

Supporting Information

Proton Translocation via Tautomerization of Asn298 During the S₂–S₃ State Transition in the Oxygen-Evolving Complex of Photosystem II

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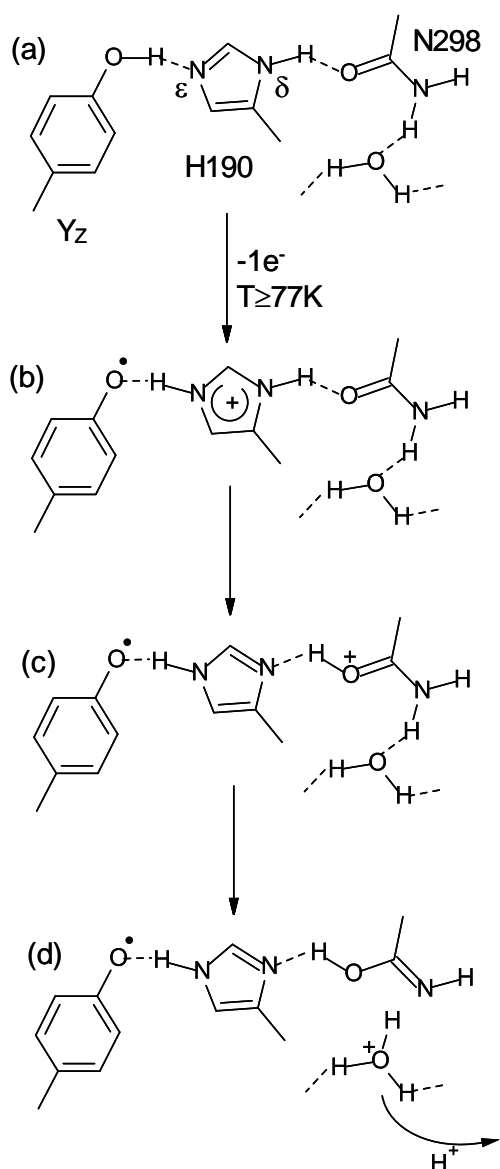
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Temperature (K)	Rate constant k (s^{-1})	Driving force $-\Delta G^0$ (meV)
212	0.00333	1219
212	0.00356	1216
193	0.00406	1208
188	0.00408	1208
150	0.00490	1197
148	0.00535	1192
123	0.00524	1193
123	0.00629	1182
77	0.00658	1179
77	0.00714	1174

Table S1. Data extracted from charge recombination kinetics of the $S_2Y_z^*$ with $Q_A^{\bullet-}$ at 10K. Driving forces were calculated using the Hopfield expression,

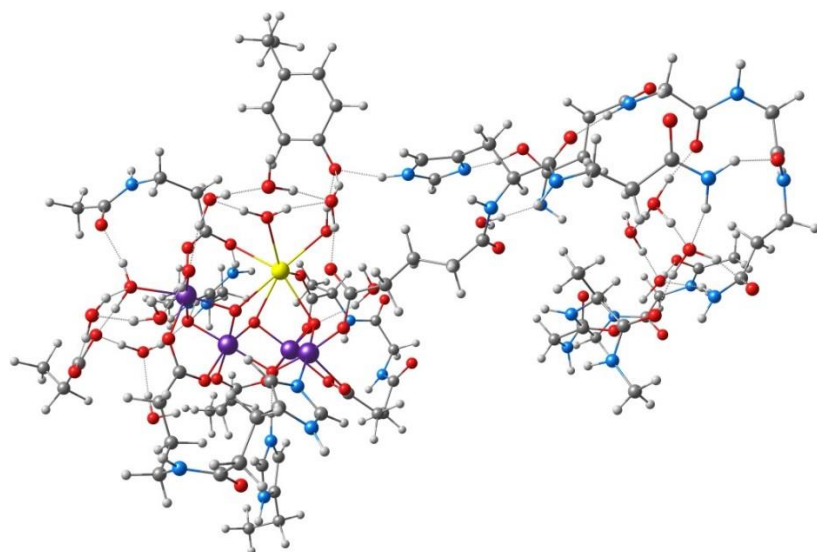
$k_{et} = (2\pi/\hbar)H_{AB}^2 \times [1/(2\lambda\pi\hbar\omega \coth(\hbar\omega/2k_B T))]^{1/2} \exp[-(\Delta G^0 + \lambda)2/2\lambda\hbar\omega \coth(\hbar\omega/2k_B T)]$, with $\hbar\omega=70$ meV, $H_{AB}=7.6 \times 10^{-6}$ meV, $\lambda=550$ meV and $T=10$ K.



Scheme S1. Schematic illustration of the suggested deprotonation events which lead to proton exit after tyrosine oxidation in the S_2 state. (a) Y_z /His190/Asn298 prior to electron transfer. Oxidation of Y_z by P_{680}^+ initially leads to a state which is characterized by the wide EPR signal (b), followed by one characterized by the narrow EPR signal (c). Finally, one proton is expelled via a mechanism that involves amide to imidic acid tautomerism (d).

Cartesian Coordinates of DFT Models

Figure depicting the full size of the 343-atom models:



Model 1

W558

Mn	25.111405000	265.901562000	349.591667000	C	31.847764000	262.949999000	343.276862000
Mn	27.549225000	265.565094000	350.861329000	O	30.694323000	262.462383000	343.295410000
Mn	27.510169000	263.652951000	348.843608000	H	32.975660000	261.493750000	344.221540000
Mn	27.783639000	263.457794000	346.102651000	N	32.089075000	264.284467000	343.265974000
Ca	28.010236000	266.965916000	347.750057000	C	31.032000000	265.273990000	343.182010000
O	26.679725000	266.851809000	349.834232000	H	31.119580000	265.798180000	342.334930000
O	28.568123000	265.036489000	349.450955000	C	30.852282000	266.123986000	344.455243000
O	26.190311000	264.413055000	350.170482000	C	30.025431000	265.523444000	345.612959000
O	28.707398000	262.935802000	347.686277000	O	30.092866000	266.068847000	346.754576000
O	26.956142000	264.606532000	347.359784000	O	29.222427000	264.564173000	345.313954000
H	30.563980000	256.790870000	345.924360000	H	21.787259000	271.372980000	347.553611000
C	30.505000000	257.418000000	346.833010000	C	22.609001000	271.709020000	348.186009000
H	31.119800000	256.955650000	347.605250000	C	22.810183000	273.210410000	348.201551000
C	29.041770000	257.722332000	347.194251000	O	23.148191000	273.810178000	349.230130000
C	28.445199000	258.833843000	346.312151000	C	23.878235000	270.865546000	347.869821000
O	29.200597000	259.884077000	346.173813000	C	23.463216000	269.377678000	347.759279000
O	27.302510000	258.701255000	345.798483000	C	24.534636000	268.317638000	347.997961000
H	31.021546000	258.363460000	346.583633000	O	25.642976000	268.316011000	347.392719000
H	33.893680000	272.587130000	341.290820000	O	24.166211000	267.389781000	348.827752000
C	33.179000000	272.187010000	342.010010000	H	23.051779000	269.181477000	346.748503000
H	33.591770000	271.381890000	342.617880000	H	24.624304000	270.997773000	348.675107000
C	31.880206000	271.686401000	341.315097000	H	22.650635000	269.164296000	348.474537000
C	30.833606000	271.399516000	342.353940000	H	24.352455000	271.205061000	346.930996000
C	29.798605000	272.351503000	342.621677000	H	19.443840000	261.850980000	348.348240000
C	30.914830000	270.220583000	343.167348000	C	20.347000000	261.696010000	347.758000000
C	28.901307000	272.162499000	343.656859000	C	21.353712000	260.915747000	348.571232000
C	30.039530000	270.013897000	344.218089000	O	21.605608000	261.171722000	349.769716000
C	29.008305000	270.992657000	344.508460000	C	20.961338000	262.992458000	347.166036000
O	28.201870000	270.828126000	345.499927000	C	21.827359000	263.748244000	348.116234000
H	30.074867000	269.120739000	344.854021000	C	23.172118000	264.074838000	348.076545000
H	32.932370000	273.017529000	342.698053000	N	21.364968000	264.250518000	349.324224000
H	32.104897000	270.768642000	340.738223000	C	22.381252000	264.851715000	349.978922000
H	29.730864000	273.249161000	341.994069000	N	23.493021000	264.764341000	349.237170000
H	31.510759000	272.448798000	340.606618000	H	20.147230000	263.639975000	346.788518000
H	34.005210000	262.615900000	343.259770000	H	23.916060000	263.882008000	347.300788000
C	33.066000000	262.063990000	343.297000000	H	22.304903000	265.352331000	350.943704000

