

**Interaction of methanol with the oxygen-evolving complex:  
atomistic models, channel identification, species dependence,  
and mechanistic implications**

Marius Retegan, Dimitrios A. Pantazis\*

Max Planck Institute for Chemical Energy Conversion,  
Stiftrasse 34-38, 45470 Mülheim and der Ruhr, Germany

dimitrios.pantazis@cec.mpg.de

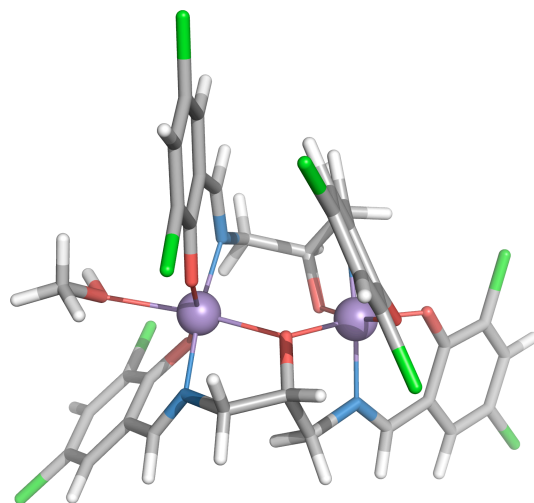
**SUPPORTING INFORMATION**

**Table S1.** Labeling of the water molecules included in the present computational model and the notation used in XRD structures.

	3ARC	3WU2	4UB6
W1	A:HOH.1000	A:HOH.595	A:HOH.608
W2	A:HOH.999	A:HOH.624	A:HOH.607
W3	A:HOH.541	A:HOH.569	A:HOH.569
W4	A:HOH.540	A:HOH.544	A:HOH.568
W5	C:HOH.538	C:HOH.633	C:HOH.665
W6	A:HOH.539	A:HOH.511	A:HOH.567
W7	A:HOH.446	A:HOH.609	A:HOH.560
W8	A:HOH.442	A:HOH.621	A:HOH.559
W9	A:HOH.542	A:HOH.564	A:HOH.570
W10	A:HOH.358	A:HOH.567	A:HOH.510
W11	A:HOH.428	A:HOH.509	A:HOH.557
W12	A:HOH.923	A:HOH.597	A:HOH.601

**Table S2.** Relative energies (kcal/mol) for the two subsets of isomeric structures, obtained at either with the BP86 functional used in the optimization, or with the TPSSh functional in the high-spin or the most stable broken-symmetry formulation.

	BP86	TPSSh (HS)	TPSSh (BS)
W1-1	7.4	5.5	5.5
W3-1	12.9	13.2	13.2
W4-1	3.2	4.0	3.9
W5-1	0.0	0.3	0.1
W6-1	3.9	3.6	3.3
W6-2	9.9	10.2	10.3
W7-1	1.4	0.0	0.0
W8-1	5.9	4.1	4.0
W8-2	6.3	5.3	5.2
W9-1	4.2	4.7	4.7
W10-1	0.9	1.6	1.5
W10-2	0.1	1.1	1.1
W11-1	11.2	10.8	10.7
W12-1	3.1	3.1	3.1
W12-2	4.4	3.9	3.9
W1-1d	0.0	0.0	0.0
W3-1d	12.6	18.2	17.9
W4-1d	14.7	22.0	21.8



**Figure S1.** The mixed-valence complex  $(2\text{-OH-}3,5\text{-Cl}_2\text{-salpn})_2\text{Mn(III)Mn(IV)}$  (salpn =  $N,N'$ -bis(3,5-dichlorosalicylidene)-1,3-diamino-2-hydroxypropane) was used as a reference compound for the interaction of methanol in the experimental study. When methanol binds to the Mn(III) ion of the complex the  $^{13}\text{C}$  of the bound methanol had an isotropic hyperfine coupling constant  $A_{\text{iso}} = 0.65 \pm 0.05$  MHz and dipolar coupling  $T = 1.25 \pm 0.05$  MHz. The computed values for an optimized model of the bound methanol were  $A_{\text{iso}} = 0.71$  MHz and  $T = 2.31$  MHz.

## Sequence alignments

### Psba (D1)

```
sp | P51765 | PSBA_THEVL      MTTTLQRRESANLWERFCNWTSTDNRLYVGVFVIMIPTLLAATICFVIAFIAAPPVDI 60
sp | P69560 | PSBA_SPIOL      MTAILERRESESLWGRFCNWTSTENRLYIGWFGVLMIPTLLTATSVFIIAFIAAPPVDI 60
                               **: *:*:* * . ** *:*:*:*:*:*:*:*:*:*:*:*:*:*:* * :*****

sp | P51765 | PSBA_THEVL      DGIREPVSGLLYGNNIITGAVVPSSNAIGLHFYPIWEAASLDEWLYNGGPYQLIIFHFL 120
sp | P69560 | PSBA_SPIOL      DGIREPVSGLLYGNNIISGAIPTSAAIGLHFYPIWEAASLDEWLYNGGPYELIVLHFL 120
                               *****: **::* * *****:*****:*****:***:***

sp | P51765 | PSBA_THEVL      LGASCYMGREQWELSYRLGMRPWICVAYSAPLASAFVFLIYPIGQGSFSDGMPLGISGTF 180
sp | P69560 | PSBA_SPIOL      LGVACYMGREWELSFRLGMRPWIAVAYSAPVAAATAVFLIYPIGQGSFSDGMPLGISGTF 180
                               **.:*****:*****:*****.*****:*:* *****

sp | P51765 | PSBA_THEVL      NFMIVFQAEHNILMHPFHQLGVAGVFGGALFCAMHGSLVTSLSLIRETTETESANYGYKFG 240
sp | P69560 | PSBA_SPIOL      NFMIVFQAEHNILMHPFHMLGVAGVFGGSLFSAMHGSLVTSLSLIRETTENESANEGYRFG 240
                               ***** *****:*. *****.*****.*** **:*

sp | P51765 | PSBA_THEVL      QEETYNIVAAGHYFGRLIFQYASFNNSRSLHFFLAAWRVGVVFAALGISTMAFNLNGF 300
sp | P69560 | PSBA_SPIOL      QEETYNIVAAGHYFGRLIFQYASFNNSRSLHFFLAAWPVVGWIWFTALGISTMAFNLNGF 300
                               ***** *****:*. ***** **:*

sp | P51765 | PSBA_THEVL      NFNHSDVIDAKGNVINTWADIINRANLGMVEMHERNAHNFPLDLASAESAPVAMIAPSING 360
sp | P69560 | PSBA_SPIOL      NFNQSVVDSQGRVINTWADIINRANLGMVEMHERNAHNFPLDLAAIEAP-----STNG 353
                               ***:*:*:*:*.* *****:*. *****: *:*
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### Psbd (D2)

```
sp | D0VWR8 | PSBD_THEVL      -----ERGFWDILDDWLKRDRFVFGWGSILLFPFCAYLALGGWLTGTTFFVTSWY 49
sp | P06005 | PSBD_SPIOL      MTIAVGKFTKDEKDLDFSMDDWLRDRFVFGWGSILLFPFCAYFALGGWFTGTTFFVTSWY 60
                               *: . ** :***:*****:*****:*****:*****

sp | D0VWR8 | PSBD_THEVL      THGLASSYLEGCNFLTAVSTPANSMGHSLLLWGPEAQGDFTRWCQLGGLWTFIALHGA 109
sp | P06005 | PSBD_SPIOL      THGLASSYLEGCNFLTAAVSTPANSLAHSLLLWGPEAQGDFTRWCQLGGLWAFVALHGA 120
                               *****.*****:. *****:*.*****

sp | D0VWR8 | PSBD_THEVL      FGLIGFMLRQFEIARLVGRVPYNAIAFSAPIAVFVSVFLIYPLGQSSWFFAPSFVAAIF 169
sp | P06005 | PSBD_SPIOL      FALIGFMLRQFELARSVQLRPYNAIAFSGPIAVFVSVFLIYPLGQSGWFFAPSFVAAIF 180
                               *.*****:* * :*****.*****.*****

sp | D0VWR8 | PSBD_THEVL      RFLFFQGFHNWTLNPFHMMGVAGVLGALLCAIHGATVENTLFDQEGEGASTFRAFNPQTQ 229
sp | P06005 | PSBD_SPIOL      RFILFFQGFHNWTLNPFHMMGVAGVLGAALLCAIHGATVENTLFDGDGANTFRAFNPQTQ 240
                               **:*****.*****:*****:***:***

sp | D0VWR8 | PSBD_THEVL      AEETYSMVTANRFWSQIFGIAFSNKRWLHFFMLFVPTGLWMSAIGVVGLALNLRSDYFI 289
sp | P06005 | PSBD_SPIOL      AEETYSMVTANRFWSQIFGVAFSNKRWLHFFMLFVPTGLWMSALGVVGLALNLRAYDFV 300
                               *****:*****:*****:*****:*****:***:

