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F -1.88456149 4.01782727 -5.14967578

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F -1.91902412 3.46732684 -5.44615199

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3\_9\_3

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H 0.17649195 0.75555118 -0.92134437

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F 6.95709362 0.97528148 0.00087284

3\_16\_1

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H 5.09268364 -0.27655829 -2.48152086

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4\_8\_1

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4\_8\_3

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4\_9\_3

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4\_11\_3

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4\_12\_1

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H -2.98498919 3.69729907 -3.85623945

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H 3.72506264 -2.19202102 0.00019072

H 2.53129290 1.91874137 -0.00028007

H 4.90464261 2.60796470 0.00028738

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6\_8\_1

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H 7.79810469 -0.47540965 -0.41470295

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6\_24\_1

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H 3.55468303 -2.15452580 -0.27952011

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8\_5\_3

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H 6.29236854 -0.94926752 -0.35354509

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H 10.66439000 1.19590167 0.54949665

H 4.44439526 -0.76265906 -1.22817302

H 4.44760039 -0.76375748 0.51912670

8\_11\_1

C -0.33085477 1.86764099 -1.21673584

C 0.97673148 1.86353810 -1.72084231

C 1.27378835 2.55358055 -2.90385565

C 0.26325831 3.24772330 -3.58276423

C -1.04432810 3.25182556 -3.07865817

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H 0.49006766 3.77458538 -4.48602160

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C 2.08720334 1.10074104 -0.97479076

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H 3.70470509 2.00774788 -2.05925378

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C 5.78613334 0.97858056 -0.96087418

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8\_11\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

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C 4.58373100 1.19454402 -0.35354509

O 3.85036102 2.21710086 -0.35354509

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C 6.80939160 2.42445696 -0.35354509

C 6.83271956 0.00841183 -0.35354509

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H 8.74461049 3.39587514 -0.35354509

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H -0.59670902 1.83470684 -0.24824377

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8\_12\_3

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C 4.58373100 1.19454402 -0.35354509

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C 6.12360252 1.20948186 -0.35354509

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8\_13\_3

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8\_14\_3

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8\_15\_1

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8\_15\_3

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8\_16\_1

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8\_16\_3

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C 6.83271956 0.00841183 -0.35354509

C 8.20398938 2.43826077 -0.35354509

H 6.25005267 3.37118026 -0.35354509

C 8.22773639 0.02205102 -0.35354509

H 6.29236854 -0.94926752 -0.35354509

C 8.91343263 1.23669404 -0.35354509

H 8.74461049 3.39587514 -0.35354509

H 8.78657444 -0.92509446 -0.35354509

O 10.34335933 1.25117299 -0.35354509

H 10.66439000 1.19590167 0.54949665

H 4.44439526 -0.76265906 -1.22817302

H 4.44760039 -0.76375748 0.51912670

8\_17\_1

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C 1.27803699 2.38920421 -3.01325346

C 0.28886593 2.98754205 -3.80537366

C -0.99924227 3.18274331 -3.28904460

C -1.29818033 2.77960371 -1.98059649

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H 0.51711117 3.29534611 -4.80440357

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C 2.06609964 1.32854899 -0.83434416

C 3.48160345 1.11404309 -1.40173836

H 3.69848001 1.87888912 -2.11789136

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C 5.93491007 0.18017295 -2.00512688

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H 9.30959887 0.43411935 -2.29173914

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O 6.66415858 2.38133432 0.92262945

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H 8.67785768 2.65114189 1.20913682

H 7.68431601 2.90652813 2.62360474

H 7.98363584 1.28430731 2.04751975

S 4.43548577 1.17274661 -0.33798913

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O -2.00859989 3.79329412 -4.09732976

C -3.02681820 2.83428927 -4.39472038

H -3.62203257 2.66380137 -3.52204992

H -3.64769170 3.20607323 -5.18287822

H -2.57261361 1.91541640 -4.70175597

8\_17\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

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H -4.44369368 -1.04091448 -0.87395912

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H 8.74461049 3.39587514 -0.35354509

H 8.78657444 -0.92509446 -0.35354509

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H 10.66439000 1.19590167 0.54949665

H 4.44439526 -0.76265906 -1.22817302

H 4.44760039 -0.76375748 0.51912670

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C 1.27563695 2.41828014 -3.01338100

C 0.28267148 3.02765476 -3.79222895

C -1.00689255 3.20239088 -3.27221561

C -1.30349061 2.76775407 -1.97335365

H -0.53698374 1.82652663 -0.20279496

H 2.26024681 2.28486225 -3.41042393

H 0.50913023 3.35950810 -4.78393949

H -2.28810166 2.90116797 -1.57631233

C 2.07021113 1.31400562 -0.85864028

C 3.48731302 1.12198308 -1.43008545

H 3.69921208 1.90427508 -2.12866832

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8\_18\_3

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H 6.25005267 3.37118026 -0.35354509

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H 6.29236854 -0.94926752 -0.35354509

C 8.91343263 1.23669404 -0.35354509

H 8.74461049 3.39587514 -0.35354509

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8\_19\_1

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8\_19\_3

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8\_20\_1

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8\_21\_1

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H 6.25005267 3.37118026 -0.35354509

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8\_22\_1

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N 6.76495765 2.15927106 0.89534369

O 5.67456043 2.30632076 1.36623701

O 7.85325486 2.67717423 1.52541156

O -2.53393013 3.04152550 -1.30585985

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H -4.48486200 3.01241546 -1.94059067

H -3.41674091 4.04017926 -2.86573213

H -3.33207425 2.30430126 -3.04635794

8\_22\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 4.58373100 1.19454402 -0.35354509

O 3.85036102 2.21710086 -0.35354509

C 6.12360252 1.20948186 -0.35354509

C 6.80939160 2.42445696 -0.35354509

C 6.83271956 0.00841183 -0.35354509

C 8.20398938 2.43826077 -0.35354509

H 6.25005267 3.37118026 -0.35354509

C 8.22773639 0.02205102 -0.35354509

H 6.29236854 -0.94926752 -0.35354509

C 8.91343263 1.23669404 -0.35354509

H 8.74461049 3.39587514 -0.35354509

H 8.78657444 -0.92509446 -0.35354509

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H 10.66439000 1.19590167 0.54949665

H 4.44439526 -0.76265906 -1.22817302

H 4.44760039 -0.76375748 0.51912670

8\_23\_1

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C 1.01933228 2.03431356 -1.69475039

C 1.29813282 2.57263273 -2.95823948

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H 2.26807373 2.44550133 -3.39177407

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8\_23\_3

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C 4.58373100 1.19454402 -0.35354509

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H 4.44760039 -0.76375748 0.51912670

8\_24\_1

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8\_24\_3

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H 10.66439000 1.19590167 0.54949665

H 4.44439526 -0.76265906 -1.22817302

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8\_25\_1

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8\_25\_3

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9\_2\_2

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H 6.36298498 -0.83536770 -0.32425376

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C 12.61647146 1.39082037 0.88354163

H 10.67181523 1.37317882 1.83604727

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9\_12\_2

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9\_12\_3

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C 4.15508565 -0.14837909 -0.32425376

9\_13\_2

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9\_13\_3

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H 10.67135242 1.36160966 -2.48464120

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H 13.16599582 1.38652853 -2.48513781

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9\_15\_2

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9\_16\_2

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C 11.22140940 1.37626960 0.88364729