H	21.586362000	262.730804000	346.294169000	C	34.984782000	264.156998000	351.621418000
N	21.995564000	259.952767000	347.870492000	C	33.901894000	264.903813000	350.831369000
C	23.071000000	259.170010000	348.449000000	N	32.922461000	263.982047000	350.233226000
H	22.721090000	258.770010000	349.400660000	C	31.996544000	264.336431000	349.315914000
C	24.360807000	259.996495000	348.646922000	N	31.822856000	265.633402000	349.001699000
C	24.942355000	260.529909000	347.333683000	N	31.291564000	263.406128000	348.656908000
C	25.943829000	261.656814000	347.475879000	H	37.585824000	261.870864000	351.030379000
O	26.181605000	262.174574000	348.618091000	H	35.401243000	262.576699000	350.181626000
O	26.483989000	262.047619000	346.384322000	H	36.465559000	263.983777000	350.040495000
H	24.153755000	260.936844000	346.667849000	N	22.557488000	273.863449000	347.012214000
H	21.744521000	259.802968000	346.895716000	C	22.951000000	275.252010000	346.817990000
H	25.116844000	259.381791000	349.169229000	C	24.157538000	275.367183000	345.841089000
H	25.451442000	259.738486000	346.749769000	C	25.316118000	274.542411000	346.305229000
H	24.129661000	260.845554000	349.309715000	C	25.808021000	273.341177000	345.817283000
H	25.458790000	259.267550000	354.767240000	N	26.031915000	274.880888000	347.444844000
C	25.515000000	259.965000000	355.603000000	C	26.932149000	273.922974000	347.646820000
H	25.321020000	259.480770000	356.560070000	N	26.825630000	272.972146000	346.680827000
C	24.578005000	261.176113000	355.346129000	H	22.482784000	273.279860000	346.176830000
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C	25.489680000	262.671171000	353.340031000	H	23.273240000	275.614399000	347.815356000
N	23.751639000	261.376627000	352.953497000	H	24.435611000	276.434294000	345.778177000
C	24.009113000	262.031913000	351.804733000	H	25.523508000	272.730905000	344.959217000
N	25.070408000	262.819145000	352.024105000	H	27.632082000	273.890661000	348.483669000
H	25.517768000	263.450215000	351.280264000	H	23.842211000	275.041237000	344.832497000
H	26.563466000	260.317773000	355.630307000	H	30.268963000	267.027238000	344.188214000
H	26.333815000	263.242799000	353.727375000	H	31.810923000	266.481397000	344.872755000
H	23.421685000	261.935245000	350.886190000	O	27.576845000	266.101952000	343.268921000
H	24.999320000	267.480390000	355.837610000	H	26.743697000	266.586618000	343.022045000
C	25.565000000	267.226990000	354.941010000	H	27.258383000	265.253895000	343.718402000
C	26.440321000	268.434904000	354.624584000	O	26.528021000	260.498206000	343.868833000
O	26.004640000	269.421292000	354.014301000	H	27.238918000	261.168276000	344.019235000
C	24.589329000	266.891397000	353.817462000	H	26.748664000	259.834249000	344.591387000
C	25.209905000	266.378774000	352.527609000	O	24.605616000	262.331063000	344.289810000
O	26.458070000	266.080181000	352.507474000	H	24.258024000	262.437478000	343.383959000
O	24.416674000	266.262322000	351.536590000	H	25.252104000	261.553924000	344.203520000
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C	28.598000000	269.534000000	355.099000000	O	28.437440000	269.416078000	347.751726000
C	29.612550000	269.648649000	353.950070000	H	28.447206000	269.895861000	346.873639000
O	30.361859000	270.636582000	353.867107000	H	29.255880000	269.672571000	348.219549000
H	29.133410000	269.629740000	356.043600000	O	27.896688000	267.579195000	345.381201000
H	28.013755000	267.549910000	355.629457000	H	27.845851000	266.953062000	344.565407000
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O	28.872701000	266.768340000	351.496468000	H	26.588751000	268.624656000	350.175690000
H	32.230495000	268.373774000	350.862268000	H	27.076935000	269.720779000	349.219649000
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H	30.155987000	269.673156000	351.328397000	H	25.910945000	263.479475000	344.571415000
H	31.884632000	267.282798000	352.261789000	O	28.642430000	262.010087000	344.998322000
H	32.264080000	269.013963000	352.530921000	H	29.427538000	262.282553000	344.435733000
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H	32.129410000	261.846910000	354.006980000	H	25.506382000	268.492479000	343.659696000
C	30.203276000	262.398759000	353.316842000	H	25.358151000	268.317433000	342.119952000
C	29.015428000	261.848833000	352.499583000	O	25.391725000	267.805327000	342.949283000
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O	28.235256000	264.076096000	352.006861000	H	28.700663000	259.969521000	349.491596000
O	28.158528000	262.510692000	350.367116000	H	31.695854000	269.480812000	342.948756000
H	28.197859000	261.495922000	353.159907000	H	28.109476000	272.889229000	343.875389000
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H	29.461851000	261.550849000	348.342792000	C	18.840793000	275.433060000	352.027591000
H	24.804824000	261.986788000	356.061746000	O	17.973123000	276.239912000	351.604931000
H	23.526930000	260.886184000	355.533148000	C	20.436398000	275.202822000	350.103016000
H	33.378753000	265.606191000	351.510731000	O	22.033366000	277.377336000	346.117698000
H	34.366968000	265.501904000	350.022943000	O	20.424898000	278.931902000	349.552979000
H	35.547601000	264.917366000	352.195862000	O	21.979430000	278.685147000	351.551762000
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H	28.958933000	258.089479000	348.235046000	H	20.518446000	274.615927000	346.486157000
H	28.399040000	256.828400000	347.119882000	H	18.703122000	275.599120000	345.412502000
H	31.125217000	265.878450000	348.284765000	H	19.636907000	277.409816000	347.631026000
H	32.110525000	266.367256000	349.640773000	H	18.044127000	276.654631000	347.432560000
H	30.379139000	263.637809000	348.226917000	H	17.411468000	280.219024000	347.248776000
H	31.393587000	262.403969000	348.849743000	H	17.442084000	278.798862000	348.249365000
H	20.423281000	264.126470000	349.693447000	H	24.844431000	279.286545000	346.794459000
H	22.987112000	260.710454000	353.070323000	H	22.962022000	278.291595000	348.230530000
C	21.820729000	276.167877000	346.349992000	H	23.577684000	279.230921000	349.596941000
N	20.618114000	275.584179000	346.181663000	H	23.871424000	277.047139000	350.587145000
C	19.446000000	276.340000000	345.755000000	H	22.815539000	279.181113000	351.465569000
H	19.680950000	276.898580000	344.959520000	H	22.326012000	279.219211000	346.489698000
C	18.841999000	277.191010000	346.890020000	H	20.516285000	280.329561000	345.695450000
C	18.358531000	278.571431000	346.429619000	H	21.532633000	281.788334000	345.486578000
N	17.555039000	279.204115000	347.315135000	H	19.795229000	283.126159000	346.077068000
O	18.719755000	279.081131000	345.349528000	H	19.724366000	283.994233000	348.715178000
H	25.275691000	280.167699000	348.188078000	H	18.814811000	283.399365000	350.541857000
C	24.481999000	279.798001000	347.704992000	H	16.825258000	281.183952000	350.508408000
C	23.419010000	280.807537000	347.296939000	H	18.342864000	281.982299000	353.052795000
O	23.475823000	282.029816000	347.518867000	H	19.261542000	281.195395000	351.759139000
C	23.880639000	278.739572000	348.656565000	H	19.460242000	279.492008000	353.744996000
C	24.786730000	277.559553000	348.969606000	H	18.209766000	278.289414000	353.655570000
N	24.658264000	276.769949000	349.987473000	H	17.455651000	278.831778000	350.636201000
O	25.712330000	277.335634000	348.033944000	H	18.102072000	277.414794000	350.603359000
N	22.353671000	280.233111000	346.656416000	H	21.427070000	283.452766000	357.018109000
C	21.223999000	281.008999000	346.209990000	H	22.728286000	282.171276000	358.199289000
C	20.461569000	281.666823000	347.349565000	H	24.184124000	280.496672000	358.772898000
O	20.447756000	281.230521000	348.530998000	H	24.787202000	280.514771000	357.093507000
N	19.744674000	282.755594000	347.024603000	H	25.035923000	278.329893000	356.942132000
C	19.011000000	283.493010000	348.032991000	H	24.445268000	276.075228000	357.609593000
C	18.055367000	282.594684000	348.829072000	H	22.742447000	276.599156000	357.703965000
O	17.259326000	281.827930000	348.258189000	H	22.519150000	274.544536000	356.516502000
H	18.434830000	284.191610000	347.608230000	H	23.427951000	274.338822000	353.736985000
N	18.103059000	282.773697000	350.168038000	H	21.819714000	274.110658000	351.952187000
C	17.337001000	281.957000000	351.103004000	H	21.459229000	275.428777000	349.759540000
H	16.641987000	282.518131000	351.552545000	H	20.239852000	274.131011000	349.923198000
C	18.238001000	281.334020000	352.162991000	H	19.723013000	275.792438000	349.505585000
C	17.737019000	279.949866000	352.599395000	H	20.511224000	279.861695000	349.074101000
N	18.502497000	279.246986000	353.458252000	H	19.405772000	278.737510000	349.824122000
O	16.676496000	279.468827000	352.130344000	H	21.716238000	278.809772000	352.532419000
O	18.065330000	278.288209000	350.067073000	H	21.049482000	278.887462000	350.393028000
H	22.031620000	283.602460000	355.441470000	H	21.418610000	278.074975000	354.459592000
C	21.583000000	282.946990000	356.049010000	H	21.890341000	279.603524000	354.593535000
C	22.466436000	281.733790000	356.209757000	N	18.545221000	274.421164000	352.840366000
O	22.731812000	280.953687000	355.263990000	C	17.201000000	274.185000000	353.303010000
H	20.684750000	282.662970000	355.713620000	H	17.041754000	274.523807000	354.230291000
N	22.995314000	281.549635000	357.439908000	H	17.005139000	273.205040000	353.266725000
C	23.874000000	280.441010000	357.715000000	H	20.532629000	276.626586000	351.718109000
C	23.199480000	279.081045000	357.499749000	H	19.304188000	273.810551000	353.140112000
O	21.987160000	278.897559000	357.673474000	H	16.505038000	274.704389000	352.624842000
N	24.079621000	278.089153000	357.195063000	O	26.691879000	274.964610000	350.579829000
C	23.678000000	276.709990000	357.126010000	H	27.077356000	275.469456000	351.319033000
C	23.458324000	276.191228000	355.704207000	H	25.890423000	275.525091000	350.326885000
O	23.783567000	276.819978000	354.688766000				