sp | D0VWR8 | PSBD_THEVL      SQEIRAAEDPEFETFYTKNLLNEGIRAWMAPQDQPHENFVFPPEEVLPRGNAL 342
sp | P06005 | PSBD_SPIOL      SQEIRAAEDPEFETFYTKNLLNEGIRAWMAAQDQPHENLIFPEEVLPRGNAL 353
                               *****:*****.*****:*****:*****
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### Psbc (CP43)

```
sp | D0VWR7 | PSBC_THEVL      -----ATNRDQESSGFAWWAGNARLINLSGKLLGAHVAHAGLI 38
sp | P06003 | PSBC_SPIOL      MKTLYSLRRFPVETLFGNGLTLAGRDQETTFGAWWAGNARLINLSGKLLGAHVAHAGLI 60
                               :.***:*****:*****:*****

sp | D0VWR7 | PSBC_THEVL      VFWAGAMTLFELAHFIPEKPMYEQGLLILPHIATLGWGVGPGGEVVDTFPFVGVVHLI 98
sp | P06003 | PSBC_SPIOL      VFWAGAMNLFVAHFVPEKPMYEQGLLILPHLATLGWGVGPGGEVIDTFPFVSGVLHLI 120
                               *****.***:*:*:* *****:***:*****:*****:***:***
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sp | D0VWR7 | PSBC_THEVL | SSAVLGFGGVYHAIRGPETLEEYSSFFGYDWKDKNKMTTILGFHLIVLGIGALLLVAKAM | 158
sp | P06003 | PSBC_SPIOL | SSAVLGFGGIYHALLGPETLEESFPFFGYVWVWDRNKMTTILGIHLILLGIGAFFLVFKAL | 180
*****:***: ***** .*** **:*:*****:***:*****:*** **

sp | D0VWR7 | PSBC_THEVL | FFGGLYDTWAPGGGDVVRVITNPTLDPRVIFGYLLKSPFGGEGWIVSVNNLEDVVGHIWI | 218
sp | P06003 | PSBC_SPIOL | YFGGVYDTWAPGGGDVVRKITNVTLSPSIIFGCLLKSPFGGEGWIVSVDDLEDIIGHVWI | 240
*:***:*****:*** ** *.* :*** *****:***:***:***

sp | D0VWR7 | PSBC_THEVL | GLICIAGGIWHILTPFGWARRAFIWSGEAYLSYSLGALSMMGFIAFCFVWFNNTVYPSE | 278
sp | P06003 | PSBC_SPIOL | GVICILGGIWHILTKPFAWARRALVWSGEAYLSYSLAALSVMGFIAFCFVWFNNTAYPSE | 300
*:*** *****:***.*****:*****:***:*** *****:***

sp | D0VWR7 | PSBC_THEVL | FYGPTGPEASQAQAMTFLIRDQKLGANVGSQAQPTGLGKYLMSRPTGEIIFGGETMRPWD | 338
sp | P06003 | PSBC_SPIOL | FYGPTGPEASQAQAFTLVRDQRLGANVGSQAQPTGLGKYLMSRPTGEVIFGGETMRPWD | 360
*****:***:***:*****:*****:*****:*****:*****:*****

sp | D0VWR7 | PSBC_THEVL | FRGPWLEPLRGPNGLDLNLKIKNDIQPWQERRAAEYMTAPLGLSLNSVGGVATEINSVNFV | 398
sp | P06003 | PSBC_SPIOL | LRAPWLEPLRGPNGLDLNLKIKNDIQPWQERRAAEYMTAPLGLSLNSVGGVATEINAVNYV | 420
:*.*****:***:***:*****:*****:*****:*****:***

sp | D0VWR7 | PSBC_THEVL | SPRSWLATSHFVLAFFFLVGHVHAGRARAAAAGFEKIDRESEPVLSMPSLD | 451
sp | P06003 | PSBC_SPIOL | SPRSWLSTSHFVLFVGHVHAGRARAAAAGFEKIDRDFEPVLSMPTLN | 473
*****:*****:***:*****:*****:*****:*****:*****:***

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**PsbB (CP47)**

```

sp | D0VWR1 | PSBB_THEVL | -GLPWYRVHTVLINDPGRLLIAAHLMTALVAGWAGSMALYELATFDPSDPVLPMPWRQGM | 59
sp | P04160 | PSBB_SPIOL | MGLPWYRVHTVVLNDPGRLLISVHIMHTALVAGWAGSMALYELAVFDPSDPVLPMPWRQGM | 60
*****:***:*****:*.***:*****:***:*****:*****:*****:*****

sp | D0VWR1 | PSBB_THEVL | FVLPFMARLGVTSWSGWSITGETGIDPGFWSFEGVALAHIVLSGLLFLAACWHVWYDLD | 119
sp | P04160 | PSBB_SPIOL | FVLPFMARLGVTSWSGWSITGGTITDPGIWSYEGVAGAHIMFSGLCFLAAIWHVWYDLD | 120
**:*:***:***:*.***:***** * **:*:***:*** **:*:*** *****

sp | D0VWR1 | PSBB_THEVL | ELFRDPRTEGEPALDLPKMFGLHFLAGLLCFGFGAFHLLTGLFGPMWVSDPYGLTGSVQP | 179
sp | P04160 | PSBB_SPIOL | EIFSDERTGKPSLDLPKIFGIHLFLSGLVACFVGFVAFHVTGLYGPVWSDPYGLTGSVQP | 180
*:* * **:*:***:***:*****:***:*****:***:*****:*****:***

sp | D0VWR1 | PSBB_THEVL | VAPEWGPDPGNPNYPPGGVVAHHIAAGIVGIIAGLPHILVRRPPQRLYKALRMGNIETVLS | 239
sp | P04160 | PSBB_SPIOL | VSPAWEVGFDPFVPGGIASHHIAAGTLGILAGLPHLSVRPPQRLYKALRMGNIETVLS | 240
*:* ** :***:***:***:*.***** :***:*****: *****:*****

sp | D0VWR1 | PSBB_THEVL | SIAAVFFAAFVAGTMWYGSATPIELFGPTRYQWDSYFQQEINRRVQASLASGATLEE | 299
sp | P04160 | PSBB_SPIOL | SIAAVFFAAFVAGTMWYGSATPIELFGPTRYQWQGYFQQEIIYRRVSAGLAENQSFSE | 300
*****:*****:*****:*****.***** **.*.***. :*.**

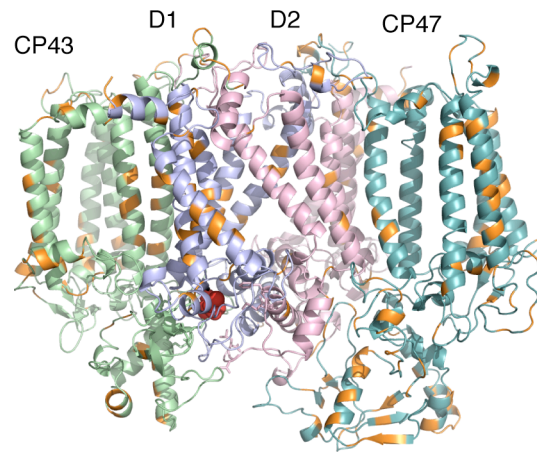
sp | D0VWR1 | PSBB_THEVL | AWSAIPKELAFYDYIGNNPAKGLFRTPGMNKGDIAGQAWKHAVFRNKEGEEELFVRRMP | 359
sp | P04160 | PSBB_SPIOL | AWSAIPKELAFYDYIGNNPAKGLFRAGSMDNGDIAVGLWGHPIFRDKEGRELFRVRRMP | 360
*** *****:*****:*.***:***** .* **.*:***:*****

sp | D0VWR1 | PSBB_THEVL | AFFESFPVILTDKNGVVKADIPFRRAESKYSFEQQGVTVSFGGELNGQTFDPTVKSYS | 419
sp | P04160 | PSBB_SPIOL | TFFETFPVVIDDGDIVRADVPFRRAESKYSVEQVGVTVSFGGELNGVSYSDPATVKYS | 420
:***:***:*** * :*:***:***:*****.*** *****:***** :*:***.***

sp | D0VWR1 | PSBB_THEVL | ARKAIFGEIFEFDTELTNSDGIFFRTSPRGWTFHAHVALLFFFGHIWHGARTLFRDVFS | 479
sp | P04160 | PSBB_SPIOL | ARRAQLGEIFEFDTRATLKSVDGFRSSPRGWTFGHASFALLFFFGHIWHGSRTRLFRDVFA | 480
**:* :*****:*** **:*:***:***:*****.*** *****:*****:*****

sp | D0VWR1 | PSBB_THEVL | GIDPELSPEQVEWGFYQKVGVDVTRK--- | 505
sp | P04160 | PSBB_SPIOL | GIDPDLV-QVEFGAFQKIGDPTTRRQGV | 508
*****:*. **:*:***:***:***:***

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**Figure S2.** Residues with variations in the four core PS-II proteins between *T. vulcanus* and *S. oleracea* indicated in orange on the crystallographic model of *T. vulcanus*.