C 12.61613149 1.38388900 -1.53280448

H 10.67135242 1.36160966 -2.48464120

C 12.61647146 1.39082037 0.88354163

H 10.67181523 1.37317882 1.83604727

C 13.31389133 1.39449325 -0.32440251

H 13.16599582 1.38652853 -2.48513781

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H 14.41351886 1.40523564 -0.32487058

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C 4.15508565 -0.14837909 -0.32425376

9\_17\_2

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9\_17\_3

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C 11.22140940 1.37626960 0.88364729

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C 12.61647146 1.39082037 0.88354163

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H 13.16609995 1.39918338 1.83607131

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9\_19\_3

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9\_20\_2

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9\_20\_3

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H 10.67135242 1.36160966 -2.48464120

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9\_21\_2

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9\_22\_2

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9\_23\_2

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9\_23\_3

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H 10.67135242 1.36160966 -2.48464120

C 12.61647146 1.39082037 0.88354163

H 10.67181523 1.37317882 1.83604727

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9\_24\_3

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9\_25\_2

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10\_0\_2

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10\_1\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_1\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_2\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_2\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_3\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

N -3.50922218 0.92854573 -0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_3\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

N -3.50922218 0.92854573 -0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_4\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_5\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_5\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_6\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_6\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_7\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_8\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_8\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_9\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_10\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_10\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_11\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_12\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_13\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_14\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_15\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_15\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_16\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_16\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_17\_2

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_17\_3

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_18\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_18\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_19\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_20\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_20\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_21\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_22\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_23\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_23\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_24\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_24\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

H 5.99468522 -0.45189361 -0.30318704

C 8.61574931 1.73406795 -0.30318704

H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

O 10.04567601 1.74854690 -0.30318704

C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

10\_25\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

O 7.65479820 1.51347856 0.00000000

C 8.13300014 1.43114733 1.34515593

H 7.83130573 0.49865229 1.77449669

H 9.20099798 1.49648052 1.34864489

H 7.72451196 2.23670476 1.91884107

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

10\_25\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 4.28604768 1.69191793 -0.30318704

O 3.55267770 2.71447477 -0.30318704

C 5.82591920 1.70685577 -0.30318704

C 6.51170828 2.92183087 -0.30318704

C 6.53503624 0.50578574 -0.30318704

C 7.90630606 2.93563468 -0.30318704

H 5.95236935 3.86855417 -0.30318704

C 7.93005307 0.51942493 -0.30318704

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H 8.44692717 3.89324905 -0.30318704

H 8.48889112 -0.42772055 -0.30318704

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C 10.52387795 1.66621567 1.04196889

H 10.22218354 0.73372063 1.47130965

H 11.59187579 1.73154886 1.04545785

H 10.11538977 2.47177310 1.61565403

H 4.14671194 -0.26528515 -1.17781497

H 4.14991707 -0.26638357 0.56948475

C 3.78678589 0.23509500 -0.30318704

11\_0\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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11\_0\_3

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O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

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C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165793 0.00006209

N 11.55248770 1.90340309 0.00006209

11\_1\_2

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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H -4.44401836 -1.04092585 0.87334351

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

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C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 6.05604936 3.65818071 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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11\_1\_3

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C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165793 0.00006209

N 11.55248770 1.90340309 0.00006209

11\_2\_2

O 0.00000000 0.00000000 0.00000000

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C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

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H -3.08467839 -5.22902992 -2.70173525

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H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

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H 7.29481665 1.50983351 0.00000000

11\_2\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H -2.01202258 -5.84317879 -0.49401571

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C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

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H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

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H -5.26359045 -5.04333756 -3.90173238

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C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

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C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165793 0.00006209

N 11.55248770 1.90340309 0.00006209

11\_3\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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N -3.50922218 0.92854573 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_3\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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N -3.50922218 0.92854573 0.00000000

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C 6.77191303 0.64778301 0.00006209

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H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

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N 11.55248770 1.90340309 0.00006209

11\_4\_2

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165793 0.00006209

N 11.55248770 1.90340309 0.00006209

11\_5\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_5\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165793 0.00006209

N 11.55248770 1.90340309 0.00006209

11\_6\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_6\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

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C 6.77191303 0.64778301 0.00006209

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C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_7\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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Br -2.80042732 -5.45300834 0.00000000

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C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

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N 11.55248770 1.90340310 0.00006209

11\_8\_2

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H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_8\_3

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C 0.10291173 -2.44429720 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

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C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

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H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_9\_2

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H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_9\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

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C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_10\_2

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C -2.68369776 -2.58154545 0.00000000

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F -2.54446440 -4.95492905 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

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H 6.05604936 3.65818071 0.00000000

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H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_10\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_11\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_11\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

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C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_12\_2

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_12\_3

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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H -4.79204763 0.43168404 -0.00036327

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C -2.63130896 -5.12392023 0.00000000

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_13\_2

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C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 1.89516987 1.45684959 0.00000000

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C 3.43504139 1.47178743 0.00000000

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C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 6.05604936 3.65818071 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_13\_3

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H 1.20115184 -2.39029979 0.00000000

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C 4.52292447 1.83391520 0.00006209

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H 4.38679386 -0.12438630 0.87273388

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N 11.55248770 1.90340310 0.00006209

11\_14\_2

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H 1.75903926 -0.50145191 0.87267179

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H 7.29481665 1.50983351 0.00000000

11\_14\_3

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N 11.55248770 1.90340310 0.00006209

11\_15\_2

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H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_15\_3

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H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

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H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

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C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_16\_2

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H 1.75903926 -0.50145191 0.87267179

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11\_16\_3

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

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H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

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C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_17\_2

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_17\_3

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_18\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_18\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_19\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_20\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_20\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_21\_2

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_21\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_22\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

H 4.38358873 -0.12328788 -0.87456584

H 4.38679386 -0.12438630 0.87273388

C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_23\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

H 7.29481665 1.50983351 0.00000000

11\_23\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

H 6.23156201 -0.30989634 0.00006209

C 8.85262610 1.87606522 0.00006209

H 8.68380396 4.03524632 0.00006209

H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

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C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

11\_24\_2

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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H 7.29481665 1.50983351 0.00000000

11\_24\_3

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

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H 6.18924614 4.01055144 0.00006209

C 8.16692986 0.66142220 0.00006209

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C 8.85262610 1.87606522 0.00006209

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H 8.72576791 -0.28572328 0.00006209

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H 4.38679386 -0.12438630 0.87273388

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N 11.55248770 1.90340310 0.00006209

11\_25\_2

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

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11\_25\_3

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C 4.52292447 1.83391520 0.00006209

O 3.78955449 2.85647204 0.00006209

C 6.06279599 1.84885304 0.00006209

C 6.74858507 3.06382814 0.00006209

C 6.77191303 0.64778301 0.00006209

C 8.14318285 3.07763195 0.00006209

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H 8.72576791 -0.28572328 0.00006209

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C 4.02366268 0.37709227 0.00006209

C 10.39254716 1.89165794 0.00006209

N 11.55248770 1.90340310 0.00006209

12\_0\_2

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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Cl 7.98478128 1.51681985 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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12\_0\_3

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H -2.43004899 -4.73228764 0.00000000

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O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

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H 6.19970007 -0.85746187 -0.32400875

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H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_1\_2

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H -2.43004899 -4.73228764 0.00000000

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H -4.44401836 -1.04092585 0.87334351

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12\_1\_3

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12\_2\_2

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C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

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12\_2\_3

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O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

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H 6.19970007 -0.85746187 -0.32400875

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H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

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C 3.99180074 -0.17047326 -0.32400875

