	-0.79500	21.25110	10.85790
H	11.25500	14.32030	12.41070	H	0.79510	21.25110	10.85790
H	11.25500	15.31290	11.12610	H	-0.79500	17.73890	14.52190
H	12.05000	13.83990	14.52190	O	4.50200	20.78010	7.79040
H	10.45990	9.55410	10.85790	O	4.50200	18.20990	11.45440
H	12.05000	9.55410	10.85790	O	6.75300	16.88110	7.79040
H	10.45990	13.83990	14.52190	O	6.75300	22.10890	11.45440
H	9.79900	9.94090	14.52190	O	6.75300	22.03320	14.19360
H	8.20890	13.45310	10.85790	O	6.75300	16.95680	10.52960
H	9.79900	13.45310	10.85790	O	4.50200	18.13420	14.19360
H	8.20890	9.94090	14.52190	O	4.50200	20.85580	10.52960
O	13.50600	12.98210	7.79040	H	4.50200	20.77070	8.74670
O	13.50600	10.41190	11.45440	H	4.50200	19.77810	7.46210
O	13.50600	10.33620	14.19360	H	4.50200	18.21930	12.41070
O	13.50600	13.05780	10.52960	H	4.50200	19.21190	11.12610
H	13.50600	12.97270	8.74670	H	6.75300	16.87170	8.74670
H	13.50600	11.98010	7.46210	H	6.75300	15.87910	7.46210
H	13.50600	10.42130	12.41070	H	6.75300	22.11830	12.41070
H	13.50600	11.41390	11.12610	H	6.75300	23.11090	11.12610
H	14.30100	9.94090	14.52190	H	7.54800	21.63790	14.52190
H	12.71090	13.45310	10.85790	H	5.95790	17.35210	10.85790
H	14.30100	13.45310	10.85790	H	7.54800	17.35210	10.85790
H	12.71090	9.94090	14.52190	H	5.95790	21.63790	14.52190
O	0.00000	20.78010	7.79040	H	5.29700	17.73890	14.52190
O	0.00000	18.20990	11.45440	H	3.70690	21.25110	10.85790
O	2.25100	16.88110	7.79040	H	5.29700	21.25110	10.85790
O	2.25100	22.10890	11.45440	H	3.70690	17.73890	14.52190
O	2.25100	22.03320	14.19360	O	9.00400	20.78010	7.79040
O	2.25100	16.95680	10.52960	O	9.00400	18.20990	11.45440
O	0.00000	18.13420	14.19360	O	11.25500	16.88110	7.79040
O	0.00000	20.85580	10.52960	O	11.25500	22.10890	11.45440
H	0.00000	20.77070	8.74670	O	11.25500	22.03320	14.19360
H	0.00000	19.77810	7.46210	O	11.25500	16.95680	10.52960
H	0.00000	18.21930	12.41070	O	9.00400	18.13420	14.19360
H	0.00000	19.21190	11.12610	O	9.00400	20.85580	10.52960
H	2.25100	16.87170	8.74670	H	9.00400	20.77070	8.74670



H	9.00400	19.77810	7.46210	H	0.79510	25.53690	14.52190
H	9.00400	18.21930	12.41070	H	-0.79500	25.53690	14.52190
H	9.00400	19.21190	11.12610	O	4.50200	28.57810	7.79040
H	11.25500	16.87170	8.74670	O	4.50200	26.00790	11.45440
H	11.25500	15.87910	7.46210	O	6.75300	24.67910	7.79040
H	11.25500	22.11830	12.41070	O	6.75300	29.90690	11.45440
H	11.25500	23.11090	11.12610	O	6.75300	29.83120	14.19360
H	12.05000	21.63790	14.52190	O	6.75300	24.75480	10.52960
H	10.45990	17.35210	10.85790	O	4.50200	25.93230	14.19360
H	12.05000	17.35210	10.85790	H	4.50200	28.56870	8.74670
H	10.45990	21.63790	14.52190	H	4.50200	27.57610	7.46210
H	9.79900	17.73890	14.52190	H	4.50200	26.01730	12.41070
H	8.20890	21.25110	10.85790	H	4.50200	27.00990	11.12610
H	9.79900	21.25110	10.85790	H	6.75300	24.66980	8.74670
H	8.20890	17.73890	14.52190	H	6.75300	23.67710	7.46210
O	13.50600	20.78010	7.79040	H	6.75300	29.91630	12.41070
O	13.50600	18.20990	11.45440	H	6.75300	30.90890	11.12610
O	13.50600	18.13420	14.19360	H	7.54800	29.43590	14.52190
O	13.50600	20.85580	10.52960	H	5.95790	25.15010	10.85790
H	13.50600	20.77070	8.74670	H	7.54800	25.15010	10.85790
H	13.50600	19.77810	7.46210	H	5.95790	29.43590	14.52190
H	13.50600	18.21930	12.41070	H	5.29700	25.53690	14.52190
H	13.50600	19.21190	11.12610	H	3.70690	29.04910	10.85790
H	14.30100	17.73890	14.52190	H	3.70690	25.53690	14.52190
H	12.71090	21.25110	10.85790	O	9.00400	28.57810	7.79040
H	14.30100	21.25110	10.85790	O	9.00400	26.00790	11.45440
H	12.71090	17.73890	14.52190	O	11.25500	24.67910	7.79040
O	0.00000	28.57810	7.79040	O	11.25500	29.90690	11.45440
O	0.00000	26.00790	11.45440	O	11.25500	29.83120	14.19360
O	2.25100	24.67910	7.79040	O	11.25500	24.75480	10.52960
O	2.25100	29.90690	11.45440	O	9.00400	25.93230	14.19360
O	2.25100	29.83120	14.19360	O	9.00400	28.65380	10.52960
O	0.00000	25.93230	14.19360	H	9.00400	28.56870	8.74670
H	0.00000	28.56870	8.74670	H	9.00400	27.57610	7.46210
H	0.00000	27.57610	7.46210	H	9.00400	26.01730	12.41070
H	0.00000	26.01730	12.41070	H	9.00400	27.00990	11.12610
H	0.00000	27.00990	11.12610	H	11.25500	24.66980	8.74670
H	2.25100	24.66980	8.74670	H	11.25500	23.67710	7.46210
H	2.25100	23.67710	7.46210	H	11.25500	29.91630	12.41070
H	2.25100	29.91630	12.41070	H	11.25500	30.90890	11.12610
H	2.25100	30.90890	11.12610	H	12.05000	29.43590	14.52190
H	3.04610	29.43590	14.52190	H	10.45990	25.15010	10.85790
H	1.45590	25.15010	10.85790	H	12.05000	25.15010	10.85790
H	1.45590	29.43590	14.52190	H	10.45990	29.43590	14.52190

H	9.79900	25.53690	14.52190	H	9.00400	5.17470	16.07470
H	8.20890	29.04910	10.85790	H	9.00400	4.18210	14.79010
H	9.79900	29.04910	10.85790	H	11.25500	6.52230	19.73870
H	8.20890	25.53690	14.52190	H	11.25500	7.51490	18.45410
O	13.50600	28.57810	7.79040	H	12.05000	6.04190	21.84990
O	13.50600	26.00790	11.45440	H	10.45990	6.04190	21.84990
O	13.50600	25.93230	14.19360	H	8.20890	5.65510	18.18590
O	13.50600	28.65380	10.52960	H	9.79900	5.65510	18.18590
H	13.50600	28.56870	8.74670	O	13.50600	5.18410	15.11840
H	13.50600	27.57610	7.46210	O	13.50600	5.25980	17.85760
H	13.50600	26.01730	12.41070	H	13.50600	5.17470	16.07470
H	13.50600	27.00990	11.12610	H	13.50600	4.18210	14.79010
H	14.30100	25.53690	14.52190	H	12.71090	5.65510	18.18590
H	12.71090	29.04910	10.85790	H	14.30100	5.65510	18.18590
H	14.30100	29.04910	10.85790	O	0.00000	12.98210	15.11840
H	12.71090	25.53690	14.52190	O	0.00000	10.41190	18.78240
O	0.00000	5.18410	15.11840	O	2.25100	9.08310	15.11840
O	2.25100	6.51290	18.78240	O	2.25100	14.31090	18.78240
O	2.25100	6.43720	21.52160	O	2.25100	14.23520	21.52160
O	0.00000	5.25980	17.85760	O	2.25100	9.15880	17.85760
H	0.00000	5.17470	16.07470	O	0.00000	10.33620	21.52160
H	0.00000	4.18210	14.79010	O	0.00000	13.05780	17.85760
H	2.25100	6.52230	19.73870	H	0.00000	12.97270	16.07470
H	2.25100	7.51490	18.45410	H	0.00000	11.98010	14.79010
H	3.04610	6.04190	21.84990	H	0.00000	10.42130	19.73870
H	1.45590	6.04190	21.84990	H	0.00000	11.41390	18.45410
H	-0.79500	5.65510	18.18590	H	2.25100	9.07370	16.07470
H	0.79510	5.65510	18.18590	H	2.25100	8.08110	14.79010
O	4.50200	5.18410	15.11840	H	2.25100	14.32030	19.73870
O	6.75300	6.51290	18.78240	H	2.25100	15.31290	18.45410
O	6.75300	6.43720	21.52160	H	3.04610	13.83990	21.84990
O	4.50200	5.25980	17.85760	H	1.45590	9.55410	18.18590
H	4.50200	5.17470	16.07470	H	3.04610	9.55410	18.18590
H	4.50200	4.18210	14.79010	H	1.45590	13.83990	21.84990
H	6.75300	6.52230	19.73870	H	0.79510	9.94090	21.84990
H	6.75300	7.51490	18.45410	H	-0.79500	13.45310	18.18590
H	7.54800	6.04190	21.84990	H	0.79510	13.45310	18.18590
H	5.95790	6.04190	21.84990	H	-0.79500	9.94090	21.84990
H	3.70690	5.65510	18.18590	O	4.50200	12.98210	15.11840
H	5.29700	5.65510	18.18590	O	4.50200	10.41190	18.78240
O	9.00400	5.18410	15.11840	O	6.75300	9.08310	15.11840
O	11.25500	6.51290	18.78240	O	6.75300	14.31090	18.78240
O	11.25500	6.43720	21.52160	O	6.75300	14.23520	21.52160
O	9.00400	5.25980	17.85760	O	6.75300	9.15880	17.85760

O	4.50200	10.33620	21.52160	O	13.50600	10.33620	21.52160
O	4.50200	13.05780	17.85760	O	13.50600	13.05780	17.85760
H	4.50200	12.97270	16.07470	H	13.50600	12.97270	16.07470
H	4.50200	11.98010	14.79010	H	13.50600	11.98010	14.79010
H	4.50200	10.42130	19.73870	H	13.50600	10.42130	19.73870
H	4.50200	11.41390	18.45410	H	13.50600	11.41390	18.45410
H	6.75300	9.07370	16.07470	H	14.30100	9.94090	21.84990
H	6.75300	8.08110	14.79010	H	12.71090	13.45310	18.18590
H	6.75300	14.32030	19.73870	H	14.30100	13.45310	18.18590
H	6.75300	15.31290	18.45410	H	12.71090	9.94090	21.84990
H	7.54800	13.83990	21.84990	O	0.00000	20.78010	15.11840
H	5.95790	9.55410	18.18590	O	0.00000	18.20990	18.78240
H	7.54800	9.55410	18.18590	O	2.25100	16.88110	15.11840
H	5.95790	13.83990	21.84990	O	2.25100	22.10890	18.78240
H	5.29700	9.94090	21.84990	O	2.25100	22.03320	21.52160
H	3.70690	13.45310	18.18590	O	2.25100	16.95680	17.85760
H	5.29700	13.45310	18.18590	O	0.00000	18.13420	21.52160
H	3.70690	9.94090	21.84990	O	0.00000	20.85580	17.85760
O	9.00400	12.98210	15.11840	H	0.00000	20.77070	16.07470
O	9.00400	10.41190	18.78240	H	0.00000	19.77810	14.79010
O	11.25500	9.08310	15.11840	H	0.00000	18.21930	19.73870
O	11.25500	14.31090	18.78240	H	0.00000	19.21190	18.45410
O	11.25500	14.23520	21.52160	H	2.25100	16.87170	16.07470
O	11.25500	9.15880	17.85760	H	2.25100	15.87910	14.79010
O	9.00400	10.33620	21.52160	H	2.25100	22.11830	19.73870
O	9.00400	13.05780	17.85760	H	2.25100	23.11090	18.45410
H	9.00400	12.97270	16.07470	H	3.04610	21.63790	21.84990
H	9.00400	11.98010	14.79010	H	1.45590	17.35210	18.18590
H	9.00400	10.42130	19.73870	H	3.04610	17.35210	18.18590
H	9.00400	11.41390	18.45410	H	1.45590	21.63790	21.84990
H	11.25500	9.07370	16.07470	H	0.79510	17.73890	21.84990
H	11.25500	8.08110	14.79010	H	-0.79500	21.25110	18.18590
H	11.25500	14.32030	19.73870	H	0.79510	21.25110	18.18590
H	11.25500	15.31290	18.45410	H	-0.79500	17.73890	21.84990
H	12.05000	13.83990	21.84990	O	4.50200	20.78010	15.11840
H	10.45990	9.55410	18.18590	O	4.50200	18.20990	18.78240
H	12.05000	9.55410	18.18590	O	6.75300	16.88110	15.11840
H	10.45990	13.83990	21.84990	O	6.75300	22.10890	18.78240
H	9.79900	9.94090	21.84990	O	6.75300	22.03320	21.52160
H	8.20890	13.45310	18.18590	O	6.75300	16.95680	17.85760
H	9.79900	13.45310	18.18590	O	4.50200	18.13420	21.52160
H	8.20890	9.94090	21.84990	O	4.50200	20.85580	17.85760
O	13.50600	12.98210	15.11840	H	4.50200	20.77070	16.07470
O	13.50600	10.41190	18.78240	H	4.50200	19.77810	14.79010

H	4.50200	18.21930	19.73870	H	13.50600	18.21930	19.73870
H	4.50200	19.21190	18.45410	H	13.50600	19.21190	18.45410
H	6.75300	16.87170	16.07470	H	14.30100	17.73890	21.84990
H	6.75300	15.87910	14.79010	H	12.71090	21.25110	18.18590
H	6.75300	22.11830	19.73870	H	14.30100	21.25110	18.18590
H	6.75300	23.11090	18.45410	H	12.71090	17.73890	21.84990
H	7.54800	21.63790	21.84990	O	0.00000	28.57810	15.11840
H	5.95790	17.35210	18.18590	O	0.00000	26.00790	18.78240
H	7.54800	17.35210	18.18590	O	2.25100	24.67910	15.11840
H	5.95790	21.63790	21.84990	O	2.25100	29.90690	18.78240
H	5.29700	17.73890	21.84990	O	2.25100	29.83120	21.52160
H	3.70690	21.25110	18.18590	O	2.25100	24.75480	17.85760
H	5.29700	21.25110	18.18590	O	0.00000	25.93230	21.52160
H	3.70690	17.73890	21.84990	O	0.00000	28.65380	17.85760
O	9.00400	20.78010	15.11840	H	0.00000	28.56870	16.07470
O	9.00400	18.20990	18.78240	H	0.00000	27.57610	14.79010
O	11.25500	16.88110	15.11840	H	0.00000	26.01730	19.73870
O	11.25500	22.10890	18.78240	H	0.00000	27.00990	18.45410
O	11.25500	22.03320	21.52160	H	2.25100	24.66980	16.07470
O	11.25500	16.95680	17.85760	H	2.25100	23.67710	14.79010
O	9.00400	18.13420	21.52160	H	2.25100	29.91630	19.73870
O	9.00400	20.85580	17.85760	H	2.25100	30.90890	18.45410
H	9.00400	20.77070	16.07470	H	3.04610	29.43590	21.84990
H	9.00400	19.77810	14.79010	H	1.45590	25.15010	18.18590
H	9.00400	18.21930	19.73870	H	3.04610	25.15010	18.18590
H	9.00400	19.21190	18.45410	H	1.45590	29.43590	21.84990
H	11.25500	16.87170	16.07470	H	0.79510	25.53690	21.84990
H	11.25500	15.87910	14.79010	H	-0.79500	29.04910	18.18590
H	11.25500	22.11830	19.73870	H	0.79510	29.04910	18.18590
H	11.25500	23.11090	18.45410	H	-0.79500	25.53690	21.84990
H	12.05000	21.63790	21.84990	O	4.50200	28.57810	15.11840
H	10.45990	17.35210	18.18590	O	4.50200	26.00790	18.78240
H	12.05000	17.35210	18.18590	O	6.75300	24.67910	15.11840
H	10.45990	21.63790	21.84990	O	6.75300	29.90690	18.78240
H	9.79900	17.73890	21.84990	O	6.75300	29.83120	21.52160
H	8.20890	21.25110	18.18590	O	6.75300	24.75480	17.85760
H	9.79900	21.25110	18.18590	O	4.50200	25.93230	21.52160
H	8.20890	17.73890	21.84990	O	4.50200	28.65380	17.85760
O	13.50600	20.78010	15.11840	H	4.50200	28.56870	16.07470
O	13.50600	18.20990	18.78240	H	4.50200	27.57610	14.79010
O	13.50600	18.13420	21.52160	H	4.50200	26.01730	19.73870
O	13.50600	20.85580	17.85760	H	4.50200	27.00990	18.45410
H	13.50600	20.77070	16.07470	H	6.75300	24.66980	16.07470
H	13.50600	19.77810	14.79010	H	6.75300	23.67710	14.79010

H	6.75300	29.91630	19.73870	H	14.30100	29.04910	18.18590
H	6.75300	30.90890	18.45410	H	12.71090	25.53690	21.84990
H	7.54800	29.43590	21.84990	O	0.00000	5.18410	22.44640
H	5.95790	25.15010	18.18590	O	2.25100	6.51290	26.11040
H	7.54800	25.15010	18.18590	O	0.00000	5.25980	25.18560
H	5.95790	29.43590	21.84990	H	0.00000	5.17470	23.40270
H	5.29700	25.53690	21.84990	H	0.00000	4.18210	22.11810
H	3.70690	29.04910	18.18590	H	2.25100	6.52230	27.06670
H	5.29700	29.04910	18.18590	H	2.25100	7.51490	25.78210
H	3.70690	25.53690	21.84990	H	-0.79500	5.65510	25.51390
O	9.00400	28.57810	15.11840	H	0.79510	5.65510	25.51390
O	9.00400	26.00790	18.78240	O	4.50200	5.18410	22.44640
O	11.25500	24.67910	15.11840	O	6.75300	6.51290	26.11040
O	11.25500	29.90690	18.78240	O	4.50200	5.25980	25.18560
O	11.25500	29.83120	21.52160	H	4.50200	5.17470	23.40270
O	11.25500	24.75480	17.85760	H	4.50200	4.18210	22.11810
O	9.00400	25.93230	21.52160	H	6.75300	6.52230	27.06670
O	9.00400	28.65380	17.85760	H	6.75300	7.51490	25.78210
H	9.00400	28.56870	16.07470	H	3.70690	5.65510	25.51390
H	9.00400	27.57610	14.79010	H	5.29700	5.65510	25.51390
H	9.00400	26.01730	19.73870	O	9.00400	5.18410	22.44640
H	9.00400	27.00990	18.45410	O	11.25500	6.51290	26.11040
H	11.25500	24.66980	16.07470	O	9.00400	5.25980	25.18560
H	11.25500	23.67710	14.79010	H	9.00400	5.17470	23.40270
H	11.25500	29.91630	19.73870	H	9.00400	4.18210	22.11810
H	11.25500	30.90890	18.45410	H	11.25500	6.52230	27.06670
H	12.05000	29.43590	21.84990	H	11.25500	7.51490	25.78210
H	10.45990	25.15010	18.18590	H	8.20890	5.65510	25.51390
H	12.05000	25.15010	18.18590	H	9.79900	5.65510	25.51390
H	10.45990	29.43590	21.84990	O	13.50600	5.18410	22.44640
H	9.79900	25.53690	21.84990	O	13.50600	5.25980	25.18560
H	8.20890	29.04910	18.18590	H	13.50600	5.17470	23.40270
H	9.79900	29.04910	18.18590	H	13.50600	4.18210	22.11810
H	8.20890	25.53690	21.84990	H	12.71090	5.65510	25.51390
O	13.50600	28.57810	15.11840	H	14.30100	5.65510	25.51390
O	13.50600	26.00790	18.78240	O	0.00000	12.98210	22.44640
O	13.50600	25.93230	21.52160	O	0.00000	10.41190	26.11040
O	13.50600	28.65380	17.85760	O	2.25100	9.08310	22.44640
H	13.50600	28.56870	16.07470	O	2.25100	14.31090	26.11040
H	13.50600	27.57610	14.79010	O	2.25100	9.15880	25.18560
H	13.50600	26.01730	19.73870	O	0.00000	13.05780	25.18560
H	13.50600	27.00990	18.45410	H	0.00000	12.97270	23.40270
H	14.30100	25.53690	21.84990	H	0.00000	11.98010	22.11810
H	12.71090	29.04910	18.18590	H	0.00000	10.42130	27.06670

H	0.00000	11.41390	25.78210	H	9.79900	13.45310	25.51390
H	2.25100	9.07370	23.40270	O	13.50600	12.98210	22.44640
H	2.25100	8.08110	22.11810	O	13.50600	10.41190	26.11040
H	2.25100	14.32030	27.06670	O	13.50600	13.05780	25.18560
H	2.25100	15.31290	25.78210	H	13.50600	12.97270	23.40270
H	1.45590	9.55410	25.51390	H	13.50600	11.98010	22.11810
H	3.04610	9.55410	25.51390	H	13.50600	10.42130	27.06670
H	-0.79500	13.45310	25.51390	H	13.50600	11.41390	25.78210
H	0.79510	13.45310	25.51390	H	12.71090	13.45310	25.51390
O	4.50200	12.98210	22.44640	H	14.30100	13.45310	25.51390
O	4.50200	10.41190	26.11040	O	0.00000	20.78010	22.44640
O	6.75300	9.08310	22.44640	O	0.00000	18.20990	26.11040
O	6.75300	14.31090	26.11040	O	2.25100	16.88110	22.44640
O	6.75300	9.15880	25.18560	O	2.25100	22.10890	26.11040
O	4.50200	13.05780	25.18560	O	2.25100	16.95680	25.18560
H	4.50200	12.97270	23.40270	O	0.00000	20.85580	25.18560
H	4.50200	11.98010	22.11810	H	0.00000	20.77070	23.40270
H	4.50200	10.42130	27.06670	H	0.00000	19.77810	22.11810
H	4.50200	11.41390	25.78210	H	0.00000	18.21930	27.06670
H	6.75300	9.07370	23.40270	H	0.00000	19.21190	25.78210
H	6.75300	8.08110	22.11810	H	2.25100	16.87170	23.40270
H	6.75300	14.32030	27.06670	H	2.25100	15.87910	22.11810
H	6.75300	15.31290	25.78210	H	2.25100	22.11830	27.06670
H	5.95790	9.55410	25.51390	H	2.25100	23.11090	25.78210
H	7.54800	9.55410	25.51390	H	1.45590	17.35210	25.51390
H	3.70690	13.45310	25.51390	H	3.04610	17.35210	25.51390
H	5.29700	13.45310	25.51390	H	-0.79500	21.25110	25.51390
O	9.00400	12.98210	22.44640	H	0.79510	21.25110	25.51390
O	9.00400	10.41190	26.11040	O	4.50200	20.78010	22.44640
O	11.25500	9.08310	22.44640	O	4.50200	18.20990	26.11040
O	11.25500	14.31090	26.11040	O	6.75300	16.88110	22.44640
O	11.25500	9.15880	25.18560	O	6.75300	22.10890	26.11040
O	9.00400	13.05780	25.18560	O	6.75300	16.95680	25.18560
H	9.00400	12.97270	23.40270	O	4.50200	20.85580	25.18560
H	9.00400	11.98010	22.11810	H	4.50200	20.77070	23.40270
H	9.00400	10.42130	27.06670	H	4.50200	19.77810	22.11810
H	9.00400	11.41390	25.78210	H	4.50200	18.21930	27.06670
H	11.25500	9.07370	23.40270	H	4.50200	19.21190	25.78210
H	11.25500	8.08110	22.11810	H	6.75300	16.87170	23.40270
H	11.25500	14.32030	27.06670	H	6.75300	15.87910	22.11810
H	11.25500	15.31290	25.78210	H	6.75300	22.11830	27.06670
H	10.45990	9.55410	25.51390	H	6.75300	23.11090	25.78210
H	12.05000	9.55410	25.51390	H	5.95790	17.35210	25.51390
H	8.20890	13.45310	25.51390	H	7.54800	17.35210	25.51390