## Cartesian coordinates of optimized structures

S<sub>2</sub>

Mn	-24.861785928	-35.538136067	203.952836733
Mn	-27.335109674	-35.218881837	205.228903286
Mn	-27.319691595	-33.337070550	203.161655355
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Ca	-27.892136398	-36.724877375	202.207552892
O	-26.433130903	-36.507855690	204.216717740
O	-28.354801738	-34.721993942	203.804147724
O	-25.993205871	-34.061808099	204.488953897
O	-28.490890642	-32.604391906	201.988704612
O	-26.758946473	-34.302260222	201.691513026
O	-28.413423888	-31.695457382	199.312428948
O	-26.563235675	-33.768942740	198.994892996
O	-27.634968089	-37.252367399	199.890742987
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H	-30.454672257	-26.816515356	200.177841532
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C	-28.185270472	-28.477022208	200.550477373
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O	-27.053969440	-28.366857946	200.001609672
C	-32.924380974	-41.850903001	196.489835023
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C	-29.959209517	-42.494978766	197.741658078
C	-30.196292183	-40.096021158	197.564999105
C	-29.101170299	-42.342324176	198.844083063
C	-29.338001382	-39.923079559	198.664011659
C	-28.784652106	-41.046915600	199.309373366
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C	-22.775252530	-42.908891989	202.609197145
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C	-20.112713046	-31.328696950	202.090234974
C	-21.154479133	-30.546219966	202.873658340



O	-21.422623390	-30.807583267	204.067098423
C	-20.723130514	-32.620743254	201.485283333
C	-21.596553322	-33.371001523	202.436634139
C	-22.941843450	-33.698187735	202.404286352
N	-21.136481113	-33.849526777	203.655488648
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C	-23.780495317	-31.695998184	206.175875225
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C	-30.997750769	-31.051073852	208.236196866
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C	-30.273882123	-32.094797835	207.373175395
C	-28.976372391	-31.550430609	206.744262571
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O	-28.012927114	-32.187399416	204.653371616
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C	-36.971478990	-32.276075031	205.926511022
C	-35.755198226	-32.775946754	205.121108235
C	-34.813655920	-33.668419535	205.953476680
C	-33.729958222	-34.411263920	205.160808226
N	-32.745671612	-33.500370025	204.553536020
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H	-25.468205000	-38.954570000	200.480015000
H	-27.656902000	-39.483583000	203.312295000
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H	-26.539393000	-38.109380000	204.848662000
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w1-1d

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Mn	-27.836451000	-32.909624000	200.466469000
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O	-25.962352000	-34.071059000	204.515272000
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C	-28.766717000	-26.741132000	200.961212000
C	-28.093062000	-27.622884000	199.886225000
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C	-31.935592000	-35.967610000	194.072818000
H	-31.190723000	-35.442655000	193.449430000
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C	-22.352883000	-41.458334000	202.717393000
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H	-22.557559000	-28.453985000	203.752879000
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W2-1

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O	-26.376360000	-33.793181000	198.958362000
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C	-28.754983000	-27.401691000	201.477842000
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O	-29.846736000	-35.629341000	201.199712000
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N	-31.861062000	-35.424455000	195.425818000
C	-31.935591000	-35.967611000	194.072817000
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H	-26.359146000	-29.780160000	209.608484000
H	-26.169752000	-33.047002000	207.866354000
H	-23.116868000	-31.522004000	205.295471000
H	-23.719303000	-33.379564000	201.745413000
H	-21.999646000	-35.060494000	205.236625000
H	-19.699391000	-30.723325000	201.262903000
H	-23.080755000	-27.940635000	202.112973000
H	-29.871954000	-34.536127000	197.380640000
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H	-32.921611000	-31.347461000	196.679241000
H	-32.148958000	-34.453439000	195.552430000
H	-30.791830000	-28.058660000	201.379175000
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C	-31.567105000	-37.916365000	206.316186000
H	-32.055186000	-37.932628000	205.325763000
H	-32.072913000	-38.655344000	206.959861000
H	-31.682469000	-36.916096000	206.771185000
H	-29.094101000	-39.310259000	210.342851000
H	-27.858742000	-40.306732000	209.536504000
H	-23.600681000	-36.034632000	208.525574000
H	-23.846757000	-37.609287000	207.767093000
H	-30.065448000	-36.764071000	198.661770000
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H	-31.383272000	-30.213488000	207.627049000
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H	-29.135477000	-30.633273000	206.170182000
H	-28.155863000	-26.417841000	201.220208000

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H	-37.548238000	-31.526089000	205.357493000
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H	-36.105722000	-33.344106000	204.234680000
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H	-24.663314000	-30.846202000	198.479959000
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H	-25.486739000	-35.564957000	199.900111000
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W3-1

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O	-26.484289000	-33.774180000	198.983433000
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C	-24.661722000	-31.109718000	209.720258000
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N	-23.640496000	-31.142337000	207.388785000
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N	-24.861781000	-32.552297000	206.290414000

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C	-29.326724000	-37.391308000	205.224024000
O	-29.461120000	-37.476583000	203.989900000
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N	-31.606631000	-35.269677000	203.386817000
N	-31.074041000	-33.063769000	202.943718000
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W3-1d

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W4-1

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W4-1d

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H	-30.041200000	-36.762684000	198.664039000
H	-31.570623000	-36.180236000	199.346237000
H	-31.368066000	-30.175594000	207.673207000
H	-30.151554000	-33.028965000	207.869661000
H	-28.289004000	-31.397584000	207.516918000
H	-31.039972000	-32.359600000	206.492318000
H	-29.137006000	-30.677416000	206.123650000
H	-28.175234000	-26.355909000	201.143305000
H	-28.456538000	-27.567079000	202.413159000
H	-25.304025000	-31.855094000	210.288101000
H	-23.680971000	-31.164495000	210.138374000
H	-25.338228000	-33.157303000	205.473420000
H	-37.548238000	-31.526089000	205.357493000
H	-35.291062000	-31.937959000	204.595727000
H	-35.219619000	-34.234997000	206.657331000
H	-32.909794000	-34.690001000	205.981178000
H	-37.646932000	-33.100899000	206.217125000
H	-36.108683000	-33.487679000	204.328549000
H	-34.245182000	-32.753051000	206.680207000
H	-33.377344000	-32.654460000	203.862509000
H	-34.067903000	-35.099373000	204.680830000
H	-31.226378000	-31.863919000	202.995351000
H	-31.546737000	-35.657041000	204.476957000
H	-30.168919000	-33.117489000	202.494591000
H	-30.033377000	-34.971280000	203.855010000
H	-23.935490000	-30.499027000	203.617853000
H	-25.366611000	-29.369326000	201.132781000
H	-24.925255000	-29.032450000	203.520295000
H	-24.001646000	-30.473958000	200.964374000
H	-20.207856000	-33.719617000	204.026436000
H	-25.825368000	-33.108407000	198.633649000
H	-29.163389000	-31.979701000	198.716295000
H	-28.583030000	-30.788902000	199.736751000
H	-29.578928000	-29.905471000	201.861733000
H	-29.156371000	-31.172050000	202.591688000
H	-27.041979000	-30.194296000	204.230685000
H	-28.361717000	-29.623359000	203.733130000
H	-32.942481000	-35.820139000	193.649354000
H	-31.697971000	-37.042558000	194.096594000
H	-26.660429000	-39.918686000	199.601477000
H	-25.685816000	-38.995368000	200.476170000
H	-27.606033000	-36.553907000	198.890204000
H	-26.528053000	-36.323374000	197.314141000
H	-27.019765000	-34.950324000	197.946386000
H	-25.359198000	-38.257066000	196.612831000
H	-25.464632000	-38.275899000	198.165106000
H	-27.118719000	-37.907345000	199.558177000
H	-24.607901000	-31.840190000	199.367178000
H	-25.122651000	-31.048115000	198.173885000
H	-27.128351000	-30.793063000	198.234041000
H	-26.631303000	-29.406068000	198.688377000
H	-25.869115000	-38.921090000	206.216084000
H	-26.004128000	-38.135076000	204.870183000
H	-24.874981000	-44.326621000	202.718946000
H	-22.937833000	-30.491394000	207.593398000

C	-27.742730000	-40.235431000	202.585170000
H	-27.527773000	-40.052139000	203.671299000
H	-28.390710000	-41.147682000	202.508817000
H	-26.742656000	-40.514212000	202.160171000

W5-1

Mn	-24.826227000	-35.561452000	203.954852000
Mn	-27.282351000	-35.234995000	205.240967000
Mn	-27.271141000	-33.344946000	203.140932000
Mn	-27.575926000	-33.173159000	200.425495000
Ca	-27.894722000	-36.726960000	202.214214000
O	-26.398955000	-36.528418000	204.232819000
O	-28.292634000	-34.754500000	203.790727000
O	-25.948571000	-34.080619000	204.490744000
O	-28.460813000	-32.607050000	202.016812000
O	-26.731848000	-34.306795000	201.674071000
O	-28.451235000	-31.652871000	199.412525000
O	-26.606467000	-33.729911000	198.959285000
O	-27.630953000	-37.260419000	199.899901000
O	-28.048809000	-39.132049000	202.509159000
H	-30.446114000	-26.826764000	200.173820000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.728478000	-27.288978000	201.449319000
C	-28.165682000	-28.487969000	200.664269000
O	-28.763833000	-29.624581000	200.874428000
O	-27.187993000	-28.325469000	199.884681000
C	-32.924381000	-41.850903000	196.489835000
C	-31.513828000	-41.561243000	195.943064000
C	-30.524241000	-41.369146000	197.081222000
C	-29.958981000	-42.482541000	197.741319000
C	-30.202248000	-40.083787000	197.571596000
C	-29.100915000	-42.330556000	198.843739000
C	-29.343939000	-39.911497000	198.670836000
C	-28.787596000	-41.035522000	199.312610000
O	-27.917988000	-40.834918000	200.370144000
H	-33.785375000	-32.318034000	197.913159000
C	-32.844739000	-31.791422000	197.688620000
C	-31.613947000	-32.672209000	197.724643000
O	-30.463710000	-32.186462000	197.668022000
H	-32.712245000	-30.956595000	198.397171000
N	-31.847058000	-34.014985000	197.749483000
C	-30.825021000	-35.049751000	197.612821000
C	-31.084606000	-35.967337000	196.396129000
O	-30.559794000	-37.087239000	196.313148000
C	-30.618482000	-35.851787000	198.908365000
C	-29.804729000	-35.206615000	200.037791000
O	-29.859016000	-35.709341000	201.185069000
O	-29.028454000	-34.226870000	199.689173000
N	-31.869343000	-35.425648000	195.425655000
C	-31.935591000	-35.967611000	194.072817000
H	-31.190723000	-35.442656000	193.449429000
H	-21.516057000	-41.187718000	202.032943000
C	-22.352883000	-41.458335000	202.717392000
C	-22.770408000	-42.910635000	202.613877000
O	-23.538256000	-43.430744000	203.443981000
C	-23.556591000	-40.514013000	202.460587000
C	-23.070606000	-39.057766000	202.334185000
C	-24.148942000	-37.992872000	202.482856000
O	-25.234068000	-38.019529000	201.855681000
O	-23.810018000	-37.036107000	203.306003000
N	-22.260239000	-43.592986000	201.548195000
C	-22.629343000	-44.962153000	201.252063000
H	-21.726399000	-45.520632000	200.924621000
C	-23.738170000	-45.085426000	200.181026000
C	-24.990501000	-44.395957000	200.606755000
C	-25.520032000	-43.162465000	200.269185000
N	-25.823540000	-44.877557000	201.607084000
C	-26.799162000	-43.962772000	201.846682000
N	-26.639179000	-42.912752000	201.043544000
H	-19.262626000	-31.517297000	202.779917000
C	-20.112713000	-31.328697000	202.090235000