12\_3\_2

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_3\_3

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N -3.50922218 0.92854573 -0.00000000

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H 6.15738420 3.46298591 -0.32400875

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H 6.19970007 -0.85746187 -0.32400875

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H 8.65194202 3.48768079 -0.32400875

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Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

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C 3.99180074 -0.17047326 -0.32400875

12\_4\_2

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H -4.79204763 0.43168404 -0.00036327

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H -3.24291089 -5.21062478 -0.87368496

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_5\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_5\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_6\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_6\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_7\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_8\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_8\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_9\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_10\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_10\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_11\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_12\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_13\_2

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_13\_3

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_14\_2

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C -2.04648885 -1.34090601 0.00000000

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H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

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F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_14\_3

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.49106253 1.28634967 -0.32400875

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C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

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C 8.13506792 0.11385667 -0.32400875

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H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

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C 3.99180074 -0.17047326 -0.32400875

12\_15\_2

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H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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N -2.68369776 -2.58154545 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_15\_3

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C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

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O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_16\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_16\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H 0.91794368 -5.00550219 0.87364974

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O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_17\_2

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_17\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_18\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_18\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_19\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_20\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_20\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_21\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_22\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_23\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_23\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

C 8.82076416 1.32849969 -0.32400875

H 8.65194202 3.48768079 -0.32400875

H 8.69390597 -0.83328881 -0.32400875

Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_24\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_24\_3

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H -2.01202258 -5.84317879 -0.49401571

C 4.49106253 1.28634967 -0.32400875

O 3.75769255 2.30890651 -0.32400875

C 6.03093405 1.30128751 -0.32400875

C 6.71672313 2.51626261 -0.32400875

C 6.74005109 0.10021748 -0.32400875

C 8.11132091 2.53006642 -0.32400875

H 6.15738420 3.46298591 -0.32400875

C 8.13506792 0.11385667 -0.32400875

H 6.19970007 -0.85746187 -0.32400875

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H 8.65194202 3.48768079 -0.32400875

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Cl 10.58067394 1.34631993 -0.32400875

H 4.35172679 -0.67085341 -1.19863668

H 4.35493192 -0.67195183 0.54866304

C 3.99180074 -0.17047326 -0.32400875

12\_25\_2

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C -2.04648885 -1.34090601 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

Cl 7.98478128 1.51681985 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

12\_25\_3

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C -1.92741092 -3.75420218 0.00000000

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F -4.19440535 -0.35777358 -0.00246802

C 4.49106253 1.28634967 -0.32400875

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C 6.03093405 1.30128751 -0.32400875

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H 4.35172679 -0.67085341 -1.19863668

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C 3.99180074 -0.17047326 -0.32400875

13\_0\_2

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C -2.04648885 -1.34090601 0.00000000

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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Br 8.13148224 1.51768753 -0.11218847

13\_0\_3

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

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H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

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H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_1\_2

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H -4.44369368 -1.04091448 -0.87395912

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Br 8.13148224 1.51768753 -0.11218847

13\_1\_3

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C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

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H 10.10818985 -0.76292232 -1.76783771

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C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_2\_2

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C 6.17040900 -0.90672700 0.24047000

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13\_2\_3

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O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

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H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

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H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

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H 5.76921580 -0.60158534 -0.89516592

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C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_3\_2

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H 0.06199400 -4.60941029 0.00000000

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N -3.50922218 0.92854573 0.00000000

C 1.89516987 1.45684959 0.00000000

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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Br 8.13148224 1.51768753 -0.11218847

13\_3\_3

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C 5.90534641 1.35671616 -1.76783771

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C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

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H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

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Br 12.14496415 1.41676734 -1.76783771

13\_4\_2

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 6.09801331 -0.66278889 0.00000000

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C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_5\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_5\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_6\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_6\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_7\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

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O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_8\_2

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H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_8\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_9\_2

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_10\_2

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_10\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_11\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_12\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_13\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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H -3.92195150 -0.29320857 -0.00195613

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_14\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_15\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_15\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_16\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_16\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

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H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_17\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_17\_3

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_18\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_18\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_19\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_20\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_20\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_21\_2

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_22\_2

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_23\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_23\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

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H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_24\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_24\_3

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

13\_25\_2

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 6.22487150 1.49899961 0.00000000

Br 8.13148224 1.51768753 -0.11218847

13\_25\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

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C 5.90534641 1.35671616 -1.76783771

O 5.17197643 2.37927300 -1.76783771

C 7.44521793 1.37165400 -1.76783771

C 8.13100701 2.58662910 -1.76783771

C 8.15433497 0.17058397 -1.76783771

C 9.52560479 2.60043291 -1.76783771

H 7.57166808 3.53335240 -1.76783771

C 9.54935180 0.18422316 -1.76783771

H 7.61398395 -0.78709538 -1.76783771

H 10.06622590 3.55804728 -1.76783771

H 10.10818985 -0.76292232 -1.76783771

H 5.76601067 -0.60048692 -2.64246564

H 5.76921580 -0.60158534 -0.89516592

C 5.40608462 -0.10010677 -1.76783771

C 10.23504804 1.39886618 -1.76783771

Br 12.14496415 1.41676734 -1.76783771

14\_0\_2

O 0.00000000 0.00000000 0.00000000

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C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H -2.43004899 -4.73228764 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

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C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

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H 7.78975175 1.73770433 -2.04602377

14\_0\_3

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C 0.10291173 -2.44429720 0.00000000

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C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

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H 6.44573898 0.56006561 -0.12275585

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C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_1\_2

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C -2.04648885 -1.34090601 0.00000000

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O 1.16179989 2.47940643 0.00000000

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H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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14\_1\_3

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C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

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H 10.78471303 0.39872863 -0.99542764

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N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_2\_2

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C -5.15700139 -4.82906594 -0.01939463

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H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

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H 1.75903926 -0.50145191 0.87267179

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H 7.78876244 1.83540754 2.03300720

14\_2\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

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O 5.84849961 3.54092395 -0.99542764

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C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

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H 6.44573898 0.56006561 -0.12275585

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C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_3\_2

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H 1.20115184 -2.39029979 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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14\_3\_3

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H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_4\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44551148 1.32189003 1.02211940

N 8.33918646 1.75795094 -1.21632406

H 9.32377026 1.78663310 -1.31205219

H 7.78801546 1.90917855 -2.01999446

14\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

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H -1.89707380 -5.90225096 0.00006691

O 1.53118641 -2.37407291 0.00000000

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_5\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44525354 1.34736353 1.02676573

N 8.33949340 1.72763742 -1.22185380

H 9.32410136 1.75393382 -1.31801757

H 7.78852521 1.85883582 -2.02917431

14\_5\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_6\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

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H 7.78957276 1.75538112 2.04402101

14\_6\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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O -3.12698910 0.60233649 1.03134164

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_7\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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14\_7\_3

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_8\_2

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 1.89516987 1.45684959 0.00000000

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

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H 9.32451316 1.71326470 -1.32427321

H 7.78915921 1.79622314 -2.03880003

14\_8\_3

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_9\_2

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44502941 1.36949870 1.03027480

N 8.33976012 1.70129650 -1.22603012

H 9.32438907 1.72551978 -1.32252294

H 7.78896816 1.81509058 -2.03610696

14\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_10\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44477861 1.39426725 1.03362533

N 8.34005857 1.67182185 -1.23001784

H 9.32471101 1.69372537 -1.32682493

H 7.78946381 1.76614114 -2.04272605

14\_10\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_11\_2

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44463401 1.40854796 1.03528290