Model 2

W628

Mn	25.110102000	265.897561000	349.593696000	C	21.353035000	260.915010000	348.571378000
Mn	27.548366000	265.563294000	350.861072000	O	21.603216000	261.169452000	349.770631000
Mn	27.508820000	263.651951000	348.842093000	C	20.960647000	262.992578000	347.166286000
Mn	27.780857000	263.458162000	346.100789000	C	21.826598000	263.747111000	348.117223000
Ca	28.008097000	266.961848000	347.750312000	C	23.171855000	264.071457000	348.078807000
O	26.677867000	266.849183000	349.834787000	N	21.364210000	264.248209000	349.325718000
O	28.566173000	265.035247000	349.449024000	C	22.381147000	264.846855000	349.981777000
O	26.190119000	264.409513000	350.170309000	N	23.493052000	264.758685000	349.240493000
O	28.706460000	262.937232000	347.682882000	H	20.146219000	263.640138000	346.789540000
O	26.952811000	264.604721000	347.357826000	H	23.916156000	263.878709000	347.303409000
H	30.563980000	256.790870000	345.924360000	H	22.305278000	265.346767000	350.946957000
C	30.505000000	257.418000000	346.833010000	H	21.585536000	262.731656000	346.294102000
H	31.119800000	256.955650000	347.605250000	N	21.995307000	259.952531000	347.870466000
C	29.042560000	257.723537000	347.194977000	C	23.071000000	259.170010000	348.449000000
C	28.446008000	258.833725000	346.311205000	H	22.721090000	258.770010000	349.400660000
O	29.201569000	259.882991000	346.169140000	C	24.359896000	259.997422000	348.646844000
O	27.302426000	258.700171000	345.799146000	C	24.943171000	260.527228000	346.752925000
H	31.022163000	258.363188000	346.583819000	C	25.943456000	261.655072000	347.474366000
H	33.893680000	272.587130000	341.290820000	O	26.180467000	262.173647000	348.616299000
C	33.179000000	272.187010000	342.010010000	O	26.483434000	262.045345000	346.382532000
H	33.591770000	271.381890000	342.617880000	H	24.155529000	260.931027000	346.664321000
C	31.879503000	271.685539000	341.319467000	H	21.746235000	259.804890000	346.894830000
C	30.832341000	271.390408000	342.357815000	H	25.115032000	259.384407000	349.172308000
C	29.772217000	272.317679000	342.604149000	H	25.454268000	259.734424000	346.752925000
C	30.935212000	270.227264000	343.189129000	H	24.127157000	260.848450000	349.306587000
C	28.868852000	272.118778000	343.634301000	H	25.458790000	259.267550000	354.767240000
C	30.054632000	270.012608000	344.235688000	C	25.515000000	259.965000000	355.603000000
C	28.995952000	270.965343000	344.501659000	H	25.321020000	259.480770000	356.560070000
O	28.179981000	270.792309000	345.488210000	C	24.578529000	261.176568000	355.346533000
H	30.109948000	269.128761000	344.883017000	C	24.652035000	261.747465000	353.951761000
H	32.932848000	273.017261000	342.698646000	C	25.490677000	262.668967000	353.338594000
H	32.104781000	270.770124000	340.738488000	N	23.750793000	261.376156000	352.954561000
H	29.687421000	273.206032000	341.965303000	C	24.008695000	262.029611000	351.804835000
H	31.505580000	272.447399000	340.612623000	N	25.071095000	262.815675000	352.022663000
H	34.005210000	262.615900000	343.259770000	H	25.518635000	263.446214000	351.278092000
C	33.066000000	262.063990000	343.297000000	H	26.563588000	260.317454000	355.630294000
C	31.847916000	262.950017000	343.276021000	H	26.335218000	263.240560000	353.725087000
O	30.694348000	262.462052000	343.293107000	H	23.420879000	261.932319000	350.886662000
H	32.975660000	261.493750000	344.221540000	H	24.999320000	267.480390000	355.837610000
N	32.089012000	264.284221000	343.265442000	C	25.565000000	267.226990000	354.941010000
C	31.032001000	265.273990000	343.182010000	C	26.440056000	268.434717000	354.623346000
H	31.119580000	265.798180000	342.334930000	O	26.004897000	269.419651000	354.010394000
C	30.853023000	266.122912000	344.455983000	C	24.589376000	266.889679000	353.818089000
C	30.022909000	265.522545000	345.611245000	C	25.209581000	266.374829000	352.528128000
O	30.091068000	266.063919000	346.754719000	O	26.458053000	266.077284000	352.508117000
O	29.216584000	264.566680000	345.309411000	O	24.415642000	266.255797000	351.538877000
H	21.787260000	271.372980000	347.553610000	N	27.722823000	268.377319000	355.110474000
C	22.609000000	271.709020000	348.186010000	C	28.598000000	269.534000000	355.099000000
C	22.837702000	273.206546000	348.195142000	C	29.614505000	269.644786000	353.951357000
O	23.246186000	273.792842000	349.202351000	O	30.371633000	270.626932000	353.872353000
C	23.874221000	270.856422000	347.876977000	H	29.133410000	269.629740000	356.043600000
C	23.454127000	269.370713000	347.767465000	H	28.012469000	267.550667000	355.630261000
C	24.526267000	268.310025000	347.999603000	N	29.582219000	268.632921000	353.058359000
O	25.630494000	268.306417000	347.388049000	C	30.261544000	268.657309000	351.767468000
O	24.161049000	267.383327000	348.833034000	C	29.532779000	267.677155000	350.837279000
H	23.037129000	269.175987000	346.758640000	O	29.627822000	267.774854000	349.599036000
H	24.618427000	270.987213000	348.684101000	C	31.754614000	268.290199000	351.866011000
H	22.645144000	269.158795000	348.487303000	O	28.871626000	266.765122000	351.495653000
H	24.352708000	271.192445000	346.939152000	H	32.232888000	268.357886000	350.872423000
H	19.443840000	261.850980000	348.348240000	H	28.883385000	267.894730000	353.179061000
C	20.347000000	261.696010000	347.758000000	H	30.163229000	269.668113000	351.327377000