H	3.70690	21.25110	25.51390	H	3.04610	25.15010	25.51390
H	5.29700	21.25110	25.51390	H	-0.79500	29.04910	25.51390
O	9.00400	20.78010	22.44640	H	0.79510	29.04910	25.51390
O	9.00400	18.20990	26.11040	O	4.50200	28.57810	22.44640
O	11.25500	16.88110	22.44640	O	4.50200	26.00790	26.11040
O	11.25500	22.10890	26.11040	O	6.75300	24.67910	22.44640
O	11.25500	16.95680	25.18560	O	6.75300	29.90690	26.11040
O	9.00400	20.85580	25.18560	O	6.75300	24.75480	25.18560
H	9.00400	20.77070	23.40270	O	4.50200	28.65380	25.18560
H	9.00400	19.77810	22.11810	H	4.50200	28.56870	23.40270
H	9.00400	18.21930	27.06670	H	4.50200	27.57610	22.11810
H	9.00400	19.21190	25.78210	H	4.50200	26.01730	27.06670
H	11.25500	16.87170	23.40270	H	4.50200	27.00990	25.78210
H	11.25500	15.87910	22.11810	H	6.75300	24.66980	23.40270
H	11.25500	22.11830	27.06670	H	6.75300	23.67710	22.11810
H	11.25500	23.11090	25.78210	H	6.75300	29.91630	27.06670
H	10.45990	17.35210	25.51390	H	6.75300	30.90890	25.78210
H	12.05000	17.35210	25.51390	H	5.95790	25.15010	25.51390
H	8.20890	21.25110	25.51390	H	7.54800	25.15010	25.51390
H	9.79900	21.25110	25.51390	H	3.70690	29.04910	25.51390
O	13.50600	20.78010	22.44640	H	5.29700	29.04910	25.51390
O	13.50600	18.20990	26.11040	O	9.00400	28.57810	22.44640
O	13.50600	20.85580	25.18560	O	9.00400	26.00790	26.11040
H	13.50600	20.77070	23.40270	O	11.25500	24.67910	22.44640
H	13.50600	19.77810	22.11810	O	11.25500	29.90690	26.11040
H	13.50600	18.21930	27.06670	O	11.25500	24.75480	25.18560
H	13.50600	19.21190	25.78210	O	9.00400	28.65380	25.18560
H	12.71090	21.25110	25.51390	H	9.00400	28.56870	23.40270
H	14.30100	21.25110	25.51390	H	9.00400	27.57610	22.11810
O	0.00000	28.57810	22.44640	H	9.00400	26.01730	27.06670
O	0.00000	26.00790	26.11040	H	9.00400	27.00990	25.78210
O	2.25100	24.67910	22.44640	H	11.25500	24.66980	23.40270
O	2.25100	29.90690	26.11040	H	11.25500	23.67710	22.11810
O	2.25100	24.75480	25.18560	H	11.25500	29.91630	27.06670
O	0.00000	28.65380	25.18560	H	11.25500	30.90890	25.78210
H	0.00000	28.56870	23.40270	H	10.45990	25.15010	25.51390
H	0.00000	27.57610	22.11810	H	12.05000	25.15010	25.51390
H	0.00000	26.01730	27.06670	H	8.20890	29.04910	25.51390
H	0.00000	27.00990	25.78210	H	9.79900	29.04910	25.51390
H	2.25100	24.66980	23.40270	O	13.50600	28.57810	22.44640
H	2.25100	23.67710	22.11810	O	13.50600	26.00790	26.11040
H	2.25100	29.91630	27.06670	O	13.50600	28.65380	25.18560
H	2.25100	30.90890	25.78210	H	13.50600	28.56870	23.40270
H	1.45590	25.15010	25.51390	H	13.50600	27.57610	22.11810

H	13.50600	26.01730	27.06670	O	6.75300	6.43720	6.86560
H	13.50600	27.00990	25.78210	O	6.75300	1.36080	3.20160
H	12.71090	29.04910	25.51390	O	4.50200	2.53820	6.86560
H	14.30100	29.04910	25.51390	O	4.50200	5.25980	3.20160
				H	4.50200	5.17470	1.41870
				H	4.50200	4.18210	0.13410
				H	4.50200	2.62330	5.08270
				H	4.50200	3.61590	3.79810
				H	6.75300	1.27570	1.41870
				H	6.75300	0.28310	0.13410
				H	6.75300	6.52230	5.08270
				H	6.75300	7.51490	3.79810
				H	7.54800	6.04190	7.19390
				H	5.95790	1.75610	3.52990
				H	7.54800	1.75610	3.52990
				H	5.95790	6.04190	7.19390
				H	5.29700	2.14290	7.19390
				H	3.70690	5.65510	3.52990
				H	5.29700	5.65510	3.52990
				H	3.70690	2.14290	7.19390
				O	9.00400	5.18410	0.46240
				O	9.00400	2.61390	4.12640
				O	11.25500	1.28510	0.46240
				O	11.25500	6.51290	4.12640
				O	11.25500	6.43720	6.86560
				O	11.25500	1.36080	3.20160
				O	9.00400	2.53820	6.86560
				O	9.00400	5.25980	3.20160
				H	9.00400	5.17470	1.41870
				H	9.00400	4.18210	0.13410
				H	9.00400	2.62330	5.08270
				H	9.00400	3.61590	3.79810
				H	11.25500	1.27570	1.41870
				H	11.25500	0.28310	0.13410
				H	11.25500	6.52230	5.08270
				H	11.25500	7.51490	3.79810
				H	12.05000	6.04190	7.19390
				H	10.45990	1.75610	3.52990
				H	12.05000	1.75610	3.52990
				H	10.45990	6.04190	7.19390
				H	9.79900	2.14290	7.19390
				H	8.20890	5.65510	3.52990
				H	9.79900	5.65510	3.52990
				H	8.20890	2.14290	7.19390

6. (H<sub>2</sub>O)<sub>512</sub>

O	0.00000	5.18410	0.46240
O	0.00000	2.61390	4.12640
O	2.25100	1.28510	0.46240
O	2.25100	6.51290	4.12640
O	2.25100	6.43720	6.86560
O	2.25100	1.36080	3.20160
O	0.00000	2.53820	6.86560
O	0.00000	5.25980	3.20160
H	0.00000	5.17470	1.41870
H	0.00000	4.18210	0.13410
H	0.00000	2.62330	5.08270
H	0.00000	3.61590	3.79810
H	2.25100	1.27570	1.41870
H	2.25100	0.28310	0.13410
H	2.25100	6.52230	5.08270
H	2.25100	7.51490	3.79810
H	3.04610	6.04190	7.19390
H	1.45590	1.75610	3.52990
H	3.04610	1.75610	3.52990
H	1.45590	6.04190	7.19390
H	0.79510	2.14290	7.19390
H	-0.79500	5.65510	3.52990
H	0.79510	5.65510	3.52990
H	-0.79500	2.14290	7.19390
O	0.00000	26.00790	4.12640
O	2.25100	29.90690	4.12640
H	0.00000	26.01730	5.08270
H	0.00000	27.00990	3.79810
H	2.25100	29.91630	5.08270
H	2.25100	30.90890	3.79810
O	15.75700	6.43720	6.86560
H	14.96190	6.04190	7.19390
O	4.50200	5.18410	0.46240
O	4.50200	2.61390	4.12640
O	6.75300	1.28510	0.46240
O	6.75300	6.51290	4.12640



O	13.50600	5.18410	0.46240	H	0.79510	13.45310	3.52990
O	13.50600	2.61390	4.12640	H	-0.79500	9.94090	7.19390
O	15.75700	1.28510	0.46240	O	4.50200	12.98210	0.46240
O	15.75700	6.51290	4.12640	O	4.50200	10.41190	4.12640
O	15.75700	1.36080	3.20160	O	6.75300	9.08310	0.46240
O	13.50600	2.53820	6.86560	O	6.75300	14.31090	4.12640
O	13.50600	5.25980	3.20160	O	6.75300	14.23520	6.86560
H	13.50600	5.17470	1.41870	O	6.75300	9.15880	3.20160
H	13.50600	4.18210	0.13410	O	4.50200	10.33620	6.86560
H	13.50600	2.62330	5.08270	O	4.50200	13.05780	3.20160
H	13.50600	3.61590	3.79810	H	4.50200	12.97270	1.41870
H	15.75700	1.27570	1.41870	H	4.50200	11.98010	0.13410
H	15.75700	0.28310	0.13410	H	4.50200	10.42130	5.08270
H	15.75700	6.52230	5.08270	H	4.50200	11.41390	3.79810
H	15.75700	7.51490	3.79810	H	6.75300	9.07370	1.41870
H	16.55200	6.04190	7.19390	H	6.75300	8.08110	0.13410
H	14.96190	1.75610	3.52990	H	6.75300	14.32030	5.08270
H	16.55200	1.75610	3.52990	H	6.75300	15.31290	3.79810
H	14.30100	2.14290	7.19390	H	7.54800	13.83990	7.19390
H	12.71090	5.65510	3.52990	H	5.95790	9.55410	3.52990
H	14.30100	5.65510	3.52990	H	7.54800	9.55410	3.52990
H	12.71090	2.14290	7.19390	H	5.95790	13.83990	7.19390
O	0.00000	12.98210	0.46240	H	5.29700	9.94090	7.19390
O	0.00000	10.41190	4.12640	H	3.70690	13.45310	3.52990
O	2.25100	9.08310	0.46240	H	5.29700	13.45310	3.52990
O	2.25100	14.31090	4.12640	H	3.70690	9.94090	7.19390
O	2.25100	14.23520	6.86560	O	9.00400	12.98210	0.46240
O	2.25100	9.15880	3.20160	O	9.00400	10.41190	4.12640
O	0.00000	10.33620	6.86560	O	11.25500	9.08310	0.46240
O	0.00000	13.05780	3.20160	O	11.25500	14.31090	4.12640
H	0.00000	12.97270	1.41870	O	11.25500	14.23520	6.86560
H	0.00000	11.98010	0.13410	O	11.25500	9.15880	3.20160
H	0.00000	10.42130	5.08270	O	9.00400	10.33620	6.86560
H	0.00000	11.41390	3.79810	O	9.00400	13.05780	3.20160
H	2.25100	9.07370	1.41870	H	9.00400	12.97270	1.41870
H	2.25100	8.08110	0.13410	H	9.00400	11.98010	0.13410
H	2.25100	14.32030	5.08270	H	9.00400	10.42130	5.08270
H	2.25100	15.31290	3.79810	H	9.00400	11.41390	3.79810
H	3.04610	13.83990	7.19390	H	11.25500	9.07370	1.41870
H	1.45590	9.55410	3.52990	H	11.25500	8.08110	0.13410
H	3.04610	9.55410	3.52990	H	11.25500	14.32030	5.08270
H	1.45590	13.83990	7.19390	H	11.25500	15.31290	3.79810
H	0.79510	9.94090	7.19390	H	12.05000	13.83990	7.19390
H	-0.79500	13.45310	3.52990	H	10.45990	9.55410	3.52990

H	12.05000	9.55410	3.52990	H	2.25100	22.11830	5.08270
H	10.45990	13.83990	7.19390	H	2.25100	23.11090	3.79810
H	9.79900	9.94090	7.19390	H	3.04610	21.63790	7.19390
H	8.20890	13.45310	3.52990	H	1.45590	17.35210	3.52990
H	9.79900	13.45310	3.52990	H	3.04610	17.35210	3.52990
H	8.20890	9.94090	7.19390	H	1.45590	21.63790	7.19390
O	13.50600	12.98210	0.46240	H	0.79510	17.73890	7.19390
O	13.50600	10.41190	4.12640	H	-0.79500	21.25110	3.52990
O	15.75700	9.08310	0.46240	H	0.79510	21.25110	3.52990
O	15.75700	14.31090	4.12640	H	-0.79500	17.73890	7.19390
O	15.75700	14.23520	6.86560	O	4.50200	20.78010	0.46240
O	15.75700	9.15880	3.20160	O	4.50200	18.20990	4.12640
O	13.50600	10.33620	6.86560	O	6.75300	16.88110	0.46240
O	13.50600	13.05780	3.20160	O	6.75300	22.10890	4.12640
H	13.50600	12.97270	1.41870	O	6.75300	22.03320	6.86560
H	13.50600	11.98010	0.13410	O	6.75300	16.95680	3.20160
H	13.50600	10.42130	5.08270	O	4.50200	18.13420	6.86560
H	13.50600	11.41390	3.79810	O	4.50200	20.85580	3.20160
H	15.75700	9.07370	1.41870	H	4.50200	20.77070	1.41870
H	15.75700	8.08110	0.13410	H	4.50200	19.77810	0.13410
H	15.75700	14.32030	5.08270	H	4.50200	18.21930	5.08270
H	15.75700	15.31290	3.79810	H	4.50200	19.21190	3.79810
H	16.55200	13.83990	7.19390	H	6.75300	16.87170	1.41870
H	14.96190	9.55410	3.52990	H	6.75300	15.87910	0.13410
H	16.55200	9.55410	3.52990	H	6.75300	22.11830	5.08270
H	14.96190	13.83990	7.19390	H	6.75300	23.11090	3.79810
H	14.30100	9.94090	7.19390	H	7.54800	21.63790	7.19390
H	12.71090	13.45310	3.52990	H	5.95790	17.35210	3.52990
H	14.30100	13.45310	3.52990	H	7.54800	17.35210	3.52990
H	12.71090	9.94090	7.19390	H	5.95790	21.63790	7.19390
O	0.00000	20.78010	0.46240	H	5.29700	17.73890	7.19390
O	0.00000	18.20990	4.12640	H	3.70690	21.25110	3.52990
O	2.25100	16.88110	0.46240	H	5.29700	21.25110	3.52990
O	2.25100	22.10890	4.12640	H	3.70690	17.73890	7.19390
O	2.25100	22.03320	6.86560	O	9.00400	20.78010	0.46240
O	2.25100	16.95680	3.20160	O	9.00400	18.20990	4.12640
O	0.00000	18.13420	6.86560	O	11.25500	16.88110	0.46240
O	0.00000	20.85580	3.20160	O	11.25500	22.10890	4.12640
H	0.00000	20.77070	1.41870	O	11.25500	22.03320	6.86560
H	0.00000	19.77810	0.13410	O	11.25500	16.95680	3.20160
H	0.00000	18.21930	5.08270	O	9.00400	18.13420	6.86560
H	0.00000	19.21190	3.79810	O	9.00400	20.85580	3.20160
H	2.25100	16.87170	1.41870	H	9.00400	20.77070	1.41870
H	2.25100	15.87910	0.13410	H	9.00400	19.77810	0.13410

H	9.00400	18.21930	5.08270	H	0.00000	28.56870	1.41870
H	9.00400	19.21190	3.79810	H	0.00000	27.57610	0.13410
H	11.25500	16.87170	1.41870	H	2.25100	24.66980	1.41870
H	11.25500	15.87910	0.13410	H	2.25100	23.67710	0.13410
H	11.25500	22.11830	5.08270	H	3.04610	29.43590	7.19390
H	11.25500	23.11090	3.79810	H	1.45590	25.15010	3.52990
H	12.05000	21.63790	7.19390	H	3.04610	25.15010	3.52990
H	10.45990	17.35210	3.52990	H	1.45590	29.43590	7.19390
H	12.05000	17.35210	3.52990	H	0.79510	25.53690	7.19390
H	10.45990	21.63790	7.19390	H	-0.79500	29.04910	3.52990
H	9.79900	17.73890	7.19390	H	0.79510	29.04910	3.52990
H	8.20890	21.25110	3.52990	H	-0.79500	25.53690	7.19390
H	9.79900	21.25110	3.52990	O	4.50200	28.57810	0.46240
H	8.20890	17.73890	7.19390	O	4.50200	26.00790	4.12640
O	13.50600	20.78010	0.46240	O	6.75300	24.67910	0.46240
O	13.50600	18.20990	4.12640	O	6.75300	29.90690	4.12640
O	15.75700	16.88110	0.46240	O	6.75300	29.83120	6.86560
O	15.75700	22.10890	4.12640	O	6.75300	24.75480	3.20160
O	15.75700	22.03320	6.86560	O	4.50200	25.93230	6.86560
O	15.75700	16.95680	3.20160	O	4.50200	28.65380	3.20160
O	13.50600	18.13420	6.86560	H	4.50200	28.56870	1.41870
O	13.50600	20.85580	3.20160	H	4.50200	27.57610	0.13410
H	13.50600	20.77070	1.41870	H	4.50200	26.01730	5.08270
H	13.50600	19.77810	0.13410	H	4.50200	27.00990	3.79810
H	13.50600	18.21930	5.08270	H	6.75300	24.66980	1.41870
H	13.50600	19.21190	3.79810	H	6.75300	23.67710	0.13410
H	15.75700	16.87170	1.41870	H	6.75300	29.91630	5.08270
H	15.75700	15.87910	0.13410	H	6.75300	30.90890	3.79810
H	15.75700	22.11830	5.08270	H	7.54800	29.43590	7.19390
H	15.75700	23.11090	3.79810	H	5.95790	25.15010	3.52990
H	16.55200	21.63790	7.19390	H	7.54800	25.15010	3.52990
H	14.96190	17.35210	3.52990	H	5.95790	29.43590	7.19390
H	16.55200	17.35210	3.52990	H	5.29700	25.53690	7.19390
H	14.96190	21.63790	7.19390	H	3.70690	29.04910	3.52990
H	14.30100	17.73890	7.19390	H	5.29700	29.04910	3.52990
H	12.71090	21.25110	3.52990	H	3.70690	25.53690	7.19390
H	14.30100	21.25110	3.52990	O	9.00400	28.57810	0.46240
H	12.71090	17.73890	7.19390	O	9.00400	26.00790	4.12640
O	0.00000	28.57810	0.46240	O	11.25500	24.67910	0.46240
O	2.25100	24.67910	0.46240	O	11.25500	29.90690	4.12640
O	2.25100	29.83120	6.86560	O	11.25500	29.83120	6.86560
O	2.25100	24.75480	3.20160	O	11.25500	24.75480	3.20160
O	0.00000	25.93230	6.86560	O	9.00400	25.93230	6.86560
O	0.00000	28.65380	3.20160	O	9.00400	28.65380	3.20160

H	9.00400	28.56870	1.41870	O	0.00000	28.65380	10.52960
H	9.00400	27.57610	0.13410	H	3.04610	25.15010	10.85790
H	9.00400	26.01730	5.08270	H	-0.79500	29.04910	10.85790
H	9.00400	27.00990	3.79810	H	0.79510	29.04910	10.85790
H	11.25500	24.66980	1.41870	O	4.50200	28.65380	10.52960
H	11.25500	23.67710	0.13410	H	5.29700	29.04910	10.85790
H	11.25500	29.91630	5.08270	O	0.00000	5.18410	7.79040
H	11.25500	30.90890	3.79810	O	0.00000	2.61390	11.45440
H	12.05000	29.43590	7.19390	O	2.25100	1.28510	7.79040
H	10.45990	25.15010	3.52990	O	2.25100	6.51290	11.45440
H	12.05000	25.15010	3.52990	O	2.25100	6.43720	14.19360
H	10.45990	29.43590	7.19390	O	2.25100	1.36080	10.52960
H	9.79900	25.53690	7.19390	O	0.00000	2.53820	14.19360
H	8.20890	29.04910	3.52990	O	0.00000	5.25980	10.52960
H	9.79900	29.04910	3.52990	H	0.00000	5.17470	8.74670
H	8.20890	25.53690	7.19390	H	0.00000	4.18210	7.46210
O	13.50600	28.57810	0.46240	H	0.00000	2.62330	12.41070
O	13.50600	26.00790	4.12640	H	0.00000	3.61590	11.12610
O	15.75700	24.67910	0.46240	H	2.25100	1.27570	8.74670
O	15.75700	29.90690	4.12640	H	2.25100	0.28310	7.46210
O	15.75700	29.83120	6.86560	H	2.25100	6.52230	12.41070
O	15.75700	24.75480	3.20160	H	2.25100	7.51490	11.12610
O	13.50600	25.93230	6.86560	H	3.04610	6.04190	14.52190
O	13.50600	28.65380	3.20160	H	1.45590	1.75610	10.85790
H	13.50600	28.56870	1.41870	H	3.04610	1.75610	10.85790
H	13.50600	27.57610	0.13410	H	1.45590	6.04190	14.52190
H	13.50600	26.01730	5.08270	H	0.79510	2.14290	14.52190
H	13.50600	27.00990	3.79810	H	-0.79500	5.65510	10.85790
H	15.75700	24.66980	1.41870	H	0.79510	5.65510	10.85790
H	15.75700	23.67710	0.13410	H	-0.79500	2.14290	14.52190
H	15.75700	29.91630	5.08270	O	4.50200	5.18410	7.79040
H	15.75700	30.90890	3.79810	O	4.50200	2.61390	11.45440
H	16.55200	29.43590	7.19390	O	6.75300	1.28510	7.79040
H	14.96190	25.15010	3.52990	O	6.75300	6.51290	11.45440
H	16.55200	25.15010	3.52990	O	6.75300	6.43720	14.19360
H	14.96190	29.43590	7.19390	O	6.75300	1.36080	10.52960
H	14.30100	25.53690	7.19390	O	4.50200	2.53820	14.19360
H	12.71090	29.04910	3.52990	O	4.50200	5.25980	10.52960
H	14.30100	29.04910	3.52990	H	4.50200	5.17470	8.74670
H	12.71090	25.53690	7.19390	H	4.50200	4.18210	7.46210
O	15.75700	24.75480	10.52960	H	4.50200	2.62330	12.41070
H	14.96190	25.15010	10.85790	H	4.50200	3.61590	11.12610
H	16.55200	25.15010	10.85790	H	6.75300	1.27570	8.74670
O	2.25100	24.75480	10.52960	H	6.75300	0.28310	7.46210

H	6.75300	6.52230	12.41070	H	13.50600	2.62330	12.41070
H	6.75300	7.51490	11.12610	H	13.50600	3.61590	11.12610
H	7.54800	6.04190	14.52190	H	15.75700	1.27570	8.74670
H	5.95790	1.75610	10.85790	H	15.75700	0.28310	7.46210
H	7.54800	1.75610	10.85790	H	15.75700	6.52230	12.41070
H	5.95790	6.04190	14.52190	H	15.75700	7.51490	11.12610
H	5.29700	2.14290	14.52190	H	16.55200	6.04190	14.52190
H	3.70690	5.65510	10.85790	H	14.96190	1.75610	10.85790
H	5.29700	5.65510	10.85790	H	16.55200	1.75610	10.85790
H	3.70690	2.14290	14.52190	H	14.96190	6.04190	14.52190
O	9.00400	5.18410	7.79040	H	14.30100	2.14290	14.52190
O	9.00400	2.61390	11.45440	H	12.71090	5.65510	10.85790
O	11.25500	1.28510	7.79040	H	14.30100	5.65510	10.85790
O	11.25500	6.51290	11.45440	H	12.71090	2.14290	14.52190
O	11.25500	6.43720	14.19360	O	0.00000	12.98210	7.79040
O	11.25500	1.36080	10.52960	O	0.00000	10.41190	11.45440
O	9.00400	2.53820	14.19360	O	2.25100	9.08310	7.79040
O	9.00400	5.25980	10.52960	O	2.25100	14.31090	11.45440
H	9.00400	5.17470	8.74670	O	2.25100	14.23520	14.19360
H	9.00400	4.18210	7.46210	O	2.25100	9.15880	10.52960
H	9.00400	2.62330	12.41070	O	0.00000	10.33620	14.19360
H	9.00400	3.61590	11.12610	O	0.00000	13.05780	10.52960
H	11.25500	1.27570	8.74670	H	0.00000	12.97270	8.74670
H	11.25500	0.28310	7.46210	H	0.00000	11.98010	7.46210
H	11.25500	6.52230	12.41070	H	0.00000	10.42130	12.41070
H	11.25500	7.51490	11.12610	H	0.00000	11.41390	11.12610
H	12.05000	6.04190	14.52190	H	2.25100	9.07370	8.74670
H	10.45990	1.75610	10.85790	H	2.25100	8.08110	7.46210
H	12.05000	1.75610	10.85790	H	2.25100	14.32030	12.41070
H	10.45990	6.04190	14.52190	H	2.25100	15.31290	11.12610
H	9.79900	2.14290	14.52190	H	3.04610	13.83990	14.52190
H	8.20890	5.65510	10.85790	H	1.45590	9.55410	10.85790
H	9.79900	5.65510	10.85790	H	3.04610	9.55410	10.85790
H	8.20890	2.14290	14.52190	H	1.45590	13.83990	14.52190
O	13.50600	5.18410	7.79040	H	0.79510	9.94090	14.52190
O	13.50600	2.61390	11.45440	H	-0.79500	13.45310	10.85790
O	15.75700	1.28510	7.79040	H	0.79510	13.45310	10.85790
O	15.75700	6.51290	11.45440	H	-0.79500	9.94090	14.52190
O	15.75700	6.43720	14.19360	O	4.50200	12.98210	7.79040
O	15.75700	1.36080	10.52960	O	4.50200	10.41190	11.45440
O	13.50600	2.53820	14.19360	O	6.75300	9.08310	7.79040
O	13.50600	5.25980	10.52960	O	6.75300	14.31090	11.45440
H	13.50600	5.17470	8.74670	O	6.75300	14.23520	14.19360
H	13.50600	4.18210	7.46210	O	6.75300	9.15880	10.52960