N 8.34023065 1.65482776 -1.23199067

H 9.32489663 1.67539377 -1.32895327

H 7.78974958 1.73791857 -2.04600043

14\_11\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_12\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.79204763 0.43168404 -0.00036327

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

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N 8.33994884 1.68265869 -1.22863540

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H 7.78928158 1.78413820 -2.04043146

14\_12\_3

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_13\_2

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

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C 7.76479256 1.51459232 0.00000000

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14\_13\_3

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

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C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_14\_2

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C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44517503 1.35511753 -1.02805057

N 8.33958730 1.71836354 1.22339049

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H 7.78867833 1.84371445 2.03167992

14\_14\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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F -1.84996634 -6.03139598 -0.62329085

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_15\_2

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H -2.64221326 -0.41663104 0.00000000

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O 1.16179989 2.47940643 0.00000000

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C 4.12083047 2.68676253 0.00000000

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H 3.56149154 3.63348583 0.00000000

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H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44463602 1.40834921 1.03526120

N 8.34022825 1.65506427 -1.23196485

H 9.32489404 1.67564889 -1.32892541

H 7.78974560 1.73831135 -2.04595756

14\_15\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_16\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44497898 1.37447933 1.03099722

N 8.33982013 1.69536954 -1.22688992

H 9.32445381 1.71912634 -1.32345050

H 7.78906783 1.80524749 -2.03753417

14\_16\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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H 0.91794368 -5.00550219 0.87364974

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C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_17\_2

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44484425 1.38778469 1.03280686

N 8.33998046 1.67953612 -1.22904370

H 9.32462675 1.70204678 -1.32577401

H 7.78933409 1.77895246 -2.04110917

14\_17\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_18\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

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H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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H 7.78825039 1.88597729 -2.02438587

14\_18\_3

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.74446035 -4.21783562 0.87459733

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_19\_2

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.79204763 0.43168404 -0.00036327

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O -2.85999570 -5.56889386 1.05506765

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

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14\_19\_3

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_20\_2

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C -0.53432909 -3.68539906 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

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H 7.78926348 1.78592574 -2.04019474

14\_20\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_21\_2

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44537854 1.33501913 1.02459586

N 8.33934466 1.74232728 -1.21927137

H 9.32394091 1.76977982 -1.31523168

H 7.78827819 1.88323178 -2.02488730

14\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_22\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44473971 1.39810939 -1.03409095

N 8.34010534 1.66720281 1.23057760

H 9.32476180 1.68870900 1.32743284

H 7.78953863 1.75875190 2.04362153

14\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_23\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44501154 1.37126355 -1.03053359

N 8.33978186 1.69914961 1.22634494

H 9.32441286 1.72317024 1.32286748

H 7.78900142 1.81180593 2.03658862

14\_23\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

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O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

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H -1.89191645 -5.27412912 -1.91662783

C 6.58186959 2.51836711 -0.99542764

O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_24\_2

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44477543 1.39458186 -1.03366400

N 8.34006284 1.67140061 1.23006962

H 9.32471595 1.69323720 1.32688493

H 7.78946804 1.76572319 2.04277743

14\_24\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -2.01202258 -5.84317879 -0.49401571

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

14\_25\_2

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.05604936 3.65818071 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 1.75583413 -0.50035349 -0.87462793

H 1.75903926 -0.50145191 0.87267179

C 1.39590808 0.00002666 0.00000000

C 7.76479256 1.51459232 0.00000000

O 8.44477678 1.39444836 -1.03364761

N 8.34006123 1.67155947 1.23005011

H 9.32471422 1.69340856 1.32686389

H 7.78946537 1.76598701 2.04274501

14\_25\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

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O 5.84849961 3.54092395 -0.99542764

C 8.12174111 2.53330495 -0.99542764

C 8.80753019 3.74828005 -0.99542764

C 8.83085815 1.33223492 -0.99542764

C 10.20212797 3.76208386 -0.99542764

H 8.24819126 4.69500335 -0.99542764

C 10.22587498 1.34587411 -0.99542764

H 8.29050713 0.37455557 -0.99542764

C 10.91157122 2.56051713 -0.99542764

H 10.74274908 4.71969823 -0.99542764

H 10.78471303 0.39872863 -0.99542764

H 6.44253385 0.56116403 -1.87005557

H 6.44573898 0.56006561 -0.12275585

C 6.08260780 1.06154418 -0.99542764

C 12.45149228 2.57610984 -0.99542764

O 13.13028396 2.57373952 -2.03680976

N 13.02818007 2.59292544 0.24382391

H 14.01294476 2.60374370 0.34135998

H 12.47852184 2.59475383 1.06261440

15\_0\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 6.00714682 4.60101080 0.87267179

H 7.32633940 3.85626133 0.00195613

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H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251793 4.04161638 0.00000000

15\_0\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

15\_1\_1

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O 0.00000000 0.00000000 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 6.00714682 4.60101080 0.87267179

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C 3.43504139 1.47178743 0.00000000

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C 8.91705787 3.92244401 -0.32520798

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15\_3\_1

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

15\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H 6.01009724 4.59934514 -0.87462793

H 6.00714682 4.60101080 0.87267179

H 7.32633940 3.85626133 0.00195613

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

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O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.27251793 4.04161638 0.00000000

15\_7\_3

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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O -2.88078860 -0.04647798 0.00000000

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O 3.80633983 2.36023406 -0.32520798

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C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

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H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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C 8.91705787 3.92244401 -0.32520798

15\_8\_1

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C 0.10291173 -2.44429720 0.00000000

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H 6.00714682 4.60101080 0.87267179

H 7.32633940 3.85626133 0.00195613

H 0.06199400 -4.60941029 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

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15\_8\_3

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C -2.63130896 -5.12392023 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

15\_9\_1

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C -2.88078860 -0.04647798 0.00000000

H 6.01009724 4.59934514 -0.87462793

H 6.00714682 4.60101080 0.87267179

H 7.32633940 3.85626133 0.00195613

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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H 1.97260279 -1.84905466 -0.87462793

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H 2.04683045 -3.35874245 0.00195613

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15\_9\_3

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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15\_10\_1

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H 1.78667599 -0.50476353 -0.87342340

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15\_10\_3

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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15\_11\_1

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15\_11\_3

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15\_12\_1

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15\_12\_3

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C 8.91705787 3.92244401 -0.32520798

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H 6.00714682 4.60101080 0.87267179

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C 4.14415843 0.27071740 0.00000000

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H 7.32445852 1.51013365 0.00000000

C 6.27251793 4.04161638 0.00000000

15\_13\_3

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C -2.68369776 -2.58154545 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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15\_14\_1

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H 6.00714682 4.60101080 0.87267179

H 7.32633940 3.85626133 0.00195613

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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C 6.27251793 4.04161638 0.00000000

15\_14\_3

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C 4.04044753 -0.11914713 -0.32520798

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15\_15\_1

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15\_15\_3

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H 4.40037407 -0.61952586 -1.19983591

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15\_16\_1

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15\_17\_1

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15\_17\_3

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15\_18\_1

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15\_18\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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15\_19\_1

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H 7.32633940 3.85626133 0.00195613

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C 6.27251793 4.04161638 0.00000000

15\_19\_3

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H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

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15\_20\_1

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H 6.00714682 4.60101080 0.87267179

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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C 6.27251793 4.04161638 0.00000000

15\_20\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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H 1.78667597 -0.50397368 0.87387943