C	-21.161721000	-30.556401000	202.873983000
O	-21.439145000	-30.828855000	204.063039000
C	-20.712020000	-32.622214000	201.477320000
C	-21.574519000	-33.386365000	202.427280000
C	-22.917668000	-33.722087000	202.399430000
N	-21.105987000	-33.865573000	203.642588000
C	-22.116078000	-34.457898000	204.312648000
N	-23.231847000	-34.388728000	203.575314000
N	-21.811984000	-29.594573000	202.175836000
C	-22.896307000	-28.815019000	202.759171000
H	-22.557559000	-28.453986000	203.752878000
C	-24.197534000	-29.623328000	202.930569000
C	-24.702233000	-30.235056000	201.623101000
C	-25.703592000	-31.365547000	201.765984000
O	-25.967339000	-31.853159000	202.914618000
O	-26.197355000	-31.791507000	200.666287000
H	-24.831897000	-28.949505000	209.209068000
C	-25.289739000	-29.704836000	209.874338000
H	-25.215628000	-29.314217000	210.902923000
C	-24.597795000	-31.076069000	209.702806000
C	-24.535944000	-31.553849000	208.278317000
C	-25.307134000	-32.454186000	207.561422000
N	-23.579229000	-31.103757000	207.368916000
C	-23.744022000	-31.698593000	206.168392000
N	-24.796320000	-32.518846000	206.274622000
H	-24.708982000	-37.374838000	210.156821000
C	-25.333665000	-37.110846000	209.273415000
C	-26.306045000	-38.218868000	208.873862000
O	-26.056629000	-39.045954000	207.975619000
C	-24.372305000	-36.727012000	208.148868000
C	-24.958455000	-36.057418000	206.913703000
O	-26.205338000	-35.738380000	206.893609000
O	-24.141185000	-35.850512000	205.962056000
N	-27.489056000	-38.237831000	209.557211000
C	-28.420988000	-39.357108000	209.469748000
C	-29.304014000	-39.439512000	208.216942000
O	-29.905439000	-40.493619000	207.947892000
N	-29.405496000	-38.302489000	207.492958000
C	-30.100963000	-38.231691000	206.212498000
C	-29.365804000	-37.252016000	205.292357000
O	-29.576368000	-37.257080000	204.067936000
O	-28.581954000	-36.428016000	205.939559000
O	-25.510900000	-37.806842000	197.290302000
O	-27.505525000	-35.872806000	197.698484000
O	-26.576805000	-30.201056000	198.005350000
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O	-29.071370000	-29.894443000	203.554561000
O	-25.762793000	-39.347033000	199.589203000
O	-26.814052000	-39.068562000	205.079465000
H	-30.307779000	-30.644744000	208.999068000
C	-30.997751000	-31.051074000	208.236197000
H	-31.843803000	-31.521736000	208.767318000
C	-30.299997000	-32.104377000	207.359818000
C	-28.995092000	-31.574981000	206.736777000
C	-28.302146000	-32.580292000	205.840883000
O	-28.039249000	-33.739028000	206.324710000
O	-28.001259000	-32.209935000	204.654649000
H	-36.690166000	-31.806964000	206.888578000
C	-36.971479000	-32.276075000	205.926511000
C	-35.719777000	-32.706623000	205.139906000
C	-34.699285000	-33.474573000	205.999386000
C	-33.545853000	-34.110915000	205.213880000
N	-32.764065000	-33.110107000	204.476204000
C	-31.554004000	-33.353117000	203.917937000
N	-30.991706000	-34.563730000	204.012898000
N	-30.896875000	-32.362410000	203.291218000
O	-26.977820000	-28.489714000	204.689506000
H	-32.902540000	-42.744041000	197.142993000
H	-33.269870000	-41.006452000	197.116021000
H	-33.700323000	-42.030393000	195.723193000
H	-31.532703000	-40.655313000	195.307737000
H	-31.184650000	-42.397500000	195.295725000
H	-30.192800000	-43.496466000	197.386818000

H	-28.669293000	-43.210883000	199.334362000
H	-29.079719000	-38.909501000	199.032887000
H	-30.607896000	-39.188991000	197.081406000
H	-27.459961000	-41.761558000	200.709203000
H	-25.170743000	-42.446912000	199.522002000
H	-27.591879000	-44.096602000	202.584455000
H	-28.806205000	-37.506879000	207.727978000
H	-27.636144000	-37.546584000	210.291042000
H	-21.520016000	-29.397648000	201.220746000
H	-21.679159000	-43.089402000	200.880612000
H	-22.969786000	-45.418211000	202.198279000
H	-23.922260000	-46.159445000	199.986701000
H	-23.393599000	-44.639791000	199.230770000
H	-22.599973000	-38.903312000	201.342489000
H	-24.092121000	-40.817768000	201.541522000
H	-21.981136000	-41.292725000	203.746141000
H	-22.293298000	-38.847822000	203.089037000
H	-24.279534000	-40.611559000	203.291100000
H	-26.359697000	-29.772524000	209.607881000
H	-26.158631000	-33.067490000	207.858027000
H	-23.106336000	-31.533841000	205.291483000
H	-23.669525000	-33.561506000	201.624375000
H	-22.033419000	-34.942674000	205.285196000
H	-19.700539000	-30.716156000	201.267913000
H	-23.059100000	-27.935804000	202.113125000
H	-29.872864000	-34.528500000	197.388878000
H	-32.809971000	-34.324867000	197.884325000
H	-32.918019000	-31.353660000	196.676275000
H	-32.161005000	-34.457516000	195.554539000
H	-30.756633000	-28.073945000	201.404691000
H	-19.890777000	-33.260665000	201.100522000
H	-21.330475000	-32.359028000	200.601153000
H	-25.918008000	-36.224110000	209.585157000
H	-30.047025000	-39.226381000	205.732918000
C	-31.576694000	-37.811001000	206.358463000
H	-32.067004000	-37.789468000	205.369490000
H	-32.107631000	-38.537886000	206.995711000
H	-31.649851000	-36.812350000	206.825684000
H	-29.094356000	-39.311804000	210.342927000
H	-27.858742000	-40.306732000	209.536504000
H	-23.590371000	-36.045898000	208.533853000
H	-23.838385000	-37.621660000	207.779030000
H	-30.041932000	-36.759850000	198.644303000
H	-31.579525000	-36.197988000	199.328959000
H	-31.379203000	-30.205437000	207.636125000
H	-30.068655000	-33.007745000	207.953900000
H	-28.279653000	-31.317774000	207.543650000
H	-30.983350000	-32.430724000	206.550974000
H	-29.176186000	-30.657133000	206.151467000
H	-28.164788000	-26.385360000	201.160131000
H	-28.524571000	-27.475559000	202.521425000
H	-25.125466000	-31.845482000	210.293801000
H	-23.565787000	-31.031774000	210.099902000
H	-25.214562000	-33.128127000	205.490101000
H	-37.548238000	-31.526089000	205.357493000
H	-35.241560000	-31.800832000	204.713889000
H	-35.211963000	-34.296252000	206.535616000
H	-32.864247000	-34.629003000	205.914864000
H	-37.626429000	-33.137257000	206.150971000
H	-36.018097000	-33.331076000	204.273668000
H	-34.286625000	-32.802276000	206.777822000
H	-33.255860000	-32.280160000	204.148015000
H	-33.948127000	-34.871395000	204.511728000
H	-31.089323000	-31.385342000	203.507531000
H	-31.548596000	-35.399047000	204.163343000
H	-30.016038000	-32.548266000	202.760380000
H	-29.976608000	-34.691267000	203.802774000
H	-24.017969000	-30.429665000	203.659878000
H	-25.165801000	-29.484223000	200.953940000
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H	-23.852225000	-30.667735000	201.054781000
H	-20.164234000	-33.732165000	204.008272000
H	-25.842328000	-33.131835000	198.704585000