O	4.50200	10.33620	14.19360	O	15.75700	9.08310	7.79040
O	4.50200	13.05780	10.52960	O	15.75700	14.31090	11.45440
H	4.50200	12.97270	8.74670	O	15.75700	14.23520	14.19360
H	4.50200	11.98010	7.46210	O	15.75700	9.15880	10.52960
H	4.50200	10.42130	12.41070	O	13.50600	10.33620	14.19360
H	4.50200	11.41390	11.12610	O	13.50600	13.05780	10.52960
H	6.75300	9.07370	8.74670	H	13.50600	12.97270	8.74670
H	6.75300	8.08110	7.46210	H	13.50600	11.98010	7.46210
H	6.75300	14.32030	12.41070	H	13.50600	10.42130	12.41070
H	6.75300	15.31290	11.12610	H	13.50600	11.41390	11.12610
H	7.54800	13.83990	14.52190	H	15.75700	9.07370	8.74670
H	5.95790	9.55410	10.85790	H	15.75700	8.08110	7.46210
H	7.54800	9.55410	10.85790	H	15.75700	14.32030	12.41070
H	5.95790	13.83990	14.52190	H	15.75700	15.31290	11.12610
H	5.29700	9.94090	14.52190	H	16.55200	13.83990	14.52190
H	3.70690	13.45310	10.85790	H	14.96190	9.55410	10.85790
H	5.29700	13.45310	10.85790	H	16.55200	9.55410	10.85790
H	3.70690	9.94090	14.52190	H	14.96190	13.83990	14.52190
O	9.00400	12.98210	7.79040	H	14.30100	9.94090	14.52190
O	9.00400	10.41190	11.45440	H	12.71090	13.45310	10.85790
O	11.25500	9.08310	7.79040	H	14.30100	13.45310	10.85790
O	11.25500	14.31090	11.45440	H	12.71090	9.94090	14.52190
O	11.25500	14.23520	14.19360	O	0.00000	20.78010	7.79040
O	11.25500	9.15880	10.52960	O	0.00000	18.20990	11.45440
O	9.00400	10.33620	14.19360	O	2.25100	16.88110	7.79040
O	9.00400	13.05780	10.52960	O	2.25100	22.10890	11.45440
H	9.00400	12.97270	8.74670	O	2.25100	22.03320	14.19360
H	9.00400	11.98010	7.46210	O	2.25100	16.95680	10.52960
H	9.00400	10.42130	12.41070	O	0.00000	18.13420	14.19360
H	9.00400	11.41390	11.12610	O	0.00000	20.85580	10.52960
H	11.25500	9.07370	8.74670	H	0.00000	20.77070	8.74670
H	11.25500	8.08110	7.46210	H	0.00000	19.77810	7.46210
H	11.25500	14.32030	12.41070	H	0.00000	18.21930	12.41070
H	11.25500	15.31290	11.12610	H	0.00000	19.21190	11.12610
H	12.05000	13.83990	14.52190	H	2.25100	16.87170	8.74670
H	10.45990	9.55410	10.85790	H	2.25100	15.87910	7.46210
H	12.05000	9.55410	10.85790	H	2.25100	22.11830	12.41070
H	10.45990	13.83990	14.52190	H	2.25100	23.11090	11.12610
H	9.79900	9.94090	14.52190	H	3.04610	21.63790	14.52190
H	8.20890	13.45310	10.85790	H	1.45590	17.35210	10.85790
H	9.79900	13.45310	10.85790	H	3.04610	17.35210	10.85790
H	8.20890	9.94090	14.52190	H	1.45590	21.63790	14.52190
O	13.50600	12.98210	7.79040	H	0.79510	17.73890	14.52190
O	13.50600	10.41190	11.45440	H	-0.79500	21.25110	10.85790

H	0.79510	21.25110	10.85790	H	12.05000	17.35210	10.85790
H	-0.79500	17.73890	14.52190	H	10.45990	21.63790	14.52190
O	4.50200	20.78010	7.79040	H	9.79900	17.73890	14.52190
O	4.50200	18.20990	11.45440	H	8.20890	21.25110	10.85790
O	6.75300	16.88110	7.79040	H	9.79900	21.25110	10.85790
O	6.75300	22.10890	11.45440	H	8.20890	17.73890	14.52190
O	6.75300	22.03320	14.19360	O	13.50600	20.78010	7.79040
O	6.75300	16.95680	10.52960	O	13.50600	18.20990	11.45440
O	4.50200	18.13420	14.19360	O	15.75700	16.88110	7.79040
O	4.50200	20.85580	10.52960	O	15.75700	22.10890	11.45440
H	4.50200	20.77070	8.74670	O	15.75700	22.03320	14.19360
H	4.50200	19.77810	7.46210	O	15.75700	16.95680	10.52960
H	4.50200	18.21930	12.41070	O	13.50600	18.13420	14.19360
H	4.50200	19.21190	11.12610	O	13.50600	20.85580	10.52960
H	6.75300	16.87170	8.74670	H	13.50600	20.77070	8.74670
H	6.75300	15.87910	7.46210	H	13.50600	19.77810	7.46210
H	6.75300	22.11830	12.41070	H	13.50600	18.21930	12.41070
H	6.75300	23.11090	11.12610	H	13.50600	19.21190	11.12610
H	7.54800	21.63790	14.52190	H	15.75700	16.87170	8.74670
H	5.95790	17.35210	10.85790	H	15.75700	15.87910	7.46210
H	7.54800	17.35210	10.85790	H	15.75700	22.11830	12.41070
H	5.95790	21.63790	14.52190	H	15.75700	23.11090	11.12610
H	5.29700	17.73890	14.52190	H	16.55200	21.63790	14.52190
H	3.70690	21.25110	10.85790	H	14.96190	17.35210	10.85790
H	5.29700	21.25110	10.85790	H	16.55200	17.35210	10.85790
H	3.70690	17.73890	14.52190	H	14.96190	21.63790	14.52190
O	9.00400	20.78010	7.79040	H	14.30100	17.73890	14.52190
O	9.00400	18.20990	11.45440	H	12.71090	21.25110	10.85790
O	11.25500	16.88110	7.79040	H	14.30100	21.25110	10.85790
O	11.25500	22.10890	11.45440	H	12.71090	17.73890	14.52190
O	11.25500	22.03320	14.19360	O	0.00000	28.57810	7.79040
O	11.25500	16.95680	10.52960	O	0.00000	26.00790	11.45440
O	9.00400	18.13420	14.19360	O	2.25100	24.67910	7.79040
O	9.00400	20.85580	10.52960	O	2.25100	29.90690	11.45440
H	9.00400	20.77070	8.74670	O	2.25100	29.83120	14.19360
H	9.00400	19.77810	7.46210	O	0.00000	25.93230	14.19360
H	9.00400	18.21930	12.41070	H	0.00000	28.56870	8.74670
H	9.00400	19.21190	11.12610	H	0.00000	27.57610	7.46210
H	11.25500	16.87170	8.74670	H	0.00000	26.01730	12.41070
H	11.25500	15.87910	7.46210	H	0.00000	27.00990	11.12610
H	11.25500	22.11830	12.41070	H	2.25100	24.66980	8.74670
H	11.25500	23.11090	11.12610	H	2.25100	23.67710	7.46210
H	12.05000	21.63790	14.52190	H	2.25100	29.91630	12.41070
H	10.45990	17.35210	10.85790	H	2.25100	30.90890	11.12610

H	3.04610	29.43590	14.52190	H	10.45990	25.15010	10.85790
H	1.45590	25.15010	10.85790	H	12.05000	25.15010	10.85790
H	1.45590	29.43590	14.52190	H	10.45990	29.43590	14.52190
H	0.79510	25.53690	14.52190	H	9.79900	25.53690	14.52190
H	-0.79500	25.53690	14.52190	H	8.20890	29.04910	10.85790
O	4.50200	28.57810	7.79040	H	9.79900	29.04910	10.85790
O	4.50200	26.00790	11.45440	H	8.20890	25.53690	14.52190
O	6.75300	24.67910	7.79040	O	13.50600	28.57810	7.79040
O	6.75300	29.90690	11.45440	O	13.50600	26.00790	11.45440
O	6.75300	29.83120	14.19360	O	15.75700	24.67910	7.79040
O	6.75300	24.75480	10.52960	O	15.75700	29.90690	11.45440
O	4.50200	25.93230	14.19360	O	15.75700	29.83120	14.19360
H	4.50200	28.56870	8.74670	O	13.50600	25.93230	14.19360
H	4.50200	27.57610	7.46210	O	13.50600	28.65380	10.52960
H	4.50200	26.01730	12.41070	H	13.50600	28.56870	8.74670
H	4.50200	27.00990	11.12610	H	13.50600	27.57610	7.46210
H	6.75300	24.66980	8.74670	H	13.50600	26.01730	12.41070
H	6.75300	23.67710	7.46210	H	13.50600	27.00990	11.12610
H	6.75300	29.91630	12.41070	H	15.75700	24.66980	8.74670
H	6.75300	30.90890	11.12610	H	15.75700	23.67710	7.46210
H	7.54800	29.43590	14.52190	H	15.75700	29.91630	12.41070
H	5.95790	25.15010	10.85790	H	15.75700	30.90890	11.12610
H	7.54800	25.15010	10.85790	H	16.55200	29.43590	14.52190
H	5.95790	29.43590	14.52190	H	14.96190	29.43590	14.52190
H	5.29700	25.53690	14.52190	H	14.30100	25.53690	14.52190
H	3.70690	29.04910	10.85790	H	12.71090	29.04910	10.85790
H	3.70690	25.53690	14.52190	H	14.30100	29.04910	10.85790
O	9.00400	28.57810	7.79040	H	12.71090	25.53690	14.52190
O	9.00400	26.00790	11.45440	O	0.00000	5.18410	15.11840
O	11.25500	24.67910	7.79040	O	0.00000	2.61390	18.78240
O	11.25500	29.90690	11.45440	O	2.25100	1.28510	15.11840
O	11.25500	29.83120	14.19360	O	2.25100	6.51290	18.78240
O	11.25500	24.75480	10.52960	O	2.25100	6.43720	21.52160
O	9.00400	25.93230	14.19360	O	2.25100	1.36080	17.85760
O	9.00400	28.65380	10.52960	O	0.00000	2.53820	21.52160
H	9.00400	28.56870	8.74670	O	0.00000	5.25980	17.85760
H	9.00400	27.57610	7.46210	H	0.00000	5.17470	16.07470
H	9.00400	26.01730	12.41070	H	0.00000	4.18210	14.79010
H	9.00400	27.00990	11.12610	H	0.00000	2.62330	19.73870
H	11.25500	24.66980	8.74670	H	0.00000	3.61590	18.45410
H	11.25500	23.67710	7.46210	H	2.25100	1.27570	16.07470
H	11.25500	29.91630	12.41070	H	2.25100	0.28310	14.79010
H	11.25500	30.90890	11.12610	H	2.25100	6.52230	19.73870
H	12.05000	29.43590	14.52190	H	2.25100	7.51490	18.45410



H	3.04610	6.04190	21.84990	H	11.25500	1.27570	16.07470
H	1.45590	1.75610	18.18590	H	11.25500	0.28310	14.79010
H	3.04610	1.75610	18.18590	H	11.25500	6.52230	19.73870
H	1.45590	6.04190	21.84990	H	11.25500	7.51490	18.45410
H	0.79510	2.14290	21.84990	H	12.05000	6.04190	21.84990
H	-0.79500	5.65510	18.18590	H	10.45990	1.75610	18.18590
H	0.79510	5.65510	18.18590	H	12.05000	1.75610	18.18590
H	-0.79500	2.14290	21.84990	H	10.45990	6.04190	21.84990
O	4.50200	5.18410	15.11840	H	9.79900	2.14290	21.84990
O	4.50200	2.61390	18.78240	H	8.20890	5.65510	18.18590
O	6.75300	1.28510	15.11840	H	9.79900	5.65510	18.18590
O	6.75300	6.51290	18.78240	H	8.20890	2.14290	21.84990
O	6.75300	6.43720	21.52160	O	13.50600	5.18410	15.11840
O	6.75300	1.36080	17.85760	O	13.50600	2.61390	18.78240
O	4.50200	2.53820	21.52160	O	15.75700	1.28510	15.11840
O	4.50200	5.25980	17.85760	O	15.75700	6.51290	18.78240
H	4.50200	5.17470	16.07470	O	15.75700	6.43720	21.52160
H	4.50200	4.18210	14.79010	O	15.75700	1.36080	17.85760
H	4.50200	2.62330	19.73870	O	13.50600	2.53820	21.52160
H	4.50200	3.61590	18.45410	O	13.50600	5.25980	17.85760
H	6.75300	1.27570	16.07470	H	13.50600	5.17470	16.07470
H	6.75300	0.28310	14.79010	H	13.50600	4.18210	14.79010
H	6.75300	6.52230	19.73870	H	13.50600	2.62330	19.73870
H	6.75300	7.51490	18.45410	H	13.50600	3.61590	18.45410
H	7.54800	6.04190	21.84990	H	15.75700	1.27570	16.07470
H	5.95790	1.75610	18.18590	H	15.75700	0.28310	14.79010
H	7.54800	1.75610	18.18590	H	15.75700	6.52230	19.73870
H	5.95790	6.04190	21.84990	H	15.75700	7.51490	18.45410
H	5.29700	2.14290	21.84990	H	16.55200	6.04190	21.84990
H	3.70690	5.65510	18.18590	H	14.96190	1.75610	18.18590
H	5.29700	5.65510	18.18590	H	16.55200	1.75610	18.18590
H	3.70690	2.14290	21.84990	H	14.96190	6.04190	21.84990
O	9.00400	5.18410	15.11840	H	14.30100	2.14290	21.84990
O	9.00400	2.61390	18.78240	H	12.71090	5.65510	18.18590
O	11.25500	1.28510	15.11840	H	14.30100	5.65510	18.18590
O	11.25500	6.51290	18.78240	H	12.71090	2.14290	21.84990
O	11.25500	6.43720	21.52160	O	0.00000	12.98210	15.11840
O	11.25500	1.36080	17.85760	O	0.00000	10.41190	18.78240
O	9.00400	2.53820	21.52160	O	2.25100	9.08310	15.11840
O	9.00400	5.25980	17.85760	O	2.25100	14.31090	18.78240
H	9.00400	5.17470	16.07470	O	2.25100	14.23520	21.52160
H	9.00400	4.18210	14.79010	O	2.25100	9.15880	17.85760
H	9.00400	2.62330	19.73870	O	0.00000	10.33620	21.52160
H	9.00400	3.61590	18.45410	O	0.00000	13.05780	17.85760

H	0.00000	12.97270	16.07470	O	11.25500	14.23520	21.52160
H	0.00000	11.98010	14.79010	O	11.25500	9.15880	17.85760
H	0.00000	10.42130	19.73870	O	9.00400	10.33620	21.52160
H	0.00000	11.41390	18.45410	O	9.00400	13.05780	17.85760
H	2.25100	9.07370	16.07470	H	9.00400	12.97270	16.07470
H	2.25100	8.08110	14.79010	H	9.00400	11.98010	14.79010
H	2.25100	14.32030	19.73870	H	9.00400	10.42130	19.73870
H	2.25100	15.31290	18.45410	H	9.00400	11.41390	18.45410
H	3.04610	13.83990	21.84990	H	11.25500	9.07370	16.07470
H	1.45590	9.55410	18.18590	H	11.25500	8.08110	14.79010
H	3.04610	9.55410	18.18590	H	11.25500	14.32030	19.73870
H	1.45590	13.83990	21.84990	H	11.25500	15.31290	18.45410
H	0.79510	9.94090	21.84990	H	12.05000	13.83990	21.84990
H	-0.79500	13.45310	18.18590	H	10.45990	9.55410	18.18590
H	0.79510	13.45310	18.18590	H	12.05000	9.55410	18.18590
H	-0.79500	9.94090	21.84990	H	10.45990	13.83990	21.84990
O	4.50200	12.98210	15.11840	H	9.79900	9.94090	21.84990
O	4.50200	10.41190	18.78240	H	8.20890	13.45310	18.18590
O	6.75300	9.08310	15.11840	H	9.79900	13.45310	18.18590
O	6.75300	14.31090	18.78240	H	8.20890	9.94090	21.84990
O	6.75300	14.23520	21.52160	O	13.50600	12.98210	15.11840
O	6.75300	9.15880	17.85760	O	13.50600	10.41190	18.78240
O	4.50200	10.33620	21.52160	O	15.75700	9.08310	15.11840
O	4.50200	13.05780	17.85760	O	15.75700	14.31090	18.78240
H	4.50200	12.97270	16.07470	O	15.75700	14.23520	21.52160
H	4.50200	11.98010	14.79010	O	15.75700	9.15880	17.85760
H	4.50200	10.42130	19.73870	O	13.50600	10.33620	21.52160
H	4.50200	11.41390	18.45410	O	13.50600	13.05780	17.85760
H	6.75300	9.07370	16.07470	H	13.50600	12.97270	16.07470
H	6.75300	8.08110	14.79010	H	13.50600	11.98010	14.79010
H	6.75300	14.32030	19.73870	H	13.50600	10.42130	19.73870
H	6.75300	15.31290	18.45410	H	13.50600	11.41390	18.45410
H	7.54800	13.83990	21.84990	H	15.75700	9.07370	16.07470
H	5.95790	9.55410	18.18590	H	15.75700	8.08110	14.79010
H	7.54800	9.55410	18.18590	H	15.75700	14.32030	19.73870
H	5.95790	13.83990	21.84990	H	15.75700	15.31290	18.45410
H	5.29700	9.94090	21.84990	H	16.55200	13.83990	21.84990
H	3.70690	13.45310	18.18590	H	14.96190	9.55410	18.18590
H	5.29700	13.45310	18.18590	H	16.55200	9.55410	18.18590
H	3.70690	9.94090	21.84990	H	14.96190	13.83990	21.84990
O	9.00400	12.98210	15.11840	H	14.30100	9.94090	21.84990
O	9.00400	10.41190	18.78240	H	12.71090	13.45310	18.18590
O	11.25500	9.08310	15.11840	H	14.30100	13.45310	18.18590
O	11.25500	14.31090	18.78240	H	12.71090	9.94090	21.84990

O	0.00000	20.78010	15.11840	H	5.29700	17.73890	21.84990
O	0.00000	18.20990	18.78240	H	3.70690	21.25110	18.18590
O	2.25100	16.88110	15.11840	H	5.29700	21.25110	18.18590
O	2.25100	22.10890	18.78240	H	3.70690	17.73890	21.84990
O	2.25100	22.03320	21.52160	O	9.00400	20.78010	15.11840
O	2.25100	16.95680	17.85760	O	9.00400	18.20990	18.78240
O	0.00000	18.13420	21.52160	O	11.25500	16.88110	15.11840
O	0.00000	20.85580	17.85760	O	11.25500	22.10890	18.78240
H	0.00000	20.77070	16.07470	O	11.25500	22.03320	21.52160
H	0.00000	19.77810	14.79010	O	11.25500	16.95680	17.85760
H	0.00000	18.21930	19.73870	O	9.00400	18.13420	21.52160
H	0.00000	19.21190	18.45410	O	9.00400	20.85580	17.85760
H	2.25100	16.87170	16.07470	H	9.00400	20.77070	16.07470
H	2.25100	15.87910	14.79010	H	9.00400	19.77810	14.79010
H	2.25100	22.11830	19.73870	H	9.00400	18.21930	19.73870
H	2.25100	23.11090	18.45410	H	9.00400	19.21190	18.45410
H	3.04610	21.63790	21.84990	H	11.25500	16.87170	16.07470
H	1.45590	17.35210	18.18590	H	11.25500	15.87910	14.79010
H	3.04610	17.35210	18.18590	H	11.25500	22.11830	19.73870
H	1.45590	21.63790	21.84990	H	11.25500	23.11090	18.45410
H	0.79510	17.73890	21.84990	H	12.05000	21.63790	21.84990
H	-0.79500	21.25110	18.18590	H	10.45990	17.35210	18.18590
H	0.79510	21.25110	18.18590	H	12.05000	17.35210	18.18590
H	-0.79500	17.73890	21.84990	H	10.45990	21.63790	21.84990
O	4.50200	20.78010	15.11840	H	9.79900	17.73890	21.84990
O	4.50200	18.20990	18.78240	H	8.20890	21.25110	18.18590
O	6.75300	16.88110	15.11840	H	9.79900	21.25110	18.18590
O	6.75300	22.10890	18.78240	H	8.20890	17.73890	21.84990
O	6.75300	22.03320	21.52160	O	13.50600	20.78010	15.11840
O	6.75300	16.95680	17.85760	O	13.50600	18.20990	18.78240
O	4.50200	18.13420	21.52160	O	15.75700	16.88110	15.11840
O	4.50200	20.85580	17.85760	O	15.75700	22.10890	18.78240
H	4.50200	20.77070	16.07470	O	15.75700	22.03320	21.52160
H	4.50200	19.77810	14.79010	O	15.75700	16.95680	17.85760
H	4.50200	18.21930	19.73870	O	13.50600	18.13420	21.52160
H	4.50200	19.21190	18.45410	O	13.50600	20.85580	17.85760
H	6.75300	16.87170	16.07470	H	13.50600	20.77070	16.07470
H	6.75300	15.87910	14.79010	H	13.50600	19.77810	14.79010
H	6.75300	22.11830	19.73870	H	13.50600	18.21930	19.73870
H	6.75300	23.11090	18.45410	H	13.50600	19.21190	18.45410
H	7.54800	21.63790	21.84990	H	15.75700	16.87170	16.07470
H	5.95790	17.35210	18.18590	H	15.75700	15.87910	14.79010
H	7.54800	17.35210	18.18590	H	15.75700	22.11830	19.73870
H	5.95790	21.63790	21.84990	H	15.75700	23.11090	18.45410

H	16.55200	21.63790	21.84990	H	6.75300	24.66980	16.07470
H	14.96190	17.35210	18.18590	H	6.75300	23.67710	14.79010
H	16.55200	17.35210	18.18590	H	6.75300	29.91630	19.73870
H	14.96190	21.63790	21.84990	H	6.75300	30.90890	18.45410
H	14.30100	17.73890	21.84990	H	7.54800	29.43590	21.84990
H	12.71090	21.25110	18.18590	H	5.95790	25.15010	18.18590
H	14.30100	21.25110	18.18590	H	7.54800	25.15010	18.18590
H	12.71090	17.73890	21.84990	H	5.95790	29.43590	21.84990
O	0.00000	28.57810	15.11840	H	5.29700	25.53690	21.84990
O	0.00000	26.00790	18.78240	H	3.70690	29.04910	18.18590
O	2.25100	24.67910	15.11840	H	5.29700	29.04910	18.18590
O	2.25100	29.90690	18.78240	H	3.70690	25.53690	21.84990
O	2.25100	29.83120	21.52160	O	9.00400	28.57810	15.11840
O	2.25100	24.75480	17.85760	O	9.00400	26.00790	18.78240
O	0.00000	25.93230	21.52160	O	11.25500	24.67910	15.11840
O	0.00000	28.65380	17.85760	O	11.25500	29.90690	18.78240
H	0.00000	28.56870	16.07470	O	11.25500	29.83120	21.52160
H	0.00000	27.57610	14.79010	O	11.25500	24.75480	17.85760
H	0.00000	26.01730	19.73870	O	9.00400	25.93230	21.52160
H	0.00000	27.00990	18.45410	O	9.00400	28.65380	17.85760
H	2.25100	24.66980	16.07470	H	9.00400	28.56870	16.07470
H	2.25100	23.67710	14.79010	H	9.00400	27.57610	14.79010
H	2.25100	29.91630	19.73870	H	9.00400	26.01730	19.73870
H	2.25100	30.90890	18.45410	H	9.00400	27.00990	18.45410
H	3.04610	29.43590	21.84990	H	11.25500	24.66980	16.07470
H	1.45590	25.15010	18.18590	H	11.25500	23.67710	14.79010
H	3.04610	25.15010	18.18590	H	11.25500	29.91630	19.73870
H	1.45590	29.43590	21.84990	H	11.25500	30.90890	18.45410
H	0.79510	25.53690	21.84990	H	12.05000	29.43590	21.84990
H	-0.79500	29.04910	18.18590	H	10.45990	25.15010	18.18590
H	0.79510	29.04910	18.18590	H	12.05000	25.15010	18.18590
H	-0.79500	25.53690	21.84990	H	10.45990	29.43590	21.84990
O	4.50200	28.57810	15.11840	H	9.79900	25.53690	21.84990
O	4.50200	26.00790	18.78240	H	8.20890	29.04910	18.18590
O	6.75300	24.67910	15.11840	H	9.79900	29.04910	18.18590
O	6.75300	29.90690	18.78240	H	8.20890	25.53690	21.84990
O	6.75300	29.83120	21.52160	O	13.50600	28.57810	15.11840
O	6.75300	24.75480	17.85760	O	13.50600	26.00790	18.78240
O	4.50200	25.93230	21.52160	O	15.75700	24.67910	15.11840
O	4.50200	28.65380	17.85760	O	15.75700	29.90690	18.78240
H	4.50200	28.56870	16.07470	O	15.75700	29.83120	21.52160
H	4.50200	27.57610	14.79010	O	15.75700	24.75480	17.85760
H	4.50200	26.01730	19.73870	O	13.50600	25.93230	21.52160
H	4.50200	27.00990	18.45410	O	13.50600	28.65380	17.85760

H	13.50600	28.56870	16.07470	O	6.75300	6.43720	28.84960
H	13.50600	27.57610	14.79010	O	6.75300	1.36080	25.18560
H	13.50600	26.01730	19.73870	O	4.50200	2.53820	28.84960
H	13.50600	27.00990	18.45410	O	4.50200	5.25980	25.18560
H	15.75700	24.66980	16.07470	H	4.50200	5.17470	23.40270
H	15.75700	23.67710	14.79010	H	4.50200	4.18210	22.11810
H	15.75700	29.91630	19.73870	H	4.50200	2.62330	27.06670
H	15.75700	30.90890	18.45410	H	4.50200	3.61590	25.78210
H	16.55200	29.43590	21.84990	H	6.75300	1.27570	23.40270
H	14.96190	25.15010	18.18590	H	6.75300	0.28310	22.11810
H	16.55200	25.15010	18.18590	H	6.75300	6.52230	27.06670
H	14.96190	29.43590	21.84990	H	6.75300	7.51490	25.78210
H	14.30100	25.53690	21.84990	H	7.54800	6.04190	29.17790
H	12.71090	29.04910	18.18590	H	5.95790	1.75610	25.51390
H	14.30100	29.04910	18.18590	H	7.54800	1.75610	25.51390
H	12.71090	25.53690	21.84990	H	5.95790	6.04190	29.17790
O	0.00000	5.18410	22.44640	H	5.29700	2.14290	29.17790
O	0.00000	2.61390	26.11040	H	3.70690	5.65510	25.51390
O	2.25100	1.28510	22.44640	H	5.29700	5.65510	25.51390
O	2.25100	6.51290	26.11040	H	3.70690	2.14290	29.17790
O	2.25100	6.43720	28.84960	O	9.00400	5.18410	22.44640
O	2.25100	1.36080	25.18560	O	9.00400	2.61390	26.11040
O	0.00000	2.53820	28.84960	O	11.25500	1.28510	22.44640
O	0.00000	5.25980	25.18560	O	11.25500	6.51290	26.11040
H	0.00000	5.17470	23.40270	O	11.25500	6.43720	28.84960
H	0.00000	4.18210	22.11810	O	11.25500	1.36080	25.18560
H	0.00000	2.62330	27.06670	O	9.00400	2.53820	28.84960
H	0.00000	3.61590	25.78210	O	9.00400	5.25980	25.18560
H	2.25100	1.27570	23.40270	H	9.00400	5.17470	23.40270
H	2.25100	0.28310	22.11810	H	9.00400	4.18210	22.11810
H	2.25100	6.52230	27.06670	H	9.00400	2.62330	27.06670
H	2.25100	7.51490	25.78210	H	9.00400	3.61590	25.78210
H	3.04610	6.04190	29.17790	H	11.25500	1.27570	23.40270
H	1.45590	1.75610	25.51390	H	11.25500	0.28310	22.11810
H	3.04610	1.75610	25.51390	H	11.25500	6.52230	27.06670
H	1.45590	6.04190	29.17790	H	11.25500	7.51490	25.78210
H	0.79510	2.14290	29.17790	H	12.05000	6.04190	29.17790
H	-0.79500	5.65510	25.51390	H	10.45990	1.75610	25.51390
H	0.79510	5.65510	25.51390	H	12.05000	1.75610	25.51390
H	-0.79500	2.14290	29.17790	H	10.45990	6.04190	29.17790
O	4.50200	5.18410	22.44640	H	9.79900	2.14290	29.17790
O	4.50200	2.61390	26.11040	H	8.20890	5.65510	25.51390
O	6.75300	1.28510	22.44640	H	9.79900	5.65510	25.51390
O	6.75300	6.51290	26.11040	H	8.20890	2.14290	29.17790