H 6.01009724 4.59934514 -0.87462793

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15\_23\_1

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15\_24\_3

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15\_25\_1

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15\_25\_3

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16\_0\_1

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H -2.43004899 -4.73228764 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 7.32445852 1.51013365 0.00000000

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

C 5.51542825 2.70056634 0.00000000

H 6.04046516 3.63077403 -0.06284824

16\_0\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_1\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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H 7.32445852 1.51013365 0.00000000

C 5.51542825 2.70056634 0.00000000

H 6.04046516 3.63077403 -0.06284824

16\_1\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_2\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H 6.04046516 3.63077403 -0.06284824

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

H 6.04046516 3.63077403 -0.06284824

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_2\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_3\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H 6.04046516 3.63077403 -0.06284824

N -3.50922218 0.92854573 -0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_3\_3

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C -0.65307274 -1.27216194 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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N -3.50922218 0.92854573 -0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

16\_4\_1

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

H 6.04046516 3.63077403 -0.06284824

C -2.63130896 -5.12392023 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 7.32445852 1.51013365 0.00000000

16\_4\_3

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_5\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

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H 6.04046516 3.63077403 -0.06284824

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

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H 1.78667599 -0.50476353 -0.87342340

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H -3.83843623 -7.47439765 2.16033398

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_5\_3

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

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C -3.58750097 -6.98533199 1.20780025

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H -3.83843623 -7.47439765 2.16033398

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_6\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_6\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H 6.04046516 3.63077403 -0.06284824

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 6.04046516 3.63077403 -0.06284824

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_8\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_9\_1

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 6.04046516 3.63077403 -0.06284824

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

16\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_10\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

H 6.04046516 3.63077403 -0.06284824

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_10\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_11\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

H 6.04046516 3.63077403 -0.06284824

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_12\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 6.04046516 3.63077403 -0.06284824

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_13\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H 6.04046516 3.63077403 -0.06284824

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_14\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

H 6.04046516 3.63077403 -0.06284824

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_15\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

H 6.04046516 3.63077403 -0.06284824

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_15\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_16\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 6.04046516 3.63077403 -0.06284824

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_16\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_17\_1

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H 6.04046516 3.63077403 -0.06284824

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_17\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

16\_18\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.74446035 -4.21783562 0.87459733

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_18\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_19\_1

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H 6.04046516 3.63077403 -0.06284824

H -4.44369368 -1.04091448 -0.87395912

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O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_20\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H 6.04046516 3.63077403 -0.06284824

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_20\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_21\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H 6.04046516 3.63077403 -0.06284824

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

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N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_22\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 6.04046516 3.63077403 -0.06284824

H 1.78667599 -0.50476353 -0.87342340

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O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_22\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_23\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

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H 6.04046516 3.63077403 -0.06284824

N -2.84286588 -0.10531562 0.00000000

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O -3.15011583 0.37516349 -1.05506215

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H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_23\_3

O 0.00000000 0.00000000 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

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C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

16\_24\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

16\_24\_3

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H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

16\_25\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 5.51542825 2.70056634 0.00000000

H 6.04046516 3.63077403 -0.06284824

16\_25\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

17\_0\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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17\_0\_3

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C 6.76537041 2.56759016 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_1\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_1\_3

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C -1.92741092 -3.75420218 0.00000000

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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H 9.96899846 1.39096128 -0.32520798

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H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_2\_1

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H 1.78667599 -0.50476353 -0.87342340

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H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

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H 7.32633940 3.85626132 0.00195613

17\_2\_3

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C 8.86941144 1.37982724 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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H 8.65168677 4.48183842 0.54746381

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17\_3\_1

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H 6.09801331 -0.66278889 0.00000000

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H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_3\_3

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C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 9.97087934 3.73708895 -0.32325185

17\_4\_1

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C 3.43504139 1.47178743 0.00000000

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17\_4\_3

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H 6.24834735 -0.80613432 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

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17\_5\_1

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

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17\_6\_1

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_6\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_8\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_9\_1

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

17\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_10\_1

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_10\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_11\_1

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O 0.00000000 0.00000000 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_12\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

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H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_13\_1

C 1.39590808 0.00002666 0.00000000

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H -3.92195150 -0.29320857 -0.00195613

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

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H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_13\_3

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H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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H 8.65463719 4.48017277 -1.19983591

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H 9.97087934 3.73708895 -0.32325185

17\_14\_1

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H 6.09801331 -0.66278889 0.00000000

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H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_14\_3

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C 6.07958133 1.35261506 -0.32520798

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C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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17\_15\_1

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H 1.78667599 -0.50476353 -0.87342340

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

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H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

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17\_15\_3

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17\_16\_1

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17\_16\_3

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17\_17\_1

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17\_17\_3

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S 0.00000000 0.00000000 0.00000000

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C 6.07958133 1.35261506 -0.32520798

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H 8.65168677 4.48183842 0.54746381

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17\_18\_1

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H 6.00714683 4.60101079 0.87267179

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17\_18\_3

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H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_19\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_19\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_20\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_20\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_21\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_21\_3

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_22\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

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C 4.14415843 0.27071740 0.00000000

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H 7.32445852 1.51013365 0.00000000

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H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_22\_3

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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O -3.15354772 0.37293328 1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

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H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_23\_1

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O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

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H -1.89191645 -5.27412912 -1.91662783

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_23\_3

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H -1.07087335 -6.22465230 -0.70194248

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H -1.89191645 -5.27412912 -1.91662783

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_24\_1

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H -2.01202258 -5.84317879 -0.49401571

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

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H 6.09801331 -0.66278889 0.00000000

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H 6.01009725 4.59934514 -0.87462793

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H 7.32633940 3.85626132 0.00195613

17\_24\_3

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H 1.20115184 -2.39029979 0.00000000

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C 4.53970981 1.33767722 -0.32520798

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

17\_25\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

H 6.01009725 4.59934514 -0.87462793

H 6.00714683 4.60101079 0.87267179

H 7.32633940 3.85626132 0.00195613

17\_25\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705788 3.92244401 -0.32520798

H 8.65463719 4.48017277 -1.19983591

H 8.65168677 4.48183842 0.54746381

H 9.97087934 3.73708895 -0.32325185

18\_0\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

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H -2.43004899 -4.73228764 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_0\_3

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_1\_1

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O 0.00000000 0.00000000 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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O 6.52025531 4.47627663 -1.05506567

18\_1\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_2\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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C -5.15700139 -4.82906594 -0.01939463

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C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

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H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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O 6.52025531 4.47627663 -1.05506567

18\_2\_3

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_3\_1

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O 0.00000000 0.00000000 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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O 6.52025531 4.47627663 -1.05506567

18\_3\_3

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H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_4\_1

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H 1.78667599 -0.50476353 -0.87342340

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H 1.74293107 -4.21843477 0.87370434

H 1.74296147 -4.21848134 -0.87359867

H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 6.22487150 1.49899961 0.00000000

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18\_4\_3

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_5\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_5\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_6\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_6\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

O -3.12698910 0.60233649 1.03134164

N -3.33789875 0.34516141 -1.22729984

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

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H -4.79204763 0.43168404 -0.00036327

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_8\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

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H -4.44369368 -1.04091448 -0.87395912

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N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_9\_1

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

18\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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O 9.16301851 4.35810731 -1.38027563

18\_10\_1

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_10\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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O 9.16301851 4.35810731 -1.38027563

18\_11\_1

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_12\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_13\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_14\_1

C 1.39590808 0.00002666 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_14\_3

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_15\_1

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C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_15\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_16\_1

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_16\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_17\_1

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_17\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_18\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