H	31.874806000	267.269422000	352.270593000	O	28.642141000	262.011186000	344.995009000
H	32.262493000	268.998969000	352.540715000	H	29.427912000	262.284179000	344.433480000
H	30.864030000	260.791230000	354.757570000	H	28.859882000	261.084024000	345.504365000
C	31.178000000	261.334020000	353.866000000	O	27.856809000	259.653353000	349.902569000
H	32.129410000	261.846910000	354.006980000	H	25.497827000	268.480141000	343.654613000
C	30.202011000	262.398029000	353.317560000	H	25.372721000	268.312243000	342.111855000
C	29.018583000	261.846691000	352.495048000	O	25.383962000	267.796536000	342.939581000
C	28.430448000	262.884641000	351.554107000	H	27.377071000	260.499537000	349.995026000
O	28.236515000	264.073659000	352.004931000	H	28.705017000	259.969280000	349.486566000
O	28.158764000	262.509344000	350.364151000	H	31.736688000	269.503897000	342.989937000
H	28.200363000	261.487615000	353.151316000	H	28.057784000	272.829039000	343.836168000
H	30.783097000	263.066416000	352.651291000	H	25.931209000	276.291474000	347.964745000
H	29.317925000	260.985369000	351.872193000	H	33.014618000	261.352396000	342.455501000
H	29.824941000	263.049816000	354.126999000	H	33.057405000	264.597063000	343.218372000
H	36.466940000	262.009610000	352.392230000	H	30.094918000	264.699228000	343.059508000
C	37.013000000	262.588010000	351.647000000	H	22.294961000	271.461404000	349.217730000
H	37.736650000	263.287660000	352.065240000	H	20.003271000	261.084562000	346.902406000
C	35.968870000	263.321337000	350.773396000	H	23.259622000	258.314163000	347.77985000
C	34.990518000	264.164229000	351.613741000	H	26.187371000	266.348828000	355.190884000
C	33.911923000	264.911529000	350.818707000	H	23.866281000	266.120890000	354.150942000
N	32.927301000	263.991253000	350.226311000	H	23.991786000	267.778200000	353.544804000
C	32.001395000	264.346292000	349.308830000	H	27.965526000	270.436456000	355.003380000
N	31.836641000	265.641986000	348.986514000	H	31.365695000	260.568639000	353.086865000
N	31.287448000	263.416673000	348.658375000	H	32.976019000	263.006674000	350.481629000
H	37.586632000	261.870118000	351.031857000	H	30.003777000	260.313982000	347.667238000
H	35.401117000	262.574858000	350.182071000	H	29.463722000	261.554621000	348.337534000
H	36.470398000	263.977231000	350.034095000	H	24.806411000	261.987278000	356.061767000
N	22.528251000	273.873275000	347.022235000	H	23.527370000	260.887433000	355.534221000
C	22.951000000	275.252010000	346.817990000	H	33.392757000	265.621540000	351.492985000
C	24.159433000	275.344375000	345.840841000	H	34.380566000	265.501303000	350.006048000
C	25.307989000	274.507168000	346.306941000	H	35.556477000	264.925289000	352.184154000
C	25.789064000	273.302478000	345.815749000	H	34.498660000	263.524388000	352.375711000
N	26.029122000	274.841981000	347.443353000	H	28.961989000	258.092809000	348.235155000
C	26.922452000	273.877780000	347.640869000	H	28.399173000	256.829868000	347.123305000
N	26.806975000	272.926160000	346.675248000	H	31.142680000	265.889472000	348.266443000
H	22.429142000	273.293112000	346.186818000	H	32.138180000	266.378950000	349.615516000
H	27.421424000	272.118158000	346.502438000	H	30.376830000	263.652319000	348.227363000
H	23.276162000	275.621102000	347.812393000	H	31.383902000	262.414437000	348.853516000
H	24.452550000	276.407206000	345.774179000	H	20.422320000	264.124494000	349.694506000
H	25.497522000	272.693712000	344.958846000	H	22.985534000	260.711056000	353.072578000
H	27.627342000	273.839906000	348.473376000	C	21.833168000	276.179236000	346.332279000
H	23.839596000	275.017908000	344.833622000	N	20.614388000	275.607861000	346.210061000
H	30.274932000	267.029601000	344.189374000	C	19.446000000	276.340000000	345.755000000
H	31.812570000	266.475512000	344.875562000	H	19.680950000	276.898580000	344.959520000
O	27.572230000	266.094491000	343.257733000	C	18.841999000	277.191010000	346.890020000
H	26.739098000	266.581096000	343.014268000	C	17.492043000	277.836749000	346.675544000
H	27.252979000	265.247532000	343.707503000	N	17.085069000	278.121106000	345.431253000
O	26.529844000	260.493885000	343.867401000	O	16.752986000	278.118417000	347.664729000
H	27.240107000	261.164735000	344.017070000	H	25.275691000	280.167700000	348.188079000
H	26.749508000	259.831547000	344.591964000	C	24.482000000	279.798000000	347.704991000
O	24.602844000	262.321479000	344.282759000	C	23.441491000	280.810615000	347.255711000
H	24.262053000	262.431142000	343.374698000	O	23.535680000	282.041431000	347.409131000
H	25.252165000	261.546201000	344.197498000	C	23.880639000	278.739572000	348.656565000
O	30.059413000	260.778502000	348.550842000	C	24.785592000	277.555167000	348.953613000
O	28.432320000	269.408549000	347.743649000	N	24.664160000	276.779163000	349.976882000
H	28.435061000	269.883152000	346.860511000	O	25.699141000	277.322922000	347.997275000
H	29.249017000	269.676041000	348.207901000	N	22.366420000	280.236266000	346.632002000
O	27.885944000	267.562412000	345.380361000	C	21.223999000	281.008999000	346.209990000
H	27.840273000	266.939799000	344.562788000	C	20.545367000	281.738445000	347.369470000
H	27.224994000	268.254026000	345.151078000	O	20.644572000	281.368128000	348.557342000
O	25.758967000	269.567787000	345.047198000	N	19.784324000	282.799502000	347.022759000
H	26.499921000	270.213762000	345.128573000	C	19.011000000	283.493010000	348.032991000
H	25.653552000	269.189044000	345.975720000	C	18.128599000	282.503986000	348.820598000
O	26.636443000	269.610854000	350.083106000	O	17.520515000	281.577410000	348.265212000
H	26.583370000	268.625622000	350.168650000	H	18.434830000	284.191610000	347.608730000
H	27.071618000	269.718461000	349.208945000	N	18.067168000	282.779284000	350.148609000
O	26.737983000	264.028100000	344.690377000	C	17.337001000	281.957000000	351.103004000
H	25.906817000	263.472862000	344.571870000	H	16.641987000	282.518131000	351.552545000