O	13.50600	5.18410	22.44640	H	0.79510	9.94090	29.17790
O	13.50600	2.61390	26.11040	H	-0.79500	13.45310	25.51390
O	15.75700	1.28510	22.44640	H	0.79510	13.45310	25.51390
O	15.75700	6.51290	26.11040	H	-0.79500	9.94090	29.17790
O	15.75700	6.43720	28.84960	O	4.50200	12.98210	22.44640
O	15.75700	1.36080	25.18560	O	4.50200	10.41190	26.11040
O	13.50600	2.53820	28.84960	O	6.75300	9.08310	22.44640
O	13.50600	5.25980	25.18560	O	6.75300	14.31090	26.11040
H	13.50600	5.17470	23.40270	O	6.75300	14.23520	28.84960
H	13.50600	4.18210	22.11810	O	6.75300	9.15880	25.18560
H	13.50600	2.62330	27.06670	O	4.50200	10.33620	28.84960
H	13.50600	3.61590	25.78210	O	4.50200	13.05780	25.18560
H	15.75700	1.27570	23.40270	H	4.50200	12.97270	23.40270
H	15.75700	0.28310	22.11810	H	4.50200	11.98010	22.11810
H	15.75700	6.52230	27.06670	H	4.50200	10.42130	27.06670
H	15.75700	7.51490	25.78210	H	4.50200	11.41390	25.78210
H	16.55200	6.04190	29.17790	H	6.75300	9.07370	23.40270
H	14.96190	1.75610	25.51390	H	6.75300	8.08110	22.11810
H	16.55200	1.75610	25.51390	H	6.75300	14.32030	27.06670
H	14.96190	6.04190	29.17790	H	6.75300	15.31290	25.78210
H	14.30100	2.14290	29.17790	H	7.54800	13.83990	29.17790
H	12.71090	5.65510	25.51390	H	5.95790	9.55410	25.51390
H	14.30100	5.65510	25.51390	H	7.54800	9.55410	25.51390
H	12.71090	2.14290	29.17790	H	5.95790	13.83990	29.17790
O	0.00000	12.98210	22.44640	H	5.29700	9.94090	29.17790
O	0.00000	10.41190	26.11040	H	3.70690	13.45310	25.51390
O	2.25100	9.08310	22.44640	H	5.29700	13.45310	25.51390
O	2.25100	14.31090	26.11040	H	3.70690	9.94090	29.17790
O	2.25100	14.23520	28.84960	O	9.00400	12.98210	22.44640
O	2.25100	9.15880	25.18560	O	9.00400	10.41190	26.11040
O	0.00000	10.33620	28.84960	O	11.25500	9.08310	22.44640
O	0.00000	13.05780	25.18560	O	11.25500	14.31090	26.11040
H	0.00000	12.97270	23.40270	O	11.25500	14.23520	28.84960
H	0.00000	11.98010	22.11810	O	11.25500	9.15880	25.18560
H	0.00000	10.42130	27.06670	O	9.00400	10.33620	28.84960
H	0.00000	11.41390	25.78210	O	9.00400	13.05780	25.18560
H	2.25100	9.07370	23.40270	H	9.00400	12.97270	23.40270
H	2.25100	8.08110	22.11810	H	9.00400	11.98010	22.11810
H	2.25100	14.32030	27.06670	H	9.00400	10.42130	27.06670
H	2.25100	15.31290	25.78210	H	9.00400	11.41390	25.78210
H	3.04610	13.83990	29.17790	H	11.25500	9.07370	23.40270
H	1.45590	9.55410	25.51390	H	11.25500	8.08110	22.11810
H	3.04610	9.55410	25.51390	H	11.25500	14.32030	27.06670
H	1.45590	13.83990	29.17790	H	11.25500	15.31290	25.78210

H	12.05000	13.83990	29.17790	H	2.25100	16.87170	23.40270
H	10.45990	9.55410	25.51390	H	2.25100	15.87910	22.11810
H	12.05000	9.55410	25.51390	H	2.25100	22.11830	27.06670
H	10.45990	13.83990	29.17790	H	2.25100	23.11090	25.78210
H	9.79900	9.94090	29.17790	H	3.04610	21.63790	29.17790
H	8.20890	13.45310	25.51390	H	1.45590	17.35210	25.51390
H	9.79900	13.45310	25.51390	H	3.04610	17.35210	25.51390
H	8.20890	9.94090	29.17790	H	1.45590	21.63790	29.17790
O	13.50600	12.98210	22.44640	H	0.79510	17.73890	29.17790
O	13.50600	10.41190	26.11040	H	-0.79500	21.25110	25.51390
O	15.75700	9.08310	22.44640	H	0.79510	21.25110	25.51390
O	15.75700	14.31090	26.11040	H	-0.79500	17.73890	29.17790
O	15.75700	14.23520	28.84960	O	4.50200	20.78010	22.44640
O	15.75700	9.15880	25.18560	O	4.50200	18.20990	26.11040
O	13.50600	10.33620	28.84960	O	6.75300	16.88110	22.44640
O	13.50600	13.05780	25.18560	O	6.75300	22.10890	26.11040
H	13.50600	12.97270	23.40270	O	6.75300	22.03320	28.84960
H	13.50600	11.98010	22.11810	O	6.75300	16.95680	25.18560
H	13.50600	10.42130	27.06670	O	4.50200	18.13420	28.84960
H	13.50600	11.41390	25.78210	O	4.50200	20.85580	25.18560
H	15.75700	9.07370	23.40270	H	4.50200	20.77070	23.40270
H	15.75700	8.08110	22.11810	H	4.50200	19.77810	22.11810
H	15.75700	14.32030	27.06670	H	4.50200	18.21930	27.06670
H	15.75700	15.31290	25.78210	H	4.50200	19.21190	25.78210
H	16.55200	13.83990	29.17790	H	6.75300	16.87170	23.40270
H	14.96190	9.55410	25.51390	H	6.75300	15.87910	22.11810
H	16.55200	9.55410	25.51390	H	6.75300	22.11830	27.06670
H	14.96190	13.83990	29.17790	H	6.75300	23.11090	25.78210
H	14.30100	9.94090	29.17790	H	7.54800	21.63790	29.17790
H	12.71090	13.45310	25.51390	H	5.95790	17.35210	25.51390
H	14.30100	13.45310	25.51390	H	7.54800	17.35210	25.51390
H	12.71090	9.94090	29.17790	H	5.95790	21.63790	29.17790
O	0.00000	20.78010	22.44640	H	5.29700	17.73890	29.17790
O	0.00000	18.20990	26.11040	H	3.70690	21.25110	25.51390
O	2.25100	16.88110	22.44640	H	5.29700	21.25110	25.51390
O	2.25100	22.10890	26.11040	H	3.70690	17.73890	29.17790
O	2.25100	22.03320	28.84960	O	9.00400	20.78010	22.44640
O	2.25100	16.95680	25.18560	O	9.00400	18.20990	26.11040
O	0.00000	18.13420	28.84960	O	11.25500	16.88110	22.44640
O	0.00000	20.85580	25.18560	O	11.25500	22.10890	26.11040
H	0.00000	20.77070	23.40270	O	11.25500	22.03320	28.84960
H	0.00000	19.77810	22.11810	O	11.25500	16.95680	25.18560
H	0.00000	18.21930	27.06670	O	9.00400	18.13420	28.84960
H	0.00000	19.21190	25.78210	O	9.00400	20.85580	25.18560

H	9.00400	20.77070	23.40270	O	2.25100	29.83120	28.84960
H	9.00400	19.77810	22.11810	O	2.25100	24.75480	25.18560
H	9.00400	18.21930	27.06670	O	0.00000	25.93230	28.84960
H	9.00400	19.21190	25.78210	O	0.00000	28.65380	25.18560
H	11.25500	16.87170	23.40270	H	0.00000	28.56870	23.40270
H	11.25500	15.87910	22.11810	H	0.00000	27.57610	22.11810
H	11.25500	22.11830	27.06670	H	0.00000	26.01730	27.06670
H	11.25500	23.11090	25.78210	H	0.00000	27.00990	25.78210
H	12.05000	21.63790	29.17790	H	2.25100	24.66980	23.40270
H	10.45990	17.35210	25.51390	H	2.25100	23.67710	22.11810
H	12.05000	17.35210	25.51390	H	2.25100	29.91630	27.06670
H	10.45990	21.63790	29.17790	H	2.25100	30.90890	25.78210
H	9.79900	17.73890	29.17790	H	3.04610	29.43590	29.17790
H	8.20890	21.25110	25.51390	H	1.45590	25.15010	25.51390
H	9.79900	21.25110	25.51390	H	3.04610	25.15010	25.51390
H	8.20890	17.73890	29.17790	H	1.45590	29.43590	29.17790
O	13.50600	20.78010	22.44640	H	0.79510	25.53690	29.17790
O	13.50600	18.20990	26.11040	H	-0.79500	29.04910	25.51390
O	15.75700	16.88110	22.44640	H	0.79510	29.04910	25.51390
O	15.75700	22.10890	26.11040	H	-0.79500	25.53690	29.17790
O	15.75700	22.03320	28.84960	O	4.50200	28.57810	22.44640
O	15.75700	16.95680	25.18560	O	4.50200	26.00790	26.11040
O	13.50600	18.13420	28.84960	O	6.75300	24.67910	22.44640
O	13.50600	20.85580	25.18560	O	6.75300	29.90690	26.11040
H	13.50600	20.77070	23.40270	O	6.75300	29.83120	28.84960
H	13.50600	19.77810	22.11810	O	6.75300	24.75480	25.18560
H	13.50600	18.21930	27.06670	O	4.50200	25.93230	28.84960
H	13.50600	19.21190	25.78210	O	4.50200	28.65380	25.18560
H	15.75700	16.87170	23.40270	H	4.50200	28.56870	23.40270
H	15.75700	15.87910	22.11810	H	4.50200	27.57610	22.11810
H	15.75700	22.11830	27.06670	H	4.50200	26.01730	27.06670
H	15.75700	23.11090	25.78210	H	4.50200	27.00990	25.78210
H	16.55200	21.63790	29.17790	H	6.75300	24.66980	23.40270
H	14.96190	17.35210	25.51390	H	6.75300	23.67710	22.11810
H	16.55200	17.35210	25.51390	H	6.75300	29.91630	27.06670
H	14.96190	21.63790	29.17790	H	6.75300	30.90890	25.78210
H	14.30100	17.73890	29.17790	H	7.54800	29.43590	29.17790
H	12.71090	21.25110	25.51390	H	5.95790	25.15010	25.51390
H	14.30100	21.25110	25.51390	H	7.54800	25.15010	25.51390
H	12.71090	17.73890	29.17790	H	5.95790	29.43590	29.17790
O	0.00000	28.57810	22.44640	H	5.29700	25.53690	29.17790
O	0.00000	26.00790	26.11040	H	3.70690	29.04910	25.51390
O	2.25100	24.67910	22.44640	H	5.29700	29.04910	25.51390
O	2.25100	29.90690	26.11040	H	3.70690	25.53690	29.17790



O	9.00400	28.57810	22.44640	H	14.30100	25.53690	29.17790
O	9.00400	26.00790	26.11040	H	12.71090	29.04910	25.51390
O	11.25500	24.67910	22.44640	H	14.30100	29.04910	25.51390
O	11.25500	29.90690	26.11040	H	12.71090	25.53690	29.17790
O	11.25500	29.83120	28.84960				
O	11.25500	24.75480	25.18560				
O	9.00400	25.93230	28.84960				
O	9.00400	28.65380	25.18560				
H	9.00400	28.56870	23.40270				
H	9.00400	27.57610	22.11810				
H	9.00400	26.01730	27.06670				
H	9.00400	27.00990	25.78210				
H	11.25500	24.66980	23.40270				
H	11.25500	23.67710	22.11810				
H	11.25500	29.91630	27.06670				
H	11.25500	30.90890	25.78210				
H	12.05000	29.43590	29.17790				
H	10.45990	25.15010	25.51390				
H	12.05000	25.15010	25.51390				
H	10.45990	29.43590	29.17790				
H	9.79900	25.53690	29.17790				
H	8.20890	29.04910	25.51390				
H	9.79900	29.04910	25.51390				
H	8.20890	25.53690	29.17790				
O	13.50600	28.57810	22.44640				
O	13.50600	26.00790	26.11040				
O	15.75700	24.67910	22.44640				
O	15.75700	29.90690	26.11040				
O	15.75700	29.83120	28.84960				
O	15.75700	24.75480	25.18560				
O	13.50600	25.93230	28.84960				
O	13.50600	28.65380	25.18560				
H	13.50600	28.56870	23.40270				
H	13.50600	27.57610	22.11810				
H	13.50600	26.01730	27.06670				
H	13.50600	27.00990	25.78210				
H	15.75700	24.66980	23.40270				
H	15.75700	23.67710	22.11810				
H	15.75700	29.91630	27.06670				
H	15.75700	30.90890	25.78210				
H	16.55200	29.43590	29.17790				
H	14.96190	25.15010	25.51390				
H	16.55200	25.15010	25.51390				
H	14.96190	29.43590	29.17790				
C. Protein Molecules							
1. 1RPB							
				N	-0.25079	4.10620	-2.90963
				C	-1.46579	4.66720	-3.57763
				C	-1.75979	4.21520	-5.05363
				O	-1.95579	5.02020	-5.96863
				C	-1.48979	6.19820	-3.36363
				S	-3.21279	6.72120	-3.33863
				H	0.61721	3.91420	-3.42163
				H	-2.34279	4.25920	-3.04163
				H	-1.04279	6.49320	-2.39463
				H	-0.91979	6.73120	-4.14663
				N	-1.89679	2.89920	-5.25463
				C	-2.42779	2.28220	-6.51363
				C	-3.55379	1.21720	-6.19063
				O	-3.94779	1.08520	-5.03063
				C	-1.25079	1.92220	-7.47263
				C	-0.63679	0.52020	-7.33363
				C	0.47521	0.30020	-8.36463
				C	-0.09479	0.30620	-5.92163
				H	-1.67079	2.34720	-4.42163
				H	-2.97179	3.03420	-7.07563
				H	-1.60479	2.03720	-8.51463
				H	-0.45279	2.69220	-7.39663
				H	-1.45279	-0.19780	-7.52363
				H	0.10421	0.43220	-9.39863
				H	1.31321	1.00920	-8.22463
				H	0.89221	-0.72080	-8.30063
				H	0.55321	1.14620	-5.60163
				H	-0.93479	0.27220	-5.20263
				H	0.46421	-0.63280	-5.81163
				N	-4.10379	0.46020	-7.16563
				C	-5.16279	-0.57380	-6.88563
				C	-4.79879	-2.07680	-6.96963
				O	-5.61379	-2.86980	-7.43863
				H	-3.73779	0.62620	-8.10663
				H	-5.63979	-0.42280	-5.90163

H	-6.01679	-0.42080	-7.56163	H	-0.21579	-4.55180	-0.24263
N	-3.60879	-2.46980	-6.49763	H	-1.43879	-4.32880	2.55137
C	-3.15479	-3.89880	-6.45263	H	0.93821	-3.46580	3.33137
C	-3.75779	-4.71480	-5.23763	H	0.71621	-5.18380	3.09237
O	-4.93379	-4.53480	-4.91063	N	-0.72679	-1.50180	2.34037
C	-1.58479	-3.87880	-6.67463	C	-1.08579	-0.05880	2.11737
C	-0.89579	-5.17380	-7.18563	C	0.18521	0.80420	1.78837
C	-0.73279	-3.37780	-5.47563	O	1.25721	0.60320	2.38037
C	-1.62579	-5.92180	-8.31263	C	-1.86279	0.43420	3.37637
H	-2.99479	-1.67780	-6.31863	C	-2.43079	1.85820	3.32737
H	-3.61879	-4.37980	-7.33863	O	-1.78179	2.81320	3.73237
H	-1.41079	-3.15380	-7.49863	N	-3.63679	2.08120	2.87037
H	0.07521	-4.83980	-7.58863	H	-0.12379	-1.80880	3.11337
H	-0.61379	-5.88280	-6.37163	H	-1.79579	0.02920	1.27037
H	-1.11679	-2.43780	-5.04763	H	-2.67979	-0.27080	3.62437
H	-0.67479	-4.11280	-4.64963	H	-1.20179	0.41420	4.26037
H	0.31121	-3.17680	-5.77863	H	-4.07779	1.33620	2.32137
H	-1.88179	-5.24980	-9.15463	H	-3.83479	3.08020	2.77537
H	-1.00379	-6.73780	-8.72463	N	0.03421	1.77120	0.85837
H	-2.56779	-6.38280	-7.96063	C	1.13421	2.69320	0.44837
N	-3.02279	-5.63280	-4.57463	C	1.40121	3.82920	1.47737
C	-3.59679	-6.43480	-3.45163	O	2.43421	3.77020	2.15137
C	-2.66179	-7.18080	-2.48663	C	1.05721	3.14620	-1.04563
O	-2.78179	-8.39380	-2.31663	C	-0.23479	3.79820	-1.59263
H	-2.08279	-5.77480	-4.95463	O	-1.19979	3.99620	-0.84863
H	-4.26979	-5.81280	-2.82963	H	-0.90579	1.83320	0.45037
H	-4.26379	-7.19480	-3.87463	H	2.06321	2.09520	0.46137
N	-1.79379	-6.43480	-1.80463	H	1.92121	3.80120	-1.25263
C	-0.94379	-6.97280	-0.69763	H	1.26321	2.26920	-1.68263
C	-1.06879	-6.13880	0.62637	N	0.52221	4.84620	1.61137
O	-1.54379	-6.65980	1.63737	C	0.75821	5.97920	2.55537
C	0.50221	-7.15980	-1.21963	C	-0.54779	6.49220	3.25637
O	1.33921	-7.76180	-0.23063	O	-1.12679	7.51520	2.88537
H	-1.79179	-5.46880	-2.13563	C	1.59321	7.08020	1.82737
H	-1.29179	-7.98780	-0.41363	C	2.33321	8.04120	2.77137
H	0.49921	-7.80480	-2.12163	C	3.60221	7.70820	3.25737
H	0.93821	-6.19880	-1.54363	C	1.74321	9.24720	3.16337
H	1.28321	-7.22880	0.56937	C	4.27021	8.56820	4.12537
N	-0.62479	-4.86880	0.64437	C	2.41121	10.10620	4.03437
C	-0.64779	-3.98980	1.85237	C	3.67421	9.76620	4.51337
C	-1.06579	-2.50780	1.50837	H	-0.29679	4.80120	0.99537
O	-1.74079	-2.28080	0.50437	H	1.40321	5.61620	3.38337
C	0.72021	-4.21880	2.55237	H	2.34321	6.61020	1.16037
S	2.09021	-4.27380	1.38137	H	0.95021	7.64920	1.13037

H	4.07121	6.77820	2.96437	C	-4.50979	-1.78380	-2.64363
H	0.75821	9.51520	2.80537	C	-5.58479	-1.03280	-3.13163
H	5.25021	8.30620	4.49837	C	-4.76279	-2.98480	-1.97963
H	1.94821	11.03420	4.33737	C	-6.88679	-1.50780	-3.01963
H	4.19221	10.43320	5.18837	C	-6.06879	-3.46280	-1.86863
N	-0.96079	5.78520	4.32537	C	-7.12779	-2.72580	-2.39363
C	-2.05179	6.19520	5.26037	O	-8.40679	-3.20180	-2.30863
C	-3.47679	6.39420	4.64537	H	-3.38279	1.29920	-3.11163
O	-3.93979	7.51720	4.43337	H	-2.52079	-0.68480	-0.96963
C	-1.55279	7.37820	6.12437	H	-2.99079	-1.00280	-3.98163
H	-0.48479	4.88320	4.39137	H	-2.44279	-2.28580	-2.96863
H	-2.16079	5.35920	5.97837	H	-5.42179	-0.07680	-3.60163
H	-0.59079	7.15820	6.62337	H	-3.93979	-3.55780	-1.57963
H	-1.40279	8.28820	5.51237	H	-7.70279	-0.93980	-3.44763
H	-2.27979	7.64120	6.91437	H	-6.24879	-4.41980	-1.40963
N	-4.17979	5.28520	4.35037	H	-8.37679	-4.09680	-1.96663
C	-5.53679	5.35120	3.72037	N	-0.09179	-1.28280	-1.86563
C	-5.67279	5.62520	2.19837	C	1.37021	-1.39380	-2.10763
O	-6.76679	5.44020	1.66737	C	1.81121	-2.88780	-2.20263
H	-3.68679	4.41220	4.56837	O	1.33521	-3.74080	-1.44663
H	-6.06379	4.40120	3.92137	C	2.13021	-0.69380	-0.96263
H	-6.15579	6.11220	4.23437	H	-0.61279	-2.04580	-1.41763
N	-4.61079	6.05420	1.49737	H	1.63921	-0.87080	-3.04963
C	-4.67979	6.40020	0.04237	H	1.87921	-1.10280	0.03337
C	-4.91679	5.21120	-0.96363	H	3.22821	-0.75780	-1.08163
O	-5.64579	5.37420	-1.94463	H	1.89621	0.37820	-0.93963
C	-3.40579	7.22420	-0.25263	N	2.77321	-3.19180	-3.08763
S	-3.45979	8.04620	-1.86163	C	3.45921	-4.53280	-3.10463
H	-3.77279	6.18320	2.08637	C	4.63921	-4.59180	-2.04763
H	-5.54079	7.08320	-0.10263	O	4.78521	-5.59080	-1.34063
H	-3.24979	8.03020	0.49337	C	3.92221	-4.93980	-4.55163
H	-2.50679	6.58320	-0.21263	C	4.51721	-6.36780	-4.61963
N	-4.32479	4.02820	-0.72863	C	2.81221	-4.89180	-5.62863
C	-4.57879	2.81820	-1.55463	H	3.09521	-2.40480	-3.65663
C	-3.69879	1.61520	-1.17163	H	2.72121	-5.30480	-2.79363
O	-3.58879	1.25520	0.00137	H	4.71721	-4.23580	-4.86663
H	-3.77179	4.01820	0.13337	H	5.39421	-6.48580	-3.95463
H	-5.63179	2.50320	-1.42463	H	3.78521	-7.14180	-4.31763
H	-4.48779	3.04020	-2.63663	H	4.86921	-6.63080	-5.63463
N	-3.11579	0.96220	-2.17863	H	1.94621	-5.52780	-5.36363
C	-2.38679	-0.32580	-2.00263	H	2.43621	-3.86480	-5.77263
C	-0.84179	-0.24080	-2.26563	H	3.17221	-5.22480	-6.62163
O	-0.32979	0.71620	-2.84863	N	5.46221	-3.52780	-1.92363
C	-3.05879	-1.36680	-2.94363	C	6.53221	-3.39880	-0.89763