H 1.74143379 -4.21908038 -0.87270226

H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_18\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

O 1.53118641 -2.37407291 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401801 -1.04092734 0.87334263

H -4.79204764 0.43168404 -0.00036151

H -4.44369403 -1.04091300 -0.87396000

C 2.07415062 -3.69698253 0.00000235

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_19\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_20\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

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H 1.78667599 -0.50476353 -0.87342340

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_20\_3

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -3.31535073 -6.38719610 1.34833652

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_21\_1

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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O 0.57029859 -5.40080634 -1.05506567

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_21\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

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O 0.57029859 -5.40080634 -1.05506567

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_22\_1

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O 0.00000000 0.00000000 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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O -3.15354772 0.37293328 1.05506567

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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O 6.52025531 4.47627663 -1.05506567

18\_22\_3

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_23\_1

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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O -3.15354772 0.37293328 1.05506567

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H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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O 6.52025531 4.47627663 -1.05506567

18\_23\_3

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C -2.68369776 -2.58154545 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_24\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_24\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -3.56601195 -5.04458316 -0.51471929

H -2.01202258 -5.84317879 -0.49401571

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

18\_25\_1

C 1.39590808 0.00002666 0.00000000

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

N 6.23810477 3.98065956 0.00000000

O 6.51669979 4.47830151 1.05506215

O 6.52025531 4.47627663 -1.05506567

18\_25\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

F -2.58786689 0.67769043 -1.10103451

F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

N 8.88264471 3.86148719 -0.32520798

O 9.16301645 4.35812610 0.72985615

O 9.16301851 4.35810731 -1.38027563

19\_0\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_0\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H -2.43004899 -4.73228764 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_1\_1

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O 0.00000000 0.00000000 0.00000000

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_1\_3

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C -2.68369776 -2.58154545 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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H -4.44369368 -1.04091448 -0.87395912

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_2\_1

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

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H -2.01202258 -5.84317879 -0.49401571

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C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

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H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_2\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

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H -5.12649991 -4.76910710 1.07820110

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H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_3\_1

C 1.39590808 0.00002666 0.00000000

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C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

N -3.50922218 0.92854573 -0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_3\_3

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_4\_1

C 1.39590808 0.00002666 0.00000000

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

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H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 1.74293107 -4.21843477 0.87370434

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_4\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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C -2.63130896 -5.12392023 0.00000000

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_5\_1

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H 0.06199400 -4.60941029 0.00000000

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H -3.83843623 -7.47439765 2.16033398

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

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H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

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H 6.56635579 3.62075923 1.99578375

19\_5\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_6\_1

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C 4.14415843 0.27071740 0.00000000

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H 6.09801331 -0.66278889 0.00000000

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O 6.21844010 3.94582709 0.00000000

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H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_6\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

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H 9.43160337 3.38458750 1.59601853

19\_7\_1

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H 6.56635579 3.62075923 1.99578375

19\_7\_3

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H -3.78200475 -2.63580705 0.00000000

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_8\_1

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H 0.06199400 -4.60941029 0.00000000

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19\_8\_3

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H 1.20115184 -2.39029979 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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C 9.84824890 3.81858088 0.71117037

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H 9.43160337 3.38458750 1.59601853

19\_9\_1

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C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

19\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_10\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_10\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_11\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_11\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_12\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_13\_1

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_13\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_14\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_15\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_15\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_16\_1

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

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C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

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H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_16\_3

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_17\_1

C 1.39590808 0.00002666 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

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S 0.00000000 0.00000000 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_17\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_18\_1

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H 7.32445852 1.51013365 0.00000000

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C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_18\_3

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C 8.18371520 0.16518422 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_19\_1

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 7.95728407 3.42493525 0.95653494

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H 6.56635579 3.62075923 1.99578375

19\_19\_3

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H 8.74255325 -0.78196126 -0.32520798

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H 9.43160337 3.38458750 1.59601853

19\_20\_1

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

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H 7.95728407 3.42493525 0.95653494

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H 6.56635579 3.62075923 1.99578375

19\_20\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_21\_1

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H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N 0.26277372 -4.92052136 0.00000000

O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_22\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_22\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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N -2.84286588 -0.10531562 0.00000000

O -3.15011583 0.37516349 -1.05506215

O -3.15354772 0.37293328 1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_23\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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O -3.15354772 0.37293328 1.05506567

O -2.58103053 -5.02608323 0.00000000

C -2.02016781 -5.85099726 -1.02462181

H -1.07087335 -6.22465230 -0.70194248

H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_23\_3

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C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

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O -3.15354772 0.37293328 1.05506567

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H -2.67804728 -6.67145343 -1.22196989

H -1.89191645 -5.27412912 -1.91662783

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_24\_1

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -2.01202258 -5.84317879 -0.49401571

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_24\_3

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C -2.04648885 -1.34090601 0.00000000

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H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

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H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

O 8.86298004 3.82665472 -0.32520798

C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

H 10.15711951 4.82204268 0.91747927

H 9.43160337 3.38458750 1.59601853

19\_25\_1

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

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C 4.14415843 0.27071740 0.00000000

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H 7.32445852 1.51013365 0.00000000

O 6.21844010 3.94582709 0.00000000

C 7.07915961 4.00806758 1.14025789

H 7.95728407 3.42493525 0.95653494

H 7.35787353 5.02507976 1.32165460

H 6.56635579 3.62075923 1.99578375

19\_25\_3

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C -2.04648885 -1.34090601 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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F -2.59145997 0.67537458 1.10350253

F -4.19440535 -0.35777358 -0.00246802

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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C 9.84824890 3.81858088 0.71117037

H 10.69325262 3.24307118 0.39548494

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20\_0\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

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20\_1\_1

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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N 6.84279328 5.05175797 0.00000000

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C 6.07958133 1.35261506 -0.32520798

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N 9.48733322 4.93258560 -0.32520798

20\_9\_1

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

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20\_9\_3

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O 3.80633983 2.36023406 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

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H 6.09801331 -0.66278889 0.00000000

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C 6.27251794 4.04161638 0.00000000

N 6.84279328 5.05175797 0.00000000

20\_13\_3

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H 0.06199400 -4.60941029 0.00000000

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H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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N 9.48733322 4.93258560 -0.32520798

20\_14\_1

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F -1.84996634 -6.03139598 -0.62329085

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H -4.79204763 0.43168404 -0.00036327

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20\_18\_1

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20\_19\_1

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N 9.48733322 4.93258560 -0.32520798

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N 6.84279328 5.05175797 0.00000000

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21\_0\_3

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H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_1\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_1\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_2\_1

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C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_2\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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C -2.63130896 -5.12392023 0.00000000

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H -5.12649991 -4.76910710 1.07820110

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C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_3\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -0.53432909 -3.68539906 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

N -3.50922218 0.92854573 -0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_3\_3

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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Cl 9.02521354 4.11402259 -0.32520798

21\_4\_1

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C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

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H 1.78667599 -0.50476353 -0.87342340

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H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_4\_3

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_5\_1

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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C -3.58795695 -6.98463655 -1.20855568

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C 4.14415843 0.27071740 0.00000000

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C 6.22487150 1.49899961 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_5\_3

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C -3.58795695 -6.98463655 -1.20855568

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C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_6\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H -3.13557388 -0.17831473 -2.03821460

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C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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H 6.09801331 -0.66278889 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_6\_3

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C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_8\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_9\_1

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

21\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_10\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_10\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_11\_1

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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O 1.16179989 2.47940643 0.00000000