C	18.238001000	281.334020000	352.162991000	H	22.318113000	279.216242000	346.526812000
C	18.005061000	279.828910000	352.310378000	H	20.487834000	280.317237000	345.762352000
N	18.914838000	279.088738000	352.956803000	H	21.501792000	281.744951000	345.429705000
O	16.969161000	279.290124000	351.814859000	H	19.718670000	283.087053000	346.048545000
O	17.868664000	277.961449000	349.867128000	H	19.701505000	284.005304000	348.731344000
H	22.031620000	283.602460000	355.441470000	H	18.648542000	283.534255000	350.509125000
C	21.583000000	282.946990000	356.049010000	H	16.823508000	281.175660000	350.520086000
C	22.495011000	281.755686000	356.208033000	H	18.075547000	281.791827000	353.157248000
O	22.832694000	281.025042000	355.248333000	H	19.306614000	281.493319000	351.923424000
H	20.684750000	282.662970000	355.713620000	H	19.834538000	279.393681000	353.326867000
N	22.983763000	281.543870000	357.452047000	H	18.708279000	278.097142000	353.083527000
C	23.874000000	280.441010000	357.715000000	H	17.375822000	278.521870000	350.593119000
C	23.202113000	279.079308000	357.506928000	H	17.948743000	277.003128000	350.326534000
O	21.991677000	278.895324000	357.694946000	H	21.424242000	283.453398000	357.017571000
N	24.080049000	278.088693000	357.194412000	H	22.653725000	282.113644000	358.227144000
C	23.678000000	276.709990000	357.126010000	H	24.197519000	280.496762000	358.769008000
C	23.441847000	276.196747000	355.705695000	H	24.777026000	280.523389000	357.080907000
O	23.730124000	276.843867000	354.690529000	H	25.030160000	278.331855000	356.920802000
N	22.926451000	274.934123000	355.663703000	H	24.450023000	276.073909000	357.600221000
C	22.540000000	274.355990000	354.399990000	H	22.748373000	276.596816000	357.712983000
C	21.437792000	275.175087000	353.714770000	H	22.561943000	274.519439000	356.519521000
O	20.800651000	276.078044000	354.275748000	H	23.416892000	274.348082000	353.722801000
H	22.252660000	273.406850000	354.528710000	H	21.815177000	274.126751000	351.975308000
N	21.178378000	274.779187000	352.435976000	H	21.712664000	275.635687000	349.964925000
C	20.285000000	275.553011000	351.592011000	H	20.476718000	274.348636000	349.767561000
C	18.821273000	275.286036000	351.853735000	H	20.053834000	276.071523000	349.491154000
O	17.909618000	275.866111000	351.190367000	H	20.702262000	279.727013000	349.047763000
C	20.650029000	275.384178000	350.110141000	H	17.327279000	277.980934000	348.913024000
O	22.054609000	277.369342000	346.030832000	H	22.101777000	278.442055000	352.230847000
O	20.603641000	278.783771000	349.362474000	H	19.648070000	278.683354000	349.567668000
O	22.259568000	277.932349000	351.398735000	H	21.720107000	278.177961000	354.338588000
O	21.560682000	279.041923000	353.900336000	H	22.067185000	279.717553000	354.429630000
H	20.505930000	274.656647000	346.564366000	N	18.540876000	274.444757000	352.843051000
H	18.704146000	275.589548000	345.428262000	C	17.201000000	274.185000000	353.303010000
H	19.560119000	277.982840000	347.189039000	H	17.041754000	274.523807000	354.230291000
H	18.736347000	276.546864000	347.779607000	H	17.005139000	273.205040000	353.266725000
H	16.189968000	278.590470000	345.293123000	H	20.452456000	276.622144000	351.844324000
H	17.646930000	277.918526000	344.608556000	H	19.328965000	273.994917000	353.306875000
H	24.856017000	279.284016000	346.799123000	H	16.501137000	274.699803000	352.626010000
H	22.952493000	278.298079000	348.245173000	O	26.662487000	274.965638000	350.578202000
H	23.579610000	279.208212000	349.609264000	H	27.047411000	275.481137000	351.310450000
H	23.884449000	277.077686000	350.588887000	H	25.865368000	275.532635000	350.309542000
H	21.650619000	278.322934000	350.714988000				

Model 3

W604

Mn	25.106951000	265.876342000	349.601059000	C	31.883922000	271.682830000	341.311648000
Mn	27.548352000	265.556347000	350.861332000	C	30.833984000	271.375258000	342.341913000
Mn	27.515528000	263.642593000	348.842776000	C	29.751487000	272.282405000	342.571010000
Mn	27.785248000	263.449110000	346.100383000	C	30.952625000	270.217625000	343.180944000
Ca	27.995083000	266.946133000	347.746801000	C	28.842489000	272.070893000	343.592417000
O	26.671090000	266.838249000	349.835316000	C	30.066878000	269.991078000	344.219009000
O	28.568217000	265.030643000	349.449525000	C	28.986042000	270.924869000	344.469149000
O	26.195869000	264.396140000	350.172902000	O	28.168870000	270.742006000	345.450304000
O	28.713350000	262.930023000	347.682885000	H	30.133431000	269.113678000	344.873889000
O	26.955110000	264.593395000	347.359230000	H	32.928484000	273.016754000	342.697398000
H	30.563980000	256.790870000	345.924360000	H	32.117388000	270.770780000	340.728270000
C	30.505000000	257.418000000	346.833010000	H	29.654866000	273.164079000	341.924854000
H	31.119800000	256.955650000	347.605250000	H	31.509339000	272.445517000	340.606355000
C	29.041596000	257.721069000	347.193293000	H	34.005210000	262.615900000	343.259770000
C	28.445101000	258.829590000	346.307836000	C	33.066000000	262.063990000	343.297000000
O	29.201194000	259.878615000	346.165014000	C	31.848150000	262.950245000	343.275207000
O	27.301863000	258.696006000	345.795549000	O	30.694573000	262.462469000	343.289163000
H	31.021589000	258.363486000	346.584130000	H	32.975660000	261.493750000	344.221540000
H	33.893680000	272.587130000	341.290820000	N	32.089276000	264.284719000	343.267260000
C	33.179000000	272.187010000	342.010011000	C	31.032000000	265.273990000	343.182010000
H	33.591770000	271.381890000	342.617880000	H	31.119580000	265.798180000	342.334930000