C	5.86321	-2.69580	0.33137	N	4.03421	-0.87880	6.38737
O	5.52121	-1.50880	0.32337	C	3.70721	-1.38180	7.74837
C	7.78621	-2.63580	-1.44663	C	4.18421	-2.85580	7.93137
C	8.89321	-2.48880	-0.37563	O	4.11121	-3.73480	7.07337
C	8.44721	-3.30780	-2.67463	C	2.20621	-1.10180	8.04337
H	5.12821	-2.69480	-2.39463	C	1.14221	-1.81280	7.18337
H	6.89321	-4.41080	-0.61263	C	0.38321	-1.19780	6.16537
H	7.46721	-1.61480	-1.74363	C	0.68621	-3.11980	7.24237
H	8.53521	-1.93080	0.51237	N	-0.54479	-2.08980	5.58837
H	9.25421	-3.46880	-0.00963	C	-0.33279	-3.27480	6.26837
H	9.77121	-1.93280	-0.75363	C	1.06721	-4.21480	8.05937
H	7.74521	-3.39580	-3.52363	C	-0.97479	-4.52280	6.10137
H	9.31621	-2.73180	-3.04663	C	0.42321	-5.43980	7.87437
H	8.80521	-4.33080	-2.44763	C	-0.58279	-5.59180	6.91137
N	5.63221	-3.50780	1.35437	O	4.69121	-3.09180	9.17437
C	4.86721	-3.12180	2.56337	H	3.62221	-1.25380	5.52937
C	5.54021	-2.09580	3.53437	H	4.25921	-0.81480	8.51537
O	6.51221	-2.39480	4.23237	H	2.00221	-1.29680	9.11237
C	4.49421	-4.44680	3.25737	H	2.04521	-0.00980	7.96737
S	3.50421	-5.45680	2.14637	H	0.49321	-0.15980	5.88137
H	5.85521	-4.46580	1.07737	H	-1.31579	-1.88580	4.94237
H	3.90521	-2.68480	2.22637	H	1.86721	-4.10880	8.78137
H	5.38721	-5.00580	3.59837	H	-1.74779	-4.64980	5.35937
H	3.88121	-4.25280	4.15937	H	0.71321	-6.28880	8.47837
N	4.95121	-0.89280	3.60837	H	-1.05979	-6.55380	6.78837
C	5.37621	0.17720	4.57037				
C	5.07921	-0.09580	6.09337				
O	5.80021	0.38320	6.97037				
C	4.77321	1.53920	4.10737	2. 2ETI			
C	5.28821	2.09920	2.76437	N	10.34000	0.13600	-1.96700
C	4.71221	1.68820	1.55737	H	10.28800	0.52100	-1.03400
C	6.32121	3.04220	2.74137	H	11.31700	0.06100	-2.21100
C	5.15821	2.21220	0.34737	H	9.82600	0.72800	-2.60200
C	6.76721	3.56820	1.52937	C	9.71100	-1.19000	-1.86600
C	6.18421	3.15320	0.33437	H	9.67500	-1.66100	-2.84800
H	4.20821	-0.75280	2.91737	H	10.37800	-1.75300	-1.21200
H	6.47421	0.25720	4.52437	C	8.30300	-1.08300	-1.29900
H	3.66621	1.48520	4.08637	O	7.61200	-0.08600	-1.49300
H	4.96721	2.29520	4.89337	N	7.81300	-2.11900	-0.61500
H	3.90821	0.96520	1.55337	H	8.39000	-2.94800	-0.59100
H	6.78121	3.37220	3.66237	C	6.42100	-2.25000	-0.23200
H	4.70421	1.88920	-0.57863	H	5.85200	-2.10800	-1.15100
H	7.56521	4.29720	1.51737	C	6.12300	-3.66400	0.26100
H	6.52921	3.56120	-0.60463	H	6.99700	-4.05600	0.78100

H	5.95300	-4.33100	-0.61500	C	4.12900	5.80900	1.55900
S	4.72100	-3.80900	1.39600	H	3.62400	4.86400	1.35500
C	5.94900	-1.19200	0.75500	C	3.24900	6.55300	2.55900
O	5.01400	-0.45300	0.45800	H	2.40300	6.92600	1.98000
N	6.53200	-1.10800	1.95500	C	2.67300	5.58400	3.58600
C	6.22100	-0.05700	2.90000	H	2.37700	4.65500	3.09800
H	5.14200	0.03700	3.02200	H	3.38200	5.33500	4.37500
C	7.53400	-2.01200	2.48400	H	1.78600	6.03900	4.03000
H	8.31900	-2.24700	1.76600	C	3.87200	7.76100	3.25300
H	7.04500	-2.93400	2.79800	H	4.52800	7.44900	4.06700
C	6.85500	-0.52800	4.20400	H	4.42100	8.39000	2.55500
H	7.12700	0.28200	4.88100	C	2.82300	8.68400	3.86700
H	6.16900	-1.20300	4.71700	H	2.16400	9.06000	3.08500
C	8.08300	-1.28700	3.71000	H	2.24700	8.16800	4.63300
H	8.81500	-0.53600	3.41400	H	3.35800	9.51500	4.32300
H	8.53600	-1.98500	4.41600	C	4.19100	6.49800	0.20200
C	6.78200	1.26900	2.40400	O	4.34000	7.71400	0.10900
O	7.49300	1.31900	1.40400	N	4.02100	5.70100	-0.85600
N	6.51300	2.34900	3.14100	H	3.97300	4.71100	-0.65400
H	5.84100	2.22300	3.88200	C	3.84200	6.12500	-2.22900
C	6.90700	3.73300	2.96400	H	3.03900	6.86400	-2.23000
H	6.57100	4.21200	3.88500	C	5.10300	6.77200	-2.79600
C	8.42000	3.91000	2.86100	H	5.04300	6.78800	-3.88400
H	8.77400	3.49000	1.91900	H	5.10200	7.82200	-2.50500
H	8.65700	4.97200	2.91400	C	6.41500	6.14700	-2.33100
C	9.26200	3.27900	3.96700	H	6.59400	6.42800	-1.29200
H	9.17800	2.19400	3.92700	C	6.41200	4.62500	-2.42700
H	10.30700	3.54200	3.79600	H	6.09400	4.34200	-3.43000
C	8.87500	3.81500	5.34200	H	7.41200	4.23500	-2.23600
H	9.75800	3.82200	5.98000	H	5.74500	4.18100	-1.68700
H	8.50100	4.83700	5.27800	C	7.61400	6.65000	-3.13100
N	7.83700	2.98000	5.94700	H	7.69500	7.73000	-3.02600
H	7.34700	2.30500	5.38000	H	8.53400	6.19700	-2.75700
C	7.44200	3.14700	7.21700	H	7.49400	6.37400	-4.17800
N	6.63500	2.26500	7.82000	C	3.28300	5.01300	-3.10500
H	6.43800	1.36600	7.40600	O	3.56900	4.92000	-4.29700
H	6.34200	2.38800	8.77900	N	2.44600	4.14600	-2.53200
N	7.86800	4.21700	7.90200	H	2.17600	4.31100	-1.57200
H	8.43900	4.93300	7.47900	C	1.61800	3.20700	-3.26300
H	7.57200	4.36000	8.85700	H	1.52100	3.48600	-4.31300
C	6.07200	4.34900	1.85000	C	2.10800	1.76400	-3.17700
O	5.91500	3.75900	0.78500	H	2.18400	1.46500	-2.13100
N	5.42700	5.48800	2.11700	H	1.30400	1.17500	-3.61500
H	5.77700	6.11200	2.82900	C	3.36500	1.39100	-3.95900

H	3.35800	0.30100	-4.00600	H	-6.38800	1.26400	-3.29500
H	3.31900	1.77400	-4.97900	C	-7.87000	1.11500	-1.84000
S	5.00000	1.81700	-3.31100	H	-7.97700	1.50100	-0.82700
C	4.66900	1.75800	-1.53200	C	-9.15200	1.39100	-2.62100
H	4.13000	0.83300	-1.32200	H	-9.02700	1.06500	-3.65400
H	5.60600	1.77700	-0.97800	H	-9.96300	0.82500	-2.16100
H	4.07300	2.63400	-1.27700	C	-9.52200	2.87200	-2.62100
C	0.28900	3.32500	-2.53200	H	-9.31900	3.29600	-1.63600
O	0.20200	2.92100	-1.37500	H	-8.92500	3.39800	-3.36800
N	-0.67500	4.01800	-3.14100	C	-11.00300	3.04800	-2.94300
H	-0.72800	3.91000	-4.14400	H	-11.58300	2.80600	-2.05100
C	-1.75000	4.69900	-2.44800	H	-11.17800	4.09800	-3.17400
H	-1.52400	4.74700	-1.38300	C	-11.42500	2.19400	-4.13500
C	-1.92500	6.14300	-2.91300	H	-10.86400	2.48300	-5.02100
H	-2.98700	6.36200	-3.02000	H	-11.29300	1.12600	-3.96300
H	-1.57700	6.74400	-2.07300	N	-12.85900	2.36800	-4.41300
C	-1.17700	6.64900	-4.14400	H	-13.12100	3.33900	-4.33400
H	-1.01300	7.71600	-3.99600	H	-13.14200	2.02600	-5.32100
H	-0.19900	6.18800	-4.27400	H	-13.40400	1.87800	-3.71700
C	-1.95000	6.63100	-5.46000	C	-7.69200	-0.38400	-1.64100
H	-2.75300	7.36700	-5.41000	O	-8.52200	-0.95300	-0.93800
H	-1.24300	6.94700	-6.22700	N	-6.71800	-1.06400	-2.25300
N	-2.48400	5.31000	-5.79400	H	-6.14300	-0.56400	-2.91400
H	-2.39700	4.58300	-5.09900	C	-6.83500	-2.50300	-2.37700
C	-2.91100	4.92300	-7.00400	H	-7.26000	-2.90400	-1.45700
N	-3.27500	3.65800	-7.25100	C	-7.66200	-2.81600	-3.62100
H	-3.61500	2.99300	-6.57100	H	-6.96100	-3.09800	-4.40800
H	-3.09800	3.28000	-8.17100	H	-8.30000	-3.67400	-3.41100
N	-2.95100	5.78900	-8.02400	C	-8.47700	-1.71000	-4.28700
H	-2.65400	6.75200	-7.95600	H	-9.27600	-1.35000	-3.63800
H	-3.32900	5.44900	-8.89700	H	-7.82900	-0.88000	-4.57200
C	-2.99900	3.85800	-2.66500	C	-9.07200	-2.26600	-5.57200
O	-3.47000	3.77800	-3.79800	O	-8.60400	-1.97000	-6.66800
N	-3.48600	3.14100	-1.64900	N	-10.07100	-3.14400	-5.44000
H	-3.20000	3.28200	-0.69100	H	-10.51700	-3.50600	-6.27000
C	-4.42100	2.08200	-1.96700	H	-10.53900	-3.29900	-4.55900
H	-4.22400	1.72600	-2.97900	C	-5.60000	-3.39100	-2.45600
C	-4.18200	0.84800	-1.10300	O	-5.76700	-4.52400	-2.90300
H	-4.58500	0.00900	-1.66900	N	-4.38900	-2.97300	-2.07800
H	-3.11800	0.66200	-0.95400	H	-4.31400	-2.04200	-1.69200
S	-5.08400	0.96400	0.46200	C	-3.15700	-3.68700	-2.34500
C	-5.87500	2.49700	-1.79600	H	-2.36800	-3.06600	-1.92200
O	-6.20900	3.34800	-0.97300	C	-3.04200	-5.00700	-1.58700
N	-6.74300	1.75600	-2.48600	H	-1.97500	-5.18800	-1.45700

H	-3.51900	-4.92900	-0.61000	H	5.86900	-4.59900	-5.69000
C	-3.59500	-6.24100	-2.28800	H	5.47100	-3.11700	-6.51700
O	-4.63800	-6.74900	-1.82200	C	5.69000	-2.88800	-4.39500
O	-2.98200	-6.73500	-3.25900	H	4.99200	-2.99300	-3.56500
C	-2.82800	-3.90700	-3.81300	C	7.05200	-3.35500	-3.88800
O	-1.65600	-3.97600	-4.17600	H	7.69800	-3.61500	-4.72700
N	-3.82600	-3.96300	-4.69800	H	7.51900	-2.55900	-3.30900
H	-4.76900	-4.03200	-4.34000	H	6.92300	-4.23200	-3.25300
C	-3.65300	-3.97100	-6.13700	C	5.77600	-1.39600	-4.70800
H	-3.04600	-4.83900	-6.40100	H	4.88500	-1.05000	-5.23400
C	-5.04600	-4.09700	-6.74900	H	5.86200	-0.87400	-3.75500
H	-5.63800	-3.21300	-6.51100	H	6.65000	-1.17100	-5.31800
H	-4.96500	-4.15700	-7.83500	C	3.56200	-5.28000	-4.68500
O	-5.68400	-5.24200	-6.22900	O	3.33100	-5.00400	-3.51000
H	-6.37400	-5.46700	-6.85900	N	3.58500	-6.53800	-5.13100
C	-2.93700	-2.70300	-6.58300	H	3.71300	-6.69900	-6.11900
O	-2.08800	-2.68700	-7.47200	C	3.32500	-7.67100	-4.26400
N	-3.23300	-1.61600	-5.86800	H	2.37500	-7.46500	-3.77000
H	-3.96100	-1.71500	-5.17600	C	3.10200	-8.97300	-5.02700
C	-2.51600	-0.35800	-5.80400	H	3.80500	-9.13700	-5.84400
H	-2.62800	0.31900	-6.65100	H	3.16000	-9.83800	-4.36600
C	-3.22400	0.40500	-4.69000	H	2.08800	-8.95300	-5.42300
H	-3.27600	-0.23100	-3.80900	C	4.36200	-7.76900	-3.15500
H	-2.65000	1.30200	-4.45600	O	5.31500	-7.00000	-3.04200
C	-4.64200	0.79000	-5.09200	N	4.13000	-8.72900	-2.25900
O	-4.81100	1.71200	-5.91900	H	3.27600	-9.25800	-2.35900
O	-5.57200	0.20200	-4.50000	C	4.72400	-8.68900	-0.93800
C	-1.00900	-0.50100	-5.63200	H	4.39400	-9.54600	-0.35100
O	-0.31200	0.47200	-5.90900	H	5.80800	-8.74100	-1.04900
N	-0.47700	-1.65100	-5.20800	C	4.30200	-7.40700	-0.23600
H	-1.10000	-2.41800	-4.99800	O	5.07200	-6.86200	0.55100
C	0.89800	-1.84000	-4.79800	N	3.08900	-6.92500	-0.52200
H	1.45000	-0.91700	-4.98500	H	2.50600	-7.46700	-1.14100
C	0.98600	-2.15400	-3.30800	C	2.43800	-5.77100	0.06400
H	0.92000	-3.23000	-3.14800	H	2.82500	-5.70600	1.08000
H	1.91600	-1.79100	-2.87100	C	2.79800	-4.52500	-0.73700
S	-0.34700	-1.37300	-2.36500	H	3.75700	-4.65700	-1.23500
C	1.62000	-2.94800	-5.55300	H	2.03200	-4.25600	-1.46300
O	1.02700	-3.67100	-6.35300	S	3.08800	-3.13100	0.37900
N	2.92100	-3.05500	-5.27400	C	0.92500	-5.90700	0.15600
H	3.25700	-2.51500	-4.48900	O	0.28000	-6.24300	-0.83600
C	3.80200	-4.13800	-5.66400	N	0.33800	-5.59400	1.31500
H	3.59900	-4.47300	-6.68200	H	0.88800	-5.08600	1.99300
C	5.26300	-3.69700	-5.61700	C	-1.09000	-5.55400	1.55000

H	-1.64100	-5.80700	0.64400	N	-3.94000	5.14700	5.81500
C	-1.54200	-6.52500	2.63800	H	-2.93700	5.13600	5.93500
H	-2.58500	-6.28100	2.83500	C	-4.51300	6.37200	5.29400
C	-1.46800	-7.94000	2.06900	H	-5.57400	6.44000	5.53700
H	-1.86600	-7.94700	1.05400	C	-3.84500	7.63100	5.83900
H	-0.42300	-8.24600	2.04500	H	-3.88800	7.60700	6.92700
H	-2.05200	-8.64500	2.66100	H	-2.79800	7.70300	5.54700
C	-0.78800	-6.41800	3.96100	C	-4.57700	8.89900	5.41900
H	-0.73100	-5.37900	4.28900	O	-5.76700	8.86900	5.11600
H	-1.29900	-6.97500	4.74700	N	-3.93000	10.06700	5.45300
H	0.21200	-6.83500	3.87100	H	-4.46000	10.90200	5.24700
C	-1.40200	-4.12400	1.96500	H	-3.00000	10.14200	5.83700
O	-0.57200	-3.50000	2.62400	C	-4.45500	6.25100	3.77800
N	-2.57300	-3.60100	1.59300	O	-3.91000	7.10200	3.07800
H	-3.24900	-4.15700	1.08800	N	-4.99400	5.13500	3.28300
C	-2.92800	-2.24400	1.95500	H	-5.33500	4.44000	3.93300
H	-2.01200	-1.72000	2.22000	C	-4.98100	4.80900	1.87300
C	-3.45900	-1.42900	0.78100	H	-5.49800	3.86800	1.68700
H	-2.92700	-0.48100	0.86900	H	-5.50400	5.59600	1.32800
H	-3.21700	-1.85000	-0.19400	C	-3.53300	4.66800	1.42500
S	-5.22200	-1.02700	0.86500	O	-3.13800	5.24800	0.41600
C	-3.80900	-2.11200	3.19000	N	-2.75900	3.86700	2.16100
O	-4.52400	-3.02900	3.58800	H	-3.17300	3.32500	2.90700
N	-3.71700	-0.92900	3.80100	C	-1.43900	3.42700	1.76300
H	-3.01600	-0.27000	3.49300	H	-1.34700	3.48700	0.67700
C	-4.63100	-0.56800	4.86400	C	-0.33000	4.26300	2.39700
H	-5.61600	-0.91200	4.55000	H	-0.54500	4.39700	3.45700
H	-4.33000	-1.14400	5.74100	H	0.60700	3.71100	2.33800
C	-4.75400	0.92500	5.13300	C	-0.12300	5.59800	1.72000
O	-5.79300	1.50600	4.82700	C	-0.47900	6.77700	2.38200
N	-3.74200	1.55200	5.73800	H	-0.63900	6.78300	3.45000
C	-3.80200	2.79800	6.47800	C	0.39500	5.66500	0.42100
H	-4.26700	2.56500	7.43500	H	0.76300	4.77800	-0.07100
C	-2.52800	0.85000	6.10300	C	-0.53600	7.98600	1.67500
H	-1.88600	0.69000	5.23600	H	-0.84700	8.87300	2.20600
H	-2.74000	-0.09400	6.60200	C	0.51400	6.90500	-0.22100
C	-2.32800	3.10800	6.72800	H	1.04700	6.98900	-1.15600
H	-1.83800	3.39100	5.79600	C	0.00100	8.05700	0.38400
H	-2.22100	3.85500	7.51300	H	0.21800	9.01300	-0.06800
C	-1.79900	1.73000	7.11300	C	-1.27700	1.95700	2.11800
H	-0.72200	1.61100	7.00700	O	-2.06900	1.36600	2.85100
H	-2.13800	1.48100	8.11900	N	-0.21400	1.41100	1.52300
C	-4.60000	4.00100	5.99700	H	0.29600	2.04000	0.92100
O	-5.82000	3.95000	5.84400	C	0.28600	0.05400	1.60500



H	-0.52300	-0.59600	1.93400
C	0.75700	-0.36500	0.21500
H	0.48100	0.39700	-0.51200
H	1.83800	-0.49700	0.18500
S	-0.04800	-1.86100	-0.40900
C	1.43000	-0.07100	2.59900
O	2.23900	0.84200	2.75300
N	1.49600	-1.24600	3.22700
H	0.75500	-1.88300	2.97000
C	2.59800	-1.68400	4.06100
H	2.46600	-2.74300	4.28400
H	3.53200	-1.57200	3.51200
C	2.70900	-0.90200	5.36300
O	1.64600	-0.51400	5.89900
O	3.84200	-0.72700	5.86000

### 3. 1CMR

N	-2.95400	3.74000	7.98500
H	-2.58800	3.66900	8.95600
H	-3.84200	4.28100	7.98700
H	-3.12700	2.78700	7.60700
C	-1.95600	4.43800	7.13200
H	-1.06400	3.83300	7.17000
C	-2.46200	4.50300	5.64900
H	-1.63200	4.85200	4.99800
H	-2.68400	3.46100	5.32800
S	-3.93900	5.54400	5.33000
C	-1.62300	5.80100	7.68800
O	-2.22200	6.26100	8.66100
N	-0.66500	6.50800	7.02500
H	-0.11900	6.11900	6.29200
C	-0.33600	7.90100	7.21700
H	-0.83200	8.29700	8.09400
C	1.17000	8.11400	7.39600
H	1.42200	9.17800	7.24600
O	1.96700	7.35600	6.48700
H	2.88000	7.57800	6.68700
C	1.55300	7.72100	8.83800
H	0.97100	8.32300	9.56700
H	1.34400	6.64600	9.02200
H	2.63300	7.90600	9.01600
C	-0.90500	8.64500	6.01700
O	-1.80000	9.47700	6.15700

N	-0.38500	8.31500	4.80600
H	0.35400	7.64800	4.75600
C	-0.82100	8.80000	3.51000
H	-1.86000	9.10100	3.55500
C	0.02100	9.98100	2.97500
H	-0.20300	10.18900	1.90700
O	1.42400	9.75200	3.08100
H	1.60200	8.95500	2.57600
C	-0.33300	11.27300	3.74400
H	-1.42600	11.46300	3.69000
H	-0.03700	11.19800	4.81100
H	0.19500	12.14200	3.29800
C	-0.76400	7.56300	2.62400
O	-0.89500	6.43900	3.10500
N	-0.51500	7.76100	1.29600
H	-0.50500	8.69100	0.95100
C	-0.26600	6.79800	0.22900
H	-1.10400	6.11800	0.18200
C	-0.23900	7.51300	-1.15900
H	-0.02100	6.80100	-1.98400
H	-1.24800	7.93900	-1.34600
O	0.69000	8.59400	-1.21500
H	1.55500	8.20800	-1.05800
C	0.98600	5.94500	0.40100
O	1.03800	4.82500	-0.10000
N	2.01300	6.48000	1.13000
H	1.88400	7.37400	1.55700
C	3.35900	5.93600	1.28400
H	3.65200	5.53200	0.33600
C	4.40000	7.05300	1.56100
H	5.43000	6.67000	1.38500
H	4.22400	7.86700	0.82200
C	4.32900	7.65600	2.97200
H	3.26500	7.87200	3.20200
H	4.69300	6.89400	3.69300
C	5.17200	8.92900	3.13900
H	6.20600	8.71200	2.78600
H	4.75500	9.73100	2.49200
C	5.26100	9.42600	4.59000
H	5.68600	8.63600	5.24400
H	5.90200	10.33100	4.64700
N	3.93000	9.78700	5.12900
H	3.51200	10.53900	4.54500
H	3.31100	8.95100	5.11200

H	4.03100	10.12300	6.10800	C	4.80300	6.58300	-2.52300
C	3.50600	4.81300	2.30100	H	4.18300	7.31100	-3.02300
O	4.57900	4.22500	2.42700	C	6.95000	5.96800	-1.53100
N	2.40700	4.49000	3.04100	H	7.96700	6.23500	-1.28200
H	1.55500	4.98900	2.90200	C	6.13000	6.89800	-2.18900
C	2.32300	3.45000	4.05400	H	6.52400	7.87200	-2.44000
H	3.31900	3.12500	4.32300	C	4.72900	-0.32700	0.29200
C	1.63300	4.00600	5.33100	O	5.46300	-1.05100	-0.37700
H	2.09200	4.99800	5.53800	N	4.55700	-0.48600	1.62800
H	0.55600	4.19800	5.13300	H	3.96100	0.14200	2.12200
C	1.77100	3.17000	6.62100	C	5.19600	-1.48000	2.45900
H	1.26400	3.70400	7.45500	H	5.66300	-2.25200	1.85900
H	1.28100	2.18300	6.50000	C	6.29400	-0.81000	3.34300
C	3.24400	2.98400	6.98500	H	6.96300	-0.22500	2.67600
O	3.92300	4.01100	7.25300	H	5.85100	-0.10000	4.07400
O	3.70900	1.81200	7.00000	O	7.11700	-1.74800	4.02900
C	1.58400	2.24600	3.49000	H	7.50500	-2.30600	3.35100
O	1.39800	1.23300	4.16300	C	4.07000	-2.09300	3.27700
N	1.17600	2.33700	2.19200	O	3.99400	-1.88200	4.48600
H	1.33500	3.18000	1.68300	N	3.14800	-2.85700	2.61800
C	0.55300	1.28800	1.40700	H	3.21700	-3.04000	1.64100
H	0.28900	0.45500	2.04300	C	1.95700	-3.40500	3.24800
C	-0.74100	1.77900	0.70500	H	2.16700	-3.57000	4.29900
H	-0.49100	2.58800	-0.01700	C	0.74700	-2.45600	3.15600
H	-1.20200	0.95500	0.11500	H	1.15600	-1.44200	3.34700
S	-1.98300	2.43600	1.86900	C	0.06500	-2.35700	1.77000
C	1.54200	0.77500	0.37100	H	0.80800	-2.20100	0.96000
O	1.18100	0.00900	-0.52000	H	-0.50800	-3.28000	1.55700
N	2.83600	1.18800	0.49700	H	-0.65100	-1.51100	1.75200
H	3.07800	1.80800	1.23900	C	-0.26400	-2.77700	4.27700
C	3.96700	0.82200	-0.34400	H	0.23900	-2.76200	5.26700
H	3.63800	0.52400	-1.32600	H	-1.07600	-2.02000	4.28200
C	4.94100	2.00700	-0.55400	H	-0.71900	-3.77800	4.12000
H	5.30400	2.36700	0.43500	C	1.70600	-4.77700	2.67400
H	5.82900	1.68200	-1.14100	O	1.55800	-5.74800	3.41000
C	4.37700	3.21200	-1.29100	N	1.66800	-4.86200	1.31800
C	5.15600	4.39200	-1.52100	H	1.73900	-4.00200	0.81500
C	3.14300	3.46200	-1.82100	C	1.46300	-6.05800	0.51300
H	2.30400	2.78700	-1.78400	H	1.15300	-6.88600	1.13700
N	3.09300	4.73300	-2.34900	C	0.39100	-5.85200	-0.59200
H	2.27600	5.18600	-2.64000	H	0.65800	-4.95600	-1.19400
C	4.32700	5.32100	-2.18300	H	0.36600	-6.72200	-1.28400
C	6.46600	4.69800	-1.18900	S	-1.30500	-5.68400	0.03900
H	7.07900	3.97400	-0.67600	C	2.76700	-6.45400	-0.15000