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_11\_3

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C 8.15996819 2.58139397 -0.32520798

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H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_12\_1

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O 0.00000000 0.00000000 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

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H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_12\_3

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H 0.06199400 -4.60941029 0.00000000

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H -4.79204763 0.43168404 -0.00036327

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_13\_1

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

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C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_13\_3

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C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_14\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_15\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_15\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_16\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_16\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_17\_1

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C -0.65307274 -1.27216194 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_17\_3

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_18\_1

C 1.39590808 0.00002666 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_18\_3

O 0.00000000 0.00000000 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H 3.14283146 -3.64390062 -0.00188621

H 1.74446035 -4.21783562 0.87459733

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_19\_1

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_19\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_20\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_20\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

O -2.58103053 -5.02608323 0.00000000

C -2.86970108 -5.41442215 1.34564564

H -3.54699404 -4.71061552 1.78248714

H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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Cl 9.02521354 4.11402259 -0.32520798

21\_21\_1

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C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

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O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_21\_3

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H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

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O 0.57029859 -5.40080634 -1.05506567

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O 3.80633983 2.36023406 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Cl 9.02521354 4.11402259 -0.32520798

21\_22\_1

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O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_22\_3

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C -0.65307274 -1.27216194 0.00000000

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O -3.15354772 0.37293328 1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

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C 8.15996819 2.58139397 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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Cl 9.02521354 4.11402259 -0.32520798

21\_23\_1

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C 3.43504139 1.47178743 0.00000000

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C 4.14415843 0.27071740 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_23\_3

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C 4.53970981 1.33767722 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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Cl 9.02521354 4.11402259 -0.32520798

21\_24\_1

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H 1.78667599 -0.50476353 -0.87342340

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O 1.16179989 2.47940643 0.00000000

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Cl 6.38067361 4.23319495 0.00000000

21\_24\_3

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C 8.15996819 2.58139397 -0.32520798

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Cl 9.02521354 4.11402259 -0.32520798

21\_25\_1

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Cl 6.38067361 4.23319495 0.00000000

21\_25\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C 6.76537041 2.56759016 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

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Cl 9.02521354 4.11402259 -0.32520798

22\_0\_1

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Br 6.45441611 4.36381671 0.00000000

22\_0\_3

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C 6.76537041 2.56759016 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

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22\_1\_1

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_1\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_2\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_2\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

H -2.80496412 -5.43568560 1.00873497

H -2.01202258 -5.84317879 -0.49401571

C -3.97658243 -5.00973416 -0.74081093

C -5.15700139 -4.82906594 -0.01939463

C -4.01495857 -5.08681552 -2.13297970

C -6.37555546 -4.72618873 -0.69003910

H -5.12649991 -4.76910710 1.07820110

C -5.23368719 -4.98293786 -2.80403848

H -3.08467839 -5.22902992 -2.70173525

C -6.41391884 -4.80278716 -2.08283394

H -7.30608942 -4.58441190 -0.12144224

H -5.26359045 -5.04333756 -3.90173238

H -7.37481597 -4.72158696 -2.61139763

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_3\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

N -3.50922218 0.92854573 -0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_3\_3

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_4\_1

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C -2.68369776 -2.58154545 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

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H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 2.07415062 -3.69698253 0.00004470

H 1.74293107 -4.21843477 0.87370434

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H 3.14283313 -3.64390048 0.00006188

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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Br 6.45441611 4.36381671 0.00000000

22\_4\_3

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H 0.06199400 -4.60941029 0.00000000

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_5\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

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C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

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H 1.78667599 -0.50476353 -0.87342340

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O 1.16179989 2.47940643 0.00000000

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C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_5\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

C -2.94995914 -5.74440251 -1.20827779

C -2.95019412 -5.74426396 1.20790482

C -3.58795695 -6.98463655 -1.20855568

H -2.69911360 -5.25471954 -2.16039590

C -3.58750097 -6.98533199 1.20780025

H -2.69896048 -5.25545026 2.16030802

C -3.90653150 -7.60550623 -0.00014861

H -3.83971591 -7.47347889 -2.16089338

H -3.83843623 -7.47439765 2.16033398

H -4.40951715 -8.58341295 -0.00061768

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_6\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

H -3.88282593 1.16559786 -1.32389272

H -3.13557388 -0.17831473 -2.03821460

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_6\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H -3.13557388 -0.17831473 -2.03821460

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

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H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.61163988 -0.97476710 0.87032494

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H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_8\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_9\_1

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 1.43000000 0.00002731 0.00000000

22\_9\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_10\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_10\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_11\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

N -1.92741092 -3.75420218 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_11\_3

O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_12\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_12\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

H -3.24301396 -5.21057181 0.87361805

H -3.24291089 -5.21062478 -0.87368496

H -1.89707380 -5.90225096 0.00006691

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_13\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_14\_1

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O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_14\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_15\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_15\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

H -2.64221326 -0.41663104 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_16\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_16\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C 0.30073100 -4.97933671 0.00000000

H 0.91793855 -5.00550550 -0.87365326

H 0.91794368 -5.00550219 0.87364974

H -0.35348543 -5.82603670 0.00000352

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_17\_1

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_17\_3

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_18\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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H 1.74446035 -4.21783562 0.87459733

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_18\_3

O 0.00000000 0.00000000 0.00000000

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H -2.43004899 -4.73228764 0.00000000

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H 1.74446035 -4.21783562 0.87459733

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

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H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_19\_1

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_19\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_20\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_20\_3

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H 1.20115184 -2.39029979 0.00000000

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H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_21\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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O 0.57374195 -5.39860238 1.05506215

O 0.57029859 -5.40080634 -1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_21\_3

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

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O 0.57029859 -5.40080634 -1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_22\_1

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C -2.68369776 -2.58154545 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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O -3.15354772 0.37293328 1.05506567

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

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H 3.56149154 3.63348583 0.00000000

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Br 6.45441611 4.36381671 0.00000000

22\_22\_3

O 0.00000000 0.00000000 0.00000000

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O -3.15354772 0.37293328 1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

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Br 9.09895605 4.24464434 -0.32520798

22\_23\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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H 1.20115184 -2.39029979 0.00000000

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H 0.06199400 -4.60941029 0.00000000

N -2.84286588 -0.10531562 0.00000000

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O -3.15354772 0.37293328 1.05506567

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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Br 6.45441611 4.36381671 0.00000000

22\_23\_3

O 0.00000000 0.00000000 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

22\_24\_1

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H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

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H 3.56149154 3.63348583 0.00000000

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Br 6.45441611 4.36381671 0.00000000

22\_24\_3

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22\_25\_1

C 1.39590808 0.00002666 0.00000000

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C 5.53917526 0.28435659 0.00000000

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H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

Br 6.45441611 4.36381671 0.00000000

22\_25\_3

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

Br 9.09895605 4.24464434 -0.32520798

23\_0\_1

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H -4.79204763 0.43168404 -0.00036327

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O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

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23\_3\_3

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C 4.04044753 -0.11914713 -0.32520798

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C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

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H 9.16852202 3.81173464 1.71467546

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_7\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -4.37928474 -0.40158556 -0.00281537

H -4.61163988 -0.97476710 0.87032494

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_7\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

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H -4.95895846 0.49779062 -0.00375250

H -4.60841834 -0.97451069 -0.87697473

Br -2.80042732 -5.45300834 0.00000000

O -2.88078860 -0.04647798 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_8\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H -3.78200475 -2.63580705 0.00000000

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H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_8\_3

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C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