C	30.848444000	266.122579000	344.455722000	O	30.359330000	270.635059000	353.861461000
C	30.021652000	265.519300000	345.612158000	H	29.133410000	269.629740000	356.043600000
O	30.088287000	266.061327000	346.755353000	H	28.008849000	267.555490000	355.644117000
O	29.218558000	264.560644000	345.310255000	N	29.581691000	268.632498000	353.057690000
H	21.787260000	271.372980000	347.553610000	C	30.253799000	268.660462000	351.763014000
C	22.609000000	271.709020000	348.186010000	C	29.524852000	267.677779000	350.835309000
C	22.925828000	273.177048000	348.114366000	O	29.616345000	267.775811000	349.596261000
O	23.530684000	273.743068000	349.036862000	C	31.749585000	268.301547000	351.853336000
C	23.860027000	270.818351000	347.918025000	O	28.869022000	266.763726000	351.494916000
C	23.421484000	269.342412000	347.800073000	H	32.223523000	268.371883000	350.857603000
C	24.497919000	268.282759000	348.013325000	H	28.887868000	267.890306000	353.183067000
O	25.597225000	268.286734000	347.392448000	H	30.148169000	269.671166000	351.324382000
O	24.144144000	267.353348000	348.847467000	H	31.877709000	267.281907000	352.258605000
H	22.993945000	269.159283000	346.793550000	H	32.256885000	269.013050000	352.525625000
H	24.586347000	270.938394000	348.742721000	H	30.864030000	260.791230000	354.757570000
H	22.619383000	269.129876000	348.527420000	C	31.178000000	261.334020000	353.866000000
H	24.368134000	271.141132000	346.990657000	H	32.129410000	261.846910000	354.006980000
H	19.443840000	261.850980000	348.348240000	C	30.202628000	262.397156000	353.317497000
C	20.347000000	261.696010000	347.758000000	C	29.016592000	261.843628000	352.500580000
C	21.354646000	260.916567000	348.571084000	C	28.432589000	262.879720000	351.556113000
O	21.606422000	261.171559000	349.769673000	O	28.237786000	264.069379000	352.005559000
C	20.957649000	262.992662000	347.164308000	O	28.166880000	262.503455000	350.365324000
C	21.823396000	263.744177000	348.116965000	H	28.198544000	261.491193000	353.160485000
C	23.172197000	264.053310000	348.087418000	H	30.782738000	263.062401000	352.647177000
N	21.358869000	264.247479000	349.323648000	H	29.312226000	260.978224000	351.881716000
C	22.378077000	264.832881000	349.987524000	H	29.828569000	263.052153000	354.125763000
N	23.493671000	264.733475000	349.253065000	H	36.466940000	262.009610000	352.392230000
H	20.142360000	263.639826000	346.788994000	C	37.013000000	262.588010000	351.647000000
H	23.918692000	263.855178000	347.315510000	H	37.736650000	263.287660000	352.065240000
H	22.301387000	265.333281000	350.952373000	C	35.965260000	263.322576000	350.777635000
H	21.582190000	262.732318000	346.291744000	C	34.981112000	264.152805000	351.624301000
N	21.996645000	259.953805000	347.870024000	C	33.896625000	264.899820000	350.836395000
C	23.071000000	259.170010000	348.449000000	N	32.918865000	263.977953000	350.235151000
H	22.721090000	258.770010000	349.400660000	C	31.994534000	264.332879000	349.316613000
C	24.361127000	259.994885000	348.647721000	N	31.818521000	265.631836000	349.008196000
C	24.945298000	260.522962000	347.333954000	N	31.295721000	263.403698000	348.650136000
C	25.950571000	261.645932000	347.475180000	H	37.585475000	261.871227000	351.029685000
O	26.190582000	262.162545000	348.617448000	H	35.401928000	262.577322000	350.180563000
O	26.490810000	262.035236000	346.383265000	H	36.463256000	263.987046000	350.043638000
H	24.158760000	260.931894000	346.666889000	N	22.525886000	273.869620000	347.002597000
H	21.745125000	259.803844000	346.895425000	C	22.951000000	275.252010000	346.817990000
H	25.114863000	259.380371000	349.173469000	C	24.196443000	275.361361000	345.893297000
H	25.451185000	259.728372000	346.751671000	C	25.326071000	274.492624000	346.353262000
H	24.130125000	260.846523000	349.307269000	C	25.775342000	273.295068000	345.816764000
H	25.458790000	259.267550000	354.767240000	N	26.077075000	274.779366000	347.486654000
C	25.515000000	259.965000000	355.603000000	C	26.958090000	273.793185000	347.628082000
H	25.321020000	259.480770000	356.560070000	N	26.803393000	272.872424000	346.639036000
C	24.575037000	261.173962000	355.347683000	H	22.280004000	273.326410000	346.173485000
C	24.647274000	261.744425000	353.953013000	H	27.404186000	272.062301000	346.426590000
C	25.488535000	262.662461000	353.338522000	H	23.238054000	275.615925000	347.823921000
N	23.744953000	261.374058000	352.956609000	H	24.502010000	276.422058000	345.875079000
C	24.004433000	262.025132000	351.805869000	H	25.455107000	272.722870000	344.944850000
N	25.069080000	262.808388000	352.022640000	H	27.709773000	273.711916000	348.415335000
H	25.519839000	263.435646000	351.277714000	H	23.908556000	275.076098000	344.864766000
H	26.562822000	260.319543000	355.630077000	H	30.262080000	267.023782000	344.188539000
H	26.334618000	263.232475000	353.724083000	H	31.805509000	266.482825000	344.874391000
H	23.415792000	261.928470000	350.888048000	O	27.556538000	266.090200000	343.264035000
H	24.999320000	267.480390000	355.837610000	H	26.716496000	266.565117000	343.019279000
C	25.565000000	267.226990000	354.941010000	H	27.246730000	265.240151000	343.716012000
C	26.443311000	268.431104000	354.618239000	O	26.527110000	260.491296000	343.866213000
O	26.014376000	269.410525000	353.992780000	H	27.238085000	261.162112000	344.012126000
C	24.590061000	266.887516000	353.818473000	H	26.748930000	259.830574000	344.591559000
C	25.209880000	266.364247000	352.531903000	O	24.603347000	262.318154000	344.296325000
O	26.459569000	266.071624000	352.510191000	H	24.248858000	262.428904000	343.393652000
O	24.414211000	266.234431000	351.545570000	H	25.250621000	261.542242000	344.201575000
N	27.723980000	268.376135000	355.112341000	O	30.066561000	260.768961000	348.545667000
C	28.598000000	269.534000000	355.099000000	O	28.413719000	269.398662000	347.741361000
C	29.609862000	269.647463000	353.947553000	H	28.435779000	269.865100000	346.856264000