O	2.81200	-7.39200	-0.94000	C	2.85000	-9.72100	3.12800
N	3.87200	-5.74100	0.18600	H	3.09100	-10.29600	4.01500
H	3.77300	-4.95700	0.79500	C	1.41400	-9.15400	3.31900
C	5.24500	-5.99700	-0.20800	H	1.54100	-8.16500	3.81300
H	5.27900	-6.55200	-1.14000	H	0.90400	-8.95400	2.35300
C	5.97500	-4.63700	-0.37500	C	0.47400	-9.95600	4.26000
H	5.42500	-4.06600	-1.15800	H	0.99800	-10.05000	5.24000
H	5.88800	-4.05400	0.57000	C	-0.81900	-9.15600	4.51800
C	7.45500	-4.71100	-0.78300	H	-0.57700	-8.15200	4.92500
H	8.04200	-5.21500	0.01400	H	-1.38600	-9.02800	3.57100
H	7.56100	-5.28100	-1.72900	H	-1.46300	-9.68900	5.24900
C	7.99600	-3.28700	-0.95900	C	0.13700	-11.38300	3.78900
O	8.60800	-2.73100	-0.04000	H	-0.32200	-11.35700	2.78100
N	7.75000	-2.69500	-2.16700	H	1.04800	-12.01500	3.75400
H	8.07300	-1.76500	-2.34200	H	-0.58100	-11.85700	4.49200
H	7.24300	-3.19000	-2.87300	C	2.94100	-10.65100	1.93900
C	5.90600	-6.83400	0.87100	O	3.14800	-11.85300	2.10300
O	6.79700	-7.64100	0.60900	N	2.79000	-10.09700	0.70100
N	5.42300	-6.63800	2.12700	H	2.61400	-9.12300	0.59500
H	4.71500	-5.95100	2.25600	C	2.83100	-10.81600	-0.56100
C	5.83600	-7.28300	3.35700	H	2.83900	-11.88300	-0.37500
H	6.83600	-7.68100	3.24100	N	-0.19600	-11.84300	-0.13200
C	5.84100	-6.26100	4.52700	H	0.24500	-12.74000	-0.19200
H	4.80600	-5.87300	4.68900	C	0.29000	-10.66600	-0.66000
H	6.18000	-6.74700	5.46900	C	1.57400	-10.54700	-1.43200
C	6.73400	-5.02700	4.27900	H	1.59400	-9.52700	-1.87000
H	6.32200	-4.45600	3.41800	H	1.50800	-11.30000	-2.24600
H	6.66800	-4.36700	5.17300	N	-1.67200	-10.26200	0.38000
C	8.21700	-5.32100	3.98900	C	-0.62500	-9.71100	-0.33600
H	8.31800	-5.92900	3.06300	H	-0.63100	-8.65500	-0.56800
H	8.76900	-4.36400	3.86300	C	-1.37200	-11.54300	0.47600
N	8.80600	-6.07200	5.15100	H	-1.97800	-12.29000	0.98500
H	8.23100	-6.23200	5.95300	C	4.14500	-10.48500	-1.25600
C	10.08700	-6.55700	5.15600	O	5.20500	-10.69100	-0.66700
N	10.91100	-6.36900	4.08500	N	4.12600	-9.98700	-2.52700
H	10.58100	-5.87100	3.28300	H	3.28400	-9.71800	-2.98500
H	11.84400	-6.72900	4.10300	C	5.30700	-9.84800	-3.36200
N	10.54300	-7.23800	6.24700	H	6.15700	-9.54000	-2.76200
H	9.94200	-7.37800	7.03400	C	5.60200	-11.14000	-4.19900
H	11.47600	-7.59500	6.25900	H	4.67800	-11.42100	-4.75800
C	4.92300	-8.44300	3.72000	H	6.42300	-10.97700	-4.93100
O	5.18000	-9.14300	4.69800	C	6.01800	-12.33200	-3.32000
N	3.83200	-8.66600	2.93200	O	5.26900	-13.30700	-3.18700
H	3.65300	-8.07700	2.14800	N	7.24500	-12.23700	-2.72400

H	7.57600	-12.97900	-2.14100	H	4.80800	5.31800	-5.39700
H	7.80900	-11.42400	-2.86800	N	4.27400	6.09400	-7.27800
C	5.04200	-8.74000	-4.35400	H	5.14700	5.75800	-7.73300
O	5.43700	-8.83600	-5.51500	H	3.48900	6.05000	-7.96000
N	4.34700	-7.64800	-3.93300	H	4.40300	7.07500	-6.96100
H	4.03900	-7.53500	-2.99600	C	1.63400	0.29800	-4.09900
C	3.90200	-6.56900	-4.79000	O	1.06000	-0.78600	-4.02000
H	4.16200	-6.76900	-5.82300	N	1.02800	1.45600	-3.76500
C	2.37600	-6.43000	-4.77400	H	1.52000	2.32000	-3.83300
H	2.04900	-5.60500	-5.43600	C	-0.30700	1.53800	-3.23900
O	1.84400	-6.16900	-3.48300	H	-1.01300	1.10500	-3.93200
H	2.24100	-5.34400	-3.19500	H	-0.31100	1.06600	-2.26800
C	1.77000	-7.74700	-5.31600	C	-0.64100	2.97600	-3.03300
H	2.17400	-7.96200	-6.32800	O	0.18100	3.86600	-3.24700
H	2.02100	-8.61200	-4.66200	N	-1.88800	3.22800	-2.57200
H	0.66500	-7.66500	-5.38700	H	-2.57000	2.51300	-2.46700
C	4.69200	-5.32900	-4.40900	C	-2.35300	4.50200	-2.10100
O	5.72800	-5.42400	-3.75400	H	-1.55100	5.00200	-1.57900
N	4.23200	-4.13800	-4.86100	C	-2.89400	5.44600	-3.21400
H	3.35600	-4.09000	-5.33200	H	-3.35300	6.32600	-2.72800
C	4.99800	-2.90600	-4.84700	H	-2.00900	5.81200	-3.77600
H	5.90600	-3.02100	-4.27800	C	-3.91600	4.86500	-4.18800
C	5.42100	-2.51400	-6.29900	C	-3.61100	4.19800	-5.42800
H	5.90700	-3.40100	-6.76000	C	-5.27600	4.83200	-4.05900
H	4.53900	-2.26500	-6.92700	H	-5.82400	5.24300	-3.22400
O	6.37500	-1.45500	-6.34900	N	-5.84400	4.16800	-5.12100
H	6.58500	-1.33100	-7.27700	H	-6.78900	3.93700	-5.20700
C	4.20000	-1.84000	-4.13000	C	-4.84000	3.76200	-5.97200
O	4.10900	-1.83200	-2.90400	C	-2.40700	3.94600	-6.08000
N	3.63600	-0.89500	-4.92400	H	-1.46000	4.28200	-5.69000
H	3.72500	-1.02600	-5.90500	C	-4.88100	3.05000	-7.16600
C	3.08200	0.39500	-4.54900	H	-5.81100	2.69100	-7.57900
H	3.65800	0.78800	-3.72100	C	-2.45100	3.23700	-7.28800
C	3.25200	1.38300	-5.74200	H	-1.53100	3.02600	-7.81400
H	4.19000	1.09100	-6.27000	C	-3.66900	2.79000	-7.82100
H	2.42900	1.27400	-6.48000	H	-3.67400	2.23600	-8.74800
C	3.44000	2.86000	-5.35000	C	-3.39700	4.16900	-1.07400
H	2.51900	3.24400	-4.86200	O	-3.92000	3.05800	-1.04700
H	4.27100	2.92800	-4.61300	N	-3.72200	5.14100	-0.18400
C	3.76400	3.77400	-6.53900	H	-3.30700	6.04600	-0.23700
H	4.69000	3.40400	-7.03300	C	-4.62500	4.94400	0.93100
H	2.93000	3.71300	-7.27400	H	-4.82900	3.88700	1.06400
C	3.96300	5.23500	-6.11300	C	-4.01100	5.43900	2.27200
H	3.04100	5.63000	-5.63700	H	-2.94200	5.13100	2.27500

H	-3.99900	6.55100	2.32900	H	-10.16500	0.90800	-0.90400
S	-4.82300	4.68400	3.72600	H	-9.54500	0.86200	0.79500
C	-5.93800	5.63400	0.64500	N	-10.72500	-0.83800	0.19200
O	-5.99600	6.84700	0.45400	H	-11.67400	-1.11800	0.33400
N	-7.03500	4.82700	0.66200	C	-9.76900	-1.81100	0.07200
H	-6.95300	3.83300	0.73800	N	-8.46000	-1.48300	-0.11800
C	-8.41900	5.23800	0.64400	H	-8.18800	-0.52200	-0.17000
H	-8.51600	6.29500	0.42600	H	-7.77100	-2.20300	-0.20100
C	-9.19500	4.39100	-0.40300	N	-10.13400	-3.12400	0.14600
H	-8.92400	3.31800	-0.29700	H	-11.09300	-3.36800	0.28700
H	-10.28900	4.47900	-0.29100	H	-9.44100	-3.84000	0.06100
C	-8.83000	4.86300	-1.81300	C	-10.33000	0.68600	3.61400
O	-9.06900	6.06300	-2.11600	O	-10.48400	-0.45300	4.05200
O	-8.31800	4.03100	-2.60600	N	-9.09400	1.22900	3.42200
C	-8.93400	5.01000	2.05400	H	-8.98300	2.14900	3.05100
O	-8.20200	4.52800	2.91900	C	-7.85100	0.54900	3.72500
N	-10.22300	5.35900	2.33300	H	-7.50800	0.89600	4.68900
H	-10.80000	5.76700	1.63400	H	-7.97400	-0.52600	3.66600
C	-10.85600	5.29700	3.64700	C	-6.83800	0.94400	2.69700
H	-10.09700	5.43500	4.40500	O	-6.99900	1.93700	1.98900
N	-10.26800	8.34400	4.35600	N	-5.75200	0.12900	2.58100
H	-9.88100	7.93300	5.18300	H	-5.66000	-0.65400	3.19100
C	-11.25300	7.79400	3.56400	C	-4.68000	0.26300	1.60700
C	-11.88000	6.44800	3.82000	H	-4.56900	1.30300	1.32500
H	-12.72500	6.32100	3.10800	C	-3.30400	-0.26000	2.12800
H	-12.29200	6.46200	4.85200	H	-3.46000	-1.20700	2.68800
N	-10.61700	9.77700	2.69300	H	-2.61100	-0.48400	1.28500
C	-11.45200	8.68300	2.55100	S	-2.39200	0.92200	3.16200
H	-12.12700	8.63600	1.70600	C	-5.00400	-0.52100	0.35400
C	-9.92600	9.52900	3.78900	O	-5.39400	-1.68700	0.40300
H	-9.16400	10.18300	4.20800	N	-4.74900	0.14200	-0.80800
C	-11.52500	3.95900	3.93200	H	-4.52900	1.11300	-0.75900
O	-12.33900	3.84200	4.84600	C	-4.72600	-0.38100	-2.16600
N	-11.15200	2.91500	3.14500	H	-5.46600	-1.16300	-2.25300
H	-10.55000	3.06200	2.37100	C	-5.04500	0.71300	-3.19300
C	-11.53900	1.53400	3.26600	H	-4.26700	1.51300	-3.16100
H	-12.23500	1.42100	4.08400	C	-5.03900	0.16000	-4.63600
C	-12.26900	1.05200	1.98200	H	-5.68400	-0.74000	-4.70700
H	-12.49400	-0.03200	2.03300	H	-5.42000	0.93300	-5.33400
H	-13.24800	1.58400	1.99600	H	-4.00900	-0.10900	-4.95100
C	-11.65600	1.41700	0.60500	C	-6.39100	1.40500	-2.84600
H	-12.45300	1.24600	-0.14900	H	-6.38900	1.72800	-1.78500
H	-11.43000	2.50300	0.56500	H	-6.46600	2.32600	-3.45800
C	-10.41500	0.63300	0.14400	C	-7.65100	0.57800	-3.10900

H	-7.60700	-0.39700	-2.58100				
H	-8.54000	1.13700	-2.74600				
H	-7.77500	0.40100	-4.19900				
C	-3.33800	-0.95700	-2.40000				
O	-2.34900	-0.37300	-1.96500				
N	-3.24900	-2.14000	-3.06000				
H	-4.05400	-2.62600	-3.38400				
C	-2.02500	-2.86800	-3.29100				
H	-1.15300	-2.29600	-2.98300				
C	-2.03800	-4.20500	-2.51000				
H	-2.97500	-4.76800	-2.71300				
H	-1.18900	-4.83500	-2.83800				
S	-1.89000	-3.90000	-0.72400				
C	-1.93700	-3.12600	-4.77700				
O	-2.74000	-3.87400	-5.33400				
N	-0.93000	-2.49900	-5.44700				
H	-0.31200	-1.88000	-4.96600				
C	-0.61800	-2.63700	-6.85800				
H	-1.36300	-3.24200	-7.36000				
C	-0.51400	-1.26500	-7.58100				
H	0.31600	-0.67000	-7.13700				
H	-0.27800	-1.41600	-8.65900				
C	-1.78900	-0.40400	-7.48500				
H	-2.02400	-0.18800	-6.42100				
H	-1.61200	0.56300	-8.00200				
C	-2.96900	-1.11100	-8.15000				
O	-2.89100	-1.36100	-9.38300				
O	-3.96500	-1.40600	-7.43800				
C	0.71300	-3.34400	-6.96200				
O	1.57500	-3.18600	-6.10200				
N	0.89300	-4.13500	-8.04700				
H	0.17400	-4.19800	-8.73300				
C	2.07700	-4.92900	-8.32900				
H	2.49500	-5.31400	-7.40300				
C	1.76500	-6.12900	-9.25200				
H	1.35800	-5.77100	-10.22200				
H	2.68900	-6.71600	-9.44400				
O	0.80600	-6.98900	-8.65100				
H	0.66400	-7.70400	-9.27600				
C	3.14800	-4.07800	-9.03500				
O	2.77700	-3.14000	-9.79000				
O	4.35400	-4.39400	-8.85100				
				4. 1CNR			
				N	6.02300	3.46900	6.20900
				C	5.94100	3.95300	4.80800
				C	7.28000	4.32500	4.18400
				O	7.88100	5.29200	5.02600
				C	7.10900	4.89900	2.78400
				C	5.26800	2.83500	4.03700
				O	5.61600	1.65400	4.23800
				N	4.37400	3.24500	3.16600
				C	3.71400	2.25300	2.29300
				C	2.18600	2.42400	2.37500
				O	1.92900	3.74400	1.93100
				C	1.64000	2.20400	3.78000
				C	4.32700	2.34400	0.87300
				O	4.62900	3.43400	0.38400
				N	4.45900	1.16200	0.27800
				C	4.99200	1.03800	-1.08600
				C	6.39600	0.45700	-1.06000
				S	7.58900	1.21400	0.08100
				C	4.08000	0.14000	-1.85400
				O	3.68700	-0.90200	-1.30300
				N	3.80900	0.46100	-3.09600
				C	2.87200	-0.36900	-3.87800
				C	1.56400	0.39200	-4.14400
				S	0.58200	0.70500	-2.64800
				C	3.49500	-0.84600	-5.17200
				O	4.32000	-0.17300	-5.78500
				N	3.08300	-2.05300	-5.61500
				C	3.69700	-2.67000	-6.77400
				C	2.19300	-3.00800	-4.90200
				C	3.30200	-4.15400	-6.66200
				C	1.95600	-4.11400	-5.95600
				C	3.27300	-2.10100	-8.08500
				O	3.96600	-2.29500	-9.09400
				N	2.13900	-1.40600	-8.08800
				C	1.56800	-0.81700	-9.29300
				C	0.79800	-1.83100	-10.13200
				O	-0.40600	-2.17700	-9.44800
				C	0.64300	0.32000	-8.89100
				O	0.26800	0.43200	-7.72400
				N	0.29500	1.10900	-9.88800
				C	-0.62900	2.25900	-9.67200
				C	-0.69000	3.12800	-10.92100

C	-1.80900	4.11900	-10.81300	C	-3.41700	0.88700	-1.14500
C	0.68600	3.76800	-11.03200	C	-2.81100	0.95900	0.22000
C	0.95100	4.66800	-12.23600	C	-2.64100	2.19200	0.84000
C	-1.99600	1.76400	-9.16800	C	-2.37600	-0.19700	0.86500
O	-2.55100	2.33600	-8.23700	C	-2.04700	2.27900	2.09600
N	-2.48800	0.73800	-9.84600	C	-1.80400	-0.13600	2.13400
C	-3.82900	0.29700	-9.42300	C	-1.65500	1.11700	2.74900
C	-4.40800	-0.61600	-10.52900	C	-5.59500	2.06400	-0.54300
C	-5.58100	-1.39700	-9.99000	O	-6.05700	2.04900	0.61100
C	-4.72200	0.20500	-11.77300	N	-5.57600	3.13200	-1.33500
C	-3.81500	-0.27400	-7.98600	C	-6.12200	4.39000	-0.82400
O	-4.77600	-0.07900	-7.20800	C	-5.76900	5.54300	-1.77300
N	-2.71000	-0.94400	-7.62400	C	-4.30600	5.93200	-1.68300
C	-2.60400	-1.41400	-6.26000	O	-3.63900	5.71500	-0.64800
C	-1.34200	-2.25200	-6.05300	N	-3.80600	6.57100	-2.72400
C	-2.67400	-0.22400	-5.27200	C	-7.61700	4.30400	-0.57400
O	-3.34100	-0.29800	-4.24000	O	-8.11100	4.89400	0.38400
N	-1.93900	0.84000	-5.61300	N	-8.31800	3.54000	-1.41800
C	-2.00000	2.03400	-4.78100	C	-9.73400	3.31200	-1.10700
C	-1.00000	3.10300	-5.26300	C	-10.50600	2.69400	-2.30000
C	-1.06500	4.42300	-4.50100	C	-11.88000	2.16500	-1.94600
C	-0.55100	4.36800	-3.08500	C	-10.58800	3.71000	-3.43300
N	0.85000	4.06900	-3.01800	C	-9.91700	2.47200	0.18400
C	1.51100	3.96100	-1.86100	O	-10.76000	2.77300	1.02700
N	0.90000	4.13000	-0.69100	N	-9.12400	1.40600	0.29200
N	2.79200	3.64100	-1.88300	C	-9.11800	0.56700	1.49100
C	-3.40400	2.65300	-4.71500	C	-8.06200	-0.51700	1.33300
O	-3.88600	3.05400	-3.64100	S	-7.87700	-1.61300	2.75200
N	-4.06400	2.68800	-5.86300	C	-8.91800	1.40400	2.76800
C	-5.40700	3.25700	-5.90200	O	-9.56100	1.12000	3.78700
C	-5.91400	3.35200	-7.32700	N	-8.08100	2.44000	2.65500
O	-5.04200	4.16500	-8.11600	C	-7.82100	3.24300	3.83900
C	-6.36900	2.43500	-5.02900	C	-6.47900	4.01100	3.63800
O	-7.16300	2.98000	-4.23300	C	-5.26000	3.11000	3.63600
N	-6.22000	1.11600	-5.11600	C	-4.86000	2.68400	5.01900
C	-7.05500	0.23700	-4.28100	N	-4.25600	3.80400	5.75700
C	-6.97400	-1.17800	-4.83400	C	-4.11900	3.91500	7.07100
C	-7.62500	-1.29600	-6.21800	N	-4.66900	3.04500	7.90300
O	-8.46000	-0.46300	-6.61400	N	-3.40300	4.92000	7.57600
N	-7.26800	-2.35300	-6.92400	C	-8.93900	4.22000	4.23600
C	-6.69100	0.38500	-2.78300	O	-8.97900	4.63700	5.39300
O	-7.58900	0.28400	-1.93100	N	-9.82100	4.53700	3.28300
N	-5.40900	0.58200	-2.51900	C	-10.84300	5.54600	3.55300
C	-4.95000	0.81800	-1.15500	C	-11.80000	5.73500	2.36500

C	-11.21100	6.38700	1.13400	N	-3.68000	-4.58900	6.79600
C	-12.26900	6.34300	0.05200	C	-4.76100	-5.26500	6.08500
C	-10.71200	7.80400	1.38000	C	-6.08500	-5.15900	6.83800
C	-11.66400	5.22600	4.83100	C	-6.19800	-6.11600	8.02100
O	-11.88200	6.17300	5.63100	C	-7.36500	-5.73800	8.93600
N	-12.11000	4.01100	5.05400	C	-6.30500	-7.55400	7.56600
C	-12.85100	3.72700	6.30300	C	-4.92900	-4.73000	4.65000
C	-12.26900	2.87000	4.07300	O	-5.16500	-5.50900	3.71600
C	-13.56700	2.41800	6.04900	N	-4.76600	-3.41800	4.51700
C	-12.77600	1.71800	4.94100	C	-4.81900	-2.88500	3.14500
C	-12.00000	3.62400	7.55500	C	-4.85100	-1.36600	3.10400
O	-12.54200	3.47500	8.64600	S	-6.39000	-0.71300	3.85200
N	-10.67600	3.67300	7.36900	C	-3.64500	-3.41900	2.28900
C	-9.74300	3.60000	8.49100	O	-3.79500	-3.59700	1.06700
C	-9.03100	2.24700	8.68100	N	-2.52100	-3.66600	2.95300
O	-8.34000	2.06000	9.67900	C	-1.35400	-4.22400	2.28400
N	-9.22800	1.33400	7.71200	C	-0.12900	-4.21600	3.21500
C	-8.63000	0.02000	7.75700	C	-1.63100	-5.63400	1.71700
C	-8.77900	-0.66400	6.39000	O	-1.44400	-5.87900	0.51000
O	-10.12400	-0.50900	5.93900	N	-2.09200	-6.53900	2.58100
C	-8.42600	-2.14200	6.44800	C	-2.36700	-7.87300	2.07000
C	-7.15500	0.08100	8.08400	C	-2.62300	-8.90900	3.22000
O	-6.45400	0.87000	7.41200	O	-3.63600	-8.33800	4.02500
N	-6.61000	-0.73200	8.97000	C	-1.35800	-9.21700	3.99900
C	-5.15900	-0.77400	9.18200	C	-3.53900	-7.89900	1.05800
C	-7.34300	-1.65800	9.87400	O	-3.57200	-8.75000	0.16600
C	-4.98400	-1.95200	10.11600	N	-4.42800	-6.93000	1.21300
C	-6.27700	-2.04700	10.91200	C	-5.56000	-6.84600	0.28800
C	-4.37900	-0.92700	7.91400	C	-6.60500	-5.90400	0.92000
O	-4.76400	-1.74300	7.02900	C	-7.64700	-5.33600	-0.01300
N	-3.23900	-0.25800	7.85400	C	-8.65000	-6.12600	-0.58000
C	-2.38800	-0.43300	6.68500	C	-7.63700	-3.97500	-0.29000
C	-1.11100	0.41700	6.83800	C	-9.59400	-5.57900	-1.44400
C	-1.36700	1.89000	6.69900	C	-8.57200	-3.41100	-1.14300
C	-0.13500	2.75600	6.71800	C	-9.53700	-4.21300	-1.72400
O	0.95800	2.29000	7.09800	O	-10.45900	-3.62600	-2.55000
O	-0.30000	4.00800	6.37100	C	-5.13900	-6.44000	-1.13800
C	-2.01000	-1.88600	6.41700	O	-5.78600	-6.80800	-2.12000
O	-1.91600	-2.23800	5.24500	N	-4.06900	-5.63000	-1.21900
N	-1.77800	-2.64000	7.48000	C	-3.62800	-5.05500	-2.49200
C	-1.34800	-4.02100	7.26800	C	-3.48500	-3.49600	-2.34600
C	-1.00600	-4.70600	8.59100	O	-2.50600	-3.23200	-1.33000
C	-2.40000	-4.84400	6.50200	C	-4.77400	-2.79500	-1.99500
O	-2.06700	-5.69600	5.66900	C	-2.30500	-5.52000	-3.08600



O	-2.03700	-5.27800	-4.26400	C	11.17400	3.90500	5.37300
N	-1.48500	-6.13500	-2.23400	O	9.93500	3.78900	5.44900
C	-0.10900	-6.39500	-2.62800	N	11.80600	4.74700	4.54600
C	0.86700	-5.26700	-2.29900	C	11.08800	5.66300	3.66700
O	2.07300	-5.39200	-2.54800	C	11.37000	7.11200	4.07800
N	0.33500	-4.15100	-1.78500	C	11.43200	5.49100	2.17800
C	1.21100	-3.12000	-1.22000	O	10.91000	6.24700	1.34400
C	0.44900	-1.83400	-0.92400	N	12.26900	4.50300	1.90300
S	-0.38900	-1.06800	-2.32700	C	12.80500	4.32500	0.54600
C	1.88700	-3.67100	0.03400	C	14.34500	4.29500	0.54400
O	1.53400	-4.73000	0.54900	O	14.84000	5.46900	1.19300
N	2.89500	-2.91800	0.49200	C	14.97700	4.27700	-0.84100
C	3.71800	-3.33200	1.61200	C	12.22100	3.05800	-0.05700
C	5.07500	-3.92400	1.19400	O	12.74100	1.96100	0.16100
C	4.83400	-5.12200	0.28700	N	11.18300	3.24600	-0.86000
C	5.97000	-2.89000	0.52800	C	10.55300	2.09500	-1.50800
C	7.38000	-3.37100	0.18700	C	9.21000	2.49600	-2.08500
C	3.94100	-2.12800	2.55500	S	7.99900	2.98500	-0.83500
O	3.81100	-0.96600	2.15600	C	11.45000	1.55300	-2.58900
N	4.22900	-2.47100	3.80000	O	12.03200	2.34100	-3.36000
C	4.66400	-1.52300	4.84600	N	11.55300	0.25500	-2.72500
C	3.95900	-1.70000	6.19000	C	12.38900	-0.40500	-3.74000
C	4.55300	-0.77800	7.26000	C	10.96100	-0.79500	-1.82200
C	2.44900	-1.46100	6.11200	C	12.53700	-1.84200	-3.27900
C	1.69600	-1.95100	7.33800	C	11.22500	-2.12100	-2.55900
C	6.10800	-1.76500	5.08200	C	11.78200	-0.27400	-5.11900
O	6.47900	-2.92300	5.34900	O	10.57000	0.03100	-5.26900
N	6.93100	-0.70700	5.00300	N	12.58800	-0.55800	-6.13700
C	8.35200	-0.81900	5.37400	C	12.17500	-0.37100	-7.52300
C	9.31900	-0.58200	4.21700	C	10.99800	-1.24900	-7.98300
C	9.08600	-1.64600	3.15100	O	10.33400	-0.87300	-8.95600
C	9.14900	0.79000	3.62900	N	10.84400	-2.36900	-7.28800
C	10.24200	1.15500	2.63300	C	9.69800	-3.22300	-7.62200
C	8.64600	0.17400	6.50000	C	10.09300	-4.72900	-7.51200
O	7.97300	1.19800	6.62800	C	10.54800	-5.17400	-6.17200
N	9.65900	-0.11900	7.31900	O	10.98100	-4.36400	-5.36600
C	9.97900	0.78200	8.42200	O	10.47700	-6.44000	-5.95100
C	10.36300	-1.42600	7.42900	C	8.40700	-2.91900	-6.81500
C	10.81100	-0.03700	9.39000	O	7.38200	-3.59000	-7.00800
C	11.31800	-1.23400	8.62100	N	8.51200	-1.90700	-5.94900
C	10.69000	2.07000	7.97300	C	7.35300	-1.35900	-5.23500
O	10.61100	3.08200	8.67600	C	7.26700	-1.78600	-3.76100
N	11.36600	1.93800	6.84600	C	6.93700	-3.24700	-3.62500
C	12.10300	3.06100	6.25000	C	7.92200	-4.23700	-3.65100