H	-29.265411000	-31.902142000	198.885674000
H	-28.608873000	-30.788820000	200.031398000
H	-29.015874000	-29.865740000	202.551019000
H	-28.686365000	-30.770600000	203.795473000
H	-27.751605000	-28.956608000	204.260391000
H	-32.943275000	-35.821170000	193.651051000
H	-31.697858000	-37.042061000	194.102631000
H	-26.515696000	-39.956641000	199.831002000
H	-25.460620000	-38.963824000	200.466278000
H	-27.685040000	-39.503536000	203.346333000
H	-27.660298000	-36.685259000	199.051107000
H	-26.728210000	-36.419397000	197.410312000
H	-27.120104000	-35.026437000	198.090971000
H	-25.755819000	-38.368540000	196.531111000
H	-25.587398000	-38.413639000	198.076525000
H	-28.021890000	-39.825094000	201.798637000
H	-26.985692000	-37.976194000	199.675358000
H	-24.208555000	-31.805270000	199.079531000
H	-25.279826000	-31.199829000	198.128859000
H	-27.248906000	-30.864424000	198.310857000
H	-26.694738000	-29.499663000	198.717273000
H	-26.737274000	-39.118207000	206.057934000
H	-26.535524000	-38.137684000	204.856047000
H	-25.698147000	-45.749879000	202.118271000
H	-22.832647000	-30.441212000	207.580672000
C	-26.369793000	-29.405657000	205.604565000
H	-26.947178000	-29.507224000	206.548383000
H	-26.242687000	-30.412328000	205.159873000
H	-25.368715000	-29.015948000	205.866792000

W6-1

Mn	-24.835153000	-35.563086000	203.952062000
Mn	-27.301401000	-35.256342000	205.232627000
Mn	-27.289971000	-33.372026000	203.138428000
Mn	-27.532571000	-33.232144000	200.418162000
Ca	-27.866454000	-36.750337000	202.194607000
O	-26.395807000	-36.545603000	204.228645000
O	-28.308197000	-34.790624000	203.776997000
O	-25.969698000	-34.094598000	204.497284000
O	-28.448177000	-32.669514000	201.970156000
O	-26.700328000	-34.348913000	201.681002000
O	-28.452713000	-31.709574000	199.422833000
O	-26.562616000	-33.767275000	198.935588000
O	-27.622538000	-37.287191000	199.875024000
O	-27.989909000	-39.156178000	202.482376000
H	-30.265174000	-26.722092000	200.188164000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.799088000	-27.457082000	201.630230000
C	-28.277611000	-28.673663000	200.854098000
O	-28.997488000	-29.751655000	200.956104000
O	-27.226499000	-28.570111000	200.164607000
C	-32.924381000	-41.850903000	196.489835000
C	-31.515057000	-41.569700000	195.935577000
C	-30.519489000	-41.380875000	197.068335000
C	-29.958530000	-42.496775000	197.727650000
C	-30.189708000	-40.096594000	197.556084000
C	-29.097456000	-42.348366000	198.827972000
C	-29.328643000	-39.927809000	198.653593000
C	-28.777458000	-41.054475000	199.295214000
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W6-2

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C	-28.891466000	-31.624983000	206.900165000
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W7-1

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H	-23.954883000	-30.467850000	203.657223000
H	-25.249878000	-29.428349000	201.055840000
H	-24.940442000	-29.007043000	203.473105000
H	-23.971588000	-30.651829000	201.034132000

H	-20.203004000	-33.747757000	203.986147000
H	-25.599883000	-33.242658000	199.084041000
H	-29.188163000	-31.979048000	198.732039000
H	-28.634011000	-30.762151000	199.770039000
H	-29.697227000	-29.922588000	201.910188000
H	-29.219620000	-31.179757000	202.613648000
H	-27.128018000	-30.139542000	204.279130000
H	-28.448919000	-29.601541000	203.745594000
H	-32.943008000	-35.819108000	193.651526000
H	-31.698937000	-37.042536000	194.097512000
H	-26.515215000	-39.962549000	199.841895000
H	-25.471028000	-38.982647000	200.516485000
H	-27.676445000	-39.485598000	203.323593000
H	-27.588577000	-36.662028000	199.063904000
H	-26.512675000	-36.393969000	197.492780000
H	-26.940509000	-35.005589000	198.163636000
H	-25.534730000	-38.325272000	196.587573000
H	-25.474613000	-38.412519000	198.140162000
H	-28.020757000	-39.817532000	201.781468000
H	-26.982105000	-37.974356000	199.703695000
H	-24.871564000	-31.350469000	198.762800000
H	-26.865061000	-30.997066000	198.368739000
H	-26.426448000	-29.620717000	198.871906000
H	-26.718708000	-39.118327000	206.035234000
H	-26.542872000	-38.111519000	204.848038000
H	-25.707558000	-45.763213000	202.102717000
H	-22.835243000	-30.456391000	207.582363000
C	-23.340112000	-32.273345000	197.878339000
H	-22.705596000	-31.377002000	197.722446000
H	-22.682554000	-33.131642000	198.103566000
H	-23.882400000	-32.487666000	196.934891000

W8-1

Mn	-24.863552000	-35.541144000	203.952709000
Mn	-27.337747000	-35.218596000	205.227168000
Mn	-27.324847000	-33.345577000	203.151023000
Mn	-27.561445000	-33.189903000	200.409260000
Ca	-27.892368000	-36.732116000	202.211507000
O	-26.435015000	-36.510852000	204.220656000
O	-28.359077000	-34.725751000	203.800723000
O	-25.996648000	-34.063873000	204.482505000
O	-28.488174000	-32.608496000	201.975682000
O	-26.773404000	-34.323545000	201.683090000
O	-28.334027000	-31.726295000	199.278254000
O	-26.552237000	-33.813128000	198.991487000
O	-27.657989000	-37.283010000	199.900372000
O	-28.033115000	-39.140603000	202.496695000
H	-30.459948000	-26.816649000	200.178746000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.731432000	-27.319153000	201.406074000
C	-28.184267000	-28.438269000	200.500196000
O	-28.915137000	-29.498985000	200.391030000
O	-27.070503000	-28.280873000	199.919893000
C	-32.924381000	-41.850903000	196.489835000
C	-31.509623000	-41.590178000	195.939715000
C	-30.519109000	-41.396903000	197.076264000
C	-29.959386000	-42.509298000	197.742485000
C	-30.194425000	-40.110350000	197.561601000
C	-29.104130000	-42.355463000	198.846756000
C	-29.339408000	-39.936304000	198.662939000
C	-28.788558000	-41.059474000	199.311301000
O	-27.922695000	-40.857113000	200.371002000
H	-33.785375000	-32.318034000	197.913159000
C	-32.844739000	-31.791422000	197.688620000
C	-31.610331000	-32.670540000	197.694472000
O	-30.463372000	-32.187593000	197.591463000
H	-32.702585000	-30.970456000	198.411795000
N	-31.843429000	-34.013563000	197.751702000
C	-30.825021000	-35.049751000	197.612821000
C	-31.088890000	-35.971647000	196.399295000
O	-30.572611000	-37.096048000	196.322558000

C	-30.629213000	-35.852626000	198.911585000
C	-29.813780000	-35.200858000	200.030118000
O	-29.863780000	-35.694209000	201.192731000
O	-29.040131000	-34.233363000	199.677542000
N	-31.866534000	-35.426257000	195.425836000
C	-31.935591000	-35.967611000	194.072817000
H	-31.190723000	-35.442656000	193.449429000
H	-21.516057000	-41.187718000	202.032943000
C	-22.352883000	-41.458335000	202.717392000
C	-22.774900000	-42.909014000	202.609532000
O	-23.547260000	-43.428101000	203.436100000
C	-23.554753000	-40.509720000	202.464513000
C	-23.074019000	-39.049252000	202.386063000
C	-24.160419000	-37.986255000	202.499638000
O	-25.234726000	-38.026195000	201.854155000
O	-23.836864000	-37.014068000	203.309642000
N	-22.262496000	-43.592051000	201.545405000
C	-22.629343000	-44.962153000	201.252063000
H	-21.726399000	-45.520632000	200.924621000
C	-23.737876000	-45.090795000	200.181258000
C	-24.993343000	-44.408232000	200.607861000
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N	-25.827510000	-44.898410000	201.603003000
C	-26.806038000	-43.987662000	201.846172000
N	-26.646273000	-42.932014000	201.050434000
H	-19.262626000	-31.517297000	202.779917000
C	-20.112713000	-31.328697000	202.090235000
C	-21.152633000	-30.543716000	202.873894000
O	-21.414154000	-30.797797000	204.070560000
C	-20.725502000	-32.619954000	201.485896000
C	-21.599871000	-33.368718000	202.437719000
C	-22.943385000	-33.703070000	202.400176000
N	-21.142719000	-33.839588000	203.660743000
C	-22.159498000	-34.426317000	204.325713000
N	-23.268689000	-34.361965000	203.577981000
N	-21.812624000	-29.590912000	202.170873000
C	-22.896307000	-28.815019000	202.759171000
H	-22.557559000	-28.453986000	203.752878000
C	-24.184322000	-29.642612000	202.953019000
C	-24.753154000	-30.189876000	201.643405000
C	-25.712993000	-31.352926000	201.783538000
O	-26.007451000	-31.829819000	202.924731000
O	-26.168956000	-31.812667000	200.674648000
H	-24.814783000	-28.958795000	209.210708000
C	-25.289739000	-29.704836000	209.874338000
H	-25.215628000	-29.314217000	210.902923000
C	-24.617173000	-31.087868000	209.712703000
C	-24.558625000	-31.568098000	208.289225000
C	-25.348671000	-32.447343000	207.566831000
N	-23.599453000	-31.123738000	207.380300000
C	-23.783538000	-31.698561000	206.173213000
N	-24.850465000	-32.500871000	206.274366000
H	-24.708982000	-37.374838000	210.156821000
C	-25.333665000	-37.110846000	209.273415000
C	-26.302822000	-38.222553000	208.875453000
O	-26.047346000	-39.055718000	207.984512000
C	-24.388708000	-36.713536000	208.140151000
C	-24.995679000	-36.041357000	206.913535000
O	-26.245869000	-35.741938000	206.895811000
O	-24.181704000	-35.814691000	205.962095000
N	-27.489748000	-38.237637000	209.552173000
C	-28.420988000	-39.357108000	209.469748000
C	-29.303154000	-39.451381000	208.216634000
O	-29.915182000	-40.504632000	207.967177000
N	-29.389153000	-38.331332000	207.465885000
C	-30.077962000	-38.288094000	206.179911000
C	-29.374272000	-37.278033000	205.266498000
O	-29.572027000	-37.296424000	204.039900000
O	-28.624555000	-36.429652000	205.920971000
O	-25.591718000	-37.882656000	197.241527000
O	-27.539559000	-35.898405000	197.701579000
O	-26.622937000	-29.336135000	197.529000000
O	-25.242021000	-31.573987000	198.070023000