H	29.233605000	269.647923000	348.210948000	N	22.363028000	280.233762000	346.635330000
O	27.878948000	267.554227000	345.380774000	C	21.223999000	281.008999000	346.209990000
H	27.822875000	266.938924000	344.556033000	C	20.483690000	281.662825000	347.376335000
H	27.247934000	268.272381000	345.152787000	O	20.546956000	281.256083000	348.554315000
O	25.710960000	269.540699000	345.044161000	N	19.709001000	282.719764000	347.028733000
H	26.441334000	270.197661000	345.109786000	C	19.011000000	283.493010000	348.032991000
H	25.621677000	269.161612000	345.974460000	C	18.034148000	282.633071000	348.843374000
O	26.624785000	269.604285000	350.077007000	O	17.173633000	281.933371000	348.281582000
H	26.574075000	268.619664000	350.171751000	H	18.434830000	284.191610000	347.608730000
H	27.050481000	269.703964000	349.197422000	N	18.127038000	282.768133000	350.188040000
O	26.740919000	264.019428000	344.692561000	C	17.337001000	281.957000000	351.103004000
H	25.907542000	263.466902000	344.573827000	H	16.641987000	282.518131000	351.552545000
O	28.644939000	262.005619000	344.992119000	C	18.238001000	281.334020000	352.162991000
H	29.429732000	262.279970000	344.429974000	C	17.648669000	280.180880000	352.929636000
H	28.862178000	261.076632000	345.500445000	N	16.362821000	279.894547000	352.856616000
O	27.875004000	259.644713000	349.915503000	O	18.345747000	279.461229000	353.753275000
H	25.456098000	268.436974000	343.662906000	O	18.188400000	278.724838000	350.436089000
H	25.283855000	268.252759000	342.125842000	H	22.031620000	283.602460000	355.441470000
O	25.342775000	267.744794000	342.956289000	C	21.583000000	282.946990000	356.049010000
H	27.389683000	260.488752000	349.997586000	C	22.412037000	281.701138000	356.221595000
H	28.718981000	259.959883000	349.490365000	O	22.544573000	280.835917000	355.319089000
H	31.770639000	269.509997000	342.993353000	H	20.684750000	282.662970000	355.713620000
H	28.014219000	272.764579000	343.781166000	N	23.017816000	281.561400000	357.417783000
H	25.880098000	276.189070000	348.122640000	C	23.874000000	280.441010000	357.715000000
H	33.014791000	261.352359000	342.455528000	C	23.188345000	279.080430000	357.540960000
H	33.057669000	264.597657000	343.221183000	O	21.988832000	278.893447000	357.784652000
H	30.095718000	264.697958000	343.058115000	N	24.063298000	278.093769000	357.203806000
H	22.279668000	271.522174000	349.225678000	C	23.678000000	276.709990000	357.126010000
H	20.002894000	261.082961000	346.903631000	C	23.398733000	276.220907000	355.700402000
H	23.258869000	258.314054000	347.777901000	O	23.610657000	276.914842000	354.689715000
H	26.186753000	266.348800000	355.193169000	N	22.944979000	274.943455000	355.654305000
H	23.862629000	266.123976000	354.153763000	C	22.540000000	274.355990000	354.399990000
H	23.997127000	267.477478000	353.539542000	C	21.399961000	275.161370000	353.743569000
H	27.964288000	270.435918000	355.005199000	O	20.694089000	275.980414000	354.353222000
H	31.365769000	260.568416000	353.087102000	H	22.252660000	273.406850000	354.528710000
H	32.973534000	262.991477000	350.481977000	N	21.224068000	274.816378000	352.433078000
H	30.008319000	260.304702000	347.662122000	C	20.285000000	275.553011000	351.592011000
H	29.469365000	261.544297000	348.333922000	C	18.829329000	275.420759000	351.984100000
H	24.800745000	261.985016000	356.063258000	O	17.966182000	276.203863000	351.521728000
H	23.524825000	260.881702000	355.535717000	C	20.509099000	275.195092000	350.112945000
H	33.372023000	265.598864000	351.518095000	O	22.068319000	277.354365000	346.007970000
H	34.359815000	265.501569000	350.029563000	O	20.740657000	278.684383000	349.532889000
H	35.541977000	264.912785000	352.201193000	O	22.483327000	277.941135000	352.145111000
H	34.493618000	263.503395000	352.380899000	O	20.827937000	279.275729000	354.039593000
H	28.958341000	258.090723000	348.233117000	H	20.496826000	274.661719000	346.584007000
H	28.399913000	256.826236000	347.120928000	H	18.708451000	275.595530000	345.409515000
H	31.120272000	265.877184000	348.291928000	H	19.609605000	277.335959000	347.677950000
H	32.080528000	266.358924000	349.666150000	H	18.003660000	276.664656000	347.381777000
H	30.382037000	263.633888000	348.221679000	H	17.628073000	280.297569000	347.405004000
H	31.401490000	262.400848000	348.837636000	H	17.869723000	278.961201000	348.494669000
H	20.413197000	264.133693000	349.685989000	H	24.854296000	279.283706000	346.798146000
H	22.977842000	260.711208000	353.075485000	H	22.982945000	278.274494000	348.203283000
C	21.835105000	276.165925000	346.309116000	H	23.530476000	279.249082000	349.573477000
N	20.619733000	275.591918000	346.185619000	H	23.817701000	277.378749000	350.711659000
C	19.446000000	276.340000000	345.755000000	H	22.884161000	277.400696000	352.866511000
H	19.680950000	276.898580000	344.959520000	H	22.331343000	279.218864000	346.480213000
C	18.841999000	277.191010000	346.890020000	H	20.512481000	280.334654000	345.697209000
C	18.393390000	278.600064000	346.501744000	H	21.525197000	281.792998000	345.488308000
N	17.846813000	279.301782000	347.519689000	H	19.704650000	283.045293000	346.064062000
O	18.542318000	279.063932000	345.350667000	H	19.739870000	283.989518000	348.702588000
H	25.275690000	280.167700000	348.188080000	H	18.901366000	283.313884000	350.563298000
C	24.482000000	279.798000000	347.704990000	H	16.861698000	281.172705000	350.487083000
C	23.426479000	280.805607000	347.278203000	H	18.563223000	282.084421000	352.911375000
O	23.497872000	282.030725000	347.483110000	H	19.155330000	280.935905000	351.688731000
C	23.880639000	278.739572000	348.656565000	H	15.737927000	280.376953000	352.214731000
C	24.741067000	277.559421000	349.066551000	H	15.993066000	279.088204000	353.361889000
N	24.554436000	276.903050000	350.167235000	H	19.405185000	279.556530000	353.798616000
O	25.632300000	277.213544000	348.132676000	H	18.095893000	277.807089000	350.810967000

H	21.428971000	283.454159000	357.017636000
H	22.875829000	282.272756000	358.130880000
H	24.186741000	280.518300000	358.770759000
H	24.789906000	280.486090000	357.094079000
H	24.995157000	278.349287000	356.882836000
H	24.474133000	276.077945000	357.562999000
H	22.767785000	276.573187000	357.737794000
H	22.664119000	274.490422000	356.522007000
H	23.390299000	274.354756000	353.690016000
H	22.105679000	274.512876000	351.965502000
H	21.550559000	275.424105000	349.823300000
H	20.321631000	274.121944000	349.926348000
H	19.834378000	275.795782000	349.482373000
H	20.882995000	279.591641000	349.143159000
H	19.155641000	278.749656000	350.183567000
H	21.921820000	278.574303000	352.650199000
H	21.460860000	278.532313000	350.177698000
H	20.868948000	278.425876000	354.534241000
H	21.425101000	279.926754000	354.545056000
N	18.537773000	274.415119000	352.818611000
C	17.201000000	274.185000000	353.303010000
H	17.041754000	274.523807000	354.230291000
H	17.005139000	273.205040000	353.266725000
H	20.504655000	276.635584000	351.707645000
H	19.304406000	273.823923000	353.136340000
H	16.500103000	274.701930000	352.626934000
O	23.951498000	274.488469000	351.520857000
H	23.845425000	273.913420000	350.722778000
H	24.279064000	275.326500000	351.074911000