C	5.61400	-3.64800	-3.42700	H	0.99300	-0.10600	-4.75000
C	7.61100	-5.58800	-3.50700	H	4.66400	-2.57700	-6.74900
C	5.28200	-4.99500	-3.30400	H	1.34800	-2.61300	-4.64600
C	6.28100	-5.96400	-3.35500	H	2.63100	-3.31100	-4.08200
O	5.93800	-7.27500	-3.20900	H	3.26300	-4.59700	-7.43600
C	7.40000	0.17900	-5.39500	H	3.95000	-4.63100	-6.14700
O	7.46400	0.89500	-4.40400	H	1.35400	-3.86800	-6.47300
N	7.37200	0.56800	-6.66800	H	1.72900	-4.93600	-5.50700
C	7.67000	1.94900	-7.03800	H	1.66400	-1.28500	-7.31700
C	8.23800	1.94200	-8.46200	H	2.27300	-0.48800	-9.87400
C	6.49600	2.91900	-7.00300	H	0.55800	-1.42200	-10.98900
O	6.70900	4.12600	-7.20300	H	1.34800	-2.63800	-10.28800
N	5.30600	2.36100	-6.78400	H	-0.18800	-2.94800	-8.90600
C	4.06100	3.13000	-6.87400	H	0.56700	0.99000	-10.73800
C	3.08900	2.52500	-7.91400	H	-0.23100	2.81000	-8.96100
C	3.76000	2.51400	-9.26000	H	-0.83900	2.52600	-11.68800
O	3.99100	1.44200	-9.81600	H	-1.87200	4.46900	-9.88200
N	4.08800	3.69000	-9.78100	H	-1.64800	4.89200	-11.42500
C	3.39700	3.28800	-5.48100	H	-2.67000	3.68000	-11.04800
O	4.08000	2.99700	-4.46000	H	0.80900	4.31400	-10.21200
O	2.22800	3.71300	-5.49800	H	1.37100	3.05000	-11.04900
H	6.23600	2.54600	6.21500	H	0.44100	4.33300	-13.03000
H	6.70400	3.92800	6.65200	H	0.68200	5.59500	-11.99500
H	5.21200	3.58100	6.65600	H	1.93000	4.65000	-12.40900
H	5.33700	4.75000	4.81900	H	-2.16000	0.46500	-10.63000
H	7.86200	3.50300	4.14700	H	-4.42900	1.06900	-9.42800
H	8.78600	4.96100	5.20600	H	-3.67500	-1.25600	-10.72800
H	6.48600	4.32900	2.23100	H	-6.15000	-0.84600	-9.41000
H	6.68700	5.79700	2.85500	H	-6.15800	-1.72500	-10.71800
H	7.96600	4.97700	2.32100	H	-5.30900	-2.18500	-9.47200
H	4.28500	4.10700	2.91600	H	-3.95600	0.74400	-12.04400
H	3.90500	1.36100	2.64000	H	-4.90900	-0.37400	-12.53700
H	1.76900	1.76400	1.73800	H	-5.47800	0.80800	-11.66300
H	1.43500	4.13200	2.67000	H	-2.04000	-1.05300	-8.21200
H	2.21200	2.69700	4.42700	H	-3.35900	-2.00700	-6.04700
H	0.71800	2.51400	3.85800	H	-0.54600	-1.73400	-6.29400
H	1.68600	1.22900	4.03700	H	-1.26600	-2.52800	-5.11300
H	4.28200	0.38500	0.70700	H	-1.37600	-3.05600	-6.61800
H	5.06800	1.91800	-1.48800	H	-1.47100	0.85400	-6.38200
H	6.35700	-0.48900	-0.80600	H	-1.72200	1.81000	-3.86700
H	6.81000	0.50400	-1.94900	H	-0.10700	2.69700	-5.22400
H	4.14900	1.20100	-3.48700	H	-1.18900	3.24700	-6.21100
H	2.60400	-1.13300	-3.33200	H	-0.52800	5.09500	-4.97300
H	1.76500	1.26100	-4.52400	H	-1.94300	4.78400	-4.49100

H	-0.71900	5.26500	-2.72300	H	-8.28600	-1.08500	0.56700
H	-1.09600	3.79400	-2.54500	H	-7.18200	-0.12300	1.16200
H	1.38100	4.15300	-3.77300	H	-7.60400	2.56600	1.90600
H	0.01500	4.35300	-0.61800	H	-7.64700	2.65400	4.60500
H	1.38400	4.04000	0.08800	H	-6.58300	4.51900	2.80800
H	3.25600	3.50800	-2.65400	H	-6.44200	4.66100	4.36100
H	3.24500	3.55100	-1.08700	H	-5.43600	2.30100	3.11600
H	-3.68400	2.41900	-6.63800	H	-4.51300	3.51200	3.20800
H	-5.38900	4.17200	-5.56900	H	-5.67200	2.42100	5.47500
H	-5.92300	2.45200	-7.72800	H	-4.29700	1.92200	5.01400
H	-6.83300	3.72500	-7.35000	H	-3.89300	4.49100	5.25000
H	-4.22100	3.67200	-8.25700	H	-5.17600	2.33300	7.63000
H	-5.53000	0.74700	-5.56200	H	-4.55500	3.14700	8.81900
H	-7.98700	0.45900	-4.39500	H	-3.00900	5.54500	7.04400
H	-6.03800	-1.46200	-4.92100	H	-3.31200	4.99400	8.48300
H	-7.41500	-1.82000	-4.22900	H	-9.65700	4.29800	2.42400
H	-7.63000	-2.49100	-7.77400	H	-10.39400	6.40900	3.72300
H	-6.65700	-2.95600	-6.60900	H	-12.15400	4.84700	2.09200
H	-4.79300	0.57900	-3.18500	H	-12.57100	6.29800	2.67700
H	-5.11000	0.05300	-0.59200	H	-10.42200	5.86800	0.82700
H	-3.09800	0.10700	-1.63700	H	-12.59400	5.41800	-0.04200
H	-3.17000	1.68100	-1.68500	H	-13.01300	6.93800	0.31700
H	-2.91800	2.97000	0.39100	H	-11.87200	6.65200	-0.80100
H	-2.49700	-1.05500	0.41700	H	-11.42600	8.32700	1.86000
H	-1.95400	3.12900	2.52300	H	-9.89800	7.78900	1.94800
H	-1.51900	-0.89300	2.58600	H	-10.50800	8.26800	0.53600
H	-1.25800	1.17900	3.62300	H	-13.47300	4.45600	6.47000
H	-5.06100	3.16800	-2.07600	H	-11.41900	2.64800	3.66500
H	-5.65500	4.65200	-0.01600	H	-12.86200	3.17100	3.35800
H	-5.96800	5.27600	-2.69900	H	-13.67500	1.86900	6.75200
H	-6.33100	6.33000	-1.57600	H	-14.47400	2.56500	5.75500
H	-2.91400	6.84500	-2.72900	H	-12.13400	1.30400	5.27300
H	-4.31300	6.73900	-3.46900	H	-13.33200	1.12500	4.41000
H	-7.90200	2.99800	-2.00600	H	-10.33400	3.84400	6.54600
H	-10.17700	4.17000	-0.96600	H	-9.05000	4.28600	8.37500
H	-9.94800	1.92500	-2.58000	H	-10.22300	3.83700	9.33500
H	-12.42300	2.84600	-1.49600	H	-9.74600	1.55500	6.99500
H	-12.37500	1.89500	-2.75000	H	-9.09400	-0.55000	8.40100
H	-11.84000	1.38300	-1.35800	H	-8.16400	-0.19500	5.74000
H	-9.72300	4.02200	-3.74600	H	-10.06800	-0.03700	5.08800
H	-11.06900	3.34900	-4.19800	H	-9.01000	-2.59000	7.11300
H	-11.10400	4.49500	-3.15900	H	-8.53800	-2.56900	5.57400
H	-8.51300	1.21800	-0.35700	H	-7.47300	-2.27400	6.75600
H	-9.96900	0.09600	1.56400	H	-4.86200	0.06000	9.58500

H	-7.65800	-2.45200	9.40800	H	-4.43400	-6.40300	1.94800
H	-8.13400	-1.20900	10.22900	H	-5.99600	-7.72200	0.23300
H	-4.78500	-2.74400	9.73100	H	-7.05900	-6.42300	1.63600
H	-4.23300	-1.82100	10.70900	H	-6.11600	-5.16600	1.38000
H	-6.40800	-2.82700	11.16800	H	-8.66700	-7.09500	-0.39600
H	-6.31100	-1.42400	11.65400	H	-6.94500	-3.38500	0.11400
H	-2.89500	0.16600	8.57300	H	-10.28000	-6.15100	-1.85400
H	-2.87200	-0.09200	5.89100	H	-8.56100	-2.44100	-1.35300
H	-0.72800	0.23300	7.73800	H	-10.29000	-2.68300	-2.55500
H	-0.47600	0.09200	6.17300	H	-3.65700	-5.35000	-0.46200
H	-1.86500	2.13700	5.88600	H	-4.33800	-5.16200	-3.15700
H	-1.92800	2.19800	7.45400	H	-3.12300	-3.17200	-3.22600
H	-1.70600	-2.27600	8.30400	H	-2.96500	-3.41000	-0.48800
H	-0.52300	-4.02300	6.73800	H	-5.53800	-3.09700	-2.59000
H	-1.75100	-4.60200	9.22500	H	-5.04200	-3.02500	-1.06400
H	-0.85400	-5.66600	8.44800	H	-4.69500	-1.81900	-2.06900
H	-0.20400	-4.30400	8.98500	H	-1.72600	-6.29400	-1.37800
H	-3.88700	-3.92000	7.37700	H	0.20800	-7.21500	-2.18100
H	-4.52500	-6.22500	6.00400	H	-0.07500	-6.60000	-3.60900
H	-6.18800	-4.23000	7.19100	H	-0.54500	-4.12700	-1.56900
H	-6.84000	-5.35800	6.22900	H	1.89000	-2.87500	-1.87300
H	-5.38300	-6.01900	8.58400	H	-0.24400	-2.01300	-0.25300
H	-8.21600	-5.73800	8.44500	H	1.05100	-1.15700	-0.55200
H	-7.42500	-6.40900	9.68000	H	3.10700	-2.12500	0.09600
H	-7.21000	-4.84200	9.32800	H	3.26400	-4.03000	2.12600
H	-7.04500	-7.63200	6.91800	H	5.50200	-4.24000	2.02600
H	-5.45500	-7.82100	7.14100	H	4.24700	-4.85400	-0.46400
H	-6.48600	-8.12800	8.35400	H	5.71300	-5.43800	-0.04900
H	-4.48900	-2.90000	5.18600	H	4.40200	-5.84400	0.80800
H	-5.65000	-3.17800	2.72600	H	5.52400	-2.62100	-0.30900
H	-4.13000	-0.98500	3.62200	H	6.06000	-2.11100	1.13100
H	-4.83500	-1.02400	2.19900	H	7.74100	-3.81600	0.99900
H	-2.45500	-3.47200	3.83700	H	7.34400	-4.00500	-0.58400
H	-1.10700	-3.64700	1.52600	H	7.93700	-2.57500	-0.01900
H	0.05100	-3.29900	3.50800	H	4.22700	-3.34600	4.07000
H	-0.31000	-4.77300	3.99900	H	4.47900	-0.61600	4.54200
H	0.65100	-4.57100	2.74100	H	4.11700	-2.63300	6.47400
H	-2.24800	-6.32100	3.43500	H	5.52500	-0.95000	7.31800
H	-1.57800	-8.22300	1.61100	H	4.39000	0.16100	6.99700
H	-2.96900	-9.74000	2.77000	H	4.11900	-0.99100	8.12100
H	-4.45700	-8.35700	3.52400	H	2.32400	-0.48900	6.02000
H	-0.96800	-8.36800	4.34000	H	2.09600	-1.93300	5.32200
H	-1.53300	-9.81700	4.75300	H	1.90900	-2.91500	7.45900
H	-0.65500	-9.63700	3.40600	H	1.96700	-1.42500	8.14600

H	0.71900	-1.86300	7.16400	H	11.28800	-2.83900	-1.91300
H	6.58000	0.12900	4.97300	H	13.41600	-0.90200	-5.99300
H	8.51900	-1.72500	5.70400	H	11.91500	0.56800	-7.65800
H	10.23100	-0.69900	4.57800	H	12.95800	-0.52200	-8.12800
H	9.09200	-2.53900	3.57500	H	11.28700	-2.52400	-6.52800
H	8.20900	-1.48600	2.71800	H	9.48800	-3.12900	-8.56600
H	9.82000	-1.58600	2.48800	H	9.34100	-5.28400	-7.82700
H	8.27900	0.81800	3.16000	H	10.80500	-4.88300	-8.16900
H	9.16100	1.47300	4.34700	H	9.29800	-1.47100	-5.84600
H	11.11300	1.09200	3.11200	H	6.53200	-1.67600	-5.65900
H	10.21900	0.52900	1.85300	H	8.13500	-1.59100	-3.33900
H	10.10400	2.09700	2.34600	H	6.58500	-1.22200	-3.30700
H	9.16300	1.11200	8.83600	H	8.87000	-3.97400	-3.77400
H	10.87600	-1.63300	6.62800	H	4.89100	-2.97600	-3.40600
H	9.70500	-2.14100	7.52900	H	8.32800	-6.26100	-3.54500
H	11.48900	0.40300	9.79800	H	4.34800	-5.28200	-3.17600
H	10.27700	-0.31900	10.14800	H	6.71000	-7.77200	-3.49100
H	12.09100	-1.09300	8.32200	H	7.13800	0.00500	-7.33600
H	11.32300	-2.05600	9.15000	H	8.38600	2.29200	-6.46300
H	11.56300	1.11700	6.49600	H	7.65300	1.41700	-9.05100
H	12.46900	3.61900	6.95800	H	8.29300	2.85700	-8.80900
H	12.86700	2.71200	5.72200	H	9.13000	1.53600	-8.46200
H	12.70000	4.65700	4.39700	H	5.23600	1.49000	-6.55800
H	10.12300	5.53400	3.77000	H	4.27100	4.02500	-7.21600
H	12.33600	7.27300	4.10000	H	2.85700	1.61600	-7.64400
H	10.96000	7.73000	3.43500	H	2.26400	3.05700	-7.93900
H	10.99900	7.28500	4.97000	H	4.50700	3.73400	-10.60900
H	12.65700	4.01600	2.56000	H	3.90300	4.46900	-9.33200
H	12.54800	5.09600	0.00100				
H	14.63900	3.48900	1.06800				
H	15.78600	5.49300	1.01700				
H	14.64600	3.49100	-1.37900				
H	14.69400	5.09700	-1.33200				
H	15.95100	4.25000	-0.79000	N	0.00000	24.29645	-3.68038
H	10.83900	4.06400	-1.02400	C	0.00000	23.04545	-4.46938
H	10.36400	1.40800	-0.83900	C	0.00000	21.87745	-3.66638
H	9.31200	3.25800	-2.68600	O	0.00000	21.82245	-3.38038
H	8.80800	1.76100	-2.59100	H	0.00000	24.49345	-3.28438
H	13.24800	0.04900	-3.78900	H	0.00000	24.21045	-2.89938
H	10.00800	-0.65800	-1.70800	H	0.00000	25.09545	-4.28738
H	11.37200	-0.71000	-0.94200	H	0.00000	22.81445	-4.79438
H	12.70300	-2.45900	-3.90700	H	0.00000	23.19045	-5.33738
H	13.27900	-1.94200	-2.67200	N	0.00000	20.93545	-3.26838
H	10.61400	-2.25700	-3.10700	C	0.00000	19.72745	-2.54138

## 5. 2KNZ

C	0.00000	18.89745	-3.35438	H	0.00000	15.77445	-5.06338
O	0.00000	18.49845	-4.48538	H	0.00000	13.48945	-5.52038
C	0.00000	18.95745	-2.34138	H	0.00000	16.40245	-5.32138
C	0.00000	19.97445	-2.50538	H	0.00000	15.09445	-6.08338
C	0.00000	20.97745	-3.49038	H	0.00000	15.03045	-7.72838
H	0.00000	19.96945	-1.57838	N	0.00000	13.68945	-2.80238
H	0.00000	18.17745	-3.08538	C	0.00000	13.37245	-1.43138
H	0.00000	18.52245	-1.35438	C	0.00000	12.00245	-1.13838
H	0.00000	19.50645	-2.88838	O	0.00000	11.85645	-0.33738
H	0.00000	20.45045	-1.55638	C	0.00000	14.40645	-0.44238
H	0.00000	20.68345	-4.50138	C	0.00000	15.83445	-0.69838
H	0.00000	21.95745	-3.27438	S	0.00000	16.97945	0.58562
N	0.00000	18.64145	-2.77238	C	0.00000	16.63045	0.62662
C	0.00000	17.97445	-3.48238	H	0.00000	13.36845	-3.13738
C	0.00000	16.45945	-3.43738	H	0.00000	13.33145	-1.35338
O	0.00000	15.83845	-2.38538	H	0.00000	14.38545	-0.49738
C	0.00000	18.37545	-2.89638	H	0.00000	14.12945	0.55562
C	0.00000	19.85845	-3.01338	H	0.00000	15.85345	-0.73738
C	0.00000	20.12245	-2.37938	H	0.00000	16.16045	-1.64938
C	0.00000	20.30645	-4.46838	H	0.00000	16.88145	-0.32638
H	0.00000	18.90045	-1.83938	H	0.00000	17.21745	1.40362
H	0.00000	18.29545	-4.51238	H	0.00000	15.57845	0.83062
H	0.00000	18.10945	-1.84938	N	0.00000	10.98545	-1.83438
H	0.00000	17.80645	-3.39538	C	0.00000	9.66945	-1.94738
H	0.00000	20.44245	-2.48138	C	0.00000	9.03145	-0.61938
H	0.00000	19.53545	-2.88238	O	0.00000	8.38445	-0.53438
H	0.00000	19.84745	-1.33538	C	0.00000	8.84245	-2.69438
H	0.00000	21.17145	-2.46738	C	0.00000	9.86345	-3.50938
H	0.00000	20.16245	-4.89038	C	0.00000	11.02545	-2.58338
H	0.00000	19.72445	-5.02538	H	0.00000	9.73445	-2.55638
H	0.00000	21.35345	-4.52138	H	0.00000	8.35745	-1.98738
N	0.00000	15.87345	-4.58338	H	0.00000	8.10645	-3.31538
C	0.00000	14.43045	-4.70538	H	0.00000	9.49445	-3.82538
C	0.00000	13.91245	-4.87138	H	0.00000	10.14845	-4.36038
O	0.00000	12.70245	-4.86538	H	0.00000	10.88145	-1.92638
H	0.00000	16.42545	-5.35838	H	0.00000	11.94645	-3.13838
H	0.00000	13.98745	-3.81638	N	0.00000	9.24245	0.42962
H	0.00000	14.14245	-5.56238	C	0.00000	8.60445	1.71562
N	0.00000	14.82945	-5.00338	C	0.00000	9.16245	2.36262
C	0.00000	14.45545	-5.05438	O	0.00000	8.53645	3.24562
C	0.00000	14.37345	-3.63338	C	0.00000	8.69645	2.68462
O	0.00000	14.87945	-3.31838	C	0.00000	7.61845	2.45662
C	0.00000	15.47945	-5.87638	C	0.00000	7.56345	3.56962
O	0.00000	15.73545	-7.10538	O	0.00000	6.82045	4.54962

O	0.00000	8.25945	3.46262	H	0.00000	13.08445	0.87662
H	0.00000	9.84445	0.34162	H	0.00000	13.17645	-2.62538
H	0.00000	7.55945	1.50762	H	0.00000	14.02345	-1.14038
H	0.00000	9.66245	2.57662	N	0.00000	6.57745	0.60062
H	0.00000	8.59845	3.69562	C	0.00000	5.29245	0.79762
H	0.00000	6.65845	2.40062	C	0.00000	4.91445	2.26262
H	0.00000	7.81945	1.52362	O	0.00000	3.87845	2.62962
N	0.00000	10.31845	1.90762	C	0.00000	5.29845	0.23362
C	0.00000	10.86045	2.39962	C	0.00000	5.31245	-1.27238
C	0.00000	9.94445	1.97662	C	0.00000	5.62045	-2.05038
O	0.00000	9.91245	2.60762	C	0.00000	5.00445	-1.90638
C	0.00000	12.30445	1.90062	C	0.00000	5.62145	-3.42838
C	0.00000	12.84545	2.41262	C	0.00000	5.00245	-3.28338
C	0.00000	13.21445	2.33362	C	0.00000	5.31045	-4.04538
H	0.00000	10.81645	1.23562	H	0.00000	7.31345	0.21362
H	0.00000	10.87745	3.47862	H	0.00000	4.55045	0.26762
H	0.00000	12.29045	0.82162	H	0.00000	6.17645	0.60162
H	0.00000	12.19745	2.08562	H	0.00000	4.41445	0.58362
H	0.00000	13.84045	2.02362	H	0.00000	5.86445	-1.56738
H	0.00000	12.87945	3.49362	H	0.00000	4.76345	-1.31238
H	0.00000	14.21545	1.96762	H	0.00000	5.86045	-4.02238
H	0.00000	12.84545	1.92662	H	0.00000	4.76045	-3.76438
H	0.00000	13.23145	3.41062	H	0.00000	5.30445	-5.12338
N	0.00000	9.19045	0.90462	N	0.00000	5.77845	3.09862
C	0.00000	8.15045	0.51362	C	0.00000	5.43145	4.48562
C	0.00000	6.79345	0.93062	C	0.00000	5.11945	5.24262
O	0.00000	5.99245	1.57562	O	0.00000	4.29445	6.15562
C	0.00000	8.17445	-1.00238	C	0.00000	6.56245	5.18162
C	0.00000	9.52945	-1.52738	C	0.00000	6.15245	6.49062
C	0.00000	9.97245	-0.91538	C	0.00000	7.31745	7.20762
N	0.00000	11.15145	-1.58338	O	0.00000	7.96645	8.05262
C	0.00000	12.21545	-0.94038	N	0.00000	7.60845	6.85762
N	0.00000	12.28145	0.38562	H	0.00000	6.67945	2.78862
N	0.00000	13.21645	-1.62538	H	0.00000	4.54745	4.47962
H	0.00000	9.33945	0.36362	H	0.00000	6.92545	4.51762
H	0.00000	8.32545	1.02162	H	0.00000	7.36445	5.38662
H	0.00000	7.89745	-1.50438	H	0.00000	5.73045	7.13962
H	0.00000	7.45245	-1.24938	H	0.00000	5.40645	6.28462
H	0.00000	10.25845	-1.27938	H	0.00000	7.06345	6.15562
H	0.00000	9.47145	-2.59738	H	0.00000	8.35645	7.31262
H	0.00000	9.16345	-0.99538	N	0.00000	5.75745	4.85262
H	0.00000	10.20645	0.12762	C	0.00000	5.52145	5.52162
H	0.00000	11.13345	-2.56838	C	0.00000	4.15245	5.12062
H	0.00000	11.53345	0.90462	O	0.00000	3.35545	5.96162