O	-29.765982000	-30.373224000	202.757130000
O	-25.776469000	-39.356343000	199.593622000
O	-26.816504000	-39.053216000	205.079566000
H	-30.318379000	-30.628900000	209.000204000
C	-30.997751000	-31.051074000	208.236197000
H	-31.843803000	-31.521736000	208.767318000
C	-30.275855000	-32.094729000	207.370890000
C	-28.986172000	-31.547573000	206.728324000
C	-28.312936000	-32.559234000	205.824262000
O	-28.066594000	-33.724546000	206.313441000
O	-28.021648000	-32.190600000	204.639095000
H	-36.654631000	-31.797146000	206.872551000
C	-36.971479000	-32.276075000	205.926511000
C	-35.751032000	-32.770331000	205.124119000
C	-34.809460000	-33.661622000	205.957761000
C	-33.720622000	-34.398841000	205.167004000
N	-32.737091000	-33.482985000	204.565982000
C	-31.798430000	-33.863394000	203.669152000
N	-31.616795000	-35.167758000	203.399854000
N	-31.081643000	-32.953536000	202.995496000
O	-27.612652000	-29.306295000	204.164586000
H	-32.916381000	-42.734552000	197.155932000
H	-33.258476000	-40.992101000	197.102375000
H	-33.700323000	-42.030393000	195.723193000
H	-31.515155000	-40.693211000	195.291570000
H	-31.192533000	-42.440189000	195.304532000
H	-30.196080000	-43.523804000	197.391635000
H	-28.676692000	-43.234895000	199.342570000
H	-29.074957000	-38.933812000	199.023095000
H	-30.596810000	-39.216328000	197.067212000
H	-27.466160000	-41.783612000	200.715233000
H	-25.175221000	-42.452411000	199.535771000
H	-27.600499000	-44.128438000	202.580747000
H	-28.785683000	-37.533482000	207.682062000
H	-27.643606000	-37.537980000	210.276523000
H	-21.544442000	-29.417557000	201.204322000
H	-21.675753000	-43.090846000	200.881034000
H	-22.969015000	-45.417276000	202.199022000
H	-23.916369000	-46.165723000	199.986821000
H	-23.395715000	-44.643100000	199.231097000
H	-22.557590000	-38.874560000	201.420548000
H	-24.072759000	-40.791864000	201.528546000
H	-21.980558000	-41.298109000	203.746851000
H	-22.333387000	-38.847901000	203.179389000
H	-24.291707000	-40.631109000	203.279514000
H	-26.358665000	-29.757244000	209.600929000
H	-26.208558000	-33.050065000	207.860781000
H	-23.145795000	-31.537351000	205.296715000
H	-23.686578000	-33.545366000	201.615984000
H	-22.086596000	-34.904011000	205.302531000
H	-19.698708000	-30.723327000	201.263407000
H	-23.075962000	-27.937982000	202.114773000
H	-29.870272000	-34.534864000	197.387791000
H	-32.802698000	-34.320867000	197.914554000
H	-32.927882000	-31.331881000	196.686881000
H	-32.157786000	-34.458220000	195.556333000
H	-30.780866000	-28.061891000	201.393689000
H	-19.910388000	-33.270742000	201.116632000
H	-21.339029000	-32.355689000	200.606814000
H	-25.922472000	-36.229296000	209.592268000
H	-29.977401000	-39.278056000	205.697579000
C	-31.572024000	-37.936386000	206.317009000
H	-32.060893000	-37.954881000	205.326911000
H	-32.070157000	-38.681557000	206.959536000
H	-31.696323000	-36.938307000	206.774708000
H	-29.094049000	-39.310240000	210.342905000
H	-27.858742000	-40.306732000	209.536504000
H	-23.607496000	-36.028271000	208.518868000
H	-23.852755000	-37.602193000	207.758850000
H	-30.057733000	-36.766473000	198.654724000
H	-31.593329000	-36.190438000	199.332090000
H	-31.384605000	-30.212790000	207.628640000
H	-30.019920000	-32.983971000	207.976292000

H	-28.258775000	-31.280816000	207.521683000
H	-30.952272000	-32.456953000	206.570792000
H	-29.170624000	-30.635628000	206.134174000
H	-28.161289000	-26.397507000	201.195724000
H	-28.491247000	-27.615684000	202.446334000
H	-25.159425000	-31.846816000	210.304069000
H	-23.586398000	-31.057371000	210.114342000
H	-25.278581000	-33.098356000	205.486347000
H	-37.548238000	-31.526089000	205.357493000
H	-35.192795000	-31.897755000	204.729365000
H	-35.404260000	-34.444212000	206.466824000
H	-33.195960000	-35.098647000	205.848005000
H	-37.645505000	-33.113381000	206.184914000
H	-36.094748000	-33.337703000	204.236021000
H	-34.339912000	-33.066549000	206.767520000
H	-32.847714000	-32.484096000	204.726669000
H	-34.186050000	-35.001304000	204.361379000
H	-31.181606000	-31.945726000	203.149587000
H	-31.918395000	-35.886779000	204.049551000
H	-30.179101000	-33.205088000	202.554427000
H	-30.893403000	-35.436756000	202.718193000
H	-23.953307000	-30.484527000	203.626091000
H	-25.295289000	-29.415115000	201.062702000
H	-24.945217000	-29.025339000	203.464323000
H	-23.940237000	-30.555237000	200.983215000
H	-20.204878000	-33.702452000	204.034862000
H	-26.168123000	-33.047762000	198.467025000
H	-29.116808000	-31.978525000	198.712736000
H	-28.520455000	-30.793780000	199.721088000
H	-29.678233000	-29.927521000	201.862258000
H	-29.202190000	-31.179755000	202.570728000
H	-27.140796000	-30.156830000	204.258648000
H	-28.446311000	-29.608284000	203.704590000
H	-32.943617000	-35.820115000	193.652282000
H	-31.698740000	-37.042313000	194.101937000
H	-26.523337000	-39.973419000	199.835001000
H	-25.472950000	-38.975489000	200.471726000
H	-27.670961000	-39.508871000	203.335728000
H	-27.683436000	-36.712579000	199.047918000
H	-26.778117000	-36.455789000	197.392747000
H	-27.130948000	-35.068260000	198.110610000
H	-25.897466000	-38.457048000	196.514604000
H	-25.653564000	-38.460401000	198.050483000
H	-28.014553000	-39.838874000	201.791475000
H	-27.006327000	-37.996894000	199.685791000
H	-25.354296000	-31.474852000	199.043391000
H	-25.818217000	-30.813293000	197.742732000
H	-26.853322000	-29.057084000	198.475802000
H	-26.713821000	-39.121407000	206.054325000
H	-26.552890000	-38.115870000	204.863836000
H	-25.701618000	-45.774219000	202.108086000
H	-22.845425000	-30.469729000	207.592687000
C	-25.714009000	-28.340630000	197.029113000
H	-24.761967000	-28.325112000	197.599490000
H	-25.485150000	-28.584166000	195.976597000
H	-26.162268000	-27.328138000	197.067755000

W8-2

Mn	-24.869857000	-35.543125000	203.950564000
Mn	-27.341772000	-35.217086000	205.233007000
Mn	-27.321878000	-33.342012000	203.157215000
Mn	-27.572485000	-33.155773000	200.407478000
Ca	-27.895236000	-36.694744000	202.207814000
O	-26.441155000	-36.510108000	204.220163000
O	-28.365992000	-34.716587000	203.816230000
O	-25.995157000	-34.066816000	204.493746000
O	-28.486787000	-32.587612000	201.989789000
O	-26.776245000	-34.318581000	201.713607000
O	-28.347359000	-31.714288000	199.345825000
O	-26.549647000	-33.872509000	199.033554000
O	-27.680007000	-37.278824000	199.897343000
O	-28.023968000	-39.110981000	202.485568000