C -2.63130896 -5.12392023 0.00000000

N -3.16151787 -6.15565591 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_9\_1

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

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H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.64105369 -2.36867104 0.00000000

H 1.97260279 -1.84905466 -0.87462793

H 1.97243641 -1.84567063 0.87267179

H 2.04683045 -3.35874245 0.00195613

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23\_9\_3

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_10\_1

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_10\_3

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C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

F -2.54446440 -4.95492905 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

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C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

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H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

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H 9.16852202 3.81173464 1.71467546

23\_11\_1

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H 1.20115184 -2.39029979 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H 1.78667599 -0.50476353 -0.87342340

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C 3.43504139 1.47178743 0.00000000

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C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

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H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

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H 6.48153382 3.95487117 2.04582571

23\_11\_3

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C -2.68369776 -2.58154545 0.00000000

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H 0.06199400 -4.60941029 0.00000000

N -1.92741092 -3.75420218 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

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H 8.74255325 -0.78196126 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

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H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_12\_1

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H 1.78667599 -0.50476353 -0.87342340

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_12\_3

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C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_13\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_13\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

C -2.88078860 -0.04647798 0.00000000

H -2.65146887 0.52565701 0.87462793

H -2.64862102 0.52749254 -0.87267179

H -3.92195150 -0.29320857 -0.00195613

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_14\_1

C 1.39590808 0.00002666 0.00000000

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C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

H -2.64221326 -0.41663104 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_14\_3

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C -2.04648885 -1.34090601 0.00000000

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C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

C -2.63130896 -5.12392023 0.00000000

F -3.81060713 -5.02382205 -0.64941218

F -2.85040659 -5.51726906 1.27270300

F -1.84996634 -6.03139598 -0.62329085

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_15\_1

C 1.39590808 0.00002666 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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H -2.64221326 -0.41663104 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -2.43004899 -4.73228764 0.00000000

N -2.68369776 -2.58154545 0.00000000

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_15\_3

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H -2.43004899 -4.73228764 0.00000000

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C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_16\_1

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C -2.04648885 -1.34090601 0.00000000

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C -1.92741092 -3.75420218 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

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H 0.91794368 -5.00550219 0.87364974

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C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

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C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

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N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_16\_3

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H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

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O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_17\_1

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

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C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_17\_3

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C -2.68369776 -2.58154545 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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H -4.79204763 0.43168404 -0.00036327

H -4.44369368 -1.04091448 -0.87395912

S 0.00000000 0.00000000 0.00000000

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_18\_1

C 1.39590808 0.00002666 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

C -1.92741092 -3.75420218 0.00000000

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H 0.06199400 -4.60941029 0.00000000

H -2.43004899 -4.73228764 0.00000000

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C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

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C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

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H 6.48153382 3.95487117 2.04582571

23\_18\_3

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_19\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

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H 0.06199400 -4.60941029 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

H -4.44401836 -1.04092585 0.87334351

H -4.79204763 0.43168404 -0.00036327

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

H -4.44369368 -1.04091448 -0.87395912

N -2.59931360 -5.06166032 0.00000000

O -2.85997830 -5.56892005 -1.05506413

O -2.85999570 -5.56889386 1.05506765

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

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N 6.67397243 4.47737851 1.23188540

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H 6.48153382 3.95487117 2.04582571

23\_19\_3

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H -4.44369368 -1.04091448 -0.87395912

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O -2.85999570 -5.56889386 1.05506765

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_20\_1

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H 1.78667599 -0.50476353 -0.87342340

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H -3.31535073 -6.38719610 1.34833652

H -1.96275660 -5.43602998 1.91299457

C 1.89516987 1.45684959 0.00000000

O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

C 5.51542825 2.70056634 0.00000000

H 3.56149154 3.63348583 0.00000000

C 5.53917526 0.28435659 0.00000000

H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

H 6.09801331 -0.66278889 0.00000000

H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_20\_3

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C -2.68369776 -2.58154545 0.00000000

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H -3.78200475 -2.63580705 0.00000000

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C -2.86970108 -5.41442215 1.34564564

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H -1.96275660 -5.43602998 1.91299457

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

H 8.74255325 -0.78196126 -0.32520798

H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_21\_1

C 1.39590808 0.00002666 0.00000000

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

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C 0.10291173 -2.44429720 0.00000000

C -2.68369776 -2.58154545 0.00000000

C -0.53432909 -3.68539906 0.00000000

H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

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H -4.44401836 -1.04092585 0.87334351

H 1.78667597 -0.50397368 0.87387943

H 1.78667599 -0.50476353 -0.87342340

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O 1.16179989 2.47940643 0.00000000

C 3.43504139 1.47178743 0.00000000

C 4.12083047 2.68676253 0.00000000

C 4.14415843 0.27071740 0.00000000

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H 3.56149154 3.63348583 0.00000000

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H 3.60380741 -0.68696195 0.00000000

C 6.22487150 1.49899961 0.00000000

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H 7.32445852 1.51013365 0.00000000

C 6.27251794 4.04161638 0.00000000

O 6.50715660 4.68857668 -1.03519445

N 6.67397243 4.47737851 1.23188540

H 7.16742042 5.32972864 1.32883970

H 6.48153382 3.95487117 2.04582571

23\_21\_3

O 0.00000000 0.00000000 0.00000000

C -0.65307274 -1.27216194 0.00000000

C -2.04648885 -1.34090601 0.00000000

C 0.10291173 -2.44429720 0.00000000

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H 1.20115184 -2.39029979 0.00000000

C -1.92741092 -3.75420218 0.00000000

H -3.78200475 -2.63580705 0.00000000

H -2.43004899 -4.73228764 0.00000000

O -2.82119576 -0.13893712 0.00000000

C -4.21282396 -0.46798253 -0.00026115

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H -4.79204763 0.43168404 -0.00036327

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O 0.57029859 -5.40080634 -1.05506567

C 4.53970981 1.33767722 -0.32520798

O 3.80633983 2.36023406 -0.32520798

C 6.07958133 1.35261506 -0.32520798

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C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

H 6.20603148 3.51431346 -0.32520798

C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_22\_1

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O 0.00000000 0.00000000 0.00000000

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C -2.04648885 -1.34090601 0.00000000

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23\_22\_3

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H 4.40357920 -0.62062428 0.54746381

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N 9.34407239 4.34377623 0.90309726

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H 9.16852202 3.81173464 1.71467546

23\_23\_1

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N 6.67397243 4.47737851 1.23188540

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H 6.48153382 3.95487117 2.04582571

23\_23\_3

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C 6.07958133 1.35261506 -0.32520798

C 6.76537041 2.56759016 -0.32520798

C 6.78869837 0.15154503 -0.32520798

C 8.15996819 2.58139397 -0.32520798

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C 8.18371520 0.16518422 -0.32520798

H 6.24834735 -0.80613432 -0.32520798

C 8.86941144 1.37982724 -0.32520798

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H 9.96899846 1.39096128 -0.32520798

C 4.04044753 -0.11914713 -0.32520798

H 4.40037407 -0.61952586 -1.19983591

H 4.40357920 -0.62062428 0.54746381

C 8.91705787 3.92244401 -0.32520798

O 9.13021759 4.58153025 -1.35739437

N 9.34407239 4.34377623 0.90309726

H 9.83953205 5.19499068 0.99976937

H 9.16852202 3.81173464 1.71467546

23\_24\_1

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C 4.14415843 0.27071740 0.00000000

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H 6.48153382 3.95487117 2.04582571

23\_24\_3

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23\_25\_1

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23\_25\_3

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