C	0.00000	6.60945	5.19062	H	0.00000	1.57545	3.91862
C	0.00000	8.02945	5.08762	H	0.00000	3.30145	4.18262
C	0.00000	8.36045	6.10662	H	0.00000	1.56545	1.46362
O	0.00000	9.19145	5.84162	H	0.00000	1.07845	2.40262
N	0.00000	7.71345	7.25962	H	0.00000	0.29645	2.67262
H	0.00000	6.39045	4.10862	N	0.00000	1.63145	6.98062
H	0.00000	5.52345	6.58662	C	0.00000	1.28845	8.29462
H	0.00000	6.36545	4.24562	C	0.00000	0.28745	8.12562
H	0.00000	6.60545	5.95662	O	0.00000	-0.58955	8.96062
H	0.00000	8.15245	4.10162	C	0.00000	2.51745	8.99862
H	0.00000	8.73145	5.21362	C	0.00000	3.70345	9.03762
H	0.00000	7.05545	7.42162	C	0.00000	4.86545	9.79762
H	0.00000	7.87845	7.88662	O	0.00000	4.87245	11.04362
N	0.00000	3.87045	3.82662	O	0.00000	5.76345	9.16162
C	0.00000	2.53745	3.31762	H	0.00000	2.55045	6.63862
C	0.00000	1.53345	3.89262	H	0.00000	0.84645	8.89862
O	0.00000	0.34445	3.99762	H	0.00000	2.81845	8.49162
C	0.00000	2.50645	1.79362	H	0.00000	2.25145	10.01462
C	0.00000	2.77745	1.05662	H	0.00000	3.40845	9.51662
C	0.00000	4.21945	1.07862	H	0.00000	4.01445	8.02262
O	0.00000	4.93845	2.05562	N	0.00000	0.43845	7.03662
N	0.00000	4.65945	-0.03038	C	0.00000	-0.45655	6.71962
H	0.00000	4.58245	3.19362	C	0.00000	-1.85855	6.41562
H	0.00000	2.26245	3.62762	O	0.00000	-2.84255	6.93962
H	0.00000	3.24845	1.47362	C	0.00000	0.10045	5.53962
H	0.00000	1.53245	1.48762	C	0.00000	-0.77355	5.08562
H	0.00000	2.48545	0.02462	C	0.00000	-0.04955	4.16362
H	0.00000	2.17245	1.50262	O	0.00000	-0.36055	4.13362
H	0.00000	4.03445	-0.78438	N	0.00000	0.93645	3.42362
H	0.00000	5.58945	-0.06438	H	0.00000	1.18245	6.42762
N	0.00000	2.02445	4.27462	H	0.00000	-0.50455	7.58062
C	0.00000	1.16545	4.83862	H	0.00000	1.07345	5.80362
C	0.00000	0.73945	6.24062	H	0.00000	0.20645	4.72562
O	0.00000	-0.38055	6.63462	H	0.00000	-1.62555	4.55862
C	0.00000	1.83645	4.85262	H	0.00000	-1.11355	5.95662
C	0.00000	2.25245	3.48362	H	0.00000	1.15645	3.50862
C	0.00000	2.46645	3.53762	H	0.00000	1.39945	2.81562
C	0.00000	1.22445	2.42962	N	0.00000	-1.94555	5.58762
H	0.00000	2.99045	4.17262	C	0.00000	-3.21955	5.32362
H	0.00000	0.27945	4.22062	C	0.00000	-3.69255	6.58562
H	0.00000	2.71745	5.47562	O	0.00000	-4.88555	6.84362
H	0.00000	1.14845	5.29962	C	0.00000	-3.06255	4.23462
H	0.00000	3.18745	3.19462	C	0.00000	-2.92555	2.81262
H	0.00000	2.67245	2.54162	C	0.00000	-2.71555	1.91462



C	0.00000	-4.16855	2.38762	C	0.00000	-7.00355	3.92362
H	0.00000	-1.13455	5.15262	H	0.00000	-5.11055	7.93862
H	0.00000	-3.94455	5.01762	H	0.00000	-7.51055	8.02662
H	0.00000	-2.19255	4.46062	H	0.00000	-6.24355	5.77062
H	0.00000	-3.91555	4.27062	H	0.00000	-7.51655	5.61362
H	0.00000	-2.07055	2.73262	H	0.00000	-5.16255	7.03462
H	0.00000	-1.77355	2.15462	H	0.00000	-4.82655	5.38762
H	0.00000	-2.72155	0.88562	H	0.00000	-7.74255	4.09062
H	0.00000	-3.51955	2.08462	H	0.00000	-6.23455	3.26162
H	0.00000	-4.00655	1.41462	H	0.00000	-7.47855	3.47162
H	0.00000	-4.38755	3.10862	N	0.00000	-7.54355	8.55762
H	0.00000	-4.99755	2.33262	C	0.00000	-8.34555	8.79462
N	0.00000	-2.71755	7.34562	C	0.00000	-8.04055	7.78762
C	0.00000	-2.93655	8.64462	O	0.00000	-8.80855	7.61162
C	0.00000	-3.70855	9.56262	H	0.00000	-6.66155	8.97462
O	0.00000	-4.45455	10.44462	H	0.00000	-8.12755	9.78362
C	0.00000	-1.57555	9.25962	H	0.00000	-9.39155	8.73262
C	0.00000	-1.63755	10.41962	N	0.00000	-6.91055	7.11862
O	0.00000	-1.56955	10.22862	C	0.00000	-6.46155	6.15562
N	0.00000	-1.73655	11.62762	C	0.00000	-5.27155	6.71862
H	0.00000	-1.79455	7.00462	O	0.00000	-4.15855	6.79262
H	0.00000	-3.49255	8.49862	C	0.00000	-6.10955	4.83962
H	0.00000	-0.93255	8.49462	C	0.00000	-7.31355	4.09062
H	0.00000	-1.13755	9.60662	C	0.00000	-8.20755	3.53062
H	0.00000	-1.76355	11.70762	C	0.00000	-7.55455	3.94862
H	0.00000	-1.77255	12.40062	C	0.00000	-9.32055	2.84762
N	0.00000	-3.52255	9.30662	C	0.00000	-8.66655	3.26462
C	0.00000	-4.16655	10.06162	C	0.00000	-9.54955	2.71262
C	0.00000	-5.58455	9.56262	H	0.00000	-6.35355	7.28362
O	0.00000	-6.44055	10.24762	H	0.00000	-7.27055	5.98462
C	0.00000	-3.36455	9.88162	H	0.00000	-5.49555	5.05862
O	0.00000	-2.06655	10.43762	H	0.00000	-5.56255	4.20462
H	0.00000	-2.93555	8.55662	H	0.00000	-8.02655	3.63562
H	0.00000	-4.18655	11.10462	H	0.00000	-6.86255	4.38062
H	0.00000	-3.26555	8.82562	H	0.00000	-10.01155	2.41362
H	0.00000	-3.87755	10.35562	H	0.00000	-8.84355	3.16062
H	0.00000	-1.63255	10.06062	H	0.00000	-10.41955	2.17762
N	0.00000	-5.80855	8.36062	N	0.00000	-5.52855	7.13862
C	0.00000	-7.03455	7.62862	C	0.00000	-4.51855	7.78662
C	0.00000	-7.96855	7.76062	C	0.00000	-4.31055	7.02262
O	0.00000	-9.03055	7.14262	O	0.00000	-3.54655	7.44562
C	0.00000	-6.64855	6.17962	C	0.00000	-4.84955	9.26762
C	0.00000	-5.59855	6.05662	C	0.00000	-6.36655	9.50762
S	0.00000	-6.26755	5.48462	C	0.00000	-4.20955	10.19562

C	0.00000	-7.02655	9.70062	H	0.00000	1.38745	5.29362
H	0.00000	-6.42455	7.00362	H	0.00000	-0.63155	5.54162
H	0.00000	-3.58755	7.76762	H	0.00000	0.79745	8.66162
H	0.00000	-4.41455	9.49362	H	0.00000	-0.24055	9.53562
H	0.00000	-6.83055	8.65462	H	0.00000	-2.00055	6.71962
H	0.00000	-6.55955	10.39062	H	0.00000	-1.81555	8.43862
H	0.00000	-3.13855	10.06162	N	0.00000	-1.40755	2.56262
H	0.00000	-4.45155	11.21962	C	0.00000	-1.53555	1.19062
H	0.00000	-4.58855	9.96462	C	0.00000	-2.20755	0.29962
H	0.00000	-6.77055	8.86662	O	0.00000	-1.62855	-0.68138
H	0.00000	-6.67055	10.61862	C	0.00000	-2.35655	1.17062
H	0.00000	-8.09655	9.74562	C	0.00000	-1.83655	2.11362
N	0.00000	-4.97655	5.88662	C	0.00000	-2.82155	2.29762
C	0.00000	-4.72655	4.99262	O	0.00000	-3.76455	3.09362
C	0.00000	-3.45955	4.24562	O	0.00000	-2.66055	1.64762
O	0.00000	-3.51255	3.15062	H	0.00000	-1.62555	3.30262
C	0.00000	-5.87755	3.99062	H	0.00000	-0.54755	0.81062
C	0.00000	-5.95255	3.43862	H	0.00000	-3.37255	1.45162
O	0.00000	-7.02455	3.06162	H	0.00000	-2.35255	0.16862
N	0.00000	-4.82255	3.39262	H	0.00000	-0.91755	1.71362
H	0.00000	-5.62055	5.63362	H	0.00000	-1.64455	3.07562
H	0.00000	-4.57755	5.57862	N	0.00000	-3.41855	0.67162
H	0.00000	-6.81255	4.46962	C	0.00000	-4.18155	-0.11838
H	0.00000	-5.74055	3.15962	C	0.00000	-3.47355	-0.17938
H	0.00000	-4.00655	3.71062	O	0.00000	-3.30355	-1.25938
H	0.00000	-4.85455	3.05462	C	0.00000	-5.58155	0.45062
N	0.00000	-2.32955	4.88462	H	0.00000	-3.79955	1.50662
C	0.00000	-1.02655	4.31762	H	0.00000	-4.27255	-1.11538
C	0.00000	-0.97155	2.85262	H	0.00000	-5.51755	1.45162
O	0.00000	-0.55855	2.02362	H	0.00000	-6.07555	0.47462
C	0.00000	0.04745	5.06662	H	0.00000	-6.14455	-0.16938
C	0.00000	0.42745	6.40462	N	0.00000	-3.07055	0.99162
C	0.00000	0.91545	6.26062	C	0.00000	-2.34755	1.11062
N	0.00000	-0.17355	6.37062	C	0.00000	-1.18455	0.11962
C	0.00000	-0.55355	7.53062	O	0.00000	-1.17955	-0.77838
N	0.00000	0.04845	8.66462	C	0.00000	-1.81055	2.54162
N	0.00000	-1.53555	7.56062	C	0.00000	-2.90055	3.59662
H	0.00000	-2.37455	5.78062	O	0.00000	-4.01155	3.43462
H	0.00000	-0.85555	4.42462	N	0.00000	-2.57955	4.70862
H	0.00000	-0.32055	5.24162	H	0.00000	-3.29255	1.81462
H	0.00000	0.93045	4.45062	H	0.00000	-3.03855	0.89562
H	0.00000	-0.43655	7.05262	H	0.00000	-1.18955	2.79162
H	0.00000	1.21445	6.84262	H	0.00000	-1.20555	2.57962
H	0.00000	1.63345	7.02762	H	0.00000	-1.67055	4.79662

H	0.00000	-3.28355	5.39462	H	0.00000	-3.61855	-3.54138
N	0.00000	-0.20755	0.25562	H	0.00000	-2.72555	-2.19738
C	0.00000	0.99745	-0.56138	H	0.00000	-4.06155	-2.92838
C	0.00000	0.75945	-2.00138	N	0.00000	-0.11655	-3.50738
O	0.00000	1.46645	-2.88538	C	0.00000	1.10945	-3.66738
C	0.00000	2.20145	0.06662	C	0.00000	1.99045	-4.75938
C	0.00000	1.94445	0.66062	O	0.00000	2.84845	-5.29138
C	0.00000	1.62745	-0.41338	C	0.00000	1.88445	-2.35838
C	0.00000	3.14745	1.47362	C	0.00000	1.54545	-1.45238
H	0.00000	-0.30355	0.90162	C	0.00000	0.55145	-0.36838
H	0.00000	1.24645	-0.59638	C	0.00000	2.81045	-0.83838
H	0.00000	2.95745	-0.69638	H	0.00000	-0.22355	-2.71838
H	0.00000	2.60445	0.85162	H	0.00000	0.84145	-3.95638
H	0.00000	1.09845	1.32962	H	0.00000	1.69645	-1.81738
H	0.00000	0.75345	-0.96438	H	0.00000	2.93945	-2.59138
H	0.00000	1.43745	0.05262	H	0.00000	1.10245	-2.04738
H	0.00000	2.46545	-1.08638	H	0.00000	-0.40555	-0.81338
H	0.00000	3.37545	2.22162	H	0.00000	0.44745	0.32262
H	0.00000	3.99745	0.81662	H	0.00000	0.91045	0.16662
H	0.00000	2.92345	1.95562	H	0.00000	3.50645	-1.61638
N	0.00000	-0.24055	-2.24738	H	0.00000	3.24645	-0.20138
C	0.00000	-0.59755	-3.62438	H	0.00000	2.57745	-0.24938
C	0.00000	-1.11155	-4.35038	N	0.00000	1.79145	-5.08338
O	0.00000	-0.88955	-5.55938	C	0.00000	2.54045	-6.16838
C	0.00000	-1.66255	-3.64738	C	0.00000	2.11945	-7.49638
C	0.00000	-1.10355	-3.43638	O	0.00000	2.95545	-8.29638
C	0.00000	-0.16855	-4.54538	C	0.00000	2.35445	-6.24038
O	0.00000	0.76645	-4.29238	C	0.00000	2.81245	-4.94338
N	0.00000	-0.41855	-5.77938	C	0.00000	3.11745	-7.43238
H	0.00000	-0.74955	-1.49838	C	0.00000	2.94345	-5.03438
H	0.00000	0.29145	-4.12038	H	0.00000	1.15245	-4.56438
H	0.00000	-2.36755	-2.85938	H	0.00000	3.58945	-6.00838
H	0.00000	-2.18255	-4.58838	H	0.00000	1.30345	-6.38938
H	0.00000	-0.55155	-2.50738	H	0.00000	3.76645	-4.65638
H	0.00000	-1.92755	-3.36138	H	0.00000	2.09245	-4.16638
H	0.00000	-1.18555	-5.92938	H	0.00000	2.73445	-8.34338
H	0.00000	0.18845	-6.50338	H	0.00000	2.99145	-7.46038
N	0.00000	-1.75855	-3.58138	H	0.00000	4.16845	-7.33638
C	0.00000	-2.27255	-4.10438	H	0.00000	1.99645	-5.32938
C	0.00000	-1.09655	-4.39238	H	0.00000	3.23145	-4.07138
O	0.00000	-1.04755	-5.41538	H	0.00000	3.69445	-5.76738
C	0.00000	-3.23955	-3.12138	N	0.00000	0.81345	-7.71838
H	0.00000	-1.84855	-2.61938	C	0.00000	0.29745	-8.97438
H	0.00000	-2.79955	-5.02738	C	0.00000	0.36245	-9.02138

O	0.00000	0.20945	-10.08838	H	0.00000	1.71645	-4.39138
C	0.00000	-1.11955	-9.22438	H	0.00000	1.58445	-6.83638
H	0.00000	0.19045	-7.03338	H	0.00000	0.18445	-6.44138
H	0.00000	0.91945	-9.76838	N	0.00000	0.32045	-2.57438
H	0.00000	-1.14255	-9.19038	C	0.00000	-0.54355	-1.52738
H	0.00000	-1.44755	-10.19638	C	0.00000	-1.94755	-1.70538
H	0.00000	-1.77655	-8.46738	O	0.00000	-2.91155	-1.25738
N	0.00000	0.57945	-7.87338	C	0.00000	0.02645	-0.16638
C	0.00000	0.70345	-7.83738	C	0.00000	-0.50955	0.86762
C	0.00000	2.16445	-7.66438	C	0.00000	-0.27155	0.19862
O	0.00000	2.50845	-7.93838	C	0.00000	-1.70755	1.65662
C	0.00000	-0.14755	-6.70538	H	0.00000	1.04845	-2.35938
O	0.00000	0.27045	-5.44738	H	0.00000	-0.57555	-1.57238
C	0.00000	-1.62355	-6.93038	H	0.00000	1.09845	-0.22638
H	0.00000	0.63945	-7.03938	H	0.00000	-0.79055	0.35562
H	0.00000	0.33145	-8.77638	H	0.00000	0.27345	1.54762
H	0.00000	-0.01255	-6.69238	H	0.00000	-1.34155	0.23462
H	0.00000	-0.31655	-5.20338	H	0.00000	0.15945	-0.54338
H	0.00000	-1.77355	-6.94338	H	0.00000	0.15545	1.16462
H	0.00000	-1.93555	-7.87338	H	0.00000	-2.54155	0.98762
H	0.00000	-2.20855	-6.13338	H	0.00000	-1.45755	2.14962
N	0.00000	3.01345	-7.20538	H	0.00000	-1.97355	2.39562
C	0.00000	4.43845	-7.05938	N	0.00000	-2.05355	-2.40238
C	0.00000	4.74745	-5.98438	C	0.00000	-3.33755	-2.66438
O	0.00000	5.68345	-6.12738	C	0.00000	-4.16455	-3.50838
H	0.00000	2.66645	-6.94038	O	0.00000	-5.29655	-3.16538
H	0.00000	4.94245	-6.79838	C	0.00000	-3.17655	-3.41338
H	0.00000	4.82545	-8.00538	C	0.00000	-1.94155	-2.99938
N	0.00000	3.97045	-4.90538	O	0.00000	-1.96255	-2.04238
C	0.00000	4.24245	-3.80538	N	0.00000	-0.85155	-3.73038
C	0.00000	3.29345	-3.80438	H	0.00000	-1.24755	-2.75938
O	0.00000	3.45445	-3.03738	H	0.00000	-3.82755	-1.71738
H	0.00000	3.18945	-4.86638	H	0.00000	-3.10655	-4.47438
H	0.00000	4.13845	-2.87438	H	0.00000	-4.04455	-3.22538
H	0.00000	5.25345	-3.88738	H	0.00000	-0.90555	-4.49138
N	0.00000	2.27145	-4.63738	H	0.00000	-0.03955	-3.49238
C	0.00000	1.27445	-4.73538	N	0.00000	-3.56655	-4.60838
C	0.00000	0.16545	-3.81238	C	0.00000	-4.21055	-5.49938
O	0.00000	-0.77755	-4.19238	C	0.00000	-4.31955	-4.84138
C	0.00000	0.74745	-6.16438	O	0.00000	-5.26355	-5.10238
C	0.00000	-0.15655	-6.31438	C	0.00000	-3.45755	-6.81738
O	0.00000	-1.10155	-5.50738	H	0.00000	-2.65855	-4.82538
O	0.00000	0.08445	-7.23838	H	0.00000	-5.20855	-5.70538
H	0.00000	2.14545	-5.13738	H	0.00000	-3.98055	-7.48538

H	0.00000	-2.46055	-6.63838	H	0.00000	-9.19055	-3.89238
H	0.00000	-3.39655	-7.26438	H	0.00000	-7.43155	-3.79938
N	0.00000	-3.34255	-3.99838	N	0.00000	-7.69155	-4.60838
C	0.00000	-3.43355	-3.18738	C	0.00000	-7.81755	-5.11638
C	0.00000	-4.75755	-2.42338	C	0.00000	-8.50755	-4.09838
O	0.00000	-5.49655	-2.49938	O	0.00000	-9.25455	-4.45438
C	0.00000	-2.26055	-2.22338	C	0.00000	-6.45755	-5.46838
H	0.00000	-2.52655	-3.94738	C	0.00000	-5.87155	-6.75438
H	0.00000	-3.38655	-3.85438	C	0.00000	-4.75855	-7.20638
H	0.00000	-2.30755	-1.69338	N	0.00000	-5.19655	-7.23338
H	0.00000	-2.30655	-1.51538	C	0.00000	-4.39155	-7.05038
H	0.00000	-1.33355	-2.77738	N	0.00000	-3.08455	-6.91438
N	0.00000	-5.06555	-1.70738	N	0.00000	-4.89255	-7.03238
C	0.00000	-6.32055	-0.96138	H	0.00000	-6.83255	-4.23138
C	0.00000	-7.49355	-1.91538	H	0.00000	-8.42455	-6.00938
O	0.00000	-8.42355	-1.68438	H	0.00000	-5.76555	-4.66938
C	0.00000	-6.47055	-0.16438	H	0.00000	-6.55255	-5.56838
C	0.00000	-5.16155	0.49162	H	0.00000	-6.64155	-7.51238
C	0.00000	-7.55255	0.89362	H	0.00000	-5.47355	-6.58838
C	0.00000	-5.12455	0.97862	H	0.00000	-4.45855	-8.19138
H	0.00000	-4.43655	-1.68738	H	0.00000	-3.92755	-6.52638
H	0.00000	-6.36255	-0.26738	H	0.00000	-6.15355	-7.37838
H	0.00000	-6.77555	-0.84338	H	0.00000	-2.69955	-6.95638
H	0.00000	-4.98255	1.33862	H	0.00000	-2.47555	-6.75538
H	0.00000	-4.37055	-0.22638	H	0.00000	-5.87455	-7.16138
H	0.00000	-8.47955	0.41762	H	0.00000	-4.28955	-6.88938
H	0.00000	-7.68155	1.41962	N	0.00000	-8.25455	-2.83138
H	0.00000	-7.26055	1.59462	C	0.00000	-8.89855	-1.76338
H	0.00000	-4.17055	1.44662	C	0.00000	-10.36455	-1.63538
H	0.00000	-5.91655	1.69562	O	0.00000	-11.23355	-1.35038
H	0.00000	-5.26055	0.14162	C	0.00000	-8.17155	-0.45138
N	0.00000	-7.43055	-3.00138	C	0.00000	-6.68755	-0.46338
C	0.00000	-8.51255	-3.97738	C	0.00000	-6.00855	0.75862
C	0.00000	-8.71055	-4.65038	C	0.00000	-6.48455	-0.52238
O	0.00000	-9.77055	-5.20438	H	0.00000	-7.61155	-2.60338
C	0.00000	-8.24755	-5.02538	H	0.00000	-8.83955	-2.00838
C	0.00000	-8.27955	-4.45538	H	0.00000	-8.27355	-0.20538
C	0.00000	-8.23155	-5.52638	H	0.00000	-8.64855	0.31962
O	0.00000	-9.02355	-6.48338	H	0.00000	-6.22555	-1.33838
O	0.00000	-7.43255	-5.40138	H	0.00000	-4.96455	0.74962
H	0.00000	-6.63155	-3.15638	H	0.00000	-6.47955	1.64762
H	0.00000	-9.41855	-3.44638	H	0.00000	-6.10555	0.74962
H	0.00000	-7.27455	-5.46438	H	0.00000	-5.42655	-0.55738
H	0.00000	-8.99855	-5.79638	H	0.00000	-6.96555	-1.40438

H	0.00000	-6.91555	0.35862	C	0.00000	-15.31955	-1.71638
N	0.00000	-10.62755	-1.85638	O	0.00000	-16.40255	-1.28338
C	0.00000	-11.98055	-1.77938	N	0.00000	-14.55455	-1.06138
C	0.00000	-12.71255	-3.08138	H	0.00000	-13.60955	-5.47438
O	0.00000	-13.89955	-3.09238	H	0.00000	-12.41655	-3.88938
C	0.00000	-11.94955	-1.56638	H	0.00000	-14.42155	-2.30838
C	0.00000	-10.94555	-0.53938	H	0.00000	-13.03455	-2.20138
C	0.00000	-10.78555	-0.68938	H	0.00000	-14.21355	-3.50338
C	0.00000	-11.36555	0.87662	H	0.00000	-15.60255	-3.65238
H	0.00000	-9.88555	-2.07138	H	0.00000	-13.69055	-1.45738
H	0.00000	-12.49955	-0.96138	H	0.00000	-14.87655	-0.20638
H	0.00000	-11.72455	-2.51538	N	0.00000	-13.76555	-5.52338
H	0.00000	-12.93555	-1.26338	C	0.00000	-14.56555	-6.38438
H	0.00000	-9.98455	-0.72938	C	0.00000	-15.01455	-5.64638
H	0.00000	-10.08155	0.04462	O	0.00000	-14.30855	-5.60638
H	0.00000	-11.74055	-0.54538	C	0.00000	-13.78355	-7.64938
H	0.00000	-10.41555	-1.68338	C	0.00000	-13.80055	-8.77438
H	0.00000	-10.61555	1.56862	C	0.00000	-15.22855	-9.21238
H	0.00000	-11.45555	0.96862	C	0.00000	-13.07755	-8.35538
H	0.00000	-12.31255	1.10162	H	0.00000	-12.79855	-5.46838
N	0.00000	-11.97855	-4.17438	H	0.00000	-15.44155	-6.66338
C	0.00000	-12.58255	-5.48938	H	0.00000	-12.75055	-7.36738
C	0.00000	-12.61755	-6.03338	H	0.00000	-14.18155	-8.03938
O	0.00000	-13.64555	-6.53238	H	0.00000	-13.27955	-9.62838
H	0.00000	-11.00555	-4.08338	H	0.00000	-15.73055	-9.47838
H	0.00000	-13.59455	-5.43038	H	0.00000	-15.20855	-10.07138
H	0.00000	-12.01955	-6.17138	H	0.00000	-15.76155	-8.40638
N	0.00000	-11.50255	-5.92938	H	0.00000	-13.52255	-7.44838
C	0.00000	-11.40855	-6.47538	H	0.00000	-13.16455	-9.14138
C	0.00000	-11.65455	-5.39038	H	0.00000	-12.03455	-8.17938
O	0.00000	-10.72255	-4.85638	N	0.00000	-16.17855	-5.02938
C	0.00000	-10.04055	-7.11138	C	0.00000	-16.76855	-4.28938
O	0.00000	-9.56555	-7.76738	C	0.00000	-18.15555	-4.85038
H	0.00000	-10.73055	-5.45338	O	0.00000	-18.28055	-5.60638
H	0.00000	-12.17155	-7.23338	C	0.00000	-16.85555	-2.80338
H	0.00000	-9.33655	-6.34838	O	0.00000	-15.61955	-2.33538
H	0.00000	-10.12655	-7.83338	O	0.00000	-19.10555	-4.56238
H	0.00000	-10.30255	-8.19138	H	0.00000	-16.66255	-5.07838
N	0.00000	-12.91455	-5.05638	H	0.00000	-16.13455	-4.40838
C	0.00000	-13.29955	-4.12038	H	0.00000	-17.63155	-2.65738
C	0.00000	-14.30055	-4.80438	H	0.00000	-17.09455	-2.23238
O	0.00000	-15.51255	-4.71238	H	0.00000	-15.45755	-2.75638
C	0.00000	-13.86155	-2.82438				
C	0.00000	-14.77355	-3.02438				