H	-30.388787000	-26.778168000	200.178550000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.756819000	-27.393992000	201.485423000
C	-28.173112000	-28.543461000	200.656877000
O	-29.041355000	-29.550802000	200.461596000
O	-27.012871000	-28.554980000	200.242646000
C	-32.924381000	-41.850903000	196.489835000
C	-31.509571000	-41.593539000	195.937849000
C	-30.517754000	-41.397236000	197.072688000
C	-29.959572000	-42.507837000	197.743215000
C	-30.190428000	-40.109225000	197.552423000
C	-29.103993000	-42.351029000	198.846851000
C	-29.335129000	-39.932223000	198.653026000
C	-28.786635000	-41.053689000	199.306533000
O	-27.922553000	-40.848506000	200.366994000
H	-33.785375000	-32.318034000	197.913159000
C	-32.844739000	-31.791422000	197.688620000
C	-31.614812000	-32.674047000	197.698371000
O	-30.468566000	-32.193630000	197.606565000
H	-32.702471000	-30.970144000	198.411186000
N	-31.849500000	-34.018970000	197.749187000
C	-30.825021000	-35.049751000	197.612821000
C	-31.078646000	-35.969909000	196.396505000
O	-30.547567000	-37.086844000	196.312553000
C	-30.625195000	-35.849986000	198.911686000
C	-29.817105000	-35.185432000	200.028017000
O	-29.876518000	-35.665363000	201.197057000
O	-29.041338000	-34.222198000	199.672765000
N	-31.865852000	-35.429814000	195.427043000
C	-31.935591000	-35.967611000	194.072817000
H	-31.190723000	-35.442656000	193.449429000
H	-21.516057000	-41.187718000	202.032943000
C	-22.352883000	-41.458335000	202.717392000
C	-22.774457000	-42.909071000	202.610140000
O	-23.546315000	-43.428382000	203.437058000
C	-23.554369000	-40.508777000	202.464210000
C	-23.071842000	-39.048924000	202.379707000
C	-24.157095000	-37.984079000	202.492901000
O	-25.224822000	-38.015555000	201.836028000
O	-23.840360000	-37.020310000	203.314756000
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C	-22.896307000	-28.815019000	202.759171000
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W9-1

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W10-1

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H	-24.037688000	-31.902405000	199.007721000
H	-25.202957000	-31.243321000	198.193962000
H	-27.150743000	-30.852537000	198.306808000
H	-26.584738000	-29.511901000	198.793044000
H	-26.700043000	-39.116819000	206.072525000
H	-26.550045000	-38.113509000	204.875983000
H	-25.690350000	-45.677220000	202.115876000
H	-22.857208000	-30.458114000	207.590137000
C	-27.514691000	-38.825806000	196.596586000
H	-27.517011000	-39.901356000	196.857337000
H	-28.394747000	-38.348633000	197.067850000
H	-27.611323000	-38.723387000	195.502067000

W10-2

Mn	-24.875176000	-35.505877000	203.945445000
Mn	-27.339726000	-35.210223000	205.236455000
Mn	-27.330186000	-33.334469000	203.162833000
Mn	-27.554750000	-33.157748000	200.426110000
Ca	-27.922260000	-36.735375000	202.231506000
O	-26.434395000	-36.490995000	204.221770000
O	-28.359161000	-34.721858000	203.806004000
O	-26.005339000	-34.043896000	204.496392000
O	-28.508564000	-32.618410000	201.985910000
O	-26.746171000	-34.290431000	201.692042000
O	-28.430509000	-31.695087000	199.318357000
O	-26.533635000	-33.699229000	198.997655000



O	-27.580679000	-37.258558000	199.915812000
O	-28.145099000	-39.153171000	202.474531000
H	-30.461885000	-26.819741000	200.178362000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.731420000	-27.323361000	201.402159000
C	-28.191839000	-28.477386000	200.536669000
O	-28.961502000	-29.519964000	200.450287000
O	-27.062737000	-28.374065000	199.982698000
C	-32.924381000	-41.850903000	196.489835000
C	-31.531524000	-41.505549000	195.931090000
C	-30.530254000	-41.321541000	197.058877000
C	-29.925206000	-42.439191000	197.674513000
C	-30.236136000	-40.043455000	197.583923000
C	-29.054415000	-42.298517000	198.767998000
C	-29.366163000	-39.882417000	198.675345000
C	-28.770262000	-41.010589000	199.272745000
O	-27.890456000	-40.817199000	200.321567000
H	-33.785375000	-32.318034000	197.913159000
C	-32.844739000	-31.791422000	197.688620000
C	-31.619435000	-32.680189000	197.700790000
O	-30.468701000	-32.203631000	197.597758000
H	-32.700073000	-30.969520000	198.409972000
N	-31.852437000	-34.023547000	197.764478000
C	-30.825021000	-35.049751000	197.612821000
C	-31.063006000	-35.957181000	196.384826000
O	-30.485393000	-37.049735000	196.282851000
C	-30.598872000	-35.860924000	198.901038000
C	-29.773336000	-35.204623000	200.009730000
O	-29.849793000	-35.663955000	201.184692000
O	-28.963635000	-34.272819000	199.641435000
N	-31.875315000	-35.435255000	195.429455000
C	-31.935591000	-35.967611000	194.072817000
H	-31.190723000	-35.442656000	193.449429000
H	-21.516057000	-41.187718000	202.032943000
C	-22.352883000	-41.458335000	202.717392000
C	-22.772256000	-42.910126000	202.608612000
O	-23.542560000	-43.430304000	203.436555000
C	-23.557370000	-40.518357000	202.472985000
C	-23.104944000	-39.053227000	202.515767000
C	-24.210087000	-38.012819000	202.609252000
O	-25.340670000	-38.154775000	202.088303000
O	-23.837039000	-36.939431000	203.250886000
N	-22.260208000	-43.592666000	201.544719000
C	-22.629343000	-44.962153000	201.252063000
H	-21.726399000	-45.520632000	200.924621000
C	-23.736615000	-45.088719000	200.179772000
C	-24.987442000	-44.391298000	200.596094000
C	-25.507231000	-43.156316000	200.249513000
N	-25.830380000	-44.863833000	201.592419000
C	-26.802770000	-43.942877000	201.820833000
N	-26.630791000	-42.897266000	201.014174000
H	-19.262626000	-31.517297000	202.779917000
C	-20.112713000	-31.328697000	202.090235000
C	-21.157430000	-30.549497000	202.873197000
O	-21.424412000	-30.810117000	204.066881000
C	-20.721347000	-32.618398000	201.477563000
C	-21.602688000	-33.364996000	202.424010000
C	-22.954123000	-33.667930000	202.399476000
N	-21.144231000	-33.851035000	203.640230000
C	-22.167568000	-34.415632000	204.313830000
N	-23.282665000	-34.321497000	203.578804000
N	-21.818085000	-29.597242000	202.169747000
C	-22.896307000	-28.815019000	202.759171000
H	-22.557559000	-28.453986000	203.752878000
C	-24.188929000	-29.634312000	202.959482000
C	-24.761350000	-30.184009000	201.654066000
C	-25.746080000	-31.326835000	201.794835000
O	-26.016740000	-31.819091000	202.938831000
O	-26.234134000	-31.751694000	200.690754000
H	-24.821265000	-28.956143000	209.209195000
C	-25.289739000	-29.704836000	209.874338000
H	-25.215628000	-29.314217000	210.902923000

C	-24.606329000	-31.082545000	209.716118000
C	-24.546247000	-31.562922000	208.293622000
C	-25.336584000	-32.441074000	207.570741000
N	-23.589058000	-31.115093000	207.384464000
C	-23.774291000	-31.687264000	206.176317000
N	-24.840400000	-32.490459000	206.277653000
H	-24.708982000	-37.374838000	210.156821000
C	-25.333665000	-37.110846000	209.273415000
C	-26.305598000	-38.219446000	208.872731000
O	-26.055937000	-39.046296000	207.974548000
C	-24.389304000	-36.712034000	208.138461000
C	-24.995727000	-36.037811000	206.911387000
O	-26.244776000	-35.731779000	206.898617000
O	-24.184583000	-35.814760000	205.956690000
N	-27.490026000	-38.237359000	209.554276000
C	-28.420988000	-39.357108000	209.469748000
C	-29.303716000	-39.448399000	208.217504000
O	-29.909452000	-40.503307000	207.960412000
N	-29.399005000	-38.322106000	207.476926000
C	-30.090939000	-38.272953000	206.193251000
C	-29.386304000	-37.263939000	205.279951000
O	-29.594689000	-37.275784000	204.054802000
O	-28.622982000	-36.425359000	205.930675000
O	-24.611506000	-37.015849000	198.538954000
O	-27.061821000	-35.923927000	197.733801000
O	-26.429238000	-30.223636000	198.064666000
O	-24.486499000	-32.010435000	198.294241000
O	-29.787414000	-30.386052000	202.832752000
O	-25.690570000	-39.317645000	199.754076000
O	-26.848789000	-39.044388000	205.058129000
H	-30.318990000	-30.629741000	209.001267000
C	-30.997751000	-31.051074000	208.236197000
H	-31.843803000	-31.521736000	208.767318000
C	-30.275525000	-32.092208000	207.371400000
C	-28.980668000	-31.543073000	206.742442000
C	-28.313679000	-32.553129000	205.834764000
O	-28.066992000	-33.718695000	206.322839000
O	-28.033331000	-32.185000000	204.647151000
H	-36.645868000	-31.794307000	206.868110000
C	-36.971479000	-32.276075000	205.926511000
C	-35.759277000	-32.781731000	205.119292000
C	-34.823439000	-33.682248000	205.949330000
C	-33.739275000	-34.422258000	205.154871000
N	-32.752684000	-33.507699000	204.557042000
C	-31.823702000	-33.882743000	203.648902000
N	-31.657249000	-35.184642000	203.355949000
N	-31.104807000	-32.968673000	202.982585000
O	-27.594990000	-29.297048000	204.177030000
H	-32.868994000	-42.761976000	197.115450000
H	-33.286925000	-41.034985000	197.143389000
H	-33.700323000	-42.030393000	195.723193000
H	-31.585063000	-40.581760000	195.324126000
H	-31.190622000	-42.312364000	195.253277000
H	-30.136553000	-43.447174000	197.290363000
H	-28.589833000	-43.181307000	199.222669000
H	-29.117862000	-38.886244000	199.064212000
H	-30.670393000	-39.146555000	197.122965000
H	-27.438847000	-41.747457000	200.667704000
H	-25.147771000	-42.446306000	199.502011000
H	-27.602050000	-44.068959000	202.552791000
H	-28.798073000	-37.523866000	207.698436000
H	-27.638735000	-37.544292000	210.286015000
H	-21.531292000	-29.403298000	201.212536000
H	-21.677571000	-43.090442000	200.877480000
H	-22.969831000	-45.416296000	202.199068000
H	-23.923996000	-46.163310000	199.992076000
H	-23.387861000	-44.650973000	199.227357000
H	-22.517127000	-38.804482000	201.608056000
H	-24.026873000	-40.749440000	201.498523000
H	-21.979902000	-41.303549000	203.747773000
H	-22.425938000	-38.880156000	203.369792000
H	-24.326683000	-40.703600000	203.244874000
H	-26.358718000	-29.766056000	209.603207000

H	-26.195643000	-33.045218000	207.864264000
H	-23.137464000	-31.524149000	205.299386000
H	-23.706854000	-33.487779000	201.629384000
H	-22.095450000	-34.902537000	205.286215000
H	-19.698187000	-30.718953000	201.266835000
H	-23.073478000	-27.939427000	202.112516000
H	-29.883428000	-34.508990000	197.389006000
H	-32.810125000	-34.334986000	197.929461000
H	-32.923254000	-31.336323000	196.684622000
H	-32.214691000	-34.485546000	195.576164000
H	-30.782123000	-28.060580000	201.396704000
H	-19.905694000	-33.269534000	201.110822000
H	-21.327246000	-32.350289000	200.594049000
H	-25.921726000	-36.228965000	209.593003000
H	-29.993838000	-39.261903000	205.708006000
C	-31.583785000	-37.918711000	206.335248000
H	-32.075421000	-37.933555000	205.346477000
H	-32.081518000	-38.664870000	206.976926000
H	-31.705423000	-36.921688000	206.795841000
H	-29.094109000	-39.311281000	210.343026000
H	-27.858742000	-40.306732000	209.536504000
H	-23.608000000	-36.027123000	208.517759000
H	-23.853289000	-37.600264000	207.756417000
H	-30.019180000	-36.765647000	198.628102000
H	-31.550577000	-36.214883000	199.335050000
H	-31.384175000	-30.211770000	207.629813000
H	-30.025591000	-32.985546000	207.973186000
H	-28.256854000	-31.287741000	207.542531000
H	-30.947200000	-32.447922000	206.564377000
H	-29.158557000	-30.625852000	206.154652000
H	-28.154600000	-26.413362000	201.161286000
H	-28.485660000	-27.590115000	202.449643000
H	-25.142320000	-31.844414000	210.309412000
H	-23.575618000	-31.042880000	210.117007000
H	-25.269986000	-33.088809000	205.491911000
H	-37.548238000	-31.526089000	205.357493000
H	-35.193805000	-31.914653000	204.722758000
H	-35.422842000	-34.463037000	206.455702000
H	-33.217692000	-35.128434000	205.831677000
H	-37.648695000	-33.108166000	206.193461000
H	-36.111653000	-33.345683000	204.232395000
H	-34.349896000	-33.093070000	206.761149000
H	-32.846865000	-32.511139000	204.740848000
H	-34.208036000	-35.017758000	204.346174000
H	-31.192560000	-31.962879000	203.158949000
H	-31.946300000	-35.909800000	204.004952000
H	-30.201627000	-33.220347000	202.542458000
H	-30.934268000	-35.444864000	202.670369000
H	-23.964795000	-30.472868000	203.638912000
H	-25.274719000	-29.405008000	201.056663000
H	-24.944959000	-29.006467000	203.465179000
H	-23.946688000	-30.573012000	201.009597000
H	-20.198689000	-33.739152000	204.003531000
H	-25.722957000	-33.135833000	198.810721000
H	-29.210404000	-31.976207000	198.757166000
H	-28.646666000	-30.766924000	199.809084000
H	-29.713488000	-29.933542000	201.941993000
H	-29.221584000	-31.187054000	202.635041000
H	-27.110532000	-30.142461000	204.249722000
H	-28.443919000	-29.604685000	203.752342000
H	-32.942965000	-35.818544000	193.651911000
H	-31.698905000	-37.042576000	194.095483000
H	-26.455757000	-39.954170000	199.815626000
H	-25.518170000	-39.064533000	200.710215000
H	-27.729513000	-39.510478000	203.293304000
H	-27.490136000	-36.699374000	199.060206000
H	-26.144188000	-36.304651000	197.751746000
H	-26.911646000	-35.010631000	198.145569000
H	-24.940859000	-37.884887000	198.884365000
H	-28.064562000	-39.829578000	201.750346000
H	-26.952930000	-38.009898000	199.749684000
H	-23.918915000	-31.770100000	199.047922000
H	-25.147947000	-31.235497000	198.238179000

H	-27.125541000	-30.886802000	198.307456000
H	-26.576599000	-29.536056000	198.785274000
H	-26.755833000	-39.109403000	206.033799000
H	-26.564918000	-38.113725000	204.842843000
H	-25.713711000	-45.734644000	202.108220000
H	-22.835588000	-30.460640000	207.597387000
C	-24.337188000	-36.154902000	199.663255000
H	-25.240566000	-35.966246000	200.277041000
H	-23.535891000	-36.566894000	200.308700000
H	-24.001102000	-35.187429000	199.254376000

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Mn	-24.862989000	-35.499307000	203.965592000
Mn	-27.334708000	-35.199582000	205.250448000
Mn	-27.334205000	-33.330905000	203.167810000
Mn	-27.503824000	-33.219723000	200.418052000
Ca	-27.892774000	-36.712338000	202.253742000
O	-26.422831000	-36.486077000	204.245550000
O	-28.359298000	-34.716379000	203.822658000
O	-26.002328000	-34.035273000	204.506862000
O	-28.488380000	-32.629005000	201.970547000
O	-26.734400000	-34.318294000	201.727156000
O	-28.355570000	-31.732484000	199.288666000
O	-26.485756000	-33.825349000	199.039827000
O	-27.487813000	-37.246729000	199.976563000
O	-28.058831000	-39.120277000	202.556744000
H	-30.458977000	-26.814873000	200.178953000
C	-30.241434000	-27.113395000	201.222163000
H	-30.724377000	-26.361921000	201.871645000
C	-28.732000000	-27.331350000	201.402217000
C	-28.187836000	-28.470813000	200.517324000
O	-28.925853000	-29.534707000	200.437572000
O	-27.073295000	-28.331458000	199.938266000
C	-32.924381000	-41.850903000	196.489835000
C	-31.510347000	-41.529326000	195.968872000
C	-30.538442000	-41.367522000	197.129314000
C	-30.071954000	-42.501448000	197.831983000
C	-30.137957000	-40.096349000	197.598983000
C	-29.247353000	-42.382956000	198.962722000
C	-29.305190000	-39.958180000	198.724054000
C	-28.861205000	-41.102289000	199.416738000
O	-28.037277000	-40.944303000	200.516044000
H	-33.785375000	-32.318034000	197.913159000
C	-32.844739000	-31.791422000	197.688620000
C	-31.616251000	-32.678284000	197.715611000
O	-30.464826000	-32.201018000	197.625721000
H	-32.705936000	-30.962153000	198.402530000
N	-31.849852000	-34.021656000	197.774454000
C	-30.825021000	-35.049751000	197.612821000
C	-31.104029000	-35.965091000	196.396180000
O	-30.606151000	-37.097047000	196.317256000
C	-30.587655000	-35.871234000	198.892707000
C	-29.760449000	-35.226067000	200.005214000
O	-29.834954000	-35.698756000	201.176394000
O	-28.952259000	-34.293351000	199.642125000
N	-31.872009000	-35.412034000	195.420730000
C	-31.935591000	-35.967611000	194.072817000
H	-31.190723000	-35.442656000	193.449429000
H	-21.516057000	-41.187718000	202.032943000
C	-22.352883000	-41.458335000	202.717392000
C	-22.784889000	-42.905644000	202.601334000
O	-23.571081000	-43.420270000	203.417530000
C	-23.545387000	-40.500767000	202.484359000
C	-23.067724000	-39.042178000	202.524242000
C	-24.159845000	-37.984810000	202.597763000
O	-25.257115000	-38.082178000	202.000654000
O	-23.815007000	-36.951462000	203.316924000
N	-22.261174000	-43.592746000	201.546003000
C	-22.629343000	-44.962153000	201.252063000
H	-21.726399000	-45.520632000	200.924621000
C	-23.737842000	-45.084615000	200.179627000
C	-25.008118000	-44.434777000	200.617045000

C	-25.563618000	-43.201011000	200.323237000
N	-25.846830000	-44.981056000	201.578889000
C	-26.851230000	-44.103928000	201.838337000
N	-26.704055000	-43.015554000	201.085131000
H	-19.262626000	-31.517297000	202.779917000
C	-20.112713000	-31.328697000	202.090235000
C	-21.154142000	-30.545267000	202.873712000
O	-21.411164000	-30.794868000	204.072242000
C	-20.721622000	-32.618848000	201.481207000
C	-21.597914000	-33.360490000	202.435275000
C	-22.947530000	-33.668806000	202.411932000
N	-21.138634000	-33.831817000	203.657334000
C	-22.160324000	-34.394341000	204.335146000
N	-23.274459000	-34.312930000	203.596789000
N	-21.820811000	-29.598905000	202.168098000
C	-22.896307000	-28.815019000	202.759171000
H	-22.557559000	-28.453986000	203.752878000
C	-24.187741000	-29.632690000	202.967284000
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O	-26.037957000	-31.794152000	202.945377000
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W12-1

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W12-